

STA 6208 – Course Notes and R Programs

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Chapter 1 - Introduction/Review

1.1 Mathematical Operations – Summation Operators

Consider sequences of numbers and numeric constants.

Sum of a sequence of Variables: $\sum_{i=1}^n Y_i = Y_1 + \dots + Y_n$

Sum of a sequence of Constants: $\sum_{i=1}^n k = k + \dots + k = nk$

Sum of a sequence of Sums of Variables: $\sum_{i=1}^n (X_i + Z_i) = \sum_{i=1}^n X_i + \sum_{i=1}^n Z_i$

Sum of a sequence of (Commonly) Linearly Transformed Variables: $\sum_{i=1}^n (a + bX_i) = na + b \sum_{i=1}^n X_i$

Sum of a sequence of (Individually) Linearly Transformed Variables: $\sum_{i=1}^n (a_i + b_i X_i) = \sum_{i=1}^n a_i + \sum_{i=1}^n b_i X_i$

Sum of a sequence of Sums of Multiples of Variables: $\sum_{i=1}^n (a_i X_i + b_i Z_i) = \sum_{i=1}^n a_i X_i + \sum_{i=1}^n b_i Z_i$

Example – Opening Weekend Box-Office Gross for Harry Potter Films

Date	Movie	Gross(\$M)	Theaters	PerTheater(\$K)	Euros/Dollar	Gross (€M)
11/16/2001	Sorcerer's Stone	90.29	3672	24.59	1.1336	102.36
11/15/2002	Chamber of Secrets	88.36	3682	24.00	0.9956	87.97
6/4/2004	Prisoner of Azkaban	93.69	3855	24.30	0.8135	76.21
11/18/2005	Goblet of Fire	102.69	3858	26.62	0.8496	87.24
7/13/2007	Order of the Phoenix	77.11	4285	18.00	0.7263	56.00
7/17/2009	Half-Blood Prince	77.84	4325	18.00	0.7085	55.15
11/19/2010	Deathly Hallows: Part I	125.02	4125	30.31	0.7353	91.93
7/15/2011	Deathly Hallows: Part II	169.19	4375	38.67	0.7042	119.14
Total		824.18	32,177.00			676.00

Total Gross (\$Millions): $\sum_{i=1}^n Y_i = 90.29 + 88.36 + \dots + 169.19 = 824.18$

Total Gross (Millions of Euros): $\sum_{i=1}^n a_i Y_i = 1.1336(90.29) + 0.9956(88.36) + \dots + 0.7042(169.19) = 676.00$

Question: What is the average gross per theater for all movies? Is it the same as the average of individual movies' gross per theater?

1.2 Basic Probability

Addition Theorem

A_i, A_j are 2 events defined on a sample space.

$$P(A_i \cup A_j) = P(A_i) + P(A_j) - P(A_i \cap A_j) \quad \text{where:}$$

$P(A_i \cup A_j) \equiv$ Probability at least one occurs $P(A_i \cap A_j) \equiv$ Probability both occur. Often written as $P(A_i A_j)$

Multiplication Theorem (Can be obtained from counts when data are in contingency table)

$$P(A_i | A_j) = \frac{P(A_i \cap A_j)}{P(A_j)} = \frac{P(A_i A_j)}{P(A_j)} \quad \text{where } P(A_i | A_j) \equiv \text{Probability } A_i \text{ occurs given } A_j \text{ has occurred}$$

$$P(A_j | A_i) = \frac{P(A_i \cap A_j)}{P(A_i)} = \frac{P(A_i A_j)}{P(A_i)}$$

$$\Rightarrow P(A_i \cap A_j) = P(A_i A_j) = P(A_i)P(A_j | A_i) = P(A_j)P(A_i | A_j)$$

Complementary Events

$$P(\bar{A}_i) = 1 - P(A_i) \quad \text{where } \bar{A}_i \equiv \text{event } A_i \text{ does not occur}$$

$$P(\overline{A_i \cup A_j}) = P(\bar{A}_i \cap \bar{A}_j) \quad \text{the complement of either } A_i \text{ and/or } A_j \text{ occurring is the intersection of them not occurring}$$

Example – New York City Sidewalk Cafes

Cafes classified by size (<100 ft², 100-199, 200-299, 300-399, 400-499, 500-599, ≥600) and type (enclosed, unenclosed).

Type\Size	<100	100-199	200-299	300-399	400-499	500-599	≥600	Total
Enclosed	2	18	31	30	23	7	9	120
Unenclosed	98	318	200	118	63	26	40	863
Total	100	336	231	148	86	33	49	983

Let $A_1 \equiv$ Size < 300ft² and $A_2 \equiv$ Type = Unenclosed.

$$P(A_1) = \frac{100 + 336 + 231}{983} = \frac{667}{983} = 0.6785$$

$$P(A_2) = \frac{863}{983} = 0.8779$$

$$P(A_1 \cap A_2) = P(A_1 A_2) = \frac{98 + 318 + 200}{983} = \frac{616}{983} = 0.6267$$

$$P(A_1 \cup A_2) = P(A_1) + P(A_2) - P(A_1 A_2) = \frac{667 + 863 - 616}{983} = \frac{914}{983} = 0.9298 = 0.6785 + 0.8779 - 0.6267$$

$$P(A_1 | A_2) = \frac{P(A_1 \cap A_2)}{P(A_2)} = \frac{616}{863} = 0.7138 = \frac{0.6267}{0.8779}$$

$$P(A_2 | A_1) = \frac{P(A_1 \cap A_2)}{P(A_1)} = \frac{616}{667} = 0.9235 = \frac{0.6267}{0.6785}$$

$$P(\overline{A_1}) = \frac{148 + 86 + 33 + 49}{983} = \frac{316}{983} = 0.3215 = 1 - 0.6785$$

$$P(\overline{A_2}) = \frac{120}{983} = 0.1221 = 1 - 0.8779$$

$$P(\overline{A_1 \cup A_2}) = \frac{30 + 23 + 7 + 9}{983} = \frac{69}{983} = 0.0702 = P(\overline{A_1} \cap \overline{A_2})$$

1.3 Univariate Random Variables

Probability (Density) Functions

Discrete (RV $\equiv Y$ takes on masses of probability at specific points y_1, \dots, y_k):

$p(y_s) = P(Y = y_s) \quad s = 1, \dots, k$ often written as $p(y)$ where y is specific point y_s

Continuous (RV $\equiv Y$ takes on density of probability over ranges of points on continuum)

$f(y) \equiv$ density at y

Expected Value (Long Run Average Outcome, aka Mean)

Discrete: $\mu_Y = E\{Y\} = \sum_{s=1}^k y_s p(y_s)$ Continuous: $\mu_Y = E\{Y\} = \int_{-\infty}^{\infty} y f(y) dy$

a, c constants $\Rightarrow E\{a + cY\} = a + cE\{Y\} = a + c\mu_Y \Rightarrow E\{a\} = a \Rightarrow E\{cY\} = cE\{Y\} = c\mu_Y$

Discrete: $\mu_{g(Y)} = E\{g(Y)\} = \sum_{s=1}^k g(y_s) p(y_s)$ Continuous: $\mu_{g(Y)} = E\{g(Y)\} = \int_{-\infty}^{\infty} g(y) f(y) dy$

Variance (Average Squared Distance from Expected Value)

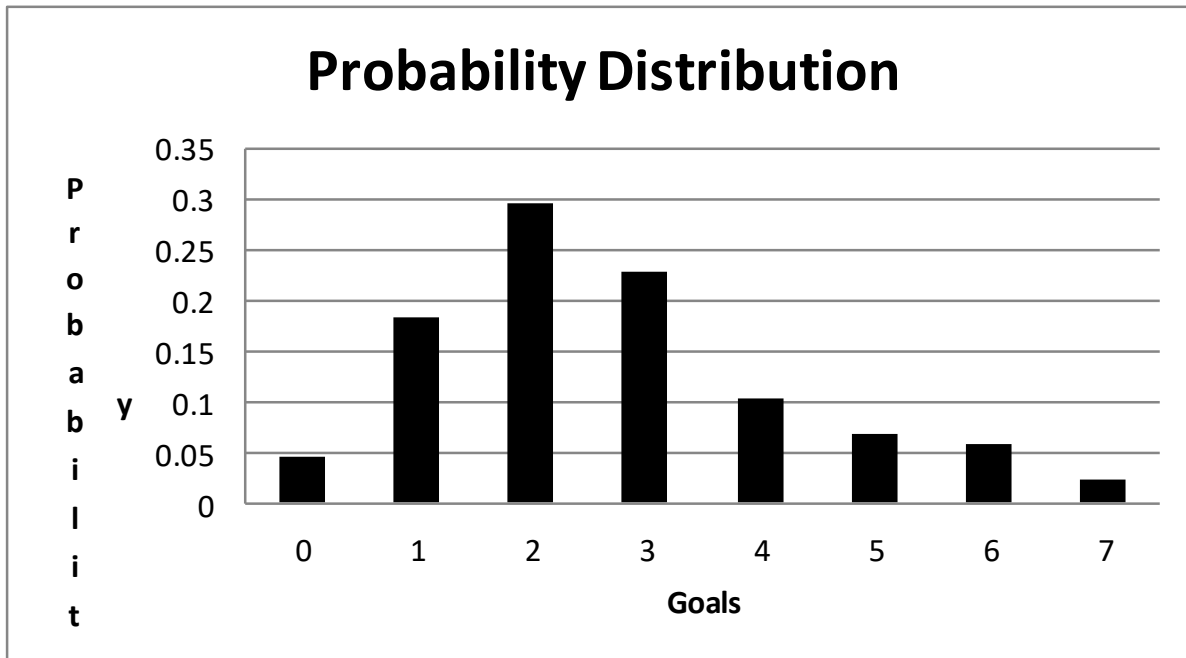
$\sigma_Y^2 = V\{Y\} = E\{(Y - E\{Y\})^2\} = E\{(Y - \mu_Y)^2\}$

Equivalently (Computationally easier): $\sigma_Y^2 = V\{Y\} = E\{Y^2\} - (E\{Y\})^2 = E\{Y^2\} - \mu_Y^2$

a, c constants $\Rightarrow V\{a + cY\} = c^2 V\{Y\} = c^2 \sigma_Y^2 \Rightarrow V\{a\} = 0 \Rightarrow V\{cY\} = c^2 V\{Y\} = c^2 \sigma_Y^2$

Example – Total Goals per Game in National Women’s Soccer League Games (2013)

Goals (y)	Frequency	Probability=p(y)	y*p(y)	(y^2)*p(y)
0	4	0.0455	0.0000	0.0000
1	16	0.1818	0.1818	0.1818
2	26	0.2955	0.5909	1.1818
3	20	0.2273	0.6818	2.0455
4	9	0.1023	0.4091	1.6364
5	6	0.0682	0.3409	1.7045
6	5	0.0568	0.3409	2.0455
7	2	0.0227	0.1591	1.1136
Total	88	1	2.7045	9.9091



Expected Value (Mean): $E\{Y\} = \mu_Y = \sum_{y=0}^7 yp(y) = 0(.0455) + \dots + 7(.0227) = 2.7045$

Variance: $\sigma_Y^2 = V\{Y\} = E\{(Y - \mu_Y)^2\} = E\{Y^2\} - \mu_Y^2 = \sum_{y=0}^7 y^2 p(y) - \mu_Y^2 = 9.9091 - 2.7045^2 = 2.5945$

Standard Deviation: $\sigma_Y = +\sqrt{V\{Y\}} = \sqrt{2.5945} = 1.6108$

1.4 Bivariate Random Variables

Joint Probability Function - Discrete Case (Generalizes to Densities in Continuous Case)

Random Variables (Outcomes observed on same unit) $\equiv y, z$ (k possibilities for y, m for z):

$$p(y_s, z_t) = P(Y = y_s \cap Z = z_t) \quad s = 1, \dots, k; t = 1, \dots, m \quad \text{Probability } Y = y_s \text{ and } Z = z_t$$

Often written as $p(y, z)$ for specific outcomes y, z

Marginal Probability Function - Discrete Case (Generalizes to Densities in Continuous Case):

$$p_Y(y_s) = \sum_{t=1}^m p(y_s, z_t) \quad \text{Probability } Y = y_s \quad p_Z(z_t) = \sum_{s=1}^k p(y_s, z_t) \quad \text{Probability } Z = z_t \quad \text{Often denoted } p_Y(y), \quad p_Z(z)$$

Continuous: Replace summations with integrals and the symbol $p(\bullet)$ with $f(\bullet)$.

Conditional Probability Function - Discrete Case (Generalizes to Densities in Continuous Case):

$$p(y_s | z_t) = \frac{p(y_s, z_t)}{p_Z(z_t)} \quad p_Z(z_t) \neq 0; s = 1, \dots, k \quad \text{Probability } Y = y_s \text{ given } Z = z_t \quad \text{Often denoted } p(y | z)$$

$$p(z_t | y_s) = \frac{p(y_s, z_t)}{p_Y(y_s)} \quad p_Y(y_s) \neq 0; t = 1, \dots, m \quad \text{Probability } Z = z_t \text{ given } Y = y_s \quad \text{Often denoted } p(z | y)$$

Example – Goals by Half Y=Home Club Z=Away Club – Irish Premier League (2012)

H\A Freq	0	1	2	3	4	5	Total(Home)
0	105	67	20	8	0	0	200
1	75	41	18	1	0	0	135
2	26	17	1	0	1	0	45
3	6	3	3	0	0	0	12
4	1	1	0	0	0	0	2
5	2	0	0	0	0	0	2
Total(Away)	215	129	42	9	1	0	396
H\A Prob	0	1	2	3	4	5	Total(Home)
0	0.26515	0.16919	0.05051	0.02020	0.00000	0.00000	0.50505
1	0.18939	0.10354	0.04545	0.00253	0.00000	0.00000	0.34091
2	0.06566	0.04293	0.00253	0.00000	0.00253	0.00000	0.11364
3	0.01515	0.00758	0.00758	0.00000	0.00000	0.00000	0.03030
4	0.00253	0.00253	0.00000	0.00000	0.00000	0.00000	0.00505
5	0.00505	0.00000	0.00000	0.00000	0.00000	0.00000	0.00505
Total(Away)	0.54293	0.32576	0.10606	0.02273	0.00253	0.00000	1.00000

Home Team
Distribution: $p_Y(y)$

Away Team Distribution: $p_Z(z)$

To obtain the conditional distribution of Away goals given a particular number of Home Goals, take the cell probabilities and divide by the total row probability. Similarly, for the conditional distribution of Home goals given Away goals, divide cell by column total.

Conditional Distribution of Home goals given Away Goals=0 $\equiv p(y|z=0)$:

$$p(y=0|z=0) = \frac{0.26515}{0.54293} = 0.48837 \quad p(y=1|z=0) = \frac{0.18939}{0.54293} = 0.34884 \quad p(y=2|z=0) = \frac{0.06566}{0.54293} = 0.12093$$

$$p(y=3|z=0) = \frac{0.01515}{0.54293} = 0.02791 \quad p(y=4|z=0) = \frac{0.00253}{0.54293} = 0.00465 \quad p(y=5|z=0) = \frac{0.00505}{0.54293} = 0.00930$$

Note: $0.48837 + 0.34884 + 0.12093 + 0.02791 + 0.00465 + 0.00930 = 1$

1.4.1 Covariance, Correlation, and Independence

Covariance - Average of Product of Distances from Means

$$\sigma_{YZ} = \text{COV}\{Y, Z\} = E\{(Y - E\{Y\})(Z - E\{Z\})\} = E\{(Y - \mu_Y)(Z - \mu_Z)\}$$

$$\text{Equivalently (for computing): } \sigma_{YZ} = \text{COV}\{Y, Z\} = E\{YZ\} - (E\{Y\})(E\{Z\}) = E\{YZ\} - \mu_Y \mu_Z$$

$$\text{Note: Discrete: } E\{YZ\} = \sum_{s=1}^k \sum_{t=1}^m y_s z_t p(y_s, z_t) \quad (\text{Replace summations with integrals in continuous case})$$

$$a_1, c_1, a_2, c_2 \text{ are constants} \Rightarrow V\{a_1 + c_1 Y, a_2 + c_2 Z\} = c_1 c_2 \sigma_{YZ} = c_1 c_2 \text{COV}\{Y, Z\}$$

$$\Rightarrow \text{COV}\{c_1 Y, c_2 Z\} = c_1 c_2 \sigma_{YZ} = c_1 c_2 \text{COV}\{Y, Z\} \Rightarrow \text{COV}\{a_1 + Y, a_2 + Z\} = \sigma_{YZ} = \text{COV}\{Y, Z\}$$

Correlation: Covariance scaled to lie between -1 and +1 for measure of association strength

Standardized Random Variables (Scaled to have mean = 0, variance = 1) $Y' = \frac{Y - \mu_Y}{\sigma_Y}$

$$\rho_{YZ} = \rho\{Y, Z\} = \text{COV}\{Y', Z'\} = \frac{\text{COV}\{Y, Z\}}{\sqrt{V\{Y\}V\{Z\}}} \quad -1 \leq \rho\{Y, Z\} \leq 1$$

$\text{COV}\{Y, Z\} = \rho\{Y, Z\} = 0 \Rightarrow Y, Z$ are uncorrelated (not necessarily independent)

Independent Random Variables

Y, Z are independent if and only if $p(y_s, z_t) = p_Y(y_s) p_Z(z_t) \quad \forall s = 1, \dots, k; t = 1, \dots, m$

If Y, Z are jointly normally distributed and $\text{COV}\{Y, Z\} = 0$ then Y, Z are independent

$$\text{Average Home Goals per Half: } \mu_Y = 0(0.50505) + \dots + 5(0.00505) = 0.70455$$

$$\text{Average Away Goals per Half: } \mu_Z = 0(0.54293) + \dots + 5(0.00000) = 0.61616$$

$$E\{Y^2\} = 0^2(0.50505) + \dots + 5^2(0.00505) = 1.27525$$

$$E\{Z^2\} = 0^2(0.54293) + \dots + 5^2(0.00000) = 0.99495$$

$$E\{YZ\} = 0(0)(0.26515) + 0(1)(0.16919) + \dots + 5(5)(0.00000) = 0.39647$$

$$\sigma_Y^2 = 1.27525 - 0.70455^2 = 0.77887 \quad \sigma_Y = \sqrt{0.77887} = 0.88254$$

$$\sigma_Z^2 = 0.99495 - 0.61616^2 = 0.61529 \quad \sigma_Z = \sqrt{0.61529} = 0.78441$$

$$\sigma_{YZ} = \text{COV}\{Y, Z\} = E\{YZ\} - \mu_Y \mu_Z = 0.39647 - 0.70455(0.61616) = -0.03765$$

$$\rho_{YZ} = \frac{\sigma_{YZ}}{\sigma_Y \sigma_Z} = \frac{-0.03765}{0.88254(0.78441)} = -0.05439$$

To see that Home and Away Goals are NOT independent (besides simply observing the correlation is not zero), you can check whether the joint probabilities in the cells of the joint distribution are all equal to the product of their row and column totals (product of the marginal probabilities).

For the case where both Home and Away goals are 0:

$$p(y = 0, z = 0) = 0.26515 \quad p_Y(y = 0) = 0.50505 \quad p_Z(z = 0) = 0.54293$$

$$0.26515 \neq 0.50505(0.54293) = 0.27421$$

1.5 Linear Functions of Random Variables

$$U = \sum_{i=1}^n a_i Y_i \quad \{a_i\} \equiv \text{constants} \quad \{Y_i\} \equiv \text{random variables}$$

$$E\{Y_i\} = \mu_i \quad V\{Y_i\} = \sigma_i^2 \quad \text{COV}\{Y_i, Y_j\} = \sigma_{ij}$$

$$\Rightarrow E\{U\} = E\left\{\sum_{i=1}^n a_i Y_i\right\} = \sum_{i=1}^n a_i E\{Y_i\} = \sum_{i=1}^n a_i \mu_i$$

$$\Rightarrow V\{U\} = V\left\{\sum_{i=1}^n a_i Y_i\right\} = \sum_{i=1}^n \sum_{j=1}^n a_i a_j \sigma_{ij} = \sum_{i=1}^n a_i^2 \sigma_i^2 + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n a_i a_j \sigma_{ij}$$

$$n = 2 \Rightarrow E\{a_1 Y_1 + a_2 Y_2\} = a_1 E\{Y_1\} + a_2 E\{Y_2\} = a_1 \mu_1 + a_2 \mu_2$$

$$V\{a_1 Y_1 + a_2 Y_2\} = a_1^2 V\{Y_1\} + a_2^2 V\{Y_2\} + 2a_1 a_2 \text{COV}\{Y_1, Y_2\} = a_1^2 \sigma_1^2 + a_2^2 \sigma_2^2 + 2a_1 a_2 \sigma_{12}$$

Total Goals, Difference (Home – Away), and Average Goals by Half $Y_1 = \text{Home}$ $Y_2 = \text{Away}$:

$$\mu_1 = \mu_Y = 0.70455 \quad \mu_2 = \mu_Z = 0.61616 \quad \sigma_1^2 = \sigma_Y^2 = 0.77887 \quad \sigma_2^2 = \sigma_Z^2 = 0.61529 \quad \sigma_{12} = \sigma_{YZ} = -0.03765$$

Total Goals: $U_1 = Y_1 + Y_2 \quad (a_1 = 1, a_2 = 1)$

Difference in Goals: $U_2 = Y_1 - Y_2 \quad (a_1 = 1, a_2 = -1)$

Average Goals: $U_3 = \frac{Y_1 + Y_2}{2} \quad \left(a_1 = \frac{1}{2}, a_2 = \frac{1}{2}\right)$

$$\mu_{U_1} = 1\mu_1 + 1\mu_2 = 1(0.70455) + 1(0.61616) = 1.32071$$

$$\sigma_{U_1}^2 = 1^2 \sigma_1^2 + 1^2 \sigma_2^2 + 2(1)(1)\sigma_{12} = 1(0.77887) + 1(0.61529) + 2(-0.03765) = 1.31886$$

$$\mu_{U_2} = 1\mu_1 + (-1)\mu_2 = 1(0.70455) - 1(0.61616) = 0.08838$$

$$\sigma_{U_2}^2 = 1^2 \sigma_1^2 + (-1)^2 \sigma_2^2 + 2(1)(-1)\sigma_{12} = 1(0.77887) + 1(0.61529) - 2(-0.03765) = 1.469461$$

$$\mu_{U_3} = \frac{1}{2} \mu_1 + \frac{1}{2} \mu_2 = \frac{1}{2}(0.70455) + \frac{1}{2}(0.61616) = 0.66035$$

$$\sigma_{U_3}^2 = \left(\frac{1}{2}\right)^2 \sigma_1^2 + \left(\frac{1}{2}\right)^2 \sigma_2^2 + 2\left(\frac{1}{2}\right)\left(\frac{1}{2}\right)\sigma_{12} = \frac{1}{4}(0.77887) + \frac{1}{4}(0.61529) + \frac{1}{2}(-0.03765) = 0.32972$$

1.5.1 Linear Functions of INDEPENDENT Random Variables

$$Y_1, \dots, Y_n \equiv \text{independent} \Rightarrow V\{U\} = V\left\{\sum_{i=1}^n a_i Y_i\right\} = \sum_{i=1}^n a_i^2 \sigma_i^2$$

Special Cases (Y_1, Y_2 independent):

$$U_1 = Y_1 + Y_2 \quad V\{U_1\} = V\{Y_1 + Y_2\} = (1)^2 \sigma_1^2 + (1)^2 \sigma_2^2 = \sigma_1^2 + \sigma_2^2$$

$$U_2 = Y_1 - Y_2 \quad V\{U_2\} = V\{Y_1 - Y_2\} = (1)^2 \sigma_1^2 + (-1)^2 \sigma_2^2 = \sigma_1^2 + \sigma_2^2$$

$$Y_1, \dots, Y_n \equiv \text{independent} \Rightarrow \text{COV}\left\{\sum_{i=1}^n a_i Y_i, \sum_{i=1}^n c_i Y_i\right\} = \sum_{i=1}^n a_i c_i \sigma_i^2$$

Special Case (Y_1, Y_2 independent):

$$\text{COV}\{U_1, U_2\} = \text{COV}\{Y_1 + Y_2, Y_1 - Y_2\} = (1)(1)\sigma_1^2 + (1)(-1)\sigma_2^2 = \sigma_1^2 - \sigma_2^2$$

Note: These do not apply for the soccer data, but are used repeatedly to obtain properties of estimators in linear models.

1.6 Central Limit Theorem

When random samples of size n are selected from any population with mean μ and finite variance σ^2 , the sampling distribution of the sample mean will be approximately normally distributed for large n :

$$\bar{Y} = \frac{\sum_{i=1}^n Y_i}{n} = \sum_{i=1}^n \left(\frac{1}{n}\right) Y_i \sim N\left(\mu, \frac{\sigma^2}{n}\right)$$

approximately, for large n

Z-table (and software packages) can be used to approximate probabilities of ranges of values for sample means, as well as percentiles of their sampling distribution.

1.7 Probability Distributions Widely Used in Linear Models

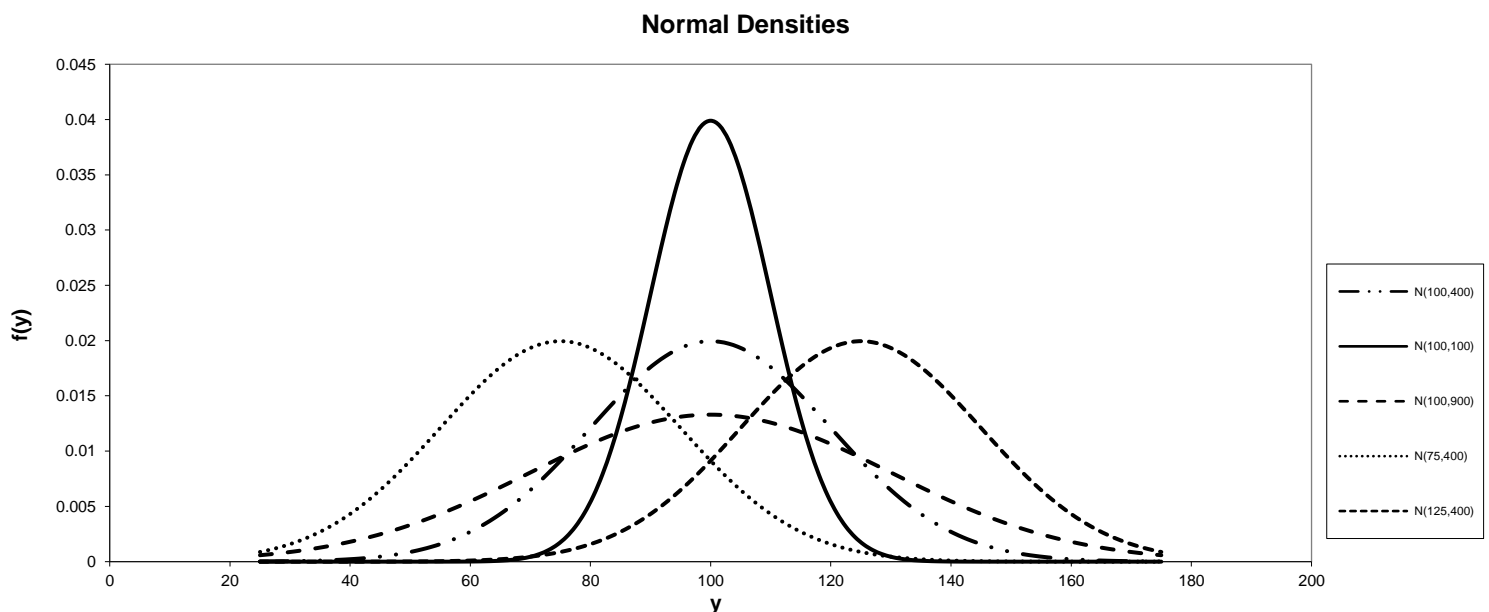
1.7.1 Normal (Gaussian) Distribution

- Bell-shaped distribution with tendency for individuals to clump around the group median/mean
- Used to model many biological phenomena
- Many estimators have approximate normal sampling distributions (see Central Limit Theorem)
- Notation: $Y \sim N(\mu, \sigma^2)$ where μ is mean and σ^2 is variance

$$f(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}\left(\frac{(y-\mu)^2}{\sigma^2}\right)\right] \quad -\infty < y < \infty, -\infty < \mu < \infty, \sigma > 0$$

Probabilities can be obtained from software packages (e.g. EXCEL, R, SPSS, SAS, STATA). Tables can be used to obtain probabilities once values have been standardized to have mean 0, and standard deviation 1.

$$Y \sim N(\mu_Y, \sigma_Y^2) \Rightarrow Z = \frac{Y - \mu_Y}{\sigma_Y} \sim N(\mu_Z = 0, \sigma_Z^2 = 1)$$



R Commands for Probabilities and Quantiles (Default are lower tail areas):

- Lower tail (cumulative) probabilities: `pnorm(y,mu,sigma)`
- Upper tail probabilities: `1 - pnorm(y,mu,sigma)`
- p^{th} quantile: `=qnorm(p,mu,sigma)` $0 < p < 1$

Second Decimal Place of Z

F(z)	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09
0.0	0.5000	0.5040	0.5080	0.5120	0.5160	0.5199	0.5239	0.5279	0.5319	0.5359
0.1	0.5398	0.5438	0.5478	0.5517	0.5557	0.5596	0.5636	0.5675	0.5714	0.5753
0.2	0.5793	0.5832	0.5871	0.5910	0.5948	0.5987	0.6026	0.6064	0.6103	0.6141
0.3	0.6179	0.6217	0.6255	0.6293	0.6331	0.6368	0.6406	0.6443	0.6480	0.6517
0.4	0.6554	0.6591	0.6628	0.6664	0.6700	0.6736	0.6772	0.6808	0.6844	0.6879
0.5	0.6915	0.6950	0.6985	0.7019	0.7054	0.7088	0.7123	0.7157	0.7190	0.7224
0.6	0.7257	0.7291	0.7324	0.7357	0.7389	0.7422	0.7454	0.7486	0.7517	0.7549
0.7	0.7580	0.7611	0.7642	0.7673	0.7704	0.7734	0.7764	0.7794	0.7823	0.7852
0.8	0.7881	0.7910	0.7939	0.7967	0.7995	0.8023	0.8051	0.8078	0.8106	0.8133
0.9	0.8159	0.8186	0.8212	0.8238	0.8264	0.8289	0.8315	0.8340	0.8365	0.8389
1.0	0.8413	0.8438	0.8461	0.8485	0.8508	0.8531	0.8554	0.8577	0.8599	0.8621
1.1	0.8643	0.8665	0.8686	0.8708	0.8729	0.8749	0.8770	0.8790	0.8810	0.8830
1.2	0.8849	0.8869	0.8888	0.8907	0.8925	0.8944	0.8962	0.8980	0.8997	0.9015
1.3	0.9032	0.9049	0.9066	0.9082	0.9099	0.9115	0.9131	0.9147	0.9162	0.9177
1.4	0.9192	0.9207	0.9222	0.9236	0.9251	0.9265	0.9279	0.9292	0.9306	0.9319
1.5	0.9332	0.9345	0.9357	0.9370	0.9382	0.9394	0.9406	0.9418	0.9429	0.9441
1.6	0.9452	0.9463	0.9474	0.9484	0.9495	0.9505	0.9515	0.9525	0.9535	0.9545
1.7	0.9554	0.9564	0.9573	0.9582	0.9591	0.9599	0.9608	0.9616	0.9625	0.9633
1.8	0.9641	0.9649	0.9656	0.9664	0.9671	0.9678	0.9686	0.9693	0.9699	0.9706
1.9	0.9713	0.9719	0.9726	0.9732	0.9738	0.9744	0.9750	0.9756	0.9761	0.9767
2.0	0.9772	0.9778	0.9783	0.9788	0.9793	0.9798	0.9803	0.9808	0.9812	0.9817
2.1	0.9821	0.9826	0.9830	0.9834	0.9838	0.9842	0.9846	0.9850	0.9854	0.9857
2.2	0.9861	0.9864	0.9868	0.9871	0.9875	0.9878	0.9881	0.9884	0.9887	0.9890
2.3	0.9893	0.9896	0.9898	0.9901	0.9904	0.9906	0.9909	0.9911	0.9913	0.9916
2.4	0.9918	0.9920	0.9922	0.9925	0.9927	0.9929	0.9931	0.9932	0.9934	0.9936
2.5	0.9938	0.9940	0.9941	0.9943	0.9945	0.9946	0.9948	0.9949	0.9951	0.9952
2.6	0.9953	0.9955	0.9956	0.9957	0.9959	0.9960	0.9961	0.9962	0.9963	0.9964
2.7	0.9965	0.9966	0.9967	0.9968	0.9969	0.9970	0.9971	0.9972	0.9973	0.9974
2.8	0.9974	0.9975	0.9976	0.9977	0.9977	0.9978	0.9979	0.9979	0.9980	0.9981
2.9	0.9981	0.9982	0.9982	0.9983	0.9984	0.9984	0.9985	0.9985	0.9986	0.9986
3.0	0.9987	0.9987	0.9987	0.9988	0.9988	0.9989	0.9989	0.9989	0.9990	0.9990

Integer and first decimal place

Table gives $F(z) = P(Z \leq z)$ for a wide range of z-values (0 to 3.09 by 0.01)

Notes:

- $P(Z \geq z) = 1 - F(z)$
- $P(Z \leq -z) = 1 - F(z)$
- $P(Z \geq -z) = F(z)$

R Program to Obtain Probabilities, Percentiles, Density Functions, and Random Sampling

```
# Obtain P(Y<=80|N(mu=100,sigma=20))
# pnorm gives lower tail probabilities (cdf) for a normal distribution
pnorm(80,mean=100,sd=20)

# Obtain P(Y>=80|N(mu=100,sigma=20))
# lower=FALSE option gives upper tail probabilities
pnorm(80,mean=100,sd=20,lower=FALSE)

# Obtain the 10th percentile of a Normal Density with mu=100, sigma=20
qnorm(0.10, mean=100, sd=20)

# Obtain a plot of a Normal Density with mu=100, sigma=20
# dnorm gives the density function for a normal distribution at point(s) y
# type="l" in plot function joins the points on the density function with a line
# The polygon command fills in the area below y=80 in green
y <- seq(40,160,0.01)
fy <- dnorm(y,mean=100,sd=20)

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\norm_dist1.png")

plot(y,fy,type="l",
main=expression(paste("Normal(",mu,"=100","sigma,"=20)"))
polygon(c(y[y<=80],80),c(fy[y<=80],fy[y==40]),col="green")

dev.off() # Close the .png file

# Obtain a random sample of 1000 items from N(mu=100,sigma=20)
# rnorm gives a random sample of size given by the first argument
# Obtain sample mean, median, variance, standard deviation

set.seed(54321) # Set the seed for random number generator for reproducing data
y.samp <- rnorm(1000,mean=100,sd=20)
mean(y.samp)
median(y.samp)
var(y.samp)
sd(y.samp)

# Plot a histogram of the sample values (Default bin size)
hist(y.samp, main = expression(paste("Sampled values, ", mu, "=100, ", sigma,
"=20")))

# Allow for more bins

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\norm_dist2.png")

hist(y.samp, breaks=23,
main = expression(paste("Sampled values, ", mu, "=100, ", sigma,
"=20")))

# Add normal density (scaled up by (n=1000 x binwidth=5), since a freq histogram)
# Makes use of y and fy defined above

lines(y,1000*5*fy)

dev.off() # Close the .png file
```

Numeric Output from R Program

```
>
> pnorm(80,mean=100,sd=20)
[1] 0.1586553
>
> pnorm(80,mean=100,sd=20,lower=FALSE)
[1] 0.8413447
>
> qnorm(0.10, mean=100, sd=20)
[1] 74.36897

> mean(y.samp)
[1] 98.80391
> median(y.samp)
[1] 98.95658
> var(y.samp)
[1] 407.2772
> sd(y.samp)
[1] 20.18111
```

Note that the first 3 values are easily computed using the z-table. The last 4 values would take lots of calculations based on a sample of 1000 observations.

$$Y \sim N(\mu = 100, \sigma^2 = 20^2 = 400)$$
$$P(Y \leq 80) = P\left(Z = \frac{Y - \mu}{\sigma} \leq \frac{80 - 100}{20} = -1\right) = P(Z \geq 1) = 1 - P(Z \leq 1) = 1 - .8413 = .1587$$
$$P(Y \geq 80) = P(Z \geq -1) = P(Z \leq 1) = .8413$$

10th-Percentile: From z-table: $P(Z \leq -1.28) = 1 - P(Z \leq 1.28) = 1 - .8997 = .1003 \approx .10$

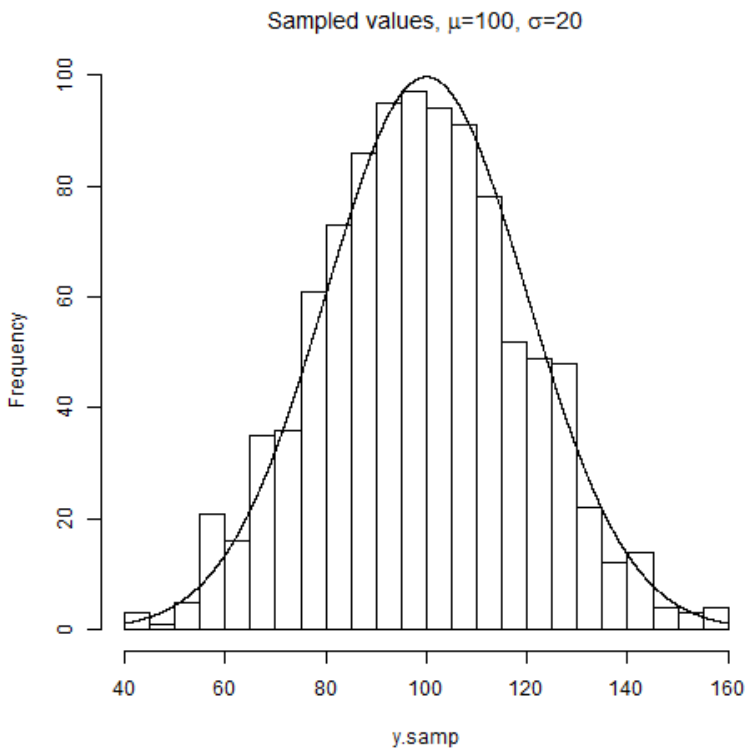
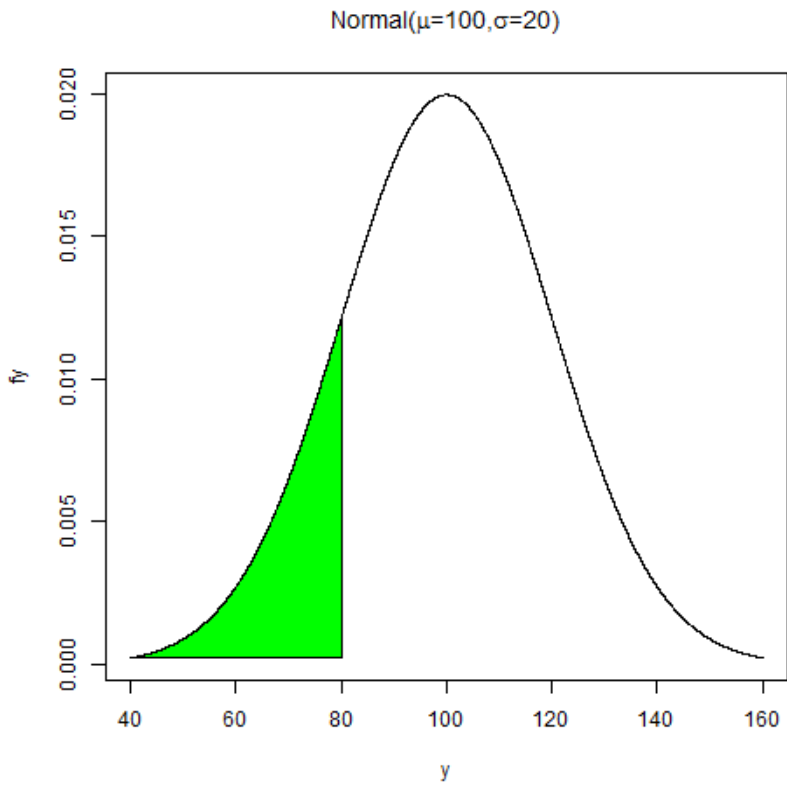
$$.10 \approx P(Z \leq -1.28) = P\left(Z = \frac{Y - \mu}{\sigma} \leq -1.28\right) = P(Y \leq -1.28\sigma + \mu) = P(Y \leq -1.28(20) + 100 = 74.4)$$

Cell	Result
A1	0.158655
A2	0.841345
A3	74.36897

EXCEL Output:

- Cell A1: =NORM.DIST(80,100,20,1)
- Cell A2: =1-NORM.DIST(80,100,20,1)
- Cell A3: =NORM.INV(0.1,100,20)

Graphics Output from R Program



1.7.2 Chi-Square Distribution

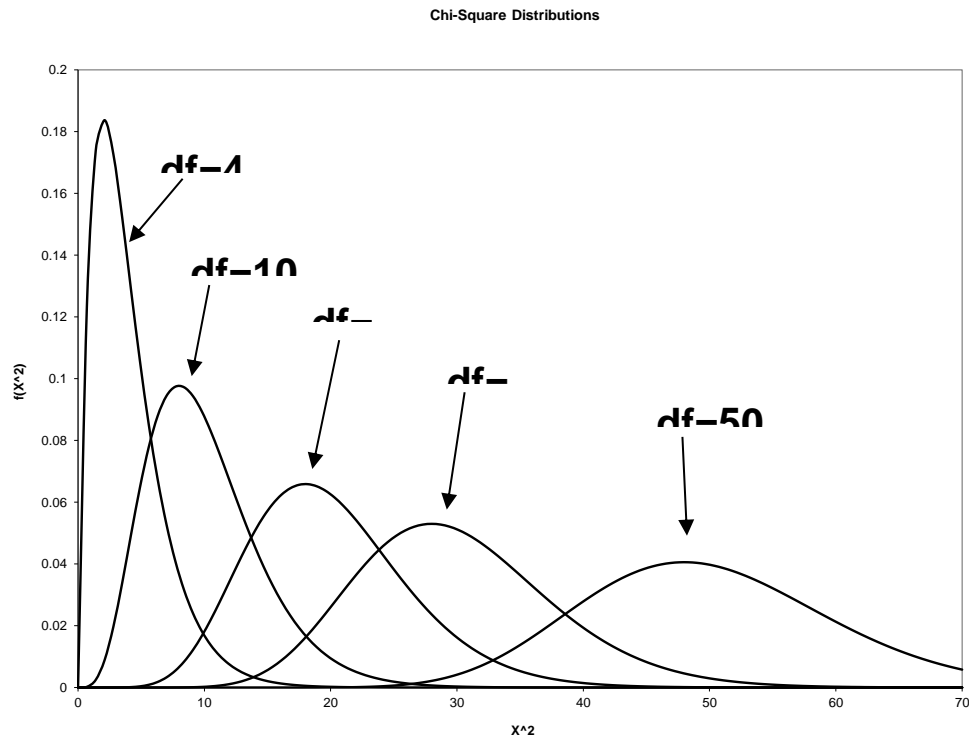
- Indexed by “degrees of freedom (ν)” $X \sim \chi_{\nu}^2$
- $Z \sim N(0,1) \Rightarrow Z^2 \sim \chi_1^2$
- Assuming Independence:

$$X_1, \dots, X_n \sim \chi_{\nu_i}^2 \quad i = 1, \dots, n \quad \Rightarrow \quad \sum_{i=1}^n X_i \sim \chi_{\sum \nu_i}^2$$

Density Function:

$$f(x) = \frac{1}{\Gamma\left(\frac{\nu}{2}\right) 2^{\nu/2}} x^{(\nu/2)-1} e^{-x/2} \quad x > 0, \nu > 0 \quad E\{X\} = \nu \quad V\{X\} = 2\nu$$

Probabilities can be obtained from software packages (e.g. EXCEL, R, SPSS, SAS, STATA). Tables can be used to obtain certain critical values for given upper and lower tail areas.



R Commands for Probabilities and Quantiles (Default are upper tail areas):

- **Density Function:** `dchisq(y,df)`
- **Lower tail (cumulative) probabilities:** `pchisq(y,df)`
- **Upper tail probabilities:** `1 - pchisq(y,df)`
- **p^{th} quantile:** `qchisq(p,df)` $0 < p < 1$
- **$(1-p)^{\text{th}}$ quantile:** `qchisq(1-p,df)` $0 < p < 1$

Critical Values for Chi-Square Distributions (Mean= v , Variance= $2v$)

df\F(x)	0.005	0.01	0.025	0.05	0.1	0.9	0.95	0.975	0.99	0.995
1	0.000	0.000	0.001	0.004	0.016	2.706	3.841	5.024	6.635	7.879
2	0.010	0.020	0.051	0.103	0.211	4.605	5.991	7.378	9.210	10.597
3	0.072	0.115	0.216	0.352	0.584	6.251	7.815	9.348	11.345	12.838
4	0.207	0.297	0.484	0.711	1.064	7.779	9.488	11.143	13.277	14.860
5	0.412	0.554	0.831	1.145	1.610	9.236	11.070	12.833	15.086	16.750
6	0.676	0.872	1.237	1.635	2.204	10.645	12.592	14.449	16.812	18.548
7	0.989	1.239	1.690	2.167	2.833	12.017	14.067	16.013	18.475	20.278
8	1.344	1.646	2.180	2.733	3.490	13.362	15.507	17.535	20.090	21.955
9	1.735	2.088	2.700	3.325	4.168	14.684	16.919	19.023	21.666	23.589
10	2.156	2.558	3.247	3.940	4.865	15.987	18.307	20.483	23.209	25.188
11	2.603	3.053	3.816	4.575	5.578	17.275	19.675	21.920	24.725	26.757
12	3.074	3.571	4.404	5.226	6.304	18.549	21.026	23.337	26.217	28.300
13	3.565	4.107	5.009	5.892	7.042	19.812	22.362	24.736	27.688	29.819
14	4.075	4.660	5.629	6.571	7.790	21.064	23.685	26.119	29.141	31.319
15	4.601	5.229	6.262	7.261	8.547	22.307	24.996	27.488	30.578	32.801
16	5.142	5.812	6.908	7.962	9.312	23.542	26.296	28.845	32.000	34.267
17	5.697	6.408	7.564	8.672	10.085	24.769	27.587	30.191	33.409	35.718
18	6.265	7.015	8.231	9.390	10.865	25.989	28.869	31.526	34.805	37.156
19	6.844	7.633	8.907	10.117	11.651	27.204	30.144	32.852	36.191	38.582
20	7.434	8.260	9.591	10.851	12.443	28.412	31.410	34.170	37.566	39.997
21	8.034	8.897	10.283	11.591	13.240	29.615	32.671	35.479	38.932	41.401
22	8.643	9.542	10.982	12.338	14.041	30.813	33.924	36.781	40.289	42.796
23	9.260	10.196	11.689	13.091	14.848	32.007	35.172	38.076	41.638	44.181
24	9.886	10.856	12.401	13.848	15.659	33.196	36.415	39.364	42.980	45.559
25	10.520	11.524	13.120	14.611	16.473	34.382	37.652	40.646	44.314	46.928
26	11.160	12.198	13.844	15.379	17.292	35.563	38.885	41.923	45.642	48.290
27	11.808	12.879	14.573	16.151	18.114	36.741	40.113	43.195	46.963	49.645
28	12.461	13.565	15.308	16.928	18.939	37.916	41.337	44.461	48.278	50.993
29	13.121	14.256	16.047	17.708	19.768	39.087	42.557	45.722	49.588	52.336
30	13.787	14.953	16.791	18.493	20.599	40.256	43.773	46.979	50.892	53.672
40	20.707	22.164	24.433	26.509	29.051	51.805	55.758	59.342	63.691	66.766
50	27.991	29.707	32.357	34.764	37.689	63.167	67.505	71.420	76.154	79.490
60	35.534	37.485	40.482	43.188	46.459	74.397	79.082	83.298	88.379	91.952
70	43.275	45.442	48.758	51.739	55.329	85.527	90.531	95.023	100.425	104.215
80	51.172	53.540	57.153	60.391	64.278	96.578	101.879	106.629	112.329	116.321
90	59.196	61.754	65.647	69.126	73.291	107.565	113.145	118.136	124.116	128.299
100	67.328	70.065	74.222	77.929	82.358	118.498	124.342	129.561	135.807	140.169

R Program to Obtain Probabilities, Percentiles, Density Functions, and Random Sampling

```
# Obtain P(Y<=5|X2(df=10))
# pchisq gives lower tail probabilities (cdf) for a chi-square distribution
pchisq(5,df=10)

# Obtain P(Y>=5|X2(df=10))
# lower=FALSE option gives upper tail probabilities
pchisq(5,df=10,lower=FALSE)

# Obtain the 95th percentile of a Chi-square Density with df=10
qchisq(0.95,df=10)

# Obtain a plot of a Chi-square Density with df=10
# dchisq gives the density function for a chi-square distribution at point(s) y
# type="l" in plot function joins the points on the density function with a line
# The polygon command fills in the area below y<5 in green

y <- seq(0,30,0.01)
fy <- dchisq(y,df=10)

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\chisq_dist1.png")

plot(y,fy,type="l",
main=expression(paste(chi^2,"(df=10)"))
polygon(c(y[y<=5],5),c(fy[y<=5],fy[y==0]),col="blue")

dev.off() # Close the .png file

# Obtain a random sample of 1000 items from Chi-square(df=10)
# rchisq gives a random sample of size given by the first argument
# Obtain sample mean, median, variance, standard deviation

set.seed(54321) # Set the seed for random number generator for reproducing data
y.samp <- rchisq(1000,df=10)
mean(y.samp)
median(y.samp)
var(y.samp)
sd(y.samp)

# Plot a histogram of the sample values (Default bin size)
hist(y.samp, main = expression(paste("Sampled values, ", chi^2, "(df=10)")))

# Allow for more bins

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\chisq_dist2.png")

hist(y.samp[y.samp<=30], breaks=29,
main = expression(paste("Sampled values, ", chi^2, "(df=10)")))

# Add chi-square density (scaled up by (n=1000 x binwidth=1), since a freq histogram)
# Makes use of y and fy defined above

lines(y,1000*1*fy)

dev.off() # Close the .png file
```

Numeric Output from R Program

```
>
> pchisq(5,df=10)
[1] 0.108822
>
> pchisq(5,df=10,lower=FALSE)
[1] 0.891178
>
> qchisq(0.95,df=10)
[1] 18.30704

> mean(y.samp)
[1] 9.834778
> median(y.samp)
[1] 9.060967
> var(y.samp)
[1] 21.78964
> sd(y.samp)
[1] 4.667937
```

Note that for the chi-square distribution, the mean is the degrees of freedom (v) and the variance is $2v$. The sample mean and variance are close to 10 and 20. As the sample size gets larger, they will tend to get closer. Also notice that the median is lower than the mean (right-skewed distribution).

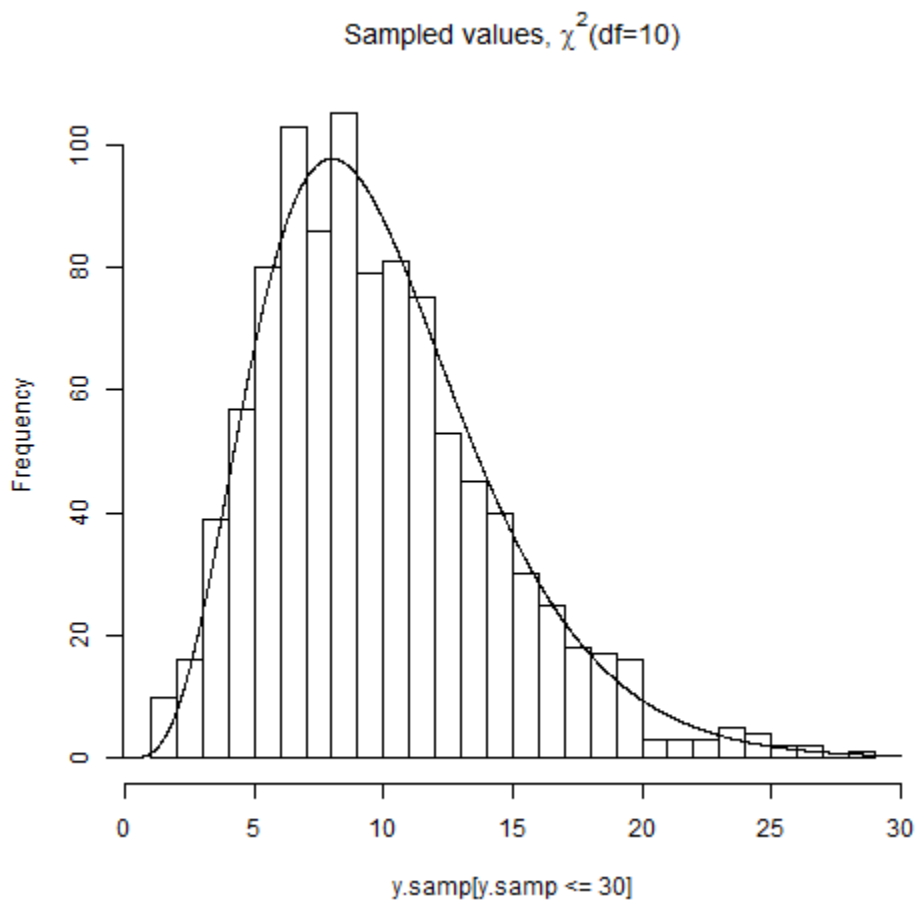
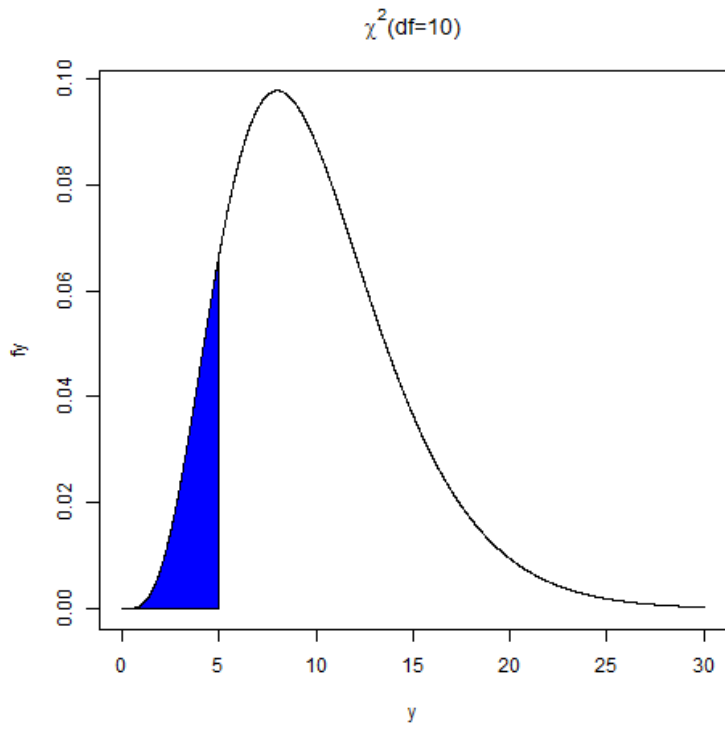
Confirm that the 95th-percentile is consistent with the table value.

Cell	Result
A1	0.108822
A2	0.891178
A3	18.30704

EXCEL Output:

- Cell A1: =CHISQ.DIST(5,10,1)
- Cell A2: =CHISQ.DIST.RT(5,10)
- Cell A3: =CHISQ.INV.RT(0.05,10)
- Cell A3: =CHISQ.INV(0.95,10)

Graphics Output from R Program

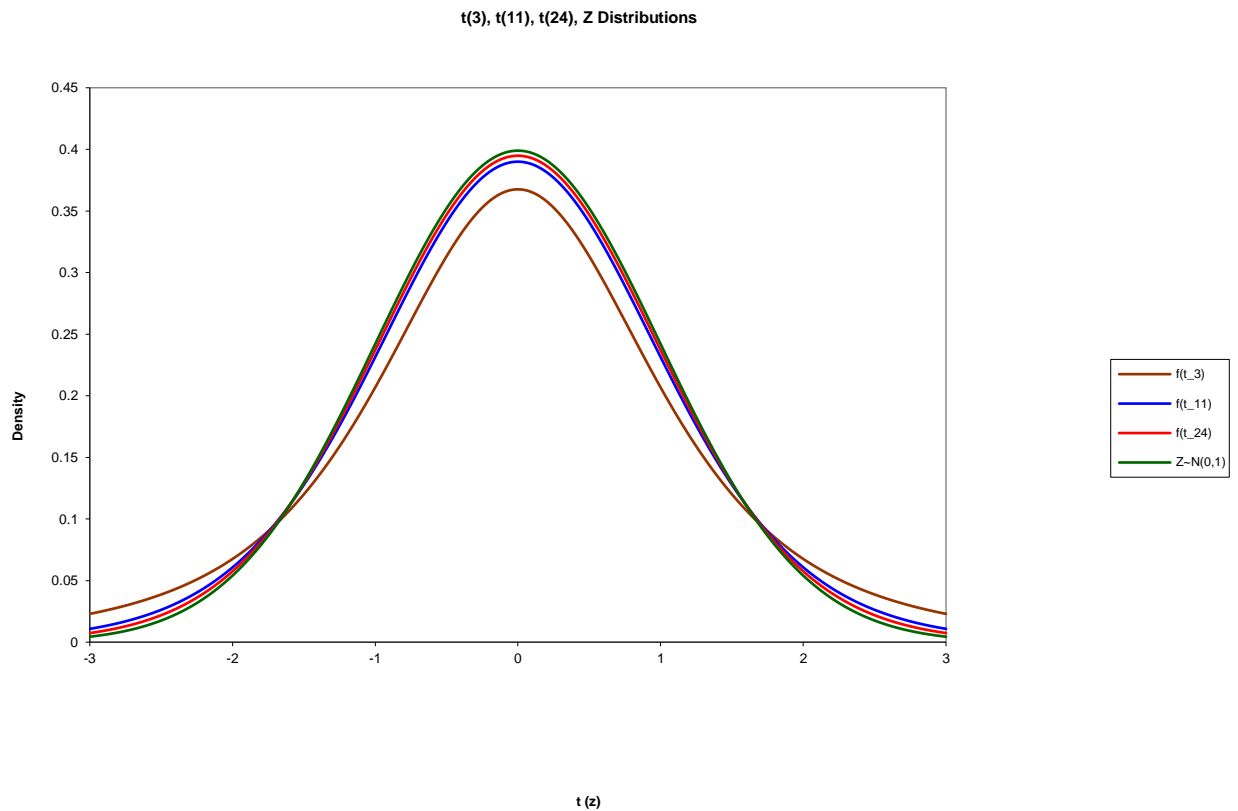


1.7.3 Student's t-Distribution

- Indexed by “degrees of freedom (ν)” $T \sim t_\nu$
- $Z \sim N(0,1)$, $X \sim \chi_\nu^2$
- Assuming Independence of Z and X :

$$T = \frac{Z}{\sqrt{X/\nu}} \sim t(\nu) \quad f(t) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)} (\nu\pi)^{-1/2} \left(1 + \frac{t^2}{\nu}\right)^{-(\nu+1)/2} \quad -\infty < t < \infty \quad \nu = 1, 2, \dots$$
$$E\{T\} = 0 \quad (\nu > 1) \quad V\{T\} = \frac{\nu}{\nu-2} \quad (\nu > 2)$$

Probabilities can be obtained from software packages (e.g. EXCEL, R, SPSS, SAS, STATA). Tables can be used to obtain certain critical values for given upper tail areas (distribution is symmetric around 0, as $N(0,1)$ is).



R Commands for Probabilities and Quantiles (Default are lower tail areas):

- Lower tail (cumulative) probabilities: $pt(y,df)$
- Upper tail probabilities: $1 - pt(y,df)$
- p^{th} quantile: $qt(p,df)$ $0 < p < 1$

Critical Values for Student's t-Distributions (Mean=0, Variance = $v/(v-2)$, $v>2$)

df\F(t)	0.9	0.95	0.975	0.99	0.995
1	3.078	6.314	12.706	31.821	63.657
2	1.886	2.920	4.303	6.965	9.925
3	1.638	2.353	3.182	4.541	5.841
4	1.533	2.132	2.776	3.747	4.604
5	1.476	2.015	2.571	3.365	4.032
6	1.440	1.943	2.447	3.143	3.707
7	1.415	1.895	2.365	2.998	3.499
8	1.397	1.860	2.306	2.896	3.355
9	1.383	1.833	2.262	2.821	3.250
10	1.372	1.812	2.228	2.764	3.169
11	1.363	1.796	2.201	2.718	3.106
12	1.356	1.782	2.179	2.681	3.055
13	1.350	1.771	2.160	2.650	3.012
14	1.345	1.761	2.145	2.624	2.977
15	1.341	1.753	2.131	2.602	2.947
16	1.337	1.746	2.120	2.583	2.921
17	1.333	1.740	2.110	2.567	2.898
18	1.330	1.734	2.101	2.552	2.878
19	1.328	1.729	2.093	2.539	2.861
20	1.325	1.725	2.086	2.528	2.845
21	1.323	1.721	2.080	2.518	2.831
22	1.321	1.717	2.074	2.508	2.819
23	1.319	1.714	2.069	2.500	2.807
24	1.318	1.711	2.064	2.492	2.797
25	1.316	1.708	2.060	2.485	2.787
26	1.315	1.706	2.056	2.479	2.779
27	1.314	1.703	2.052	2.473	2.771
28	1.313	1.701	2.048	2.467	2.763
29	1.311	1.699	2.045	2.462	2.756
30	1.310	1.697	2.042	2.457	2.750
40	1.303	1.684	2.021	2.423	2.704
50	1.299	1.676	2.009	2.403	2.678
60	1.296	1.671	2.000	2.390	2.660
70	1.294	1.667	1.994	2.381	2.648
80	1.292	1.664	1.990	2.374	2.639
90	1.291	1.662	1.987	2.368	2.632
100	1.290	1.660	1.984	2.364	2.626

R Program to Obtain Probabilities, Percentiles, Density Functions, and Random Sampling

```
# Obtain P(Y<=1|t(df=8))
# pt gives lower tail probabilities (cdf) for a t distribution
pt(1,df=8)

# Obtain P(Y>=1|t(df=8))
# lower=FALSE option gives upper tail probabilities
pt(1,df=8,lower=FALSE)

# Obtain the 90th percentile of a t Density with df=8
qt(0.90,df=8)

# Obtain a plot of a t Density with df=8
# dt gives the density function for a t-distribution at point(s) y
# type="l" in plot function joins the points on the density function with a line
# The polygon command fills in the area below y<1 in red
y <- seq(-4,4,0.01)
fy <- dt(y,df=8)

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\t_dist1.png")
plot(y,fy,type="l",
main="t(df=8)")
polygon(c(y[y<=1],1),c(fy[y<=1],fy[y==4]),col="red")
dev.off() # Close the .png file

# Obtain a random sample of 1000 items from t(df=8)
# rt gives a random sample of size given by the first argument
# Obtain sample mean, median, variance, standard deviation

set.seed(54321) # Set the seed for random number generator for reproducing data
y.samp <- rt(1000,df=8)
mean(y.samp)
median(y.samp)
var(y.samp)
sd(y.samp)

# Plot a histogram of the sample values (Default bin size)
hist(y.samp, main = "Sampled values, t(df=8)")

# Allow for more bins

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\t_dist2.png")

hist(y.samp[abs(y.samp)<=4], breaks=31,
main = "Sampled values, t(df=8)")

# Add t density (scaled up by (n=1000 x binwidth=0.25), since a freq histogram)
# Makes use of y and fy defined above

lines(y,1000*0.25*fy)

dev.off() # Close the .png file
```

Numeric Output from R Program

```
> pt(1,df=8)
[1] 0.8267032
>
> pt(1,df=8,lower=FALSE)
[1] 0.1732968
>
> qt(0.90,df=8)
[1] 1.396815

> mean(y.samp)
[1] -0.03754771
> median(y.samp)
[1] 0.0007432709
> var(y.samp)
[1] 1.43555
> sd(y.samp)
[1] 1.198145
```

Note that for the t distribution, the mean is 0, and the variance is $v/(v-2)$. The sample mean and variance are close to 0 and $8/6=1.333$. As the sample size gets larger, they will tend to get closer.

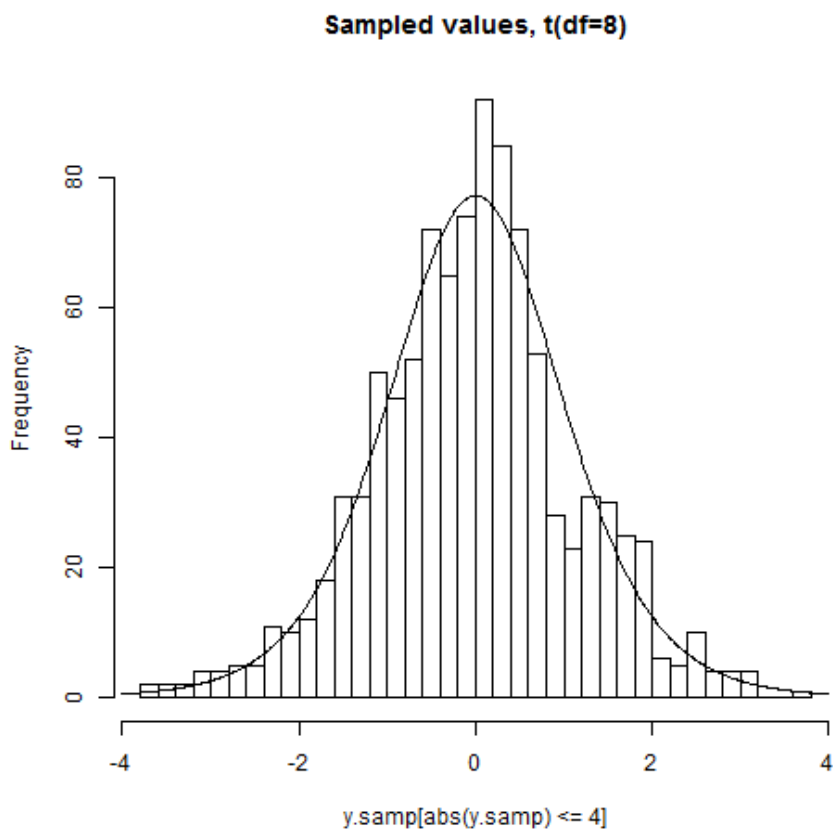
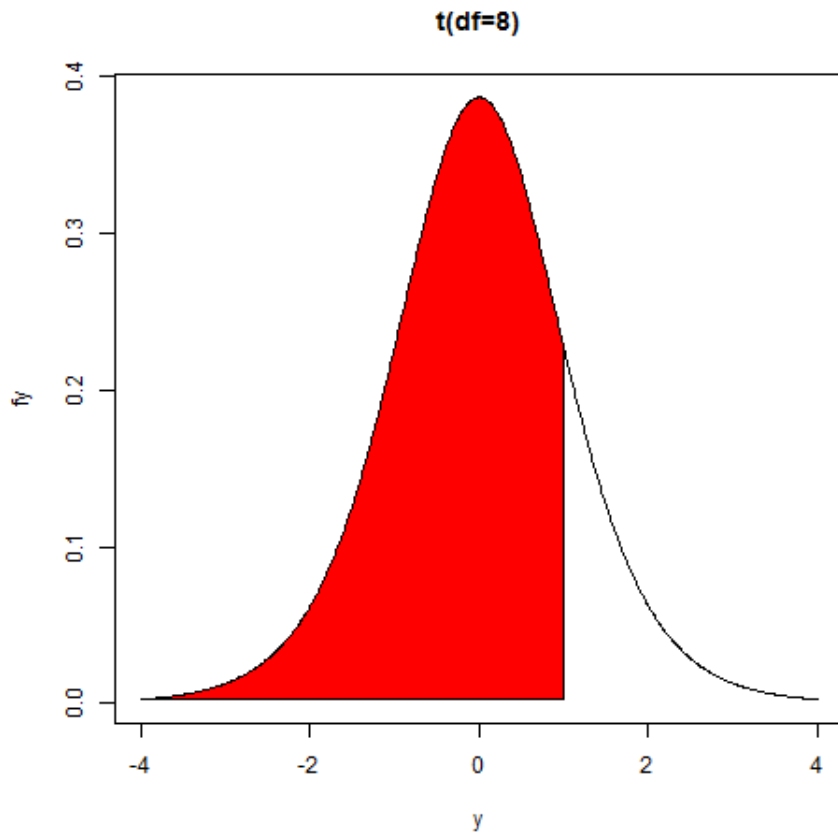
Confirm that the 90th-percentile is consistent with the table value.

Cell	Result
A1	0.826703
A2	0.173297
A3	1.396815

EXCEL Output:

- Cell A1: =T.DIST(1,8,1)
- Cell A2: =1-T.DIST(1,8,1) or =T.DIST.RT(1,8)
- Cell A3: =T.INV(0.9,8)

Graphics Output from R Program



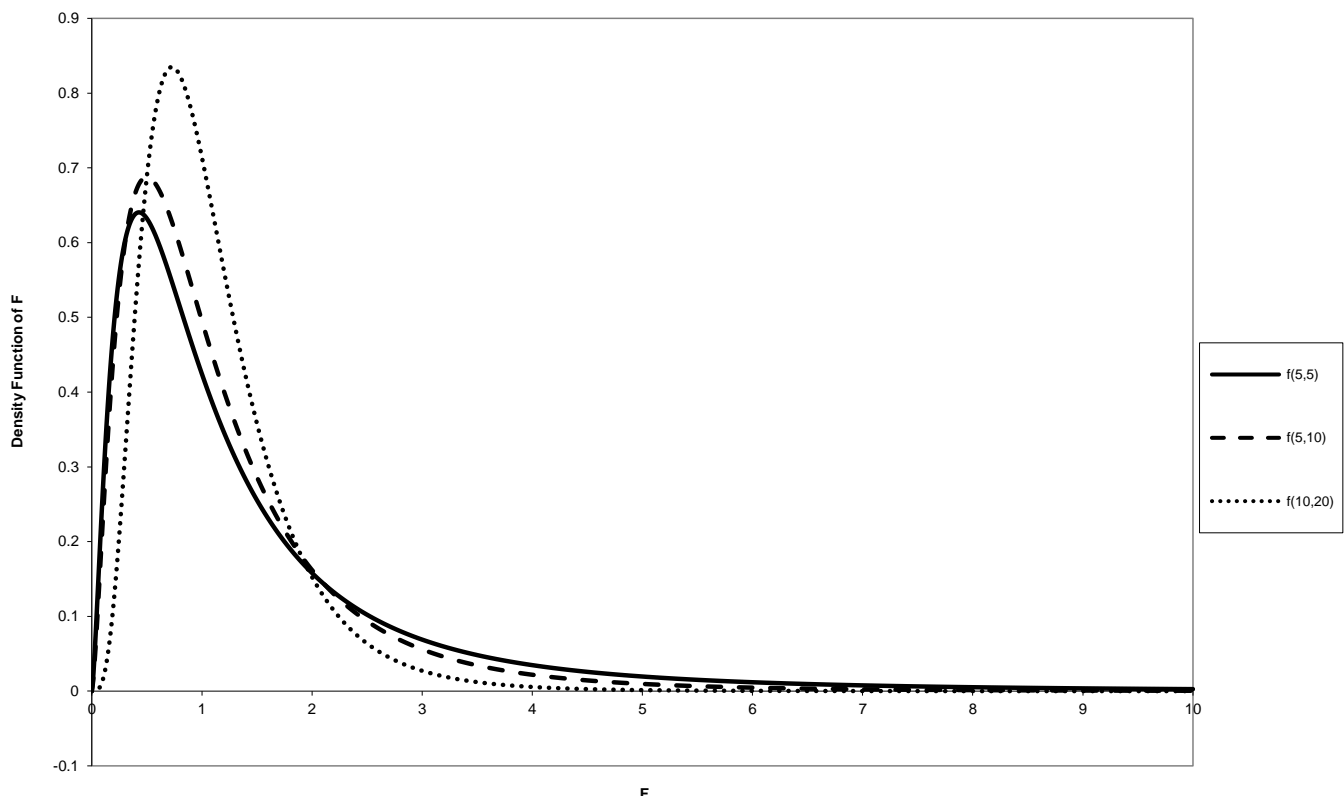
1.7.4 F-Distribution

- Indexed by 2 “degrees of freedom (ν_1, ν_2)” $W \sim F_{\nu_1, \nu_2}$
- $X_1 \sim \chi_{\nu_1}^2$, $X_2 \sim \chi_{\nu_2}^2$
- Assuming Independence of X_1 and X_2 :

$$W = \frac{X_1/\nu_1}{X_2/\nu_2} \sim F(\nu_1, \nu_2) \quad E\{W\} = \frac{\nu_2}{\nu_2 - 2} \quad (\nu_2 > 2) \quad V\{W\} = \frac{2\nu_2^2(\nu_1 + \nu_2 - 2)}{\nu_1(\nu_2 - 2)(\nu_2 - 4)} \quad (\nu_2 > 4)$$

Probabilities can be obtained from software packages (e.g. EXCEL, R, SPSS, SAS, STATA). Tables can be used to obtain certain critical values for given upper tail areas. Lower tails are obtained by taking the reciprocal of the upper tail with the degrees of freedom reversed.

F-Distributions



R Commands for Probabilities and Quantiles:

- Density function: `df(y,df1,df2)`
- Lower tail (cumulative) probabilities: `pf(y,df1,df2)`
- Upper tail probabilities: `1 - pf(y,df1,df2)`
- p^{th} quantile: `qf(p,df1,df2)` $0 < p < 1$

Critical Values for F-distributions $P(F \leq \text{Table Value}) = 0.95$

df2\df1	1	2	3	4	5	6	7	8	9	10
1	161.45	199.50	215.71	224.58	230.16	233.99	236.77	238.88	240.54	241.88
2	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40
3	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79
4	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96
5	6.61	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74
6	5.99	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06
7	5.59	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64
8	5.32	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35
9	5.12	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14
10	4.96	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98
11	4.84	3.98	3.59	3.36	3.20	3.09	3.01	2.95	2.90	2.85
12	4.75	3.89	3.49	3.26	3.11	3.00	2.91	2.85	2.80	2.75
13	4.67	3.81	3.41	3.18	3.03	2.92	2.83	2.77	2.71	2.67
14	4.60	3.74	3.34	3.11	2.96	2.85	2.76	2.70	2.65	2.60
15	4.54	3.68	3.29	3.06	2.90	2.79	2.71	2.64	2.59	2.54
16	4.49	3.63	3.24	3.01	2.85	2.74	2.66	2.59	2.54	2.49
17	4.45	3.59	3.20	2.96	2.81	2.70	2.61	2.55	2.49	2.45
18	4.41	3.55	3.16	2.93	2.77	2.66	2.58	2.51	2.46	2.41
19	4.38	3.52	3.13	2.90	2.74	2.63	2.54	2.48	2.42	2.38
20	4.35	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35
21	4.32	3.47	3.07	2.84	2.68	2.57	2.49	2.42	2.37	2.32
22	4.30	3.44	3.05	2.82	2.66	2.55	2.46	2.40	2.34	2.30
23	4.28	3.42	3.03	2.80	2.64	2.53	2.44	2.37	2.32	2.27
24	4.26	3.40	3.01	2.78	2.62	2.51	2.42	2.36	2.30	2.25
25	4.24	3.39	2.99	2.76	2.60	2.49	2.40	2.34	2.28	2.24
26	4.23	3.37	2.98	2.74	2.59	2.47	2.39	2.32	2.27	2.22
27	4.21	3.35	2.96	2.73	2.57	2.46	2.37	2.31	2.25	2.20
28	4.20	3.34	2.95	2.71	2.56	2.45	2.36	2.29	2.24	2.19
29	4.18	3.33	2.93	2.70	2.55	2.43	2.35	2.28	2.22	2.18
30	4.17	3.32	2.92	2.69	2.53	2.42	2.33	2.27	2.21	2.16
40	4.08	3.23	2.84	2.61	2.45	2.34	2.25	2.18	2.12	2.08
50	4.03	3.18	2.79	2.56	2.40	2.29	2.20	2.13	2.07	2.03
60	4.00	3.15	2.76	2.53	2.37	2.25	2.17	2.10	2.04	1.99
70	3.98	3.13	2.74	2.50	2.35	2.23	2.14	2.07	2.02	1.97
80	3.96	3.11	2.72	2.49	2.33	2.21	2.13	2.06	2.00	1.95
90	3.95	3.10	2.71	2.47	2.32	2.20	2.11	2.04	1.99	1.94
100	3.94	3.09	2.70	2.46	2.31	2.19	2.10	2.03	1.97	1.93

R Program to Obtain Probabilities, Percentiles, Density Functions, and Random Sampling

```
# Obtain P(Y<=2.5|F(df1=10,df2=8))
# pf gives lower tail probabilities (cdf) for a F distribution
pf(2.5,df1=10,df2=8)

# Obtain P(Y>=2.5|F(df1=10,df2=8))
# lower=FALSE option gives upper tail probabilities
pf(2.5,df1=10,df2=8,lower=FALSE)

# Obtain the 5th and 95th percentiles of a F Density with df1=10,df2=8
qf(0.05,df1=10,df2=8)
qf(0.95,df1=10,df2=8)

# Obtain a plot of a F Density with df1=10, df2=8
# df gives the density function for a F distribution at point(s) y
# type="l" in plot function joins the points on the density function with a line
# The polygon command fills in the area below y<2.5 in purple
y <- seq(0,10,0.01)
fy <- df(y,df1=10,df2=8)

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\f_dist1.png")
plot(y,fy,type="l",
main="F(df1=10,df2=8)")
polygon(c(y[y<=2.5],2.5),c(fy[y<=2.5],fy[y==0]),col="purple")
dev.off() # Close the .png file

# Obtain a random sample of 1000 items from F(df1=10,df2=8)
# rf gives a random sample of size given by the first argument
# Obtain sample mean, median, variance, standard deviation

set.seed(54321) # Set the seed for random number generator for reproducing data
y.samp <- rf(1000,df1=10,df2=8)
mean(y.samp)
median(y.samp)
var(y.samp)
sd(y.samp)

# Plot a histogram of the sample values (Default bin size)

hist(y.samp, main = "Sampled values, F(df1=10,df2=8)")

# Allow for more bins

# Output graph to a .png file in the following directory/file
png("E:\\blue_drive\\Rmisc\\graphs\\f_dist2.png")

hist(y.samp[y.samp<=10], breaks=19, ylim=c(0,400),
main = "Sampled values, F(df1=10,df2=8)")

# Add chi-square density (scaled up by (n=1000 x binwidth=0.5), since a freq histogram)
# Makes use of y and fy defined above

lines(y,1000*0.5*fy)

dev.off() # Close the .png file
```

Numeric Output from R Program

```
> pf(2.5,df1=10,df2=8)
[1] 0.8964058
>
> pf(2.5,df1=10,df2=8,lower=FALSE)
[1] 0.1035942
>
> qf(0.05,df1=10,df2=8)
[1] 0.325557
> qf(0.95,df1=10,df2=8)
[1] 3.347163

> mean(y.samp)
[1] 1.369505
> median(y.samp)
[1] 1.059021
> var(y.samp)
[1] 1.50341
> sd(y.samp)
[1] 1.226136
```

Note that for the F distribution, the mean and variance formulas are given below.

$$W \sim F(v_1, v_2) \quad E\{W\} = \frac{v_2}{v_2 - 2} \quad (v_2 > 2) \quad V\{W\} = \frac{2v_2^2(v_1 + v_2 - 2)}{v_1(v_2 - 2)(v_2 - 4)} \quad (v_2 > 4)$$

For this case, the mean is $8/6 = 1.333$ and the variance is $2048/1440 = 1.422$. Again the sample mean and variance would tend to be closer to the theoretical values as the sample size increases.

Confirm the 5th and 95th percentiles based on the F-table. Again note that the lower percentile can be obtained by taking the reciprocal of the upper percentile with the degrees of freedom reversed.

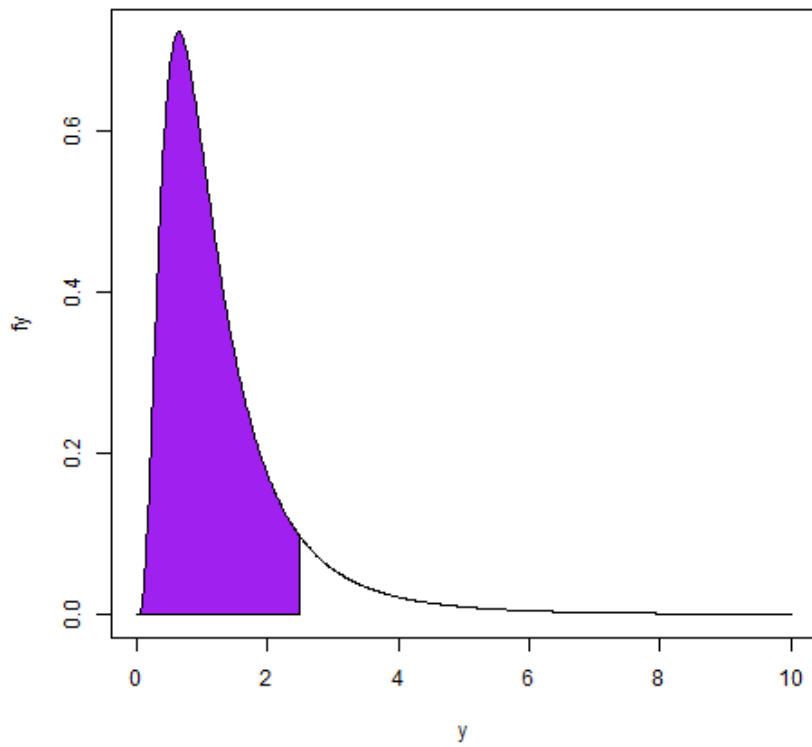
Cell	Result
A1	0.896406
A2	0.103594
A3	0.325557
A4	3.347163

EXCEL Output:

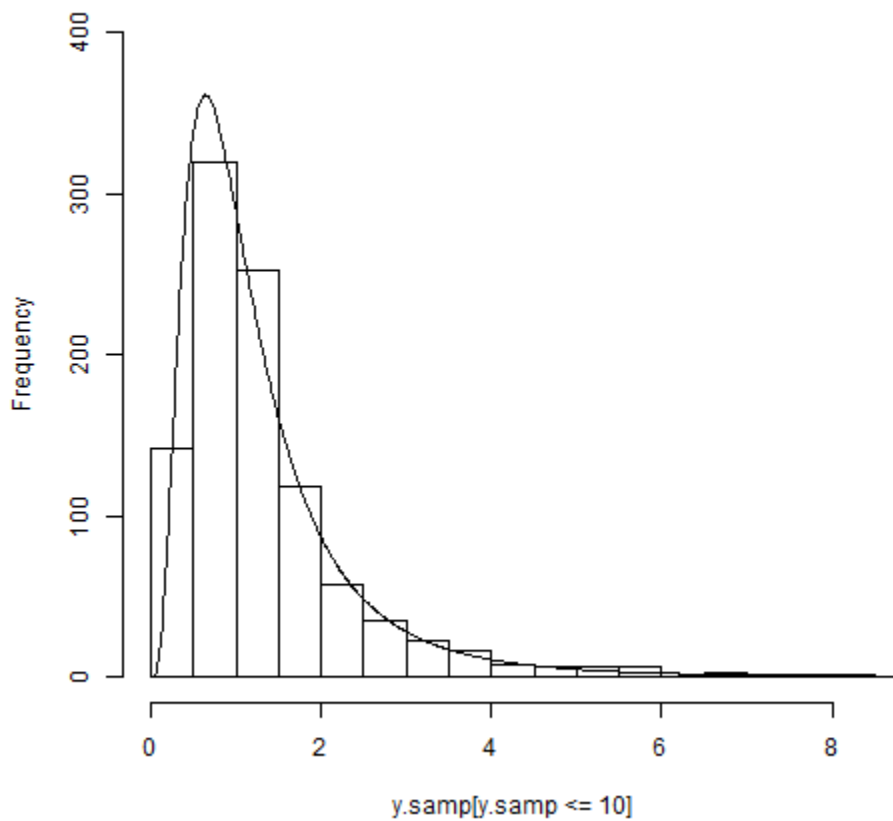
- Cell A1: =F.DIST(2.5,10,8,1)
- Cell A2: =F.DIST.RT(2.5,10,8)
- Cell A3: =F.INV(0.05,10,8)
- Cell A4: =F.INV.RT(0.05,10,8)

Graphics Output from R Program

F(df1=10,df2=8)



Sampled values, F(df1=10,df2=8)



1.8. Statistical Estimation: Properties

Properties of Estimators:

Parameter: θ Estimator: $\hat{\theta} \equiv$ function of Y_1, \dots, Y_n

1) Unbiased: $E\left\{\hat{\theta}\right\} = \theta$

2) Consistent: $\lim_{n \rightarrow \infty} P\left(\left|\hat{\theta} - \theta\right| \geq \varepsilon\right) = 0$ for any $\varepsilon > 0$

3) Sufficient if conditional joint probability of sample, given $\hat{\theta}$ does not depend on θ

4) Minimum Variance: $\sigma^2\left\{\hat{\theta}\right\} \leq \sigma^2\left\{\hat{\theta}^*\right\}$ for all $\hat{\theta}^*$

Note: If an estimator is unbiased (easy to show) and its variance goes to zero as its sample size gets infinitely large (often easy to show), it is consistent. It is tougher to show that it is Minimum Variance, but general results have been obtained in many standard cases.

1.9. Statistical Estimation: Methods

Maximum Likelihood (ML) Estimators:

$Y \sim f(y; \theta) \equiv$ Probability function for Y that depends on parameter θ

Random Sample (independent) Y_1, \dots, Y_n with joint probability function:

$$f(y_1, \dots, y_n) = \prod_{i=1}^n f(y_i; \theta)$$

When viewed as function of θ , given the observed data (sample):

Likelihood function: $L(\theta) = \prod_{i=1}^n f(y_i; \theta)$ Goal: maximize $L(\theta)$ with respect to θ .

Under general conditions, ML estimators are consistent and sufficient

Least Squares (LS) Estimators

$$Y_i = f_i(\theta) + \varepsilon_i$$

where $f_i(\theta)$ is a known function of the parameter θ and ε_i are random variables, usually with $E\{\varepsilon_i\} = 0$

Sum of Squares: $Q = \sum_{i=1}^n [Y_i - f_i(\theta)]^2$ Goal: minimize Q with respect to θ .

In many settings, LS estimators are unbiased and consistent.

1.10. Sampling Distribution of t-statistic and Inference Concerning Mean(s)

$$Y_1, \dots, Y_n \sim NID(\mu, \sigma^2)$$

$$\text{Sample Mean: } \bar{Y} = \frac{1}{n} \sum_{i=1}^n Y_i \Rightarrow \bar{Y} \sim N\left(\mu, \frac{\sigma^2}{n}\right) \quad Z = \frac{\bar{Y} - \mu}{\sigma/\sqrt{n}} \sim N(0,1)$$

$$\text{Sample Variance: } S^2 = \frac{1}{n-1} \sum_{i=1}^n (Y_i - \bar{Y})^2 \Rightarrow W = \frac{(n-1)S^2}{\sigma^2} \sim \chi_{n-1}^2$$

$$\bar{Y}, S^2 \text{ are independent (independent, normal data)} \quad t = \frac{Z}{\sqrt{W/v}} \sim t_v \quad (Z \perp W)$$

$$t = \frac{\left[\frac{\bar{Y} - \mu}{\sigma/\sqrt{n}} \right]}{\left[\sqrt{\frac{(n-1)S^2}{\sigma^2}} / (n-1) \right]} = \frac{\bar{Y} - \mu}{S/\sqrt{n}} \sim t_{n-1}$$

One-Sample Confidence Interval for μ

- **Simple Random Sample (SRS) from a population with mean μ is obtained.**
- **Sample mean, sample standard deviation are obtained (Lower case used for observed data)**
- **Degrees of freedom are $df = n-1$, and confidence level $(1-\alpha)$ are selected**
- **Level $(1-\alpha)$ confidence interval of form:**

$$V\{\bar{Y}\} = \frac{\sigma^2}{n} \Rightarrow \hat{V}\{\bar{Y}\} = \frac{S^2}{n} \Rightarrow \hat{SE}\{\bar{Y}\} = \frac{S}{\sqrt{n}} \quad \hat{SE}\{\bullet\} \text{ is the standard error of the estimator}$$

$$P\left\{-t(1-(\alpha/2); n-1) \leq \frac{\bar{Y} - \mu}{\hat{SE}\{\bar{Y}\}} \leq t(1-(\alpha/2); n-1)\right\} = 1 - \alpha =$$

$$= P\left\{\bar{Y} - t(1-(\alpha/2); n-1)\hat{SE}\{\bar{Y}\} \leq \mu \leq \bar{Y} + t(1-(\alpha/2); n-1)\hat{SE}\{\bar{Y}\}\right\}$$

$$\Rightarrow (1-\alpha)100\% \text{ CI for } \mu: \bar{y} \pm t(1-(\alpha/2); n-1)\hat{SE}\{\bar{Y}\} \quad \bar{y} = \frac{\sum_{i=1}^n y_i}{n} \quad s^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1} \quad \hat{SE}\{\bar{Y}\} = \frac{s}{\sqrt{n}}$$

Procedure is theoretically derived based on normally distributed data, but has been found to work well for most distributions for moderate to large n .

Example: Mercury Levels of Albacore Fish in the Eastern Mediterranean

Sample: $n = 34$ albacore fish caught in the Eastern Mediterranean Sea. Response is Mercury level (mg/kg).
 Goal: Treating this as a random sample of all albacore in the area, obtain 95% Confidence Interval for the population mean mercury level.

Fish	1	2	3	4	5	6	7	8	9	10	11	12
Mercury	1.007	1.447	0.763	2.01	1.346	1.243	1.586	0.821	1.735	1.396	1.109	0.993
Fish	13	14	15	16	17	18	19	20	21	22	23	24
Mercury	2.007	1.373	2.242	1.647	1.35	0.948	1.501	1.907	1.952	0.996	1.433	0.866
Fish	25	26	27	28	29	30	31	32	33	34	Mean	StdDev
Mercury	1.049	1.665	2.139	0.534	1.027	1.678	1.214	0.905	1.525	0.763	1.358147	0.440703

$$(1 - \alpha) = 0.95 \Rightarrow \alpha = 0.05 \quad n = 34$$

$$\Rightarrow t(1 - \alpha / 2; n - 1) = t(1 - 0.05 / 2; 34 - 1) = t(0.975; 33) = 2.0345$$

$$\bar{y} = 1.3581 \quad s = 0.4407 \Rightarrow \hat{SE}\{\bar{Y}\} = \frac{s}{\sqrt{n}} = \frac{0.4407}{\sqrt{34}} = 0.0756$$

$$\bar{y} \pm t(1 - \alpha / 2; n - 1) \hat{SE}\{\bar{Y}\} \equiv 1.3581 \pm 2.0345(0.0756)$$

$$\equiv 1.3581 \pm 0.1538 \equiv (1.2043, 1.5119)$$

If all possible random samples of size 34 had been obtained, and this calculation had been made for each sample, then approximately 95% of all sample Confidence Intervals would contain the true unknown population mean level μ . Thus we can be 95% confident that μ is between 1.2043 and 1.5119. Note that 90% and 99% Confidence Intervals based on this same sample are as follow (confirm them, and why the lengths differ):

90% Confidence Interval for μ : (1.2302 , 1.4861) 99% Confidence Interval for μ : (1.1516 , 1.5647)

1-Sample t -test (2-tailed alternative)

- **2-sided Test:** $H_0: \mu = \mu_0$ $H_a: \mu \neq \mu_0$
- **Decision Rule :**
 - Conclude $\mu > \mu_0$ if Test Statistic (t_{obs}) $> t(1 - \alpha / 2; n - 1)$
 - Conclude $\mu < \mu_0$ if Test Statistic (t_{obs}) $< - t(1 - \alpha / 2; n - 1)$
 - Do not conclude Conclude $\mu \neq \mu_0$ otherwise
- **P-value:** $2P(t(n-1) \geq |t_{obs}|)$
- **Test Statistic:**

$$t_{obs} = \frac{\bar{y} - \mu_0}{\hat{SE}\{\bar{Y}\}} \quad \hat{SE}\{\bar{Y}\} = \frac{s}{\sqrt{n}}$$

1-tailed alternative tests

Upper Tailed $H_0^+ : \mu \leq \mu_0$ $H_A^+ : \mu > \mu_0$

Decision Rule: Reject H_0^+ if $t_{obs} \geq t(1 - \alpha; n - 1)$

P-value: $P(t_{n-1} \geq t_{obs})$

Lower Tailed $H_0^- : \mu \geq \mu_0$ $H_A^- : \mu < \mu_0$

Decision Rule: Reject H_0^- if $t_{obs} \leq -t(1 - \alpha; n - 1)$

P-value: $P(t_{n-1} \leq t_{obs})$

Note: Tests for μ are generally used when trying to show whether a mean differs from, is above or below some pre-specified value; or when the data are paired differences (such as before/after treatment measures).

Example: The European Union has a permissible limit of 1 mg/kg of Mercury in fish. Is $\mu > 1$?

$$H_0 : \mu \leq \mu_0 = 1 \quad H_A : \mu > \mu_0 = 1$$
$$TS : t_{obs} = \frac{\bar{y} - \mu_0}{\hat{SE}\{\bar{Y}\}} = \frac{1.3581 - 1}{0.0756} = 4.7836 \geq t(0.95; 33) = 1.6924 \quad \text{Reject } H_0, \text{ Conclude } \mu > 1$$
$$P\text{-value: } P(t_{33} \geq 4.7836) = .00002$$

Comparing 2 Means - Independent Samples

- Observed individuals/items from the 2 groups are samples from distinct populations (identified by (μ_1, σ_1^2) and (μ_2, σ_2^2))
- Measurements across groups are independent
- Summary statistics obtained from the 2 groups

$$\text{Sample 1: } Y_{11}, Y_{12}, \dots, Y_{1n_1} \quad Y_{1\bullet} = \sum_{j=1}^{n_1} Y_{1j} \quad \bar{Y}_{1\bullet} = \frac{Y_{1\bullet}}{n_1} \quad S_1^2 = \frac{1}{n_1 - 1} \sum_{j=1}^{n_1} (Y_{1j} - \bar{Y}_{1\bullet})^2$$

$$\text{Sample 2: } Y_{21}, Y_{22}, \dots, Y_{2n_2} \quad Y_{2\bullet} = \sum_{j=1}^{n_2} Y_{2j} \quad \bar{Y}_{2\bullet} = \frac{Y_{2\bullet}}{n_2} \quad S_2^2 = \frac{1}{n_2 - 1} \sum_{j=1}^{n_2} (Y_{2j} - \bar{Y}_{2\bullet})^2$$

Sampling Distribution of $\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}$

- Underlying distributions normal \Rightarrow sampling distribution is normal, and resulting t-distribution with estimated std. dev. (when $\sigma_1^2 = \sigma_2^2 = \sigma^2$)
- Mean, variance, standard error (Std. Dev. of estimator)

$$E\{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}\} = \mu_{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}} = \mu_1 - \mu_2$$

$$V\{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}\} = \sigma_{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}}^2 = \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} \quad SE\{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}\} = \sigma_{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}} = \sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}$$

$$\hat{SE}\{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}\} = \sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}$$

$$\sigma_1^2 = \sigma_2^2 \Rightarrow \frac{(\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}) - (\mu_1 - \mu_2)}{\hat{SE}\{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}\}} \sim t \text{ with } df = n_1 + n_2 - 2$$

$$\text{where: } \hat{SE}\{\bar{Y}_{1\bullet} - \bar{Y}_{2\bullet}\} = S \sqrt{\left(\frac{1}{n_1} + \frac{1}{n_2}\right)} \quad S^2 = \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{n_1 + n_2 - 2}$$

Inference for $\mu_1 - \mu_2$ - Normal Populations – Equal variances

$(1 - \alpha)100\%$ Confidence Interval:

$$\left(\bar{y}_{1\cdot} - \bar{y}_{2\cdot}\right) \pm t(1 - \alpha / 2; n_1 + n_2 - 2) \hat{SE}\left\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\right\}$$

- Interpretation (at the α significance level):
 - If interval contains 0, do not reject $H_0: \mu_1 = \mu_2$
 - If interval is strictly positive, conclude that $\mu_1 > \mu_2$
 - If interval is strictly negative, conclude that $\mu_1 < \mu_2$

$$H_0 : \mu_1 - \mu_2 = 0 \quad H_A : \mu_1 - \mu_2 \neq 0$$

$$\text{Test Stat : } t_{obs} = \frac{\bar{y}_{1\cdot} - \bar{y}_{2\cdot}}{\hat{SE}\left\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\right\}}$$

$$\text{Reject Reg : } |t_{obs}| \geq t(1 - \alpha / 2; n_1 + n_2 - 2)$$

Example – Children’s Participation in Meal Preparation and Caloric Intake

Experiment had 2 conditions: Child participated in Cooking Meal, and Parent only cooking meal. Response measured: Total Energy Intake (kcal). Total of 47 participants: 25 Child cooks (Y_{1j}), 22 Parent cooks (Y_{2j}).

Child Cooks: $\bar{y}_{1\cdot} = 431.4$ $s_1 = 105.7$ $n_1 = 25$ Parent Cooks: $\bar{y}_{2\cdot} = 346.8$ $s_2 = 99.5$ $n_2 = 22$

$$\bar{y}_{1\cdot} - \bar{y}_{2\cdot} = 431.4 - 346.8 = 84.6 \quad t(1 - .05 / 2; 25 + 22 - 2) = t(.975; 45) = 2.0141$$

$$s^2 = \frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{n_1 + n_2 - 2} = \frac{(25 - 1)105.7^2 + (22 - 1)99.5^2}{25 + 22 - 2} = \frac{476045}{45} = 10578.78 \Rightarrow s = 102.8532$$

$$\hat{SE}\left\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\right\} = s \sqrt{\left(\frac{1}{n_1} + \frac{1}{n_2}\right)} = 102.8532 \sqrt{\left(\frac{1}{25} + \frac{1}{22}\right)} = 102.8532(0.2923) = 30.0667$$

$$95\% \text{ CI for } \mu_1 - \mu_2 : \left(\bar{y}_{1\cdot} - \bar{y}_{2\cdot}\right) \pm t(.975; 45) \hat{SE}\left\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\right\} \equiv 84.6 \pm 2.0141(30.0667) \equiv 84.6 \pm 60.6 \equiv (24.0, 145.2)$$

Testing: $H_0 : \mu_1 - \mu_2 = 0$ vs $H_A : \mu_1 - \mu_2 \neq 0$

$$TS : t_{obs} = \frac{\bar{y}_{1\cdot} - \bar{y}_{2\cdot}}{\hat{SE}\left\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\right\}} = \frac{84.6}{30.0667} = 2.8137 > t(.975; 45) = 2.0141 \quad P = 2P(t_{45} \geq 2.8137) = 2(.0036) = .0072$$

Power & Sample Size Computation for Independent Sample t-test

Consider the case where we test $H_0: \mu_1 - \mu_2 = 0$ versus $H_A: \mu_1 - \mu_2 \neq 0$ at significance level of α . Assuming equal variances ($\sigma_1^2 = \sigma_2^2 = \sigma^2$) and sample sizes ($n_1 = n_2 = n$), we have the following (we will need an estimate of σ or keep Δ in standard deviation units).

$$\text{Under } H_0: \mu_1 - \mu_2 = 0 \quad t_{obs} = \frac{\frac{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}}{\sigma\sqrt{\frac{2}{n}}}}{(s/\sigma)} = \frac{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}}{s\sqrt{\frac{2}{n}}} \sim t_{2(n-1)} \quad \text{Reject } H_0 \text{ if } |t_{obs}| \geq t(1 - (\alpha/2); 2(n-1))$$

$$\text{Under } H_A: \mu_1 - \mu_2 = \Delta \neq 0 \quad t_\delta = \frac{(\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot})}{s\sqrt{\frac{2}{n}}} \sim t_{2(n-1),\delta} \quad \text{where: } \delta = \frac{\Delta}{\sigma\sqrt{\frac{2}{n}}} = \frac{\Delta}{SE\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\}}$$

$T = \frac{Z + \delta}{\sqrt{\chi^2/\nu}} \sim t_{\nu,\delta}$ is the Non-central t -distribution with ν degrees of freedom and non-centrality parameter δ

Power: $\pi_\delta = P(t_{obs} \geq t(1 - (\alpha/2); 2(n-1)) | t_{obs} \sim t_{2(n-1),\delta}) + P(t_{obs} \leq t(\alpha/2; 2(n-1)) | t_{obs} \sim t_{2(n-1),\delta})$

The necessary quantiles and probabilities needed for these computations are available in R, with the **qt** and **pt** functions. These functions are given below.

$$t((1 - \alpha/2), 2(n-1)) \equiv qt((1 - \alpha/2), 2(n-1))$$

$$\pi_\delta = P(t_{obs} \geq t(1 - (\alpha/2); 2(n-1)) | t_{obs} \sim t_{2(n-1),\delta}) + P(t_{obs} \leq t(\alpha/2; 2(n-1)) | t_{obs} \sim t_{2(n-1),\delta})$$

$$\equiv 1 - pt(qt((1 - \alpha/2), 2(n-1)), 2(n-1), \delta) + pt(qt(\alpha/2, 2(n-1)), 2(n-1), \delta)$$

An R Program to compute power for the independent sample t-test is given here.

```
### Power of 2-sample t-test
library(power)
alt.side <- 1
group1.n <- 20
group2.n <- 20
alpha <- 0.05
alt.diff <- 5
sigma <- 10

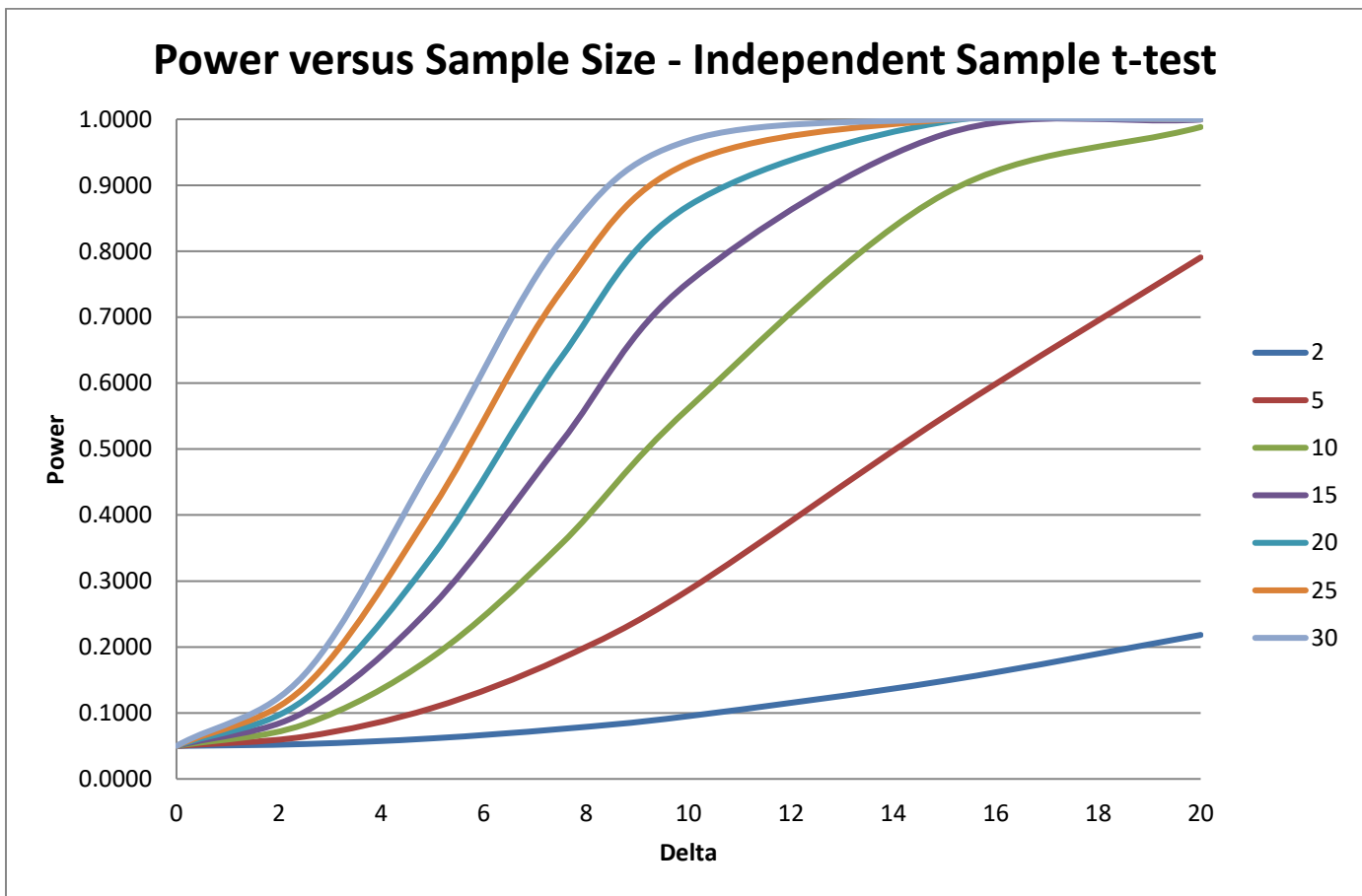
se.diff <- sigma*sqrt((1/group1.n)+(1/group2.n))
df.diff <- group1.n + group2.n - 2
delta.diff <- alt.diff / se.diff

power.2ttest <- function(alt.side, alpha, df.diff, delta.diff) {
  if (alt.side == 2) {
    power.diff <- 1-pt(qt(1-alpha/2,df.diff), df.diff, delta.diff) +
      pt(qt(alpha/2,df.diff), df.diff, delta.diff)
  }
  else power.diff <- 1-pt(qt(1-alpha,df.diff), df.diff, delta.diff)
  return(power.diff)
}

power.2ttest(alt.side, alpha, df.diff, delta.diff)
```

For $\sigma = 10$, and $\Delta = (0, 2.5, 5, 7.5, 10, 15, 20)$ we have the following powers for selected sample sizes n .

n\Delta	0	2.5	5	7.5	10	15	20
2	0.0500	0.0529	0.0615	0.0757	0.0952	0.1487	0.2183
5	0.0500	0.0642	0.1077	0.1822	0.2863	0.5494	0.7905
10	0.0500	0.0827	0.1851	0.3551	0.5620	0.8870	0.9882
15	0.0500	0.1014	0.2624	0.5093	0.7529	0.9774	0.9996
20	0.0500	0.1203	0.3379	0.6374	0.8690	0.9961	1.0000
25	0.0500	0.1394	0.4101	0.7384	0.9337	0.9994	1.0000
30	0.0500	0.1586	0.4779	0.8150	0.9677	0.9999	1.0000



Comparing 2 Means – Paired (Matched) Samples

- Individual or matched pair observations are made in 2 conditions (or before/after treatment exposure) for n individuals or matched pairs:

$$Y_{1j} \sim NID(\mu_1, \sigma_1^2) \quad Y_{2j} \sim NID(\mu_2, \sigma_2^2) \quad \text{COV}\{Y_{1j}, Y_{2j}\} = \sigma_{12} = \rho\sigma_1\sigma_2$$

- Measurements across groups are dependent (due to matched pairs/individuals)
- Summary statistics obtained from the 2 conditions

Condition 1: $Y_{11}, Y_{12}, \dots, Y_{1n}$	Condition 2: $Y_{21}, Y_{22}, \dots, Y_{2n}$
$D_j = Y_{1j} - Y_{2j}$	$E\{D_j\} = \mu_1 - \mu_2 = \mu_D$
$\bar{D} = \frac{1}{n} \sum_{j=1}^n d_j$	$V\{D_j\} = \sigma_1^2 + \sigma_2^2 - 2\sigma_{12} = \sigma_D^2$
$S_D^2 = \frac{1}{n-1} \sum_{j=1}^n (D_j - \bar{D})^2$	$S_D^2 = S_1^2 + S_2^2 - 2S_{12}$
$\frac{\bar{D} - \mu_D}{\sigma_D/\sqrt{n}} \sim N(0,1)$	$S_{12} = \frac{1}{n-1} \sum_{j=1}^n (Y_{1j} - \bar{Y}_{1\cdot})(Y_{2j} - \bar{Y}_{2\cdot})$
$\frac{(n-1)S_D^2}{\sigma_D^2} \sim \chi_{n-1}^2$	$\bar{d} \pm s_d^2 \Rightarrow t = \frac{\bar{D} - \mu_D}{S_D/\sqrt{n}} \sim t_{n-1}$
(1- α)100% CI for μ_D : $\bar{d} \pm t(1-(\alpha/2); n-1) \hat{SE}\{\bar{D}\}$	$s_d^2 = \frac{1}{n-1} \sum_{j=1}^n (d_j - \bar{d})^2$
Test Statistic for testing $H_0: \mu_D = \mu_{D0}$:	$\hat{SE}\{\bar{D}\} = \frac{s_d}{\sqrt{n}}$
$t_{obs} = \frac{\bar{d} - \mu_{D0}}{s_d/\sqrt{n}}$	

Example – Interference Effect in Reading Task Times (Stroop Effect)

Subjects read a list of color names. In condition 1, the word was written in a different color (e.g. the word “Blue” was written in Red ink. In condition 2, the word was written in standard black ink. Each subject read a list of color names under each condition (hopefully, in random order). Inference is interested in the difference of the true population mean reading times for the 2 conditions.

Data: $n = 70$	$\bar{d} = \bar{y}_1 - \bar{y}_2 = 2.39$	$s_d = 7.81$	$\hat{SE}\{\bar{d}\} = \frac{7.81}{\sqrt{70}} = 0.93$
$t(.975; 70-1 = 69) = 1.995$			
95% CI for μ_D : $2.39 \pm 1.995(0.93) \equiv 2.39 \pm 1.86 \equiv (0.53, 4.25)$			
$H_0: \mu_D = 0 \quad H_A: \mu_D \neq 0 \quad TS: t_{obs} = \frac{2.39 - 0}{0.93} = 2.57 \quad RR: t_{obs} \geq 1.995$			
P-value: $2P(t_{69} \geq 2.57) = .0123$			

Power & Sample Size Computation for Paired Sample t-test

Consider the case where we test $H_0: \mu_1 - \mu_2 = 0$ versus $H_A: \mu_1 - \mu_2 \neq 0$ at significance level of α . We have (with a ball-park estimate of $\sigma_1 = \sigma_2 = \sigma$ and ρ which provides an estimate of σ_D):

Under $H_0: \mu_1 - \mu_2 = \mu_\delta = 0$ $t = \frac{\bar{D}}{\left(\frac{S_D}{\sqrt{n}}\right)} \sim t_{n-1}$ Reject H_0 if $|t| \geq t(1 - (\alpha/2); n-1)$

Under $H_A: \mu_1 - \mu_2 = \mu_D = \Delta \neq 0$ $t_\delta = \frac{\bar{D}}{\left(\frac{S_D}{\sqrt{n}}\right)} \sim t_{n-1,\delta}$ $\delta = \sqrt{n} \frac{\Delta}{\sigma_D}$ $\sigma_D = \sqrt{\sigma_1^2 + \sigma_2^2 + 2\rho\sigma_1\sigma_2}$

Power: $\pi_\Delta = P(t \geq t(1 - (\alpha/2); n-1) | t \sim t_{n-1,\delta}) + P(t \leq t(\alpha/2; n-1) | t \sim t_{n-1,\delta})$

For $\sigma = 10$, $\rho = (0.0, 0.4, 0.8)$ and $\Delta = (5, 10, 15, 20)$, we obtain the following powers.

Rho	0				0.4				0.8			
n\Delta	5	10	15	20	5	10	15	20	5	10	15	20
5	0.0949	0.2313	0.4402	0.6625	0.1253	0.3471	0.6360	0.8566	0.2757	0.7528	0.9712	0.9989
10	0.1706	0.5144	0.8464	0.9772	0.2527	0.7292	0.9696	0.9991	0.6061	0.9930	1.0000	1.0000
15	0.2477	0.7215	0.9680	0.9991	0.3772	0.9073	0.9984	1.0000	0.8123	0.9999	1.0000	1.0000
20	0.3236	0.8506	0.9943	1.0000	0.4912	0.9718	0.9999	1.0000	0.9180	1.0000	1.0000	1.0000

2-Sample Permutation/Randomization Tests

Independent Samples

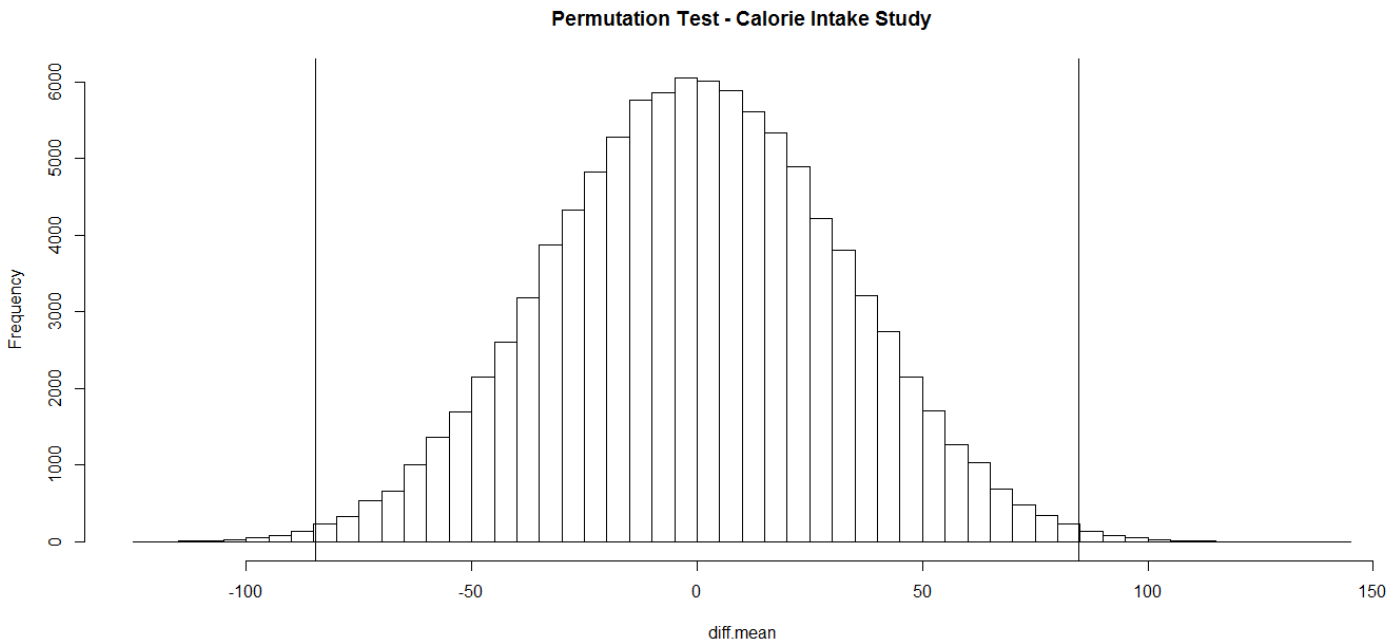
Under the null hypothesis of no differences between the two treatments/conditions, all experimental units can be thought of as coming from the same population. Then their assignment to treatments or groups can be considered to be random, having no effect on their measurements. We can obtain a measure of the magnitude of the difference between their sample means, and compare the magnitude of the difference with the reference distribution of all possible permutations of the measurements to the groups. If the observed difference is sufficiently large compared to the reference distribution, we can conclude that the true population means differ. We can consider both 1-tailed ($\mu_1 - \mu_2 > 0$) and 2-tailed alternatives ($\mu_1 - \mu_2 \neq 0$). Note that unless n_1 and n_2 are very small, there will be very many possible permutations of the data which would be virtually impossible to cycle through. We can computationally obtain many resamples to approximate the reference distribution.

No distributional assumptions are necessary to conduct the test.

Example – Children’s Participation in Meal Preparation and Caloric Intake

The observed sample means for the Child Cooks and Parent Cooks conditions are 431.4 and 346.8 calories per child, respectively. The observed mean difference is $431.4 - 346.8 = 84.6$ calories per child. The $N=47$ observations were permuted 99999 times into samples of $n_1 = 25$ and $n_2 = 22$ subjects per treatment and the mean difference was computed for each resample. Of the 99999 mean differences, only 706 were as large or larger in absolute value than the observed mean difference, resulting in a P -value of:

$$P\text{-Value} = \frac{[\# \text{ of permutation samples with } \text{abs}(\text{mean difference}) \geq \text{abs}(\text{observed mean difference})] + 1}{[\# \text{ of permutation samples}] + 1} = \frac{706 + 1}{99999 + 1} = 0.00707$$



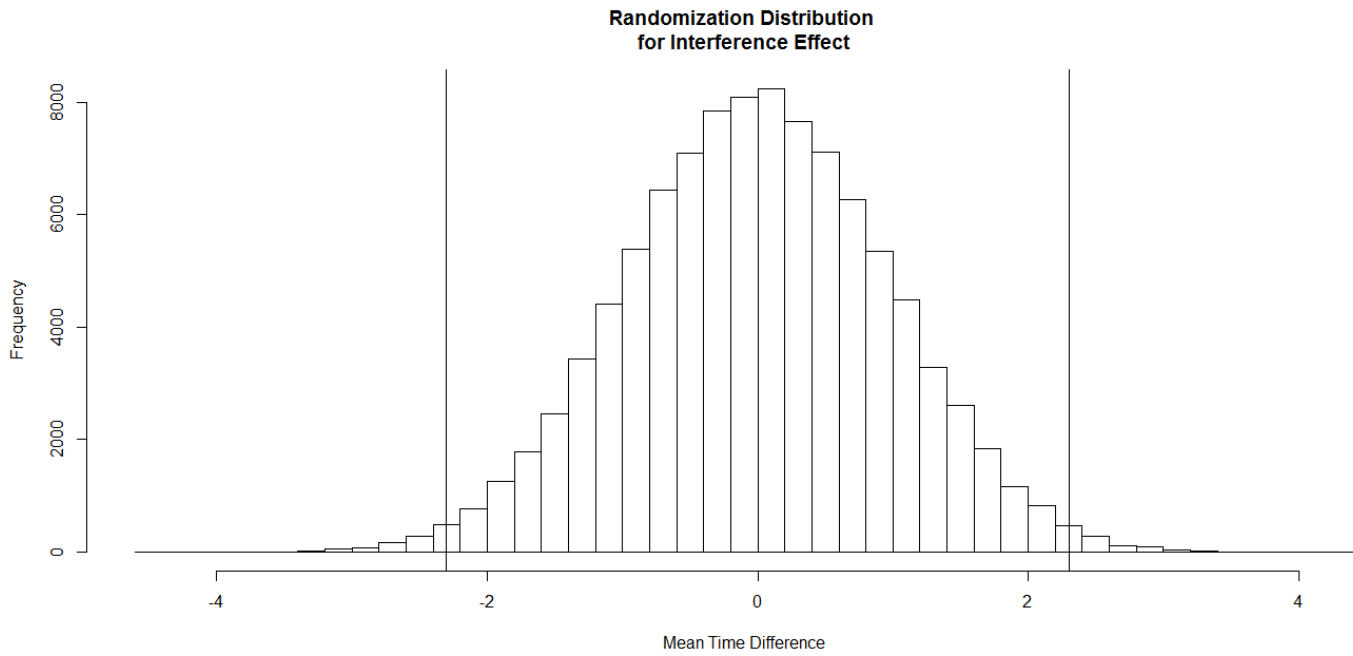
Paired Samples

Under the null hypothesis of no differences between the two treatments/conditions, all observed differences within pairs are equally likely to have been positive ($\text{Trt 1} > \text{Trt 2}$) or negative ($\text{Trt 1} < \text{Trt 2}$). Thus, we can generate a random sign (positive or negative, each with probability 0.5) for each pair. If the sign is positive, we keep the difference in its original value, if the sign is negative, we reverse its sign. We do this for many resamples to determine how extreme the observed mean difference is within its reference distribution.

Example – Interference Effect in Reading Task Times (Stroop Effect)

Based on the $n = 70$ observed differences, 99999 resamples with each observed difference having its sign (+/-) switched with .5 probability, we observed that the absolute value of the mean difference was as large or larger than the observed absolute value of the mean difference in 1602 of the samples. The P -value is:

$$P\text{-Value} = \frac{[\# \text{ of permutation samples with } \text{abs}(\text{mean difference}) \geq \text{abs}(\text{observed mean difference})] + 1}{[\# \text{ of permutation samples}] + 1} = \frac{1602 + 1}{99999 + 1} = 0.01603$$



1.11. Sampling Distribution of S^2 (Normal Data)

- Population variance (σ^2) is a fixed (unknown) parameter based on the population of measurements
- Sample variance (S^2) varies from sample to sample (just as sample mean does)
- When $Y \sim N(\mu, \sigma^2)$, the distribution of (a multiple of) S^2 is Chi-Square with $n-1$ degrees of freedom. Unlike inference on means, the normality assumption is very important.
- $(n-1)S^2/\sigma^2 \sim \chi^2$ with $df = n-1$

$$1 - \alpha = P\left(\chi_L^2 \leq \frac{(n-1)S^2}{\sigma^2} \leq \chi_U^2\right) = P\left(\frac{1}{\chi_U^2} \leq \frac{\sigma^2}{(n-1)S^2} \leq \frac{1}{\chi_L^2}\right) = P\left(\frac{(n-1)S^2}{\chi_U^2} \leq \sigma^2 \leq \frac{(n-1)S^2}{\chi_L^2}\right)$$

(1- α)100% Confidence Interval for σ^2 (or σ)

- Step 1: Obtain a random sample of n items from the population, compute s^2
- Step 2: Obtain χ_L^2 and χ_U^2 from table of critical values for chi-square distribution with $n-1$ df
- Step 3: Compute the confidence interval for σ^2 based on the formula below and take square roots of bounds for σ^2 to obtain confidence interval for σ

$$(1 - \alpha)100\% \text{ CI for } \sigma^2: \left(\frac{(n-1)s^2}{\chi_U^2}, \frac{(n-1)s^2}{\chi_L^2}\right) \text{ with: } \chi_U^2 = \chi^2(1 - \alpha/2; n-1) \quad \chi_L^2 = \chi^2(\alpha/2; n-1)$$

Example: Mercury Levels in Albacore Fish from Eastern Mediterranean (Continued)

$$\begin{aligned} (1 - \alpha) &= 0.95 \Rightarrow \alpha = 0.05 \Rightarrow \alpha/2 = 0.025 \Rightarrow 1 - \alpha/2 = 0.975 \\ n = 34 &\Rightarrow \chi_U^2 = \chi^2(.975; 33) = 50.73 \quad \chi_L^2 = \chi^2(.025; 33) = 19.05 \\ s = 0.4407 &\Rightarrow s^2 = 0.4407^2 = 0.1942 \Rightarrow (n-1)s^2 = 33(0.1942) = 6.4092 \\ (1 - \alpha)100\% \text{ CI for } \sigma^2 &: \left(\frac{(n-1)s^2}{\chi_U^2}, \frac{(n-1)s^2}{\chi_L^2}\right) \equiv \left(\frac{6.4092}{50.73}, \frac{6.4092}{19.05}\right) \equiv (0.1263, 0.3364) \\ (1 - \alpha)100\% \text{ CI for } \sigma &: \left(\sqrt{0.1263}, \sqrt{0.3364}\right) \equiv (0.3364, 0.5800) \end{aligned}$$

Statistical Test for σ^2

- **Null and alternative hypotheses**

1-sided (upper tail):	$H_0 : \sigma^2 \leq \sigma_0^2$	$H_A : \sigma^2 > \sigma_0^2$
1-sided (lower tail):	$H_0 : \sigma^2 \geq \sigma_0^2$	$H_A : \sigma^2 < \sigma_0^2$
2-sided:	$H_0 : \sigma^2 = \sigma_0^2$	$H_A : \sigma^2 \neq \sigma_0^2$

- **Test Statistic**

$$\chi_{obs}^2 = \frac{(n-1)s^2}{\sigma_0^2}$$

- **Decision Rule based on chi-square distribution w/ df=n-1:**

1-sided (upper tail) Rejection Region:	$\chi_{obs}^2 \geq \chi^2(1-\alpha; n-1)$
1-sided (lower tail) Rejection Region:	$\chi_{obs}^2 \leq \chi^2(\alpha; n-1)$
2-sided Rejection Region:	$\{\chi_{obs}^2 \leq \chi^2(\alpha/2; n-1)\} \cup \{\chi_{obs}^2 \geq \chi^2(1-\alpha/2; n-1)\}$

There are not too many practical cases where there is a null value to test, except in cases where firms may need to demonstrate that variation in purity of a chemical or compound is below some nominal level, or that variation in measurements of manufactured parts is below some nominal level.

Note that most decisions can be obtained based on the confidence interval for the population variance (or standard deviation).

1.12. Inferences Regarding 2 Population Variances

- **Goal:** Compare variances between 2 populations
- **Parameter:** $\frac{\sigma_1^2}{\sigma_2^2}$ (Ratio is 1 when variances are equal)
- **Estimator:** $\frac{S_1^2}{S_2^2}$ (Ratio of sample variances)
- **Distribution of (multiple) of estimator (Normal Data):**

$$X_i = \frac{(n_i - 1)S_i^2}{\sigma_i^2} \sim \chi_{n_i}^2 \quad S_1^2 \perp S_2^2 \Rightarrow \frac{X_1/\nu_1}{X_2/\nu_2} = \frac{S_1^2/\sigma_1^2}{S_2^2/\sigma_2^2} = \frac{S_1^2/S_2^2}{\sigma_1^2/\sigma_2^2} \sim F_{\nu_1, \nu_2} = F_{n_1-1, n_2-1}$$

$$\Rightarrow 1 - \alpha = P\left(F_{\alpha/2; n_1-1, n_2-1} \leq \frac{S_1^2/S_2^2}{\sigma_1^2/\sigma_2^2} \leq F_{1-\alpha/2; n_1-1, n_2-1}\right) = P\left(\frac{1}{F_{1-\alpha/2; n_1-1, n_2-1}} \leq \frac{\sigma_1^2/\sigma_2^2}{S_1^2/S_2^2} \leq \frac{1}{F_{\alpha/2; n_1-1, n_2-1}}\right) =$$

$$= P\left(\frac{S_1^2/S_2^2}{F_{1-\alpha/2; n_1-1, n_2-1}} \leq \frac{\sigma_1^2}{\sigma_2^2} \leq \frac{S_1^2/S_2^2}{F_{\alpha/2; n_1-1, n_2-1}}\right) = P\left(\left(\frac{S_1^2}{S_2^2}\right) \frac{1}{F_{1-\alpha/2; n_1-1, n_2-1}} \leq \frac{\sigma_1^2}{\sigma_2^2} \leq \left(\frac{S_1^2}{S_2^2}\right) F_{1-\alpha/2; n_2-1, n_1-1}\right)$$

Test Comparing Two Population Variances

1-Sided Test: $H_0 : \sigma_1^2 \leq \sigma_2^2 \quad H_a : \sigma_1^2 > \sigma_2^2$

Test Statistic: $F_{obs} = \frac{S_1^2}{S_2^2}$ Rejection Region: $F_{obs} \geq F(1 - \alpha; n_1 - 1, n_2 - 1)$ P - value: $P(F \geq F_{obs})$

2-Sided Test: $H_0 : \sigma_1^2 = \sigma_2^2 \quad H_a : \sigma_1^2 \neq \sigma_2^2$

Test Statistic: $F_{obs} = \frac{S_1^2}{S_2^2}$

Rejection Region: $F_{obs} \geq F(1 - \alpha / 2; n_1 - 1, n_2 - 1) \quad (\sigma_1^2 > \sigma_2^2)$

or $F_{obs} \leq F(\alpha / 2; n_1 - 1, n_2 - 1) = 1/F(1 - \alpha / 2; n_2 - 1, n_1 - 1) \quad (\sigma_1^2 < \sigma_2^2)$

P - value: $2\min(P(F \geq F_{obs}), P(F \leq F_{obs}))$

(1- α)100% Confidence Interval for σ_1^2/σ_2^2

$$(1 - \alpha)100\% \text{ Confidence Interval for } \frac{\sigma_1^2}{\sigma_2^2} : \left[\left(\frac{S_1^2}{S_2^2}\right) \frac{1}{F_{1-\alpha/2; n_1-1, n_2-1}}, \left(\frac{S_1^2}{S_2^2}\right) F_{1-\alpha/2; n_2-1, n_1-1} \right]$$

Conclude population variances unequal if interval does not contain 1

Example – Children’s Participation in Meal Preparation and Caloric Intake (Continued)

2-Sided Test: $H_0 : \sigma_1^2 = \sigma_2^2$ $H_a : \sigma_1^2 \neq \sigma_2^2$

$$\text{Test Statistic: } F_{obs} = \frac{s_1^2}{s_2^2} = \frac{105.7^2}{99.5^2} = 1.13$$

Rejection Region: $F_{obs} \geq F(1 - \alpha / 2; n_1 - 1, n_2 - 1) = F(1 - .025; 25 - 1, 22 - 1) = F(.975; 24, 21) = 2.3675$ ($\sigma_1^2 > \sigma_2^2$)

or $F_{obs} \leq F(.025; 24, 21) = 1 / F(.975; 21, 24) = 0.4327$ ($\sigma_1^2 < \sigma_2^2$)

$$P\text{-value: } 2\min(P(F \geq F_{obs}), P(F \leq F_{obs})) = 2\min(.3912, .6088) = 0.7824$$

95% Confidence Interval for $\frac{\sigma_1^2}{\sigma_2^2}$

$$F_L = F(.025; 24, 21) = 1 / F(.975; 21, 24) = 0.4327$$

$$F_U = F(.975; 24, 21) = 2.3675$$

$$\left[\frac{s_1^2}{s_2^2} F_L, \frac{s_1^2}{s_2^2} F_U \right] \equiv [1.13(0.4327), 1.13(2.3675)] \equiv [0.49, 2.68]$$

What do you conclude?

1.13. Comparing 2 Means – Unequal Variances

An approximate t-test and confidence interval can be used when the population variances are unequal. The method is commonly referred to as “Welch’s Test” and makes use of a special case of Satterthwaite’s approximation for degrees of freedom, which will be covered in more detail later for Analysis of Variance models containing random effects. For this case, we have the following model.

$$Y_{11}, \dots, Y_{1n_1} \sim NID(\mu_1, \sigma_1^2) \quad Y_{21}, \dots, Y_{2n_2} \sim NID(\mu_2, \sigma_2^2)$$

$$E\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\} = \mu_{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}} = \mu_1 - \mu_2$$

$$V\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\} = \sigma_{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}}^2 = \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} \quad SE\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\} = \sigma_{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}} = \sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}$$

$$\hat{SE}\{\bar{Y}_{1\cdot} - \bar{Y}_{2\cdot}\} = \sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}$$

A brief derivation of the approximate degrees of freedom is given below. First we consider the equal variance case and the exact t-distribution.

$$\begin{aligned}
 & Y_{11}, \dots, Y_{1n_1} \sim N(\mu_1, \sigma_1^2) \quad Y_{21}, \dots, Y_{2n_2} \sim N(\mu_2, \sigma_2^2) \quad \sigma_1^2 = \sigma_2^2 = \sigma^2 \quad \{Y_1\} \perp \{Y_2\} \\
 & \bar{Y}_i = \frac{\sum_{j=1}^{n_i} Y_{ij}}{n_i} \quad S_i^2 = \frac{\sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2}{n_i - 1} \quad i = 1, 2 \quad S^2 = \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{n_1 + n_2 - 2} \\
 & \bar{Y}_i \sim N\left(\mu_i, \frac{\sigma^2}{n_i}\right) \quad \frac{(n_i - 1)S_i^2}{\sigma^2} \sim \chi_{n_i - 1}^2 \\
 & Z = \frac{(\bar{Y}_1 - \bar{Y}_2) - (\mu_1 - \mu_2)}{\sqrt{\sigma^2 \left(\frac{1}{n_1} + \frac{1}{n_2}\right)}} \sim N(0, 1) \quad W = \frac{(n_1 + n_2 - 2)S^2}{\sigma^2} \sim \chi_{n_1 + n_2 - 2}^2 \quad Z \perp W \\
 & \sqrt{\frac{W}{df_w}} = \sqrt{\frac{\frac{(n_1 + n_2 - 2)S^2}{\sigma^2}}{n_1 + n_2 - 2}} = \sqrt{\frac{S^2}{\sigma^2}} \quad \frac{Z}{\sqrt{\frac{W}{df_w}}} = \frac{\frac{(\bar{Y}_1 - \bar{Y}_2) - (\mu_1 - \mu_2)}{\sqrt{\sigma^2 \left(\frac{1}{n_1} + \frac{1}{n_2}\right)}}}{\sqrt{\frac{S^2}{\sigma^2}}} = \frac{(\bar{Y}_1 - \bar{Y}_2) - (\mu_1 - \mu_2)}{\sqrt{S^2 \left(\frac{1}{n_1} + \frac{1}{n_2}\right)}} \sim t_{n_1 + n_2 - 2} \\
 & \Rightarrow P \left(-t_{\alpha/2, n_1 + n_2 - 2} \leq \frac{(\bar{Y}_1 - \bar{Y}_2) - (\mu_1 - \mu_2)}{\sqrt{S^2 \left(\frac{1}{n_1} + \frac{1}{n_2}\right)}} \leq t_{\alpha/2, n_1 + n_2 - 2} \right) = 1 - \alpha
 \end{aligned}$$

Now we consider the unequal variance case and the derivation of the approximate degrees of freedom for the approximate t-distribution.

$$Y_{11}, \dots, Y_{1n_1} \sim N(\mu_1, \sigma_1^2) \quad Y_{21}, \dots, Y_{2n_2} \sim N(\mu_2, \sigma_2^2) \quad \sigma_1^2 \neq \sigma_2^2 \quad \{Y_1\} \perp \{Y_2\}$$

$$\frac{(n_i - 1)S_i^2}{\sigma_i^2} \sim \chi_{n_i - 1}^2 \Rightarrow E\left[\frac{(n_i - 1)S_i^2}{\sigma_i^2}\right] = n_i - 1, \quad V\left[\frac{(n_i - 1)S_i^2}{\sigma_i^2}\right] = 2(n_i - 1) \Rightarrow E(S_i^2) = \sigma_i^2, \quad V(S_i^2) = \frac{2\sigma_i^4}{n_i - 1}$$

$$Z = \frac{(\bar{Y}_1 - \bar{Y}_2) - (\mu_1 - \mu_2)}{\sqrt{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)}} \sim N(0, 1)$$

Problem: Replacing Denominator with estimated variances, consider :

$$\frac{W^*}{df_{W^*}} = \frac{\left(\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}\right)}{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)} \quad \text{which is NOT a chi-square divided by its degrees of freedom.}$$

$$\text{Aside: } W \sim \chi_\nu^2 \Rightarrow E(W) = \nu, V(W) = 2\nu \Rightarrow E\left\{\frac{W}{\nu}\right\} = 1, \quad V\left\{\frac{W}{\nu}\right\} = \frac{2}{\nu}$$

$$E\left\{\frac{W^*}{df_{W^*}}\right\} = E\left\{\frac{\left(\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}\right)}{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)}\right\} = \frac{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)}{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)} = 1 \quad V\left\{\frac{W^*}{df_{W^*}}\right\} = \frac{1}{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)^2} \left\{\frac{1}{n_1^2} \frac{2\sigma_1^4}{n_1 - 1} + \frac{1}{n_2^2} \frac{2\sigma_2^4}{n_2 - 1}\right\} = \frac{2}{\nu^*}$$

$$\Rightarrow \frac{2}{\nu^*} = \frac{2\left(\frac{\sigma_1^4}{n_1^2(n_1 - 1)} + \frac{\sigma_2^4}{n_2^2(n_2 - 1)}\right)}{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)^2} \Rightarrow \nu^* = \frac{\left(\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}\right)^2}{\left(\frac{\sigma_1^2/n_1}{n_1 - 1} + \frac{\sigma_2^2/n_2}{n_2 - 1}\right)}$$

Replacing the unknown variances with their estimates:

$$\hat{\nu}^* = \frac{\left(\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}\right)^2}{\left(\frac{(S_1^2/n_1)^2}{n_1 - 1} + \frac{(S_2^2/n_2)^2}{n_2 - 1}\right)}$$

So, we have the approximate degrees of freedom if our denominator were the square root of the ratio of a chi-square random variable to its degrees of freedom.

Example: Art Instruction Effect on Reading Development

A study had a group of $N = 52$ children. They were randomized so that $n_1 = 26$ received art instruction (treatment group) and $n_2 = 26$ did not (control group). Each child was given a pre-“treatment” exam and a post-“treatment” exam. The response Y was the difference between the post and pre exam scores.

$$\begin{aligned} \bar{y}_T &= 7.77 & s_T^2 &= 70.49 & n_T &= 26 \\ \bar{y}_C &= -1.58 & s_C^2 &= 26.00 & n_C &= 26 \\ H_0: \sigma_T^2 &= \sigma_C^2 & H_A: \sigma_T^2 &\neq \sigma_C^2 & TS: F_{obs} &= \frac{s_T^2}{s_C^2} = 2.71 & RR: \max(F_{obs}, 1/F_{obs}) &\geq F_{.975, 25, 25} = 2.23 \\ H_0: \mu_T &= \mu_C & H_A: \mu_T &\neq \mu_C & TS: t_{obs} &= \frac{\bar{y}_T - \bar{y}_C}{\sqrt{\frac{s_T^2}{n_T} + \frac{s_C^2}{n_C}}} = \frac{7.77 - (-1.58)}{\sqrt{\frac{70.49}{26} + \frac{26.00}{26}}} = 4.85 \\ \hat{v}^* &= \frac{\left(\frac{70.49}{26} + \frac{26}{26}\right)^2}{\left(\frac{(70.49/26)^2}{25} + \frac{(26.00/26)^2}{25}\right)} = \frac{13.77}{0.33} = 41.23 & RR: |t_{obs}| &\geq t_{.025, 41.23} = 2.020 \end{aligned}$$

The following R program first generates 2 samples of raw data that have the same means, variances, and sample sizes for the 2 groups. Then, it conducts the F-test for variances as well as t-tests and confidence intervals for the equal and unequal variance cases.

R Program

```
set.seed(12345) # Makes random samples reproducible in future runs

### Assign summary statistics for 2 groups
mean1 <- 7.77; var1 <- 70.49; n1 <- 26; std1 <- sqrt(var1)
mean2 <- -1.58; var2 <- 26.00; n2 <- 26; std2 <- sqrt(var2)

### z1 and z2 and random samples of sizes n1 and n2 from N(0,1)
### z1a and z2a have been scaled to have mean=0, SD=1
z1 <- rnorm(26); z2 <- rnorm(26)
z1a <- (z1-mean(z1))/sd(z1)
z2a <- (z2-mean(z2))/sd(z2)

### y1 and y2 are scaled to have means and SDs for the 2 groups
y1 <- mean1 + std1*z1a
y2 <- mean2 + std2*z2a

### create single response vector y and group vector for the 2 groups
y <- cbind(y1,y2)
group <- cbind(rep(1,n1),rep(2,n2))

var.test(y ~ group)
t.test(y ~ group, var.equal=T)
t.test(y ~ group, var.equal=F)
```


R Output

```
> var.test(y ~ group)
      F test to compare two variances
data:  y by group
F = 2.7112, num df = 25, denom df = 25, p-value = 0.01549
alternative hypothesis: true ratio of variances is not equal to 1
95 percent confidence interval:
 1.215599 6.046692
sample estimates:
ratio of variances
      2.711154

> t.test(y ~ group, var.equal=T)
      Two Sample t-test
data:  y by group
t = 4.8535, df = 50, p-value = 1.23e-05
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 5.48064 13.21936
sample estimates:
mean in group 1 mean in group 2
      7.77      -1.58

> t.test(y ~ group, var.equal=F)
      welch Two Sample t-test
data:  y by group
t = 4.8535, df = 41.234, p-value = 1.774e-05
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 5.460154 13.239846
sample estimates:
mean in group 1 mean in group 2
      7.77      -1.58
```

Data Sources:

New York City Street Café's:

<https://nycopendata.socrata.com/Business/Sidewalk-Cafes/6k68-kc8u>

Women's Professional Soccer:

<http://www.nwslsoccer.com/>

Irish Premier League Soccer:

www.soccerpunter.com/

Mercury Levels in Albacore:

S. Mol, O. Ozden, S. Karakulak (2012). "Levels of Selected Metals in Albacore (Thunnus alalunga, Bonaterre, 1788) from the Eastern Mediterranean, *Journal of Aquatic Food Product Technology*, Vol. 21, #2, pp. 111-117.

Children/Parent Cooking Effects on Food Intake:

K. van der Horst, A. Ferrage, A. Rytz (2014). "Involving Children in Meal Preparation: Effects on Food Intake," *Appetite*, Vol. 79, pp. 18-24.

Interference Effect:

Source: J.R. Stroop (1935). "Studies of Interference in Serial Verbal Reactions", *Journal of Experimental Psychology*, Vol 18, pp643-662

Art Instruction and Reading Development:

Source: J.C. Mills (1973), "The Effect of Art Instruction Upon a Reading Development Test: An Experimental Study with Rural Appalachian Children," *Studies in Art Education*, Vol. 14, #3, pp.4-8

R Programs for Randomization/Permutation Tests

Example – Children’s Participation in Meal Preparation and Caloric Intake

```
kidcal <- read.csv("http://www.stat.ufl.edu/~winner/data/kid_calories.csv",header=T)
attach(kidcal); names(kidcal)

Trt.f <- factor(Trt)
t.test(Calories ~ Trt.f, var.equal=T)
n.kids <- length(Calories)
n.kids1 <- length(Calories[Trt.f=="1"])
diff.mean.obs <- mean(Calories[Trt.f=="1"]) - mean(Calories[Trt.f=="2"])
diff.mean.obs

### Choose the number of samples and initialize diff.mean, and set seed
N <- 99999; diff.mean <- rep(0,N); set.seed(97531)
diff.mean <- numeric(N)

for (i in 1:N) {
  sample1 <- sample(1:n.kids,n.kids1,replace=F)
  diff.mean[i] <- mean(Calories[sample1]) - mean(Calories[-sample1])
}

p.value.2t <- (sum(abs(diff.mean) >= diff.mean.obs) + 1)/(N+1)
p.value.2t
hist(diff.mean,main="Permutation Test - Calorie Intake Study",breaks=50)
abline(v = diff.mean.obs)
abline(v = -diff.mean.obs)
```

Example – Interference Effect in Reading Task Times (Stroop Effect)

```
stroop <- read.csv("http://www.stat.ufl.edu/~winner/data/interference.csv",header=T)
attach(stroop); names(stroop)

t.test(DiffCol,Black,paired=T)

diff.t.obs <- DiffCol - Black

### Obtain Sample Size and Test Statistic (Average of diff.t.obs)
(n <- length(diff.t.obs))
(TS.obs <- mean(diff.t.obs))

### Choose the number of samples and initialize TS, and set seed
N <- 99999; TS <- rep(0,N); set.seed(86420)

### Loop through samples and compute each TS
for (i in 1:N) {
  diff.t <- diff.t.obs      # Initialize difference
  u <- runif(n)-0.5         # Generate n U(-0.5,0.5)'s
  u.s <- sign(u)           # -1 if u.s < 0, +1 if u.s > 0
  diff.t <- u.s * diff.t
  TS[i] <- mean(diff.t)    # Compute Test Statistic for this sample
}
summary(TS)
(num.exceed1 <- sum(TS >= TS.obs)) # Count for 1-sided (Upper Tail) P-value
(num.exceed2 <- sum(abs(TS) >= abs(TS.obs))) # Count for 2-sided P-value
(p.val.1sided <- (num.exceed1 + 1)/(N+1)) # 1-sided p-value
(p.val.2sided <- (num.exceed2 + 1)/(N+1)) # 2-sided p-value

### Draw histogram of distribution of TS, with vertical line at TS.obs
hist(TS,xlab="Mean Time Difference",main="Randomization Distribution
for Interference Effect",breaks=50)
abline(v=TS.obs)
abline(v=-TS.obs)
```

Chapter 2 – Completely Randomized Design – Fixed Effects

This model can be used to analyze data from $g \geq 2$ independent samples of treatments or populations. In controlled experiments, experimental units are randomly assigned to treatments. In observational studies, independent random samples are obtained from pre-existing populations. The sample sizes can all be equal (balanced design) or not all equal (unbalanced design). Even if an experiment is set up as a balanced design, due to factors beyond the experimenters' control, some observations may be missing or need to be discarded. The statistical model assumes that all treatments/populations of interest are included, and is as follows.

$$\text{Cell Means Model: } Y_{ij} = \mu_i + \varepsilon_{ij} \quad i = 1, \dots, g; j = 1, \dots, n_i \quad \varepsilon_{ij} \sim NID(0, \sigma^2) \quad N = n_1 + \dots + n_g$$

$$\Rightarrow Y_{ij} \sim N(\mu_i, \sigma^2)$$

$$\text{Treatment Effects Model: } Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad i = 1, \dots, g; j = 1, \dots, n_i \quad \varepsilon_{ij} \sim NID(0, \sigma^2)$$

$$\Rightarrow Y_{ij} \sim N(\mu + \alpha_i, \sigma^2) \quad \mu + \alpha_i = \mu_i$$

$$\text{Two of several possible parameterizations for } \{\alpha_i\} \quad i): \sum_{i=1}^g \alpha_i = 0 \quad ii): \sum_{i=1}^g n_i \alpha_i = 0$$

We will see that the second has nicer computational properties (they are the same for balanced data).

In practice, the goal is to test whether the population means are all equal (H_0), or whether there exist differences among them (H_A). First, we consider least squares estimation of the model parameters:

$$\text{Cell Means Model: } Q = \sum_{i=1}^g \sum_{j=1}^{n_i} \varepsilon_{ij}^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \mu_i)^2$$

$$\Rightarrow \frac{\partial Q}{\partial \mu_k} = -2 \sum_{j=1}^{n_k} (Y_{kj} - \mu_k) \stackrel{\text{setting}}{=} 0 \Rightarrow \sum_{j=1}^{n_k} Y_{kj} = Y_{k\bullet} = n_k \hat{\mu}_k \Rightarrow \hat{\mu}_k = \frac{Y_{k\bullet}}{n_k} = \bar{Y}_{k\bullet} \quad k = 1, \dots, g$$

$$\text{Treatment Effects Model with } \sum_{i=1}^g n_i \alpha_i = 0: Q = \sum_{i=1}^g \sum_{j=1}^{n_i} \varepsilon_{ij}^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \mu - \alpha_i)^2$$

$$\Rightarrow \frac{\partial Q}{\partial \mu} = -2 \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \mu - \alpha_i) = -2 \left[\sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij} - N\mu - \sum_{i=1}^g n_i \alpha_i \right] = -2 [Y_{\bullet\bullet} - N\mu - 0] \stackrel{\text{setting}}{=} 0 \Rightarrow \hat{\mu} = \frac{Y_{\bullet\bullet}}{N} = \bar{Y}_{\bullet\bullet}$$

$$\Rightarrow \frac{\partial Q}{\partial \alpha_k} = -2 \sum_{j=1}^{n_k} (Y_{kj} - \mu - \alpha_k) \stackrel{\text{setting}}{=} 0 \Rightarrow Y_{k\bullet} = n_k \hat{\mu} + n_k \hat{\alpha}_k \Rightarrow \hat{\alpha}_k = \frac{Y_{k\bullet}}{n_k} - \frac{n_k \bar{Y}_{\bullet\bullet}}{n_k} = \bar{Y}_{k\bullet} - \bar{Y}_{\bullet\bullet} \quad k = 1, \dots, g$$

$$\text{Treatment Effects Model with } \sum_{i=1}^g \alpha_i = 0: Q = \sum_{i=1}^g \sum_{j=1}^{n_i} \varepsilon_{ij}^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \mu - \alpha_i)^2$$

$$\Rightarrow \frac{\partial Q}{\partial \alpha_k} = -2 \sum_{j=1}^{n_k} (Y_{kj} - \mu - \alpha_k) \stackrel{\text{setting}}{=} 0 \Rightarrow Y_{k\bullet} = n_k \hat{\mu} + n_k \hat{\alpha}_k \Rightarrow \hat{\alpha}_k = \frac{Y_{k\bullet}}{n_k} - \frac{n_k \hat{\mu}}{n_k} = \bar{Y}_{k\bullet} - \hat{\mu} \quad k = 1, \dots, g$$

$$\sum_{i=1}^g \hat{\alpha}_i = 0 \Rightarrow \sum_{i=1}^g (\bar{Y}_{i\bullet} - \hat{\mu}) = 0 \Rightarrow \sum_{i=1}^g \bar{Y}_{i\bullet} = g \hat{\mu} \Rightarrow \hat{\mu} = \frac{1}{g} \sum_{i=1}^g \bar{Y}_{i\bullet}$$

$$\Rightarrow \hat{\alpha}_k = \bar{Y}_{k\bullet} - \frac{1}{g} \sum_{i=1}^g \bar{Y}_{i\bullet} = \frac{g-1}{g} \bar{Y}_{k\bullet} - \frac{1}{g} \sum_{\substack{i=1, \\ i \neq k}}^g \bar{Y}_{i\bullet} \quad k = 1, \dots, g$$

Under the hypothesis that all population means are equal, we have the following:

$$H_0 : \mu_1 = \dots = \mu_g = \mu \quad (\alpha_1 = \dots = \alpha_g) = 0 \Rightarrow Y_{ij} = \mu + \varepsilon_{ij} \quad i = 1, \dots, g; j = 1, \dots, n_i$$

$$Q = \sum_{i=1}^g \sum_{j=1}^{n_i} \varepsilon_{ij}^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \mu)^2 \Rightarrow \frac{\partial Q}{\partial \mu} = -2 \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \mu) \stackrel{\text{setting}}{=} 0$$

$$\Rightarrow \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij} = N \hat{\mu} \Rightarrow \hat{\mu} = \frac{Y_{..}}{N} = \bar{Y}_{..}$$

Using the general linear test approach, we can test whether the means are equal, or whether there exist differences among them. We will use the cell means model, which gives the exact same predicted values as the two treatment effects formulations for the test.

$$H_0 : \mu_1 = \dots = \mu_g = \mu \quad (\alpha_1 = \dots = \alpha_g) = 0 \Rightarrow Y_{ij} = \mu + \varepsilon_{ij} \quad i = 1, \dots, g; j = 1, \dots, n_i$$

$$H_A : \text{Not all } \mu_i \text{ are equal} \Rightarrow Y_{ij} = \mu_i + \varepsilon_{ij} \quad i = 1, \dots, g; j = 1, \dots, n_i$$

$$\text{Under } H_0 : \hat{Y}_{ij} = \hat{\mu} = \bar{Y}_{..} \quad \text{Under } H_A : \hat{Y}_{ij} = \hat{\mu}_i = \bar{Y}_{i.}$$

$$\text{Reduced Model}(H_0) : SSE_R = \sum_{i=1}^g \sum_{j=1}^{n_i} \left(Y_{ij} - \hat{Y}_{ij} \right)^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} \left(Y_{ij} - \bar{Y}_{..} \right)^2 \quad df_{E(R)} = N - 1$$

$$\text{Complete Model}(H_A) : SSE_C = \sum_{i=1}^g \sum_{j=1}^{n_i} \left(Y_{ij} - \hat{Y}_{ij} \right)^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} \left(Y_{ij} - \bar{Y}_{i.} \right)^2 \quad df_{E(C)} = N - g$$

$$\text{Test Statistic: } F = \frac{\left[\frac{SSE_R - SSE_C}{df_{E(R)} - df_{E(C)}} \right]}{\left[\frac{SSE_C}{df_{E(C)}} \right]} = \frac{\left[\frac{SSE_R - SSE_C}{g - 1} \right]}{\left[\frac{SSE_C}{N - g} \right]} \stackrel{H_0}{\sim} F_{g-1, N-g}$$

This approach (while very general in terms of hypotheses to be tested) can be shown to provide the standard Analysis of Variance provided by many software packages and EXCEL. We partition the deviations of the observed data from the overall mean into: i) deviations of data from the treatment means and ii) the deviations of the treatment means from the overall mean.

$$Y_{ij} - \bar{Y}_{..} = (Y_{ij} - \bar{Y}_{i\cdot}) + (\bar{Y}_{i\cdot} - \bar{Y}_{..}) \Rightarrow (Y_{ij} - \bar{Y}_{..})^2 = (Y_{ij} - \bar{Y}_{i\cdot})^2 + (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 + 2(Y_{ij} - \bar{Y}_{i\cdot})(\bar{Y}_{i\cdot} - \bar{Y}_{..})$$

$$\sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{..})^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} \left[(Y_{ij} - \bar{Y}_{i\cdot})^2 + (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 + 2(Y_{ij} - \bar{Y}_{i\cdot})(\bar{Y}_{i\cdot} - \bar{Y}_{..}) \right] =$$

$$= \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})^2 + \sum_{i=1}^g \sum_{j=1}^{n_i} (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 + 2 \sum_{i=1}^g (\bar{Y}_{i\cdot} - \bar{Y}_{..}) \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})$$

Consider the last term: $\sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot}) = \sum_{j=1}^{n_i} Y_{ij} - n_i \bar{Y}_{i\cdot} = Y_{i\cdot} - Y_{i\cdot} = 0 \quad i = 1, \dots, g$

$$\Rightarrow \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{..})^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})^2 + \sum_{i=1}^g \sum_{j=1}^{n_i} (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2$$

Total Sum of Squares (Corrected for the Mean): $SS_{\text{Total}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{..})^2 \quad df_{\text{Total}} = N - 1$

Error (Within Treatments) Sum of Squares: $SS_{\text{Error}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})^2 = \sum_{i=1}^g (n_i - 1) S_i^2 \quad df_{\text{Error}} = N - g$

Treatment Sum of Squares: $SS_{\text{Trts}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 = \sum_{i=1}^g n_i (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 \quad df_{\text{Trts}} = g - 1$

$$\Rightarrow SS_{\text{Total}} = SS_{\text{Trts}} + SS_{\text{Error}} \quad df_{\text{Total}} = df_{\text{Trts}} + df_{\text{Error}}$$

Next, we consider the Expectations of the Treatment and Error Sums of Squares, along with their sampling distributions. This will lead to the traditional F-test for treatment effects (mean differences).

$$SS_{\text{Total}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{..})^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 + N(\bar{Y}_{..})^2 - 2\bar{Y}_{..} \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij} = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 + N(\bar{Y}_{..})^2 - 2\bar{Y}_{..} (N\bar{Y}_{..}) =$$

$$= \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 - N(\bar{Y}_{..})^2 \quad df_{\text{Total}} = N - 1$$

$$SS_{\text{Error}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 + \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 - 2 \sum_{i=1}^g \bar{Y}_{i\cdot} \sum_{j=1}^{n_i} Y_{ij} = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 + \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 - 2 \sum_{i=1}^g \bar{Y}_{i\cdot} (n_i \bar{Y}_{i\cdot}) =$$

$$= \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 - \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 \quad df_{\text{Error}} = N - g$$

$$SS_{\text{Trts}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 = \sum_{i=1}^g n_i (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 = \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 + \bar{Y}_{..}^2 \sum_{i=1}^g n_i - 2\bar{Y}_{..} \sum_{i=1}^g n_i \bar{Y}_{i\cdot} =$$

$$= \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 + N\bar{Y}_{..}^2 - 2\bar{Y}_{..} (N\bar{Y}_{..}) = \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 - N\bar{Y}_{..}^2 \quad df_{\text{Trts}} = g - 1$$

$$E\{Y_{ij}\} = \mu_i \quad V\{Y_{ij}\} = \sigma^2 \Rightarrow E\{Y_{ij}^2\} = \mu_i^2 + \sigma^2$$

$$E\{\bar{Y}_{i\cdot}\} = \mu_i \quad V\{\bar{Y}_{i\cdot}\} = \frac{\sigma^2}{n_i} \Rightarrow E\{\bar{Y}_{i\cdot}^2\} = \mu_i^2 + \frac{\sigma^2}{n_i}$$

$$E\{\bar{Y}_{..}\} = E\left\{\frac{1}{N} \sum_{i=1}^g n_i \mu_i\right\} = \mu \quad V\{\bar{Y}_{..}\} = \frac{\sigma^2}{N} \Rightarrow E\{\bar{Y}_{..}^2\} = \mu^2 + \frac{\sigma^2}{N}$$

$$SS_{\text{Error}} = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 - \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 \quad df_{\text{Error}} = N - g \quad SS_{\text{Trts}} = \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 - N \bar{Y}_{\cdot\cdot}^2 \quad df_{\text{Trts}} = g - 1$$

$$E\{Y_{ij}\} = \mu_i \quad V\{Y_{ij}\} = \sigma^2 \Rightarrow E\{Y_{ij}^2\} = \mu_i^2 + \sigma^2$$

$$E\{\bar{Y}_{i\cdot}\} = \mu_i \quad V\{\bar{Y}_{i\cdot}\} = \frac{\sigma^2}{n_i} \Rightarrow E\{\bar{Y}_{i\cdot}^2\} = \mu_i^2 + \frac{\sigma^2}{n_i}$$

$$E\{\bar{Y}_{\cdot\cdot}\} = E\left\{\frac{1}{N} \sum_{i=1}^g n_i \mu_i\right\} = \mu \quad V\{\bar{Y}_{\cdot\cdot}\} = \frac{\sigma^2}{N} \Rightarrow E\{\bar{Y}_{\cdot\cdot}^2\} = \mu^2 + \frac{\sigma^2}{N}$$

$$E\left\{\sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2\right\} = \sum_{i=1}^g \sum_{j=1}^{n_i} (\mu_i^2 + \sigma^2) = \sum_{i=1}^g n_i \mu_i^2 + N\sigma^2$$

$$E\left\{\sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2\right\} = \sum_{i=1}^g n_i \left(\mu_i^2 + \frac{\sigma^2}{n_i}\right) = \sum_{i=1}^g n_i \mu_i^2 + g\sigma^2$$

$$E\{N\bar{Y}_{\cdot\cdot}^2\} = N\left(\mu^2 + \frac{\sigma^2}{N}\right) = N\mu^2 + \sigma^2$$

$$\Rightarrow E\{SS_{\text{Error}}\} = \left(\sum_{i=1}^g n_i \mu_i^2 + N\sigma^2\right) - \left(\sum_{i=1}^g n_i \mu_i^2 + g\sigma^2\right) = (N - g)\sigma^2 \Rightarrow E\{MS_{\text{Error}}\} = E\left\{\frac{SS_{\text{Error}}}{N - g}\right\} = \sigma^2$$

$$\Rightarrow E\{SS_{\text{Trts}}\} = \left(\sum_{i=1}^g n_i \mu_i^2 + g\sigma^2\right) - (N\mu^2 + \sigma^2) = \sum_{i=1}^g n_i (\mu_i - \mu)^2 + (g - 1)\sigma^2 \Rightarrow$$

$$\Rightarrow E\{MS_{\text{Trts}}\} = E\left\{\frac{SS_{\text{Trts}}}{g - 1}\right\} = \sigma^2 + \frac{\sum_{i=1}^g n_i (\mu_i - \mu)^2}{g - 1} \geq \sigma^2 \quad \text{with equality iff } \mu_i = \mu \quad i = 1, \dots, g$$

Note: $\sum_{i=1}^g n_i (\mu_i - \mu)^2 = \sum_{i=1}^g n_i [\mu_i^2 + \mu^2 - 2\mu\mu_i] = \sum_{i=1}^g n_i \mu_i^2 + N\mu^2 - 2\mu \sum_{i=1}^g n_i \mu_i =$

$$= \sum_{i=1}^g n_i \mu_i^2 + N\mu^2 - 2\mu N\mu = \sum_{i=1}^g n_i \mu_i^2 - N\mu^2$$

The distributions can easily be obtained by using the matrix form of the model. Here we simply state the results that lead to the F-test.

$$\frac{SS_{\text{ERROR}}}{\sigma^2} \sim \chi_{N-g}^2 \quad \frac{SS_{\text{TRTS}}}{\sigma^2} \sim \text{Noncentral-}\chi^2 \left(df = g - 1, \Omega = \frac{\sum_{i=1}^g n_i (\mu_i - \mu)^2}{\sigma^2} \right) \quad SS_{\text{ERROR}} \perp SS_{\text{TRTS}}$$

$$\Rightarrow F = \frac{\left[\left(\frac{SS_{\text{TRTS}}}{\sigma^2} \right) / (g - 1) \right]}{\left[\left(\frac{SS_{\text{ERROR}}}{\sigma^2} \right) / (N - g) \right]} = \frac{MS_{\text{TRTS}}}{MS_{\text{ERROR}}} \sim \text{Noncentral-F} \left(df_1 = g - 1, df_2 = N - g, \Omega = \frac{\sum_{i=1}^g n_i (\mu_i - \mu)^2}{\sigma^2} \right)$$

Under $H_0: \mu_1 = \dots = \mu_g = \mu \quad F = \frac{MS_{\text{TRTS}}}{MS_{\text{ERROR}}} \sim F_{g-1, N-g}$

The sampling distributions of least squares estimators can be obtained by making use of the fact that they are linear functions of normally distributed random variables. Note that these make use of a specific model restriction.

Working with the restriction: $\sum_{i=1}^g n_i \alpha_i = 0 \Rightarrow \alpha_g = -\sum_{i=1}^{g-1} \frac{n_i \alpha_i}{n_g}$ and independent $Y_{ij} \sim N(\mu + \alpha_i, \sigma^2)$

$$\hat{\mu} = \frac{1}{N} \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij} = \bar{Y}_{..} \Rightarrow E\{\hat{\mu}\} = \frac{1}{N} \sum_{i=1}^g \sum_{j=1}^{n_i} E\{Y_{ij}\} = \frac{1}{N} \sum_{i=1}^g \sum_{j=1}^{n_i} (\mu + \alpha_i) = \frac{1}{N} N\mu + \frac{1}{N} \sum_{i=1}^g n_i \alpha_i = \mu + 0 = \mu$$

$$V\{\hat{\mu}\} = \frac{1}{N^2} \sum_{i=1}^g \sum_{j=1}^{n_i} V\{Y_{ij}\} = \frac{1}{N^2} N\sigma^2 = \frac{\sigma^2}{N}$$

$$\hat{\alpha}_i = \bar{Y}_{i\cdot} - \bar{Y}_{..} \Rightarrow E\{\hat{\alpha}_i\} = E\{\bar{Y}_{i\cdot} - \bar{Y}_{..}\} = \mu + \alpha_i - \mu = \alpha_i$$

Noting that $\bar{Y}_{..} = \frac{1}{N} \sum_{i=1}^g n_i \bar{Y}_{i\cdot} \Rightarrow \text{COV}\{\bar{Y}_{i\cdot}, \bar{Y}_{..}\} = \frac{n_i}{N} V\{\bar{Y}_{i\cdot}\} = \frac{n_i}{N} \frac{\sigma^2}{n_i} = \frac{\sigma^2}{N}$

$$\Rightarrow V\{\hat{\alpha}_i\} = V\{\bar{Y}_{i\cdot} - \bar{Y}_{..}\} = V\{\bar{Y}_{i\cdot}\} + V\{\bar{Y}_{..}\} - 2\text{COV}\{\bar{Y}_{i\cdot}, \bar{Y}_{..}\} = \frac{\sigma^2}{n_i} + \frac{\sigma^2}{N} - 2\frac{\sigma^2}{N} = \frac{\sigma^2}{n_i} - \frac{\sigma^2}{N} = \sigma^2 \left(\frac{1}{n_i} - \frac{1}{N} \right)$$

(1- α)100% CI for μ : $\hat{\mu} \pm t(1-(\alpha/2); N-g) \sqrt{\frac{MS_{\text{ERR}}}{N}}$

(1- α)100% CI for α_i : $\hat{\alpha}_i \pm t(1-(\alpha/2); N-g) \sqrt{MS_{\text{ERR}} \left(\frac{1}{n_i} - \frac{1}{N} \right)}$

These parameters are ambiguous, unless specific restrictions (as above) are made.

Two types of parameters are "estimable" regardless of restrictions: $\mu + \alpha_i$ and $C = \sum_{i=1}^g w_i (\mu + \alpha_i)$ s.t. $\sum_{i=1}^g w_i = 0$

$$\hat{\mu} + \hat{\alpha}_i = \hat{\mu} + \hat{\alpha}_i = \bar{Y}_{..} + \bar{Y}_{i\cdot} - \bar{Y}_{..} = \bar{Y}_{i\cdot} \Rightarrow E\{\hat{\mu} + \hat{\alpha}_i\} = \mu + \alpha_i \quad V\{\hat{\mu} + \hat{\alpha}_i\} = \frac{\sigma^2}{n_i}$$

$$\hat{C} = \sum_{i=1}^g w_i (\hat{\mu} + \hat{\alpha}_i) = \sum_{i=1}^g w_i (\bar{Y}_{i\cdot}) = \sum_{i=1}^g w_i \bar{Y}_{i\cdot} = 0 + \sum_{i=1}^g w_i \bar{Y}_{i\cdot} = \sum_{i=1}^g w_i \bar{Y}_{i\cdot} - 0 = \sum_{i=1}^g w_i \bar{Y}_{i\cdot}$$

$$\Rightarrow E\{\hat{C}\} = \sum_{i=1}^g w_i (\mu + \alpha_i) = \sum_{i=1}^g w_i \alpha_i = C \quad V\{\hat{C}\} = \sum_{i=1}^g w_i^2 \frac{\sigma^2}{n_i} = \sigma^2 \sum_{i=1}^g \frac{w_i^2}{n_i}$$

(1- α)100% CI for $\mu + \alpha_i$: $\bar{y}_{i\cdot} \pm t(1-(\alpha/2); N-g) \sqrt{\frac{MS_{\text{ERR}}}{n_i}}$

(1- α)100% CI for $C = \sum_{i=1}^g w_i (\mu + \alpha_i)$: $\sum_{i=1}^g w_i \bar{y}_{i\cdot} \pm t(1-(\alpha/2); N-g) \sqrt{MS_{\text{ERR}} \sum_{i=1}^g \frac{w_i^2}{n_i}}$

The model can also be written in **matrix form**. This form is simpler to write out, however it also depends on the restrictions among the parameters. We will consider the cell means and treatment effects models below. It turns the model into a regression model, with Ordinary Least Squares being used to estimate parameters. The data vector will be labelled as \mathbf{Y} , the design or model matrix as \mathbf{X} , the parameter vector as $\boldsymbol{\beta}$ and the error vector as $\boldsymbol{\epsilon}$. Because of the treatment structure, many of the calculations involve blocks of values. Throughout, we assume the data are ordered by treatment and replicate id within treatment.

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \\ \vdots \\ \mathbf{Y}_g \end{bmatrix} \quad \mathbf{Y}_i = \begin{bmatrix} Y_{i1} \\ Y_{i2} \\ \vdots \\ Y_{in_i} \end{bmatrix} \quad \mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \quad \boldsymbol{\varepsilon} \sim N(\mathbf{0}_N, \sigma^2 \mathbf{I}_N) \quad \mathbf{Y} \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_N)$$

The forms of \mathbf{X} and $\boldsymbol{\beta}$ depend on the model restrictions

$$\text{Cell Means Model: } \mathbf{X} = \begin{bmatrix} \mathbf{1}_{n_1} & \mathbf{0}_{n_1} & \cdots & \mathbf{0}_{n_1} \\ \mathbf{0}_{n_2} & \mathbf{1}_{n_2} & \cdots & \mathbf{0}_{n_2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g} & \mathbf{0}_{n_g} & \cdots & \mathbf{1}_{n_g} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_g \end{bmatrix} \quad \text{where } \mathbf{1}_{n_i} \equiv n_i \times 1 \text{ vector of } 1^s \text{ and similarly for } \mathbf{0}_{n_i}$$

$$\Rightarrow \mathbf{X}'\mathbf{X} = \begin{bmatrix} n_1 & 0 & \cdots & 0 \\ 0 & n_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & n_g \end{bmatrix} \quad (\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} 1/n_1 & 0 & \cdots & 0 \\ 0 & 1/n_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/n_g \end{bmatrix} \quad \mathbf{X}'\mathbf{Y} = \begin{bmatrix} Y_{1\bullet} \\ Y_{2\bullet} \\ \vdots \\ Y_{g\bullet} \end{bmatrix}$$

$$\Rightarrow \hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y} = \begin{bmatrix} \bar{Y}_{1\bullet} \\ \bar{Y}_{2\bullet} \\ \vdots \\ \bar{Y}_{g\bullet} \end{bmatrix} \quad \Rightarrow E\left\{\hat{\boldsymbol{\beta}}\right\} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \boldsymbol{\beta} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_g \end{bmatrix}$$

$$V\left\{\hat{\boldsymbol{\beta}}\right\} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\sigma^2 \mathbf{I}_N \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1} = \sigma^2 \begin{bmatrix} 1/n_1 & 0 & \cdots & 0 \\ 0 & 1/n_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/n_g \end{bmatrix}$$

$$\text{Treatment Effects Model with } \sum_{i=1}^g n_i \alpha_i = 0: \quad \mathbf{X} = \begin{bmatrix} \mathbf{1}_{n_1} & \mathbf{1}_{n_1} & \cdots & \mathbf{0}_{n_1} & \mathbf{0}_{n_1} \\ \mathbf{1}_{n_2} & \mathbf{0}_{n_2} & \cdots & \mathbf{0}_{n_2} & \mathbf{0}_{n_2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_{n_{g-1}} & \mathbf{0}_{n_{g-1}} & \cdots & \mathbf{0}_{n_{g-1}} & \mathbf{1}_{n_{g-1}} \\ \mathbf{1}_{n_g} & -\frac{n_1}{n_g} \mathbf{1}_{n_g} & \cdots & -\frac{n_{g-2}}{n_g} \mathbf{1}_{n_g} & -\frac{n_{g-1}}{n_g} \mathbf{1}_{n_g} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \vdots \\ \alpha_{g-1} \end{bmatrix}$$

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} N & 0 & \cdots & 0 & 0 \\ 0 & n_1 \left(1 + \frac{n_1}{n_g}\right) & \cdots & \frac{n_1 n_{g-2}}{n_g} & \frac{n_1 n_{g-1}}{n_g} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \frac{n_1 n_{g-2}}{n_g} & \cdots & n_{g-2} \left(1 + \frac{n_{g-2}}{n_g}\right) & \frac{n_{g-2} n_{g-1}}{n_g} \\ 0 & \frac{n_1 n_{g-1}}{n_g} & \cdots & \frac{n_{g-2} n_{g-1}}{n_g} & n_{g-1} \left(1 + \frac{n_{g-1}}{n_g}\right) \end{bmatrix} \quad \mathbf{X}'\mathbf{Y} = \begin{bmatrix} Y_{\bullet\bullet} \\ Y_{1\bullet} - n_1 \bar{Y}_{g\bullet} \\ \vdots \\ Y_{g-1\bullet} - n_{g-1} \bar{Y}_{g\bullet} \end{bmatrix}$$

Through some very tedious algebra, we obtain the following:

$$(\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} \frac{1}{N} & 0 & \cdots & 0 & 0 \\ 0 & \frac{N-n_1}{Nn_1} & \cdots & -\frac{1}{N} & -\frac{1}{N} \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & -\frac{1}{N} & \cdots & \frac{N-n_{g-2}}{Nn_{g-2}} & -\frac{1}{N} \\ 0 & -\frac{1}{N} & \cdots & -\frac{1}{N} & \frac{N-n_{g-1}}{Nn_{g-1}} \end{bmatrix} \quad \hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y} = \begin{bmatrix} \hat{\mu} \\ \hat{\alpha}_1 \\ \vdots \\ \hat{\alpha}_{g-1} \end{bmatrix}$$

$$\hat{\mu} = \frac{Y_{..}}{N} = \bar{Y}_{..}$$

$$\hat{\alpha}_1 = \frac{(N-n_1)}{Nn_1} \left(Y_{1\cdot} - \frac{n_1}{n_g} Y_{g\cdot} \right) - \frac{1}{N} \left(Y_{2\cdot} - \frac{n_2}{n_g} Y_{g\cdot} \right) - \cdots - \frac{1}{N} \left(Y_{g-1\cdot} - \frac{n_{g-1}}{n_g} Y_{g\cdot} \right) =$$

$$= \frac{N-n_1}{N} \bar{Y}_{1\cdot} - \frac{n_2}{N} \bar{Y}_{2\cdot} - \cdots - \frac{n_g}{N} \bar{Y}_{g\cdot} = \bar{Y}_{1\cdot} - \bar{Y}_{..}$$

$$E\left\{ \hat{\mu} \right\} = E\left\{ \bar{Y}_{..} \right\} = \mu \quad V\left\{ \hat{\mu} \right\} = \frac{\sigma^2}{N}$$

For all i , we get: $\hat{\alpha}_i = \bar{Y}_{i\cdot} - \bar{Y}_{..} \quad i=1, \dots, g$

$$E\left\{ \hat{\alpha}_i \right\} = \alpha_i \quad V\left\{ \hat{\alpha}_i \right\} = \sigma^2 \left(\frac{N-n_i}{Nn_i} \right) = \sigma^2 \left(\frac{1}{n_i} - \frac{1}{N} \right) \quad \text{COV}\left\{ \hat{\alpha}_i, \hat{\alpha}_k \right\} = \text{COV}\left\{ \bar{Y}_{i\cdot} - \bar{Y}_{..}, \bar{Y}_{k\cdot} - \bar{Y}_{..} \right\} = -\frac{\sigma^2}{N}$$

$$\text{COV}\left\{ \hat{\mu}, \hat{\alpha}_i \right\} = \text{COV}\left\{ \bar{Y}_{..}, \bar{Y}_{i\cdot} - \bar{Y}_{..} \right\} = \text{COV}\left\{ \bar{Y}_{..}, \bar{Y}_{i\cdot} \right\} - \text{COV}\left\{ \bar{Y}_{..}, \bar{Y}_{..} \right\} = \frac{\sigma^2}{N} - \frac{\sigma^2}{N} = 0$$

$$E\left\{ \hat{\mu} + \hat{\alpha}_i \right\} = \mu + \alpha_i \quad V\left\{ \hat{\mu} + \hat{\alpha}_i \right\} = \frac{\sigma^2}{N} + \sigma^2 \left(\frac{1}{n_i} - \frac{1}{N} \right) - 2(0) = \sigma^2 \left(\frac{1}{n_i} \right)$$

$$E\left\{ \hat{\alpha}_i - \hat{\alpha}_k \right\} = \alpha_i - \alpha_k \quad V\left\{ \hat{\alpha}_i - \hat{\alpha}_k \right\} = \sigma^2 \left(\frac{1}{n_i} - \frac{1}{N} \right) + \sigma^2 \left(\frac{1}{n_k} - \frac{1}{N} \right) - 2 \left(-\frac{\sigma^2}{N} \right) = \sigma^2 \left(\frac{1}{n_i} + \frac{1}{n_k} \right)$$

The Analysis of Variance can be obtained based on either form of the model, as follows, where \mathbf{I} is an $N \times N$ identity matrix, \mathbf{J} is a matrix of 1^s and $\mathbf{0}$ is a matrix of 0^s :

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y} = \mathbf{P}\mathbf{Y} \quad \mathbf{P} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'$$

$$\mathbf{P} = \begin{bmatrix} \frac{1}{n_1} \mathbf{J}_{n_1 \times n_1} & \mathbf{0}_{n_1 \times n_2} & \cdots & \mathbf{0}_{n_1 \times n_g} \\ \mathbf{0}_{n_2 \times n_1} & \frac{1}{n_2} \mathbf{J}_{n_2 \times n_2} & \cdots & \mathbf{0}_{n_2 \times n_g} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g \times n_1} & \mathbf{0}_{n_g \times n_2} & \cdots & \frac{1}{n_g} \mathbf{J}_{n_g \times n_g} \end{bmatrix} \quad \text{trace}(\mathbf{P}) = n_1 \left(\frac{1}{n_1} \right) + \cdots + n_g \left(\frac{1}{n_g} \right) = g$$

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{P}\mathbf{Y} \quad \mathbf{P} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' \Rightarrow$$

$$\mathbf{P}\mathbf{P} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' = \mathbf{P} \quad \mathbf{P}\mathbf{X} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X} = \mathbf{X} \quad \mathbf{P}\mathbf{J} = \mathbf{J}$$

$$\text{Total Corrected SS: } SS_{\text{Total}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{..})^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 - N(\bar{Y}_{..})^2 = \mathbf{Y}'\left(\mathbf{I} - \frac{1}{N}\mathbf{J}\right)\mathbf{Y}$$

$$df_{\text{Total}} = \text{trace}\left(\mathbf{I} - \frac{1}{N}\mathbf{J}\right) = N - 1$$

$$\text{Treatment SS: } SS_{\text{Trt}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (\bar{Y}_{i\cdot} - \bar{Y}_{..})^2 = \sum_{i=1}^g n_i (\bar{Y}_{i\cdot})^2 - N(\bar{Y}_{..})^2 = \mathbf{Y}'\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right)\mathbf{Y}$$

$$df_{\text{Trt}} = \text{trace}\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right) = g - 1$$

$$\text{Error SS: } SS_{\text{Err}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 - \sum_{i=1}^g n_i (\bar{Y}_{i\cdot})^2 = \mathbf{Y}'(\mathbf{I} - \mathbf{P})\mathbf{Y}$$

$$df_{\text{Err}} = \text{trace}(\mathbf{I} - \mathbf{P}) = N - g$$

Under independence, constant variance, and normality of the error terms, we have:

$$(\mathbf{I} - \mathbf{P})(\mathbf{I} - \mathbf{P}) = \mathbf{I} - \mathbf{P} - \mathbf{P} + \mathbf{P}\mathbf{P} = \mathbf{I} - \mathbf{P} \Rightarrow \frac{1}{\sigma^2} SS_{\text{Err}} = \frac{1}{\sigma^2} \mathbf{Y}'(\mathbf{I} - \mathbf{P})\mathbf{Y} \sim \chi^2$$

$$\text{with degrees of freedom} = df_{\text{Err}} = \text{trace}(\mathbf{I} - \mathbf{P}) = N - g \quad \text{and}$$

$$\text{Non-centrality parameter: } \Omega_{\text{Err}} = \frac{1}{2\sigma^2} \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P})\mathbf{X}\boldsymbol{\beta} = 0$$

$$\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right)\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right) = \mathbf{P}\mathbf{P} - \frac{1}{N}\mathbf{P}\mathbf{J} - \frac{1}{N}\mathbf{J}\mathbf{P} + \frac{1}{N}\mathbf{J}\frac{1}{N}\mathbf{J} = \mathbf{P} - \frac{1}{N}\mathbf{J} \Rightarrow \frac{1}{\sigma^2} SS_{\text{Trt}} = \frac{1}{\sigma^2} \mathbf{Y}'\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right)\mathbf{Y} \sim \chi^2$$

$$\text{with degrees of freedom} = df_{\text{Trt}} = \text{trace}\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right) = g - 1 \quad \text{and}$$

$$\text{Non-centrality parameter: } \Omega_{\text{Trt}} = \frac{1}{2\sigma^2} \boldsymbol{\beta}'\mathbf{X}'\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right)\mathbf{X}\boldsymbol{\beta} = \frac{1}{2\sigma^2} \boldsymbol{\beta}'\mathbf{X}'\left(\mathbf{I} - \frac{1}{N}\mathbf{J}\right)\mathbf{X}\boldsymbol{\beta} = \frac{1}{2\sigma^2} \left[\boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} - \boldsymbol{\beta}'\mathbf{X}'\left(\frac{1}{N}\mathbf{J}\right)\mathbf{X}\boldsymbol{\beta} \right]$$

$$= \frac{1}{2\sigma^2} \left[\sum_{i=1}^g n_i \mu_i^2 - N\mu^2 \right] = \frac{1}{2\sigma^2} \sum_{i=1}^g n_i (\mu_i - \mu)^2 = 0 \Leftrightarrow \mu_1 = \dots = \mu_g = \mu \quad \mu = \frac{1}{N} \sum_{i=1}^g n_i \mu_i$$

$$(\mathbf{I} - \mathbf{P})\left(\mathbf{P} - \frac{1}{N}\mathbf{J}\right) = \mathbf{P} - \frac{1}{N}\mathbf{J} - \mathbf{P}\mathbf{P} + \frac{1}{N}\mathbf{P}\mathbf{J} = \mathbf{P} - \frac{1}{N}\mathbf{J} - \mathbf{P} + \frac{1}{N}\mathbf{J} = \mathbf{0} \Rightarrow SS_{\text{Err}} \perp SS_{\text{Trt}}$$

$$\Rightarrow F = \frac{\left(\frac{SS_{\text{Trt}}}{\sigma^2} / (g - 1)\right)}{\left(\frac{SS_{\text{Err}}}{\sigma^2} / (N - g)\right)} = \frac{MS_{\text{TRT}}}{MS_{\text{Err}}} \sim \text{Non-Central-} F\left(g - 1, N - g, \Omega_{\text{Trt}} = \frac{1}{2\sigma^2} \sum_{i=1}^g n_i (\mu_i - \mu)^2 = \frac{1}{2\sigma^2} \sum_{i=1}^g n_i \alpha_i^2\right)$$

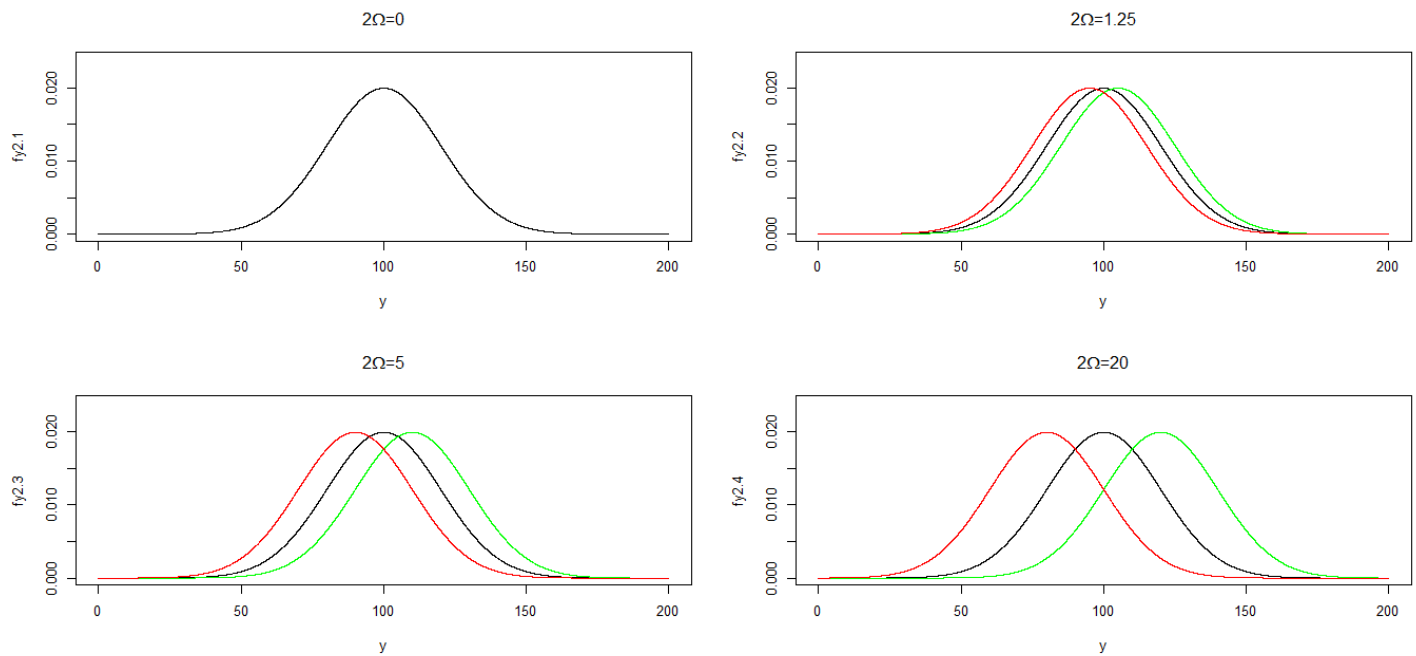
$$\text{Under } H_0 : \mu_1 = \dots = \mu_g = \mu \quad (\alpha_1 = \dots = \alpha_g = 0) \quad F \sim F(g - 1, N - g)$$

Note that when using R or SAS for power computations, use $2\Omega_{\text{Trt}}$ as the non-centrality parameter

Consider an experiment with $g = 3$ treatments, $n_1 = n_2 = n_3 = 10$, and the following cases of treatment effects relative to the experimental error variance:

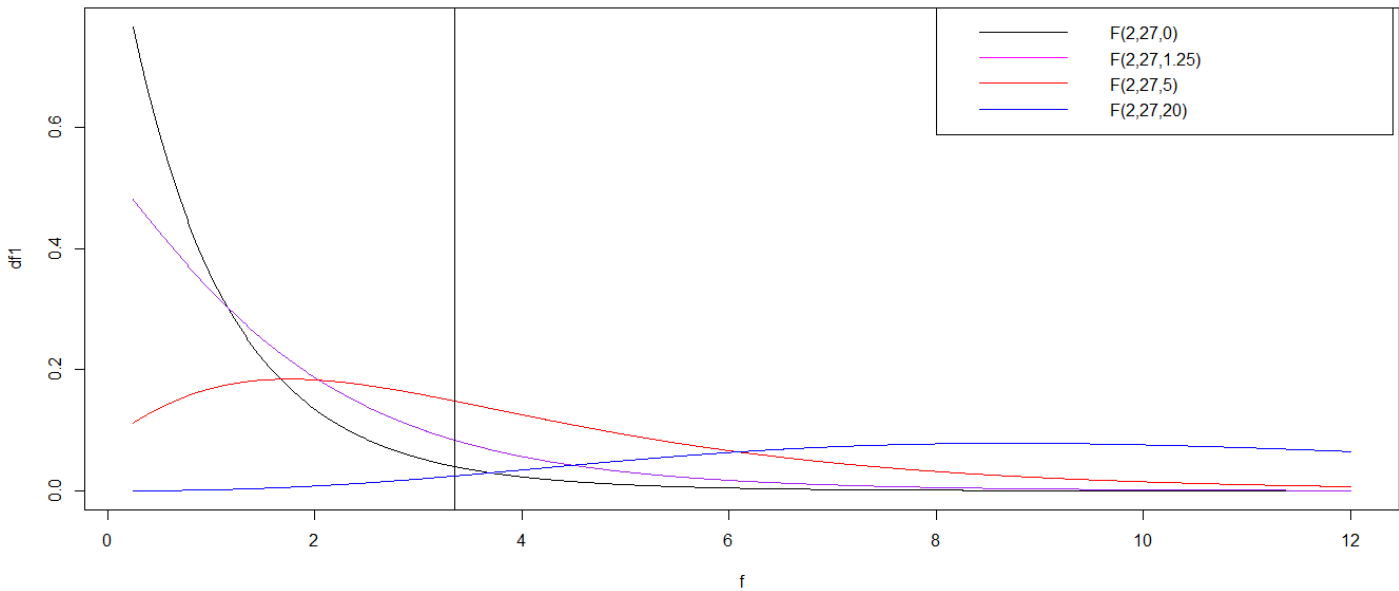
Scenario 1:	$\frac{1}{\sigma^2} \sum_{i=1}^3 \alpha_i^2 = 0 \Rightarrow 2\Omega_{\text{Ttt}} = \frac{1}{\sigma^2} \sum_{i=1}^3 n_i \alpha_i^2 = 0$	$\alpha_1 = \alpha_2 = \alpha_3 = 0$
Scenario 2:	$\frac{1}{\sigma^2} \sum_{i=1}^3 \alpha_i^2 = 0.125 \Rightarrow 2\Omega_{\text{Ttt}} = 10(0.125) = 1.25$	$\alpha_1 = 0.25\sigma \quad \alpha_2 = 0 \quad \alpha_3 = -0.25\sigma$
Scenario 3:	$\frac{1}{\sigma^2} \sum_{i=1}^3 \alpha_i^2 = 0.50 \Rightarrow 2\Omega_{\text{Ttt}} = 10(0.50) = 5$	$\alpha_1 = 0.50\sigma \quad \alpha_2 = 0 \quad \alpha_3 = -0.50\sigma$
Scenario 4:	$\frac{1}{\sigma^2} \sum_{i=1}^3 \alpha_i^2 = 2.00 \Rightarrow 2\Omega_{\text{Ttt}} = 10(2.00) = 20$	$\alpha_1 = \sigma \quad \alpha_2 = 0 \quad \alpha_3 = -\sigma$

The distributions of individual measurements under the 4 scenarios are as shown below:



In these plots, we use $n=10$, $\mu = 100$, $\sigma = 20$. The central and 3 non-central F-distributions are given in the following plot. The vertical line represents $F_{.95;2,27} = 3.354$, the critical value for the F-test with $\alpha = 0.05$.

F(2,27) and non-central F-Distributions



For each scenario, we can compute the power of the F-test, making use of the probability functions in R or SAS:

$$\pi_1 = P(F_{2,27,0} \geq F_{.95;2,27}) = 0.0500 \quad \pi_2 = P(F_{2,27,1.25} \geq F_{.95;2,27}) = 0.1435$$

$$\pi_3 = P(F_{2,27,5} \geq F_{.95;2,27}) = 0.4580 \quad \pi_4 = P(F_{2,27,20} \geq F_{.95;2,27}) = 0.9733$$

In most applications, researchers have a particular set of treatment effects that they would like to be able to detect with a high probability. That is, they feel these effects are of practical importance. Once the effects, and an estimate of σ are obtained (or the effects have been determined in standard deviation units as in the previous example), the researchers choose treatment sample sizes that achieve a chosen power, when the test is conducted at a given significance level (typically $\alpha = 0.05$). Note that the distribution of the F-statistic used for testing $H_0: \mu_1 = \dots = \mu_g = \mu$ has degrees of freedom: $df_1 = g-1$ and $df_2 = N-g$, where $N = ng$ in the balanced case. Thus, the critical value and the F-distributions shapes depend on the sample sizes.

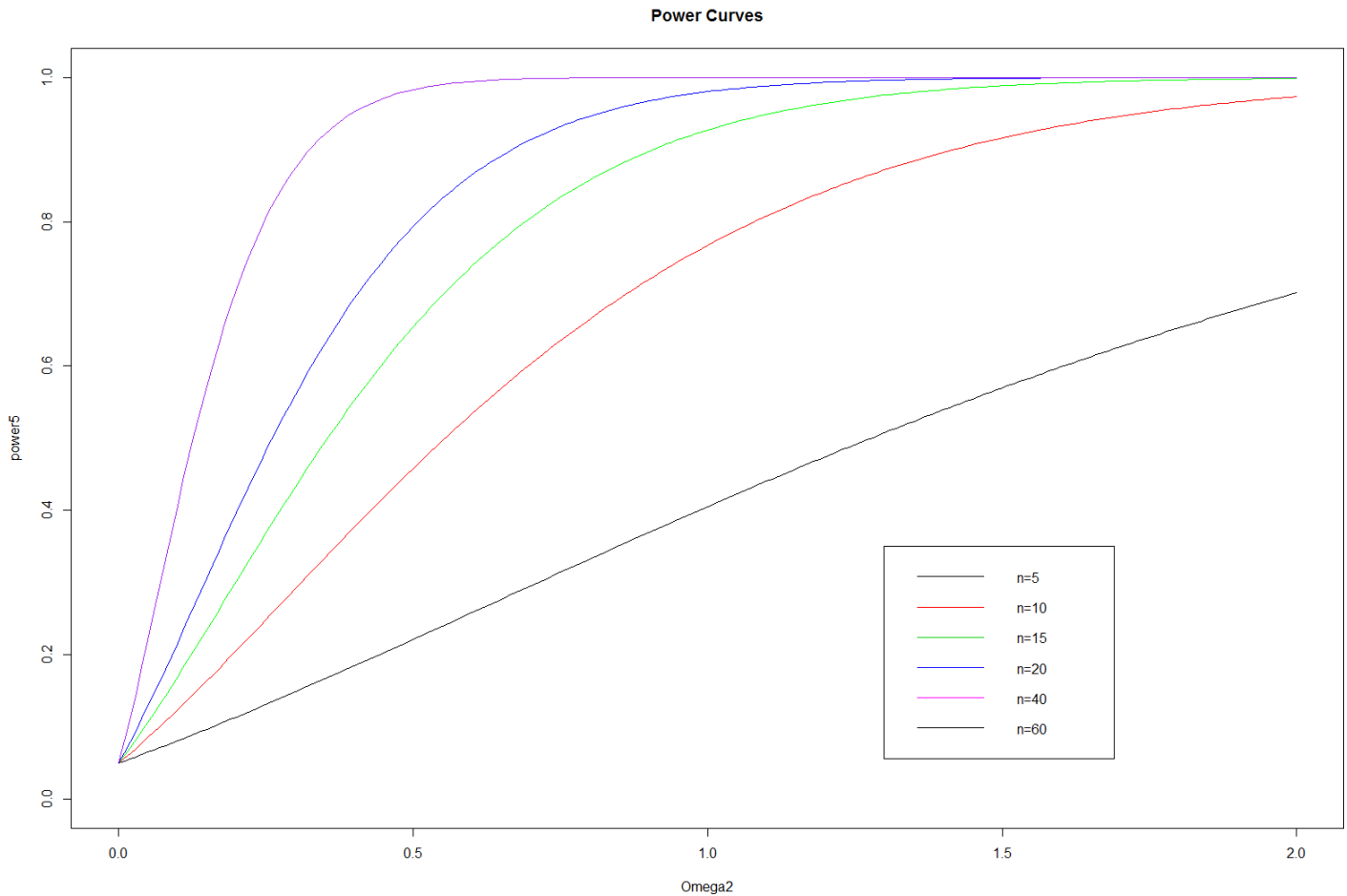
Suppose we wish to detect the treatment effects described by scenarios 2 and 3, previously described with power $= \pi^*$ (say 0.80, with significance level α). What sample sizes are needed for this power to be met? Consider the following algorithm for a given 2Ω :

1. Set n at a low value (say 2)
2. Compute 2Ω for the given sample size, treatment effects, and σ
3. Obtain $\pi_n = P(F_{g-1, N-g, 2\Omega} \geq F_{1-\alpha; g-1, N-g})$
4. If $\pi_n \geq \pi^*$ stop, otherwise go back to step 1, and increase n by 1.

The algorithm is run below with:

$$2\Omega_2 = 0.125n \quad 2\Omega_3 = 0.50n \quad \text{with } \alpha = 0.05 \quad \pi^* = 0.80$$

For scenario 2, we find that sample sizes of $n = 80$ (per treatment) will be needed to meet the requirements. For scenario 3, we will need $n = 22$ per treatment. The following plot gives power curves for a range of 2Ω values for $n = 5, 10, 15, 20, 40$, and 60 observations per treatment (60 is not given in R program).



R Program – Normal Distributions

```
## Plot data norml distributions
y <- seq(0,200,.01)
fy1.1 <- dnorm(y,100,20); fy2.1 <- dnorm(y,100,20); fy3.1 <- dnorm(y,100,20)
fy1.2 <- dnorm(y,105,20); fy2.2 <- dnorm(y,100,20); fy3.2 <- dnorm(y,95,20)
fy1.3 <- dnorm(y,110,20); fy2.3 <- dnorm(y,100,20); fy3.3 <- dnorm(y,90,20)
fy1.4 <- dnorm(y,120,20); fy2.4 <- dnorm(y,100,20); fy3.4 <- dnorm(y,80,20)

par(mfrow=c(2,2))
plot(y,fy2.1,type="l",main=expression(paste("2",Omega,"=0")),col="black",
xlim=c(0,200),ylim=c(0,1.2*dnorm(100,100,20)))

plot(y,fy2.2,type="l",main=expression(paste("2",Omega,"=1.25")),col="black",
xlim=c(0,200),ylim=c(0,1.2*dnorm(100,100,20)))
lines(y,fy1.2,type="l",col="green")
lines(y,fy3.2,type="l",col="red")

plot(y,fy2.3,type="l",main=expression(paste("2",Omega,"=5")),col="black",
xlim=c(0,200),ylim=c(0,1.2*dnorm(100,100,20)))
lines(y,fy1.3,type="l",col="green")
lines(y,fy3.3,type="l",col="red")

plot(y,fy2.4,type="l",main=expression(paste("2",Omega,"=20")),col="black",
xlim=c(0,200),ylim=c(0,1.2*dnorm(100,100,20)))
lines(y,fy1.4,type="l",col="green")
lines(y,fy3.4,type="l",col="red")
```

R Program - F and non-central F distributions and Power Calculations

```
### Plot F-distributions
par(mfrow=c(1,1))
f <- seq(0.25,12,.01); df1 <- df(f,2,27); df2 <- df(f,2,27,1.25)
df3 <- df(f,2,27,5); df4 <- df(f,2,27,20)

f1.crit <- qf(.95,2,27)

plot(f,df1,main="F(2,27) and non-central F-Distributions",type="l")
lines(f,df2,col="purple")
lines(f,df3,col="red")
lines(f,df4,col="blue")
abline("v"=f1.crit)
legend(8,0.8,c("F(2,27,0)", "F(2,27,1.25)", "F(2,27,5)", "F(2,27,20)"),
lty=c(1,1,1,1),col=c(1,6,2,4))

### Power Computations for fixed n, Omega

(pi1 <- 1-pf(qf(.95,2,27),2,27,0))
(pi2 <- 1-pf(qf(.95,2,27),2,27,1.25))
(pi3 <- 1-pf(qf(.95,2,27),2,27,5))
(pi4 <- 1-pf(qf(.95,2,27),2,27,20))

### Power Computations for fixed power, alpha, Omega (2xOmega)

## Scenario 2

Omega_n <- 0.125; power_star <- 0.80; alpha <- 0.05; n <- 2; power_n <- 0
g <- 3
while (power_n < power_star) {
N <- n*g; df1 <- g-1; df2 <- N-g
Omega <- n*Omega_n
n.new <- n
power_n <- 1-pf(qf(1-alpha,df1,df2),df1,df2,Omega)
n <- n.new + 1
# print(cbind(n,power_n))
}

print(cbind(n,power_n))

## Scenario 3

Omega_n <- 0.500; power_star <- 0.80; alpha <- 0.05; n <- 2; power_n <- 0
g <- 3
while (power_n < power_star) {
N <- n*g; df1 <- g-1; df2 <- N-g
Omega <- n*Omega_n
n.new <- n
power_n <- 1-pf(qf(1-alpha,df1,df2),df1,df2,Omega)
n <- n.new + 1
# print(cbind(n,power_n))
}
print(cbind(n,power_n))

### Power curves for n = 5,10,15,20,40 with sum(a_i^2/sigma^2) < 2, alpha=.05
g <- 3; Omega2 <- seq(0,2,0.01)

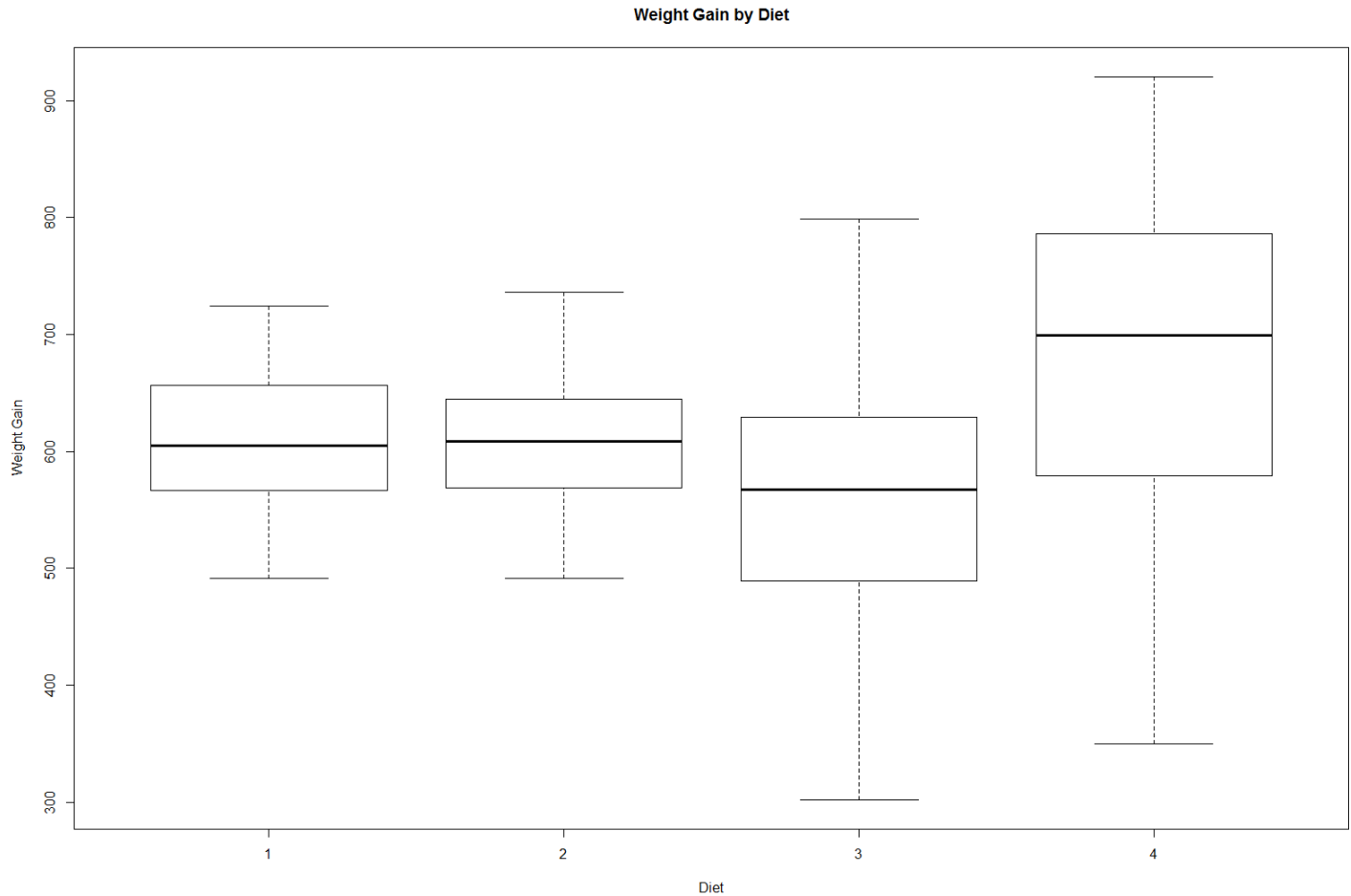
power5 <- 1-pf(qf(.95,g-1,(g*(5-1))),g-1,(g*(5-1)),(5*Omega2))
power10 <- 1-pf(qf(.95,g-1,(g*(10-1))),g-1,(g*(10-1)),(10*Omega2))
power15 <- 1-pf(qf(.95,g-1,(g*(15-1))),g-1,(g*(15-1)),(15*Omega2))
power20 <- 1-pf(qf(.95,g-1,(g*(20-1))),g-1,(g*(20-1)),(20*Omega2))
power40 <- 1-pf(qf(.95,g-1,(g*(40-1))),g-1,(g*(40-1)),(40*Omega2))

plot(Omega2,power5,main="Power Curves",type="l",col="black",ylim=c(0,1))
lines(Omega2,power10,col="red")
lines(Omega2,power15,col="green")
lines(Omega2,power20,col="blue")
lines(Omega2,power40,col="purple")
legend(1.3,0.35,c("n=5", "n=10", "n=15", "n=20", "n=40"),lty=c(rep(1,5)),
col=c(1,2,3,4,6))

1-pf(qf(.95,g-1,(g*(20-1))),g-1,(g*(20-1)),(20*0.5))
```

Example: Whole Breast Weight of Broiler Chickens

An experiment was conducted to compare $g = 4$ treatments for weight gain in broiler chickens. A total of $N = 240$ chicks were randomized to 4 diets ($n = 60$ for each treatment). The 4 diets were: Base Sorghum (BS, $i=1$), Base Sorghum + Methionine (BSM, $i=2$), Base Corn (BC, $i=3$), and Base Corn + Methionine (BCM, $i=4$). Data have been simulated to match the published means and standard deviations. Side-by-side box-plots are shown here, along with the sample means, standard deviations, and sums of squares.



Diet (i)	n	Mean	SD	$(y_{b_i} - \bar{y})^2$	$(n_i - 1)S_i^2$
BS(1)	60	606.33	54.18	88.74	173192.87
BSM(2)	60	610.67	53.68	25.81	170011.00
BC(3)	60	566.00	102.41	2475.06	618780.68
BCM(4)	60	680.00	135.06	4128.06	1076231.01
Summary	240	615.75		403060.07	2038215.56
	N	ybar		SS_Trts	SS_Err

Below, we give the ANOVA table, along with F-test at $\alpha = 0.05$ significance level.

ANOVA						
Source	df	SumSq	MeanSq	F	F(0.05)	P-value
Diets	3	403060	134353.36	15.56	2.64	0.0000
Error	236	2038216	8636.51			
Total	239	2441276				

Clearly, we reject $H_0: \mu_1 = \mu_2 = \mu_3 = \mu_4$. There is strong evidence that the means are not all equal. Consider the treatment effects model, subject to the treatment effects summing to 0. Note: there is no need to assume the sample size weighted means sum to 0, as all sample sizes are equal.

$$Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad i = 1, \dots, g = 4; j = 1, \dots, n = 60 \quad \varepsilon_{ij} \sim NID(0, \sigma^2) \quad s^2 = MS_{\text{Err}} = 8636.5 \quad t_{.975, 240-4} = 1.970$$

$$\hat{\mu} = \bar{y}_{..} = 615.75 \quad \hat{\alpha}_1 = \bar{y}_{1.} - \bar{y}_{..} = 606.33 - 615.75 = -9.42$$

$$\hat{\alpha}_2 = 610.67 - 615.75 = -5.08 \quad \hat{\alpha}_3 = 566.00 - 615.75 = -49.75 \quad \hat{\alpha}_4 = 680.00 - 615.75 = 64.25$$

$$V\left\{\hat{\mu}\right\} = \frac{MS_{\text{Err}}}{N} = \frac{8636.5}{240} = 35.99 \Rightarrow SE\left\{\hat{\mu}\right\} = \sqrt{35.99} = 6.00$$

$$95\% \text{ CI for } \mu: 615.75 \pm 1.970(6.00) \equiv 615.75 \pm 11.82 \equiv (603.93, 627.57)$$

$$V\left\{\hat{\alpha}_i\right\} = MS_{\text{Err}} \left(\frac{1}{n_i} - \frac{1}{N} \right) = 8636.5 \left(\frac{1}{60} - \frac{1}{240} \right) = 8636.5 \left(\frac{3}{240} \right) = 107.96 \Rightarrow SE\left\{\hat{\alpha}_i\right\} = \sqrt{107.96} = 10.39$$

$$95\% \text{ CI for } \alpha_1: -9.42 \pm 1.970(10.39) \equiv -9.42 \pm 20.47 \equiv (-29.89, 11.05)$$

$$95\% \text{ CI for } \alpha_2: -5.08 \pm 1.970(10.39) \equiv -5.08 \pm 20.47 \equiv (-25.55, 15.39)$$

$$95\% \text{ CI for } \alpha_3: -49.75 \pm 1.970(10.39) \equiv -49.75 \pm 20.47 \equiv (-70.22, -29.28)$$

$$95\% \text{ CI for } \alpha_4: 64.25 \pm 1.970(10.39) \equiv 64.25 \pm 20.47 \equiv (43.78, 84.72)$$

Below is the R program for this analysis. Note that it uses the **contrasts** = “**contr.sum**” options to make the treatment effects sum to zero. The 4th estimated treatment effect is the negative of the sum of the first 3, and will have the same standard error, as all sample sizes are equal.

R Program:

```
wbw <-
read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F, col.names=c("trt", "repnum", "base", "meth", "wtg"))
attach(wbw); names(wbw)

trt.f <- factor(trt)

plot(trt.f, wtg, main="Weight Gain by Diet", xlab="Diet", ylab="Weight Gain")

tapply(wtg, trt.f, mean)
tapply(wtg, trt.f, sd)

options(contrasts=c("contr.sum", "contr.poly"))

wbw.mod2 <- aov(wtg ~ trt.f)
summary.lm(wbw.mod2)
confint(wbw.mod2)
```

R Output:

```
> tapply(wtg,trt.f,mean)
      1      2      3      4
606.3300 610.6697 566.0003 679.9997
> tapply(wtg,trt.f,sd)
      1      2      3      4
 54.17975  53.68048 102.40992 135.05940
> options(contrasts=c("contr.sum","contr.poly"))
>
> wbw.mod2 <- aov(wtg ~ trt.f)
> summary.lm(wbw.mod2)

Call:
aov(formula = wtg ~ trt.f)

Residuals:
    Min       1Q   Median       3Q      Max
-330.05  -58.17    2.07   57.44  240.66

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)   615.750      5.999  102.646 < 2e-16 ***
trt.f1         -9.420     10.390  -0.907   0.366
trt.f2        -5.080     10.390  -0.489   0.625
trt.f3        -49.750     10.390  -4.788 2.97e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 92.93 on 236 degrees of freedom
Multiple R-squared:  0.1651,    Adjusted R-squared:  0.1545
F-statistic: 15.56 on 3 and 236 DF,  p-value: 2.887e-09

> confint(wbw.mod2)
              2.5 %    97.5 %
(Intercept) 603.93193 627.56790
trt.f1      -29.88927  11.04943
trt.f2      -25.54960  15.38910
trt.f3      -70.21893 -29.28023
```

Note that the default for R is to set the intercept as the first treatment mean, and the remaining $g-1$ estimates represent the differences between the other group means and the first mean. This is the **contr.treatment** option.

$$\begin{aligned} \text{Intercept: } \mu + \alpha_1 \quad \mu + \alpha_1 = \bar{y}_{1\cdot} = 606.33 \quad SE\left\{\hat{\mu} + \hat{\alpha}_1\right\} &= \sqrt{\frac{MS_{\text{Err}}}{n_1}} = \sqrt{\frac{8636.5}{60}} = 12.00 \\ \text{trt.f2: } \alpha_2 - \alpha_1 \quad \alpha_2 - \alpha_1 = \bar{y}_{2\cdot} - \bar{y}_{1\cdot} = 610.67 - 606.33 = 4.34 \quad SE\left\{\hat{\alpha}_2 - \hat{\alpha}_1\right\} &= \sqrt{MS_{\text{Err}} \left(\frac{1}{n_1} + \frac{1}{n_2}\right)} = \sqrt{\frac{2(8636.5)}{60}} = 16.97 \\ \text{trt.f3: } \alpha_3 - \alpha_1 \quad \alpha_3 - \alpha_1 = \bar{y}_{3\cdot} - \bar{y}_{1\cdot} = 566.0 - 606.33 = -40.33 \quad SE\left\{\hat{\alpha}_3 - \hat{\alpha}_1\right\} &= \sqrt{MS_{\text{Err}} \left(\frac{1}{n_1} + \frac{1}{n_3}\right)} = \sqrt{\frac{2(8636.5)}{60}} = 16.97 \\ \text{trt.f4: } \alpha_4 - \alpha_1 \quad \alpha_4 - \alpha_1 = \bar{y}_{4\cdot} - \bar{y}_{1\cdot} = 680.00 - 606.33 = 73.67 \quad SE\left\{\hat{\alpha}_4 - \hat{\alpha}_1\right\} &= \sqrt{MS_{\text{Err}} \left(\frac{1}{n_1} + \frac{1}{n_4}\right)} = \sqrt{\frac{2(8636.5)}{60}} = 16.97 \end{aligned}$$

R Program:

```
options(contrasts=c("contr.treatment","contr.poly"))

wbw.mod1 <- aov(wtg ~ trt.f)
summary.lm(wbw.mod1)
confint(wbw.mod1)
```

R Output:

```
> options(contrasts=c("contr.treatment","contr.poly"))
>
> wbw.mod1 <- aov(wtg ~ trt.f)
> summary.lm(wbw.mod1)

Call:
aov(formula = wtg ~ trt.f)

Residuals:
    Min       1Q   Median       3Q      Max
-330.05  -58.17    2.07   57.44  240.66

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)    606.33     12.00   50.538 < 2e-16 ***
trt.f2         4.34      16.97    0.256  0.7984
trt.f3        -40.33     16.97   -2.377  0.0183 *
trt.f4         73.67     16.97    4.342  2.1e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 92.93 on 236 degrees of freedom
Multiple R-squared:  0.1651,    Adjusted R-squared:  0.1545
F-statistic: 15.56 on 3 and 236 DF,  p-value: 2.887e-09

> confint(wbw.mod1)
              2.5 %      97.5 %
(Intercept) 582.69403 629.965970
trt.f2      -29.08664  37.765977
trt.f3      -73.75598  -6.903357
trt.f4       40.24336 107.095977
>
```

We can decompose the sum of squares for treatments into any $g-1$ pairwise orthogonal contrasts. There will be many possibilities, depending on research questions of interest among the treatments. For two contrasts to be orthogonal, we need:

$$C_A = \sum_{i=1}^g a_i \mu_i \quad \text{s.t.} \quad \sum_{i=1}^g a_i = 0 \quad C_B = \sum_{i=1}^g b_i \mu_i \quad \text{s.t.} \quad \sum_{i=1}^g b_i = 0 \quad C_A \perp C_B \Leftrightarrow \sum_{i=1}^g \frac{a_i b_i}{n_i} = 0$$

Note that when the experiment is balanced (equal sample sizes among treatments), we simply need $\sum_{i=1}^g a_i b_i = 0$.

Consider the Broiler Chicken Diet Experiment, with the following 3 Contrasts:

- Corn – Sorghum (Across Methionine levels):
- Methionine – No Methionine (Across Base Levels)
- (Corn – Sorghum)_{Meth+} - (Corn – Sorghum)_{Meth-}

The forms of the contrasts are given below.

Corn - Sorghum: $[(\mu_C + \mu_{CM}) - (\mu_S + \mu_{SM})] = [-\mu_1 - \mu_2 + \mu_3 + \mu_4] = \sum_{i=1}^g a_i \mu_i = C_A$			
Meth ⁺ – Meth ⁻ : $[(\mu_{SM} + \mu_{CM}) - (\mu_S + \mu_C)] = [-\mu_1 + \mu_2 - \mu_3 + \mu_4] = \sum_{i=1}^g b_i \mu_i = C_B$			
(C - S) _{M+} – (C - S) _{M-} : $[(\mu_{CM} - \mu_{SM}) - (\mu_C - \mu_S)] = [+ \mu_1 - \mu_2 - \mu_3 + \mu_4] = \sum_{i=1}^g c_i \mu_i = C_C$			
$\sum_{i=1}^g a_i b_i = ((-1)(-1) + (-1)(+1) + (+1)(-1) + (+1)(+1)) = 0$			
$\sum_{i=1}^g a_i c_i = ((-1)(+1) + (-1)(-1) + (+1)(-1) + (+1)(+1)) = 0$			
$\sum_{i=1}^g b_i c_i = ((-1)(+1) + (+1)(-1) + (-1)(-1) + (+1)(+1)) = 0$			
$\hat{C}_A = [-606.33 - 610.67 + 566 + 680] = 29.00$	$\hat{V}\{\hat{C}_A\} = MS_{\text{Err}} \sum_{i=1}^g \frac{a_i^2}{n_i} = 8636.5 \left(4 \left(\frac{1}{60} \right) \right) = 575.77$	$\hat{SE}\{\hat{C}_A\} = 24.00$	
$\hat{C}_B = [-606.33 + 610.67 - 566 + 680] = 118.34$	$\hat{V}\{\hat{C}_B\} = MS_{\text{Err}} \sum_{i=1}^g \frac{b_i^2}{n_i} = 8636.5 \left(4 \left(\frac{1}{60} \right) \right) = 575.77$	$\hat{SE}\{\hat{C}_B\} = 24.00$	
$\hat{C}_C = [606.33 - 610.67 - 566 + 680] = 109.66$	$\hat{V}\{\hat{C}_C\} = MS_{\text{Err}} \sum_{i=1}^g \frac{c_i^2}{n_i} = 8636.5 \left(4 \left(\frac{1}{60} \right) \right) = 575.77$	$\hat{SE}\{\hat{C}_C\} = 24.00$	
95% CI for C_A : $29.00 \pm 1.970(24) \equiv 29.00 \pm 47.28 \equiv (-18.28, 76.28)$			
95% CI for C_B : $118.34 \pm 1.970(24) \equiv 118.34 \pm 47.28 \equiv (71.06, 165.62)$			
95% CI for C_C : $109.66 \pm 1.970(24) \equiv 109.66 \pm 47.28 \equiv (62.38, 156.94)$			

Clearly, Contrasts B and C are important, while Contrast A is not. There is evidence of a Methionine main effect, and the fact that the Corn – Sorghum effect depends on whether Methionine is present or absent. The sum of squares for a contrast is given below, along with its corresponding F-test. Note that below, we replace the weights of +/-1 with +/- (1/4), so that the sum of the absolute values of the weights is 1, which is common in the description of contrasts.

$$SSC = \frac{\left(\sum_{i=1}^g w_i \bar{Y}_{i\cdot}\right)^2}{\sum_{i=1}^g \frac{w_i^2}{n_i}} = \frac{\left(\hat{C}\right)^2}{\sum_{i=1}^g \frac{w_i^2}{n_i}} \quad \text{when the experiment is balanced: } SSC = \frac{\left(\hat{C}\right)^2}{\sum_{i=1}^g \frac{w_i^2}{n}} = n \frac{\left(\hat{C}\right)^2}{\sum_{i=1}^g w_i^2}$$

$$H_0 : C = 0 \quad H_A : C \neq 0 \quad TS : F = \frac{(SSC/1)}{MS_{Err}} \stackrel{H_0}{\sim} F_{1, N-g}$$

$$SSC_A = n \frac{\left(\hat{C}_A\right)^2}{\sum_{i=1}^g w_i^2} = 60 \left(\frac{(7.25)^2}{1/4} \right) = 12615 \quad SSC_B = 60 \left(\frac{(29.585)^2}{1/4} \right) = 210065.3 \quad SSC_C = 60 \left(\frac{(27.415)^2}{1/4} \right) = 180379.7$$

$$F_A = \frac{12615}{8636.5} = 1.46 \quad F_B = \frac{210065.3}{8636.5} = 24.32 \quad F_C = \frac{180379.7}{8636.5} = 20.89 \quad F_{.95; 1, 236} = 3.88$$

Note: $SSC_A + SSC_B + SSC_C = 403060 = SS_{Tt}$ They are pairwise orthogonal contrasts.

R Program: Note that we need to divide each weight by $g = 4$ in R to obtain same scale for C as we had above.

```
contrasts(trt.f) <- cbind(c(-1/4, -1/4, 1/4, 1/4),
                        c(-1/4, 1/4, -1/4, 1/4), c(1/4, -1/4, -1/4, 1/4))

wbw.mod4 <- aov(wtg ~ trt.f)
summary.lm(wbw.mod4)
anova(wbw.mod4)
confint(wbw.mod4)
```

R Output:

```
> wbw.mod4 <- aov(wtg ~ trt.f)
> summary.lm(wbw.mod4)

Call: aov(formula = wtg ~ trt.f)

Residuals:
    Min       1Q   Median       3Q      Max
-330.05  -58.17    2.07   57.44  240.66

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  615.750     5.999  102.646 < 2e-16 ***
trt.f1       29.000     23.995   1.209  0.228
trt.f2      118.339     23.995   4.932 1.54e-06 ***
trt.f3      109.660     23.995   4.570 7.86e-06 ***

Residual standard error: 92.93 on 236 degrees of freedom
Multiple R-squared:  0.1651,    Adjusted R-squared:  0.1545
F-statistic: 15.56 on 3 and 236 DF,  p-value: 2.887e-09

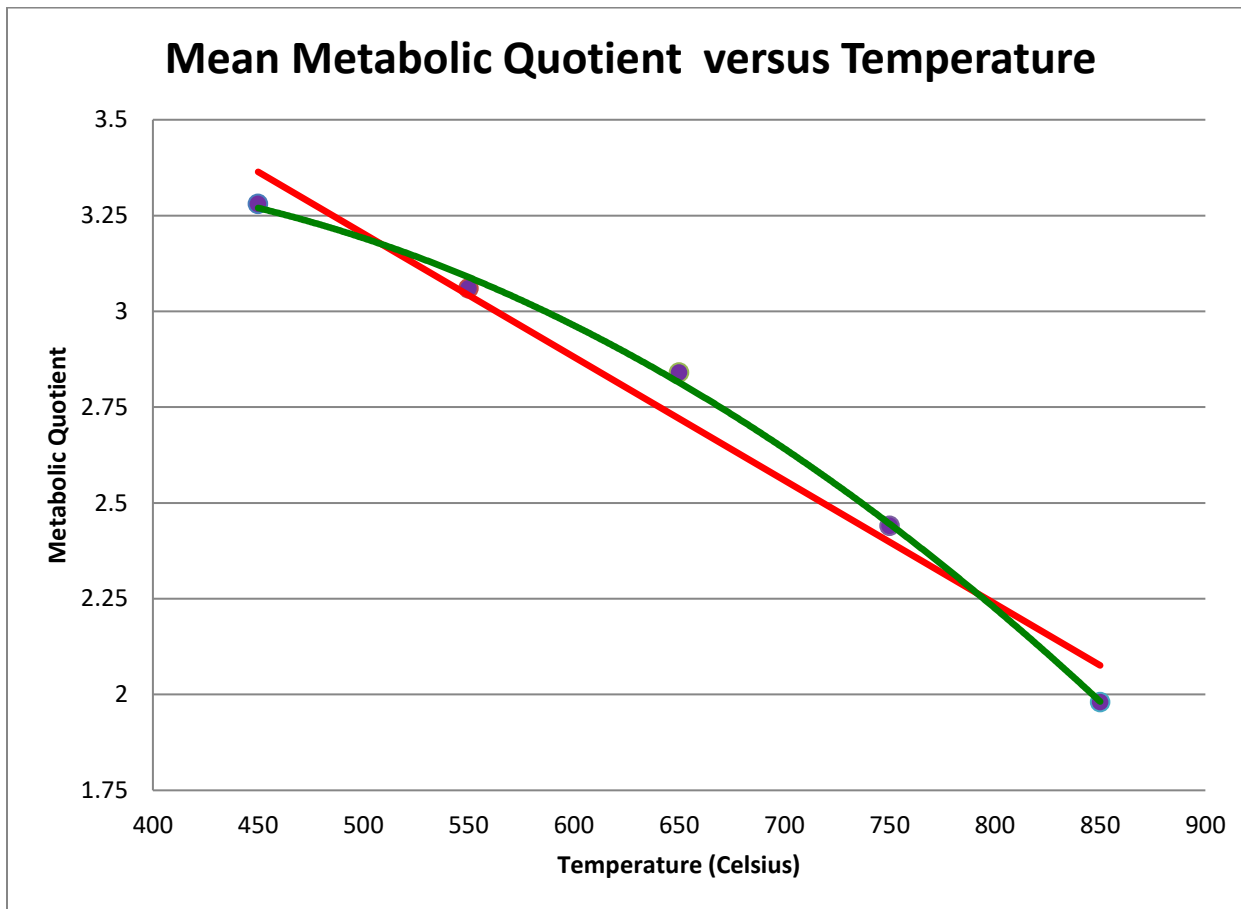
> anova(wbw.mod4)
Analysis of Variance Table

Response: wtg
          Df Sum Sq Mean Sq F value    Pr(>F)
trt.f      3  403056  134352  15.556 2.887e-09 ***
Residuals 236 2038207    8636
> confint(wbw.mod4)
          2.5 %    97.5 %
(Intercept) 603.93193 627.56790
trt.f1     -18.27161  76.27227
trt.f2      71.06706 165.61094
trt.f3      62.38773 156.93161
```

When the treatments are numeric levels of a factor, we can decompose the Treatment sum of squares into contrasts representing linear, quadratic, cubic, etc., components (up to order $g-1$). When the levels are equally spaced and design is balanced, there are tables that give orthogonal polynomial contrasts. When they are not equally spaced, and/or the design is unbalanced, the **orpol** function in SAS/IML can be used to obtain them.

Example: Characteristics of Soil Charcoal Generated at 5 Temperatures

Soil charcoal was produced at $g = 5$ equally spaced temperatures (450°C, 550, 650, 750, 850) with $n_i = 24$ replicates per temperature. One reported characteristic is Metabolic Quotient (MQ). The following plot gives the mean MQ for each treatment, along with linear and quadratic curves.



Note that while the quadratic curve (Green) appears to fit better than the linear (Red), we need to take into account the variation in the measurements within the temperatures. The following table gives the summary statistics, sums of squares, and F-test for the study. We find strong evidence of differences among temperature effects ($F_{obs} = 10.175$, $F(.95;4,115) = 2.451$)

Temp	Mean	SEM	n	SD		SSTrts	SSErr
450	3.28	0.19	24	0.9308		25.6704	72.5328
550	3.06	0.18	24	0.8818		dfTrts	dfErr
650	2.84	0.17	24	0.8328		4	115
750	2.44	0.14	24	0.6859		MSTrts	MSErr
850	1.98	0.12	24	0.5879		6.4176	0.6307
						F*	F(0.95)
						10.1750	2.4506

The following table gives the coefficients for orthogonal polynomials (linear, quadratic, cubic, and quartic), along with the estimates, sums of squares and 1 degree of freedom F-tests. Although the plot shows a quadratic effect, the experimental error is large so that the F-test for the quadratic contrast is not significant. Recall that the Sum of Squares for a contrast is:

$$SSC = \frac{\left(\hat{C}\right)^2}{\sum_{i=1}^g \frac{w_i^2}{n_i}} \quad \text{and for a balanced design, } SSC = n \left[\frac{\left(\hat{C}\right)^2}{\sum_{i=1}^g w_i^2} \right]$$

Linear	Quad	Cubic	Quartic
-2	2	-1	1
-1	-1	2	-4
0	-2	0	6
1	-1	-2	-4
2	2	1	1
C1	C2	C3	C4
-3.22	-0.66	-0.06	0.30
sum(w^2)	sum(w^2)	sum(w^2)	sum(w^2)
10	14	10	70
SSC1	SSC2	SSC3	SSC4
24.8842	0.7467	0.0086	0.0309
F_C1	F_C2	F_C3	F_C4
39.4536	1.1840	0.0137	0.0489
P-val1	P-val2	P-val3	P-val4
0.0000	0.2788	0.9070	0.8253

Below is the R program and output for this analysis. Note that the tests for polynomial effects are tested by t-tests as opposed to the F-test above conducted in EXCEL. The square of the t-statistic is the F-statistic, and the p-values are identical.

R Program

```
tapply(y, trt.y, mean)
tapply(y, trt.y, sd)
trt.y <- factor(trt.y, ordered=T)

charcoal.mod1 <- lm(y ~ trt.y)
summary.aov(charcoal.mod1)
summary.lm(charcoal.mod1)
```

R Output

```
> tapply(y, trt.y, mean)
  1     2     3     4     5
3.28 3.06 2.84 2.44 1.98
> tapply(y, trt.y, sd)
  1     2     3     4     5
0.9308 0.8818 0.8328 0.6859 0.5879
>
>
> trt.y <- factor(trt.y, ordered=T)
>
> charcoal.mod1 <- lm(y ~ trt.y)
>
> summary.aov(charcoal.mod1)
      Df Sum Sq Mean Sq F value    Pr(>F)
trt.y    4   25.67   6.418   10.18 4.35e-07 ***
Residuals 115   72.53   0.631
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary.lm(charcoal.mod1)

Call:
lm(formula = y ~ trt.y)

Residuals:
    Min       1Q   Median       3Q      Max
-1.68892 -0.56933 -0.02668  0.53526  1.84450

Coefficients:
(Intercept)  2.72000  0.07250  37.518 < 2e-16 ***
trt.y.L      -1.01825  0.16211  -6.281 6.18e-09 ***
trt.y.Q      -0.17639  0.16211  -1.088  0.279
trt.y.C      -0.01897  0.16211  -0.117  0.907
trt.y^4       0.03586  0.16211   0.221  0.825
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.7942 on 115 degrees of freedom
Multiple R-squared:  0.2614, Adjusted R-squared:  0.2357
F-statistic: 10.18 on 4 and 115 DF, p-value: 4.35e-07
```

Data Sources:

M.I. Aksu, H. Imik, M. Karoglu (2007). "Influence of Dietary Sorghum(*Sorghum vulgare*) and Corn Supplemented with Methionine on Cut-Up Pieces Weights of Broiler Carcass and Quality Properties of Breast and Drumsticks Meat," *Food Science and Technology International*, Vol. 13, #5, pp. 361-367.

S.P. Bergeron, R.L. Bradley, A. Munson, W. Parsons (2013). "Physico-Chemical and Functional Characteristics of Soil Charcoal Produced at Five Different Temperatures," *Soil Biology & Biochemistry*, Vol. 58, pp. 140-146.

Chapter 3 – Multiple Comparison Methods

In practice, there are typically multiple contrasts that are to be simultaneously tested and/or estimated. These may be **pre-planned** or **data-generated** by the observed responses. In the first case, we would want to adjust the error rates on the individual pre-planned tests, so that the overall error rate is some acceptable level. In the second case, we would want to use a very conservative method to detect the data-generated effects.

There can be individual hypotheses or there can be simultaneous hypotheses. The simultaneous hypotheses can be considered as the intersection of individual hypotheses. $H_0 : H_{01} \cap H_{02} \cap \dots \cap H_{0S}$ where S is the number of simultaneous hypotheses. The **comparison-wise error rate** is the probability we reject a given single H_{0i} when it is true. This will be labelled as α_c . The **experiment-wise error rate** is the probability we reject at least one of the H_{0i} when all of the null hypotheses are true. This will be labelled as α_E , and the comparison-wise error rates will have to be less than or equal to the experiment-wise error rate: $\alpha_c \leq \alpha_E$. The experiment-wise error rate only considers false rejections, if one of the null hypotheses is false, and the test rejects it, no error has occurred.

The **false discovery rate** is the expected proportion of all rejected null hypotheses that are false rejections. Note that null hypotheses can either be true or false and a test can end in either rejecting or accepting the null hypotheses. The FDR represents the expected ratio of false rejections to total rejections.

The **strong family-wise error rate** is the probability that any false rejections have occurred among the true null hypotheses. This acknowledges that some of the null hypotheses can be true, and others false.

Two special classes of multiple comparisons are all pairwise comparisons of treatment means, with:

$$S = \binom{g}{2} = \frac{g!}{2!(g-2)!} = \frac{g(g-1)}{2} \text{ and comparisons of all treatments with a Control, with } S = g - 1.$$

When estimating means, and contrasts among means, confidence intervals can be computed based on the estimates and their standard errors. Each confidence interval can be computed at a given level of confidence, such that all confidence intervals will contain their true parameter values with confidence $1 - \alpha_E$. These are referred to as **simultaneous confidence intervals**. Consider the case where we have $S = 2$ contrasts or parameters we wish to estimate simultaneously. Note that these will not be independent in the case of an ANOVA model, as the intervals will both make use of MS_{Err} . Let $E_1 \equiv$ the event that the first confidence interval does not contain its target parameter, and similarly E_2 for the second confidence interval. Then:

$$\begin{aligned} P(E_1) &= \alpha & P(E_2) &= \alpha & P(E_1 \cup E_2) &= P(E_1) + P(E_2) - P(E_1 \cap E_2) = \alpha + \alpha - \alpha^2 = 2\alpha - \alpha^2 \\ \Rightarrow P(\overline{E_1 \cup E_2}) &= 1 - (2\alpha - \alpha^2) = 1 - 2\alpha + \alpha^2 \geq 1 - 2\alpha \end{aligned}$$

Thus, the probability that both are correct exceeds $1 - 2\alpha$. This is the Bonferroni Inequality and generalizes for any number S confidence intervals. The lack of independence makes the probability higher than this. The Bonferroni approach has each confidence interval computed with $\alpha_c = \alpha_E / S$. That is, we lower the error rate (increase the confidence level) for the individual confidence intervals.

Now, we consider several of the many methods available for making multiple comparisons.

3.1. Scheffe's Method for All Contrasts

Scheffe's method is the most conservative of the methods, but can be used for all possible contrasts, even those generated from the data. To understand the method, consider the F-test for treatment effects:

$$H_0 : \mu_1 = \dots = \mu_g = \mu \Rightarrow \sum_{i=1}^g w_i \mu_i = 0 \quad \forall \quad \{w_i\} \ni \sum_{i=1}^g w_i = 0 \quad \text{Reject } H_0 \text{ if: } F = \frac{\left[\frac{SS_{\text{Trt}}}{g-1} \right]}{MS_{\text{Err}}} \geq F_{1-\alpha; g-1, N-g}$$

If any contrast, when replacing SS_{Trt} with SSC for the contrast in the F-statistic, exceeds the critical F-value, then that contrast "single handedly" rejects the F-test for treatment effects. The procedure can be interpreted to conclude a contrast is significantly different from 0 if:

$$H_0 : C = 0 \quad \text{Reject } H_0 \text{ if: } F_C = \frac{\left[\frac{SSC}{g-1} \right]}{MS_{\text{Err}}} \geq F_{1-\alpha; g-1, N-g} \Rightarrow SSC \geq MS_{\text{Err}} (g-1) F_{1-\alpha; g-1, N-g} \quad SSC = \frac{\left(\hat{C} \right)^2}{\sum_{i=1}^g \frac{w_i^2}{n_i}}$$

Simultaneous confidence Intervals can be computed for any number of contrasts as:

$$\hat{C} \pm S_{\alpha_E; g-1, N-g} \hat{SE} \left\{ \hat{C} \right\} \quad S_{\alpha_E; g-1, N-g} = \sqrt{(g-1) F_{\alpha_E; g-1, N-g}} \quad \hat{SE} \left\{ \hat{C} \right\} = \sqrt{MS_{\text{Err}} \sum_{i=1}^g \frac{w_i^2}{n_i}}$$

Example: Whole Breast Weight of Broiler Chickens

Recall the $g = 4$ treatments: BS, BSM, BC, and BCM (Base Sorghum, Base Sorghum + Methionine, Base Corn, and Base Corn + Methionine). We considered the 3 orthogonal contrasts: (Corn - Sorghum, Meth⁺ - Meth⁻, (C-S)_{M+} - (C-S)_{M-}). In this case, we have:

$$g = 4 \quad n_1 = n_2 = n_3 = n_4 = 60 \quad N = 240 \quad MS_{\text{Err}} = 8636.5 \quad F_{.95; 3, 236} = 2.643 \quad (4-1)2.643 = 7.929$$

The conclusion for any contrast is, reject $H_0: C = 0$ if $SSC \geq 8636.5(7.929) = 68478.8$.

Below is an EXCEL spreadsheet giving the estimated contrasts and their sums of squares:

Diet	BS	BSM	BC	BCM	C-hat	SSC
Mean	606.33	610.67	566.00	680.00		
C1	-1	-1	1	1	29	12615
C2	-1	1	-1	1	118.34	210065.3
C3	1	-1	-1	1	109.66	180379.7

Thus, the Methionine versus non-Methionine contrast is significant and the corn versus sorghum within Methionine versus corn versus sorghum within non-Methionine contrasts are significantly different than 0. We can also compute simultaneous 95% Confidence Intervals for each contrast.

$$S_{1-\alpha_E;g-1,N-g} = \sqrt{(g-1)F_{1-\alpha_E;g-1,N-g}} = \sqrt{(4-1)2.643} = 2.816 \quad \hat{SE}\{\hat{C}\} = \sqrt{MS_{\text{Err}} \sum_{i=1}^g \frac{w_i^2}{n_i}} = \sqrt{8636.5 \left(\frac{4}{60}\right)} = 24.00$$

$$S_{1-\alpha_E;g-1,N-g} \hat{SE}\{\hat{C}\} 2.816(24.00) = 67.58$$

$$C_1 : 29 \pm 67.58 \equiv (-38.58, 96.58) \quad C_2 : 118.34 \pm 67.58 \equiv (50.76, 185.92) \quad C_3 : 109.66 \pm 67.58 \equiv (42.08, 177.24)$$

3.2. Tukey's Method for All Pairwise Comparisons

Tukey's method is based on the studentized range and its corresponding distribution. Suppose we take a random sample from a normal population, and obtain an independent estimate of the standard deviation. Note that in this setting, the sample standard deviation cannot be based on the same sample as the original sample, and assume the standard deviation has ν degrees of freedom. Then the studentized range statistic, q , follows the studentized range distribution.

$$Y_1, \dots, Y_n \sim NID(\mu, \sigma^2) \quad q = \frac{\max(Y_1, \dots, Y_n) - \min(Y_1, \dots, Y_n)}{s} \quad P(q \geq q_{1-\alpha; n, \nu}) = \alpha$$

Critical values for the studentized range distribution for $\alpha = 0.05$ and 0.01 are widely available in textbooks and the internet. General quantiles can be obtained using the **qtukey** function in **R**. This method is highly useful in comparing all pairs of treatments in Analysis of Variance models. First, consider the testing procedure for a balanced design.

$$H_0 : \mu_1 = \dots = \mu_g = \mu \Rightarrow \bar{Y}_{1\bullet}, \dots, \bar{Y}_{g\bullet} \sim NID\left(\mu, \frac{\sigma^2}{n}\right) \quad s_{\bar{Y}_{i\bullet}} = \sqrt{\frac{MS_{\text{Err}}}{n}} \perp \{\bar{Y}_{i\bullet}\}$$

$$\Rightarrow P_{H_0} \left(\frac{|\bar{Y}_{i\bullet} - \bar{Y}_{j\bullet}|}{\sqrt{\frac{MS_{\text{Err}}}{n}}} \geq q_{1-\alpha; g, N-g} \right) \leq \alpha \Rightarrow \text{Conclude } \mu_i \neq \mu_j \text{ if } |\bar{Y}_{i\bullet} - \bar{Y}_{j\bullet}| \geq q_{1-\alpha; g, N-g} \sqrt{\frac{MS_{\text{Err}}}{n}}$$

This is referred to as **Tukey's Honest Significant Difference**. We can also obtain simultaneous confidence intervals for all pairs of mean as follows (under any configuration of the $\{\mu_i\}$), as follows:

$$\bar{Y}_{i\cdot} - \mu_i \sim N\left(0, \frac{\sigma^2}{n}\right) \Rightarrow P\left(\frac{|\left(\bar{Y}_{i\cdot} - \mu_i\right) - \left(\bar{Y}_{j\cdot} - \mu_j\right)|}{\sqrt{\frac{MS_{\text{Err}}}{n}}} \leq q_{1-\alpha;g,N-g}\right) \geq 1-\alpha \quad \forall i, j$$

$$\Rightarrow P\left(-q_{1-\alpha;g,N-g}\sqrt{\frac{MS_{\text{Err}}}{n}} \leq \left(\bar{Y}_{i\cdot} - \bar{Y}_{j\cdot}\right) - (\mu_i - \mu_j) \leq q_{1-\alpha;g,N-g}\sqrt{\frac{MS_{\text{Err}}}{n}}\right) \geq 1-\alpha$$

$$\Rightarrow P\left(\left(\bar{Y}_{i\cdot} - \bar{Y}_{j\cdot}\right) - q_{1-\alpha;g,N-g}\sqrt{\frac{MS_{\text{Err}}}{n}} \leq \mu_i - \mu_j \leq \left(\bar{Y}_{i\cdot} - \bar{Y}_{j\cdot}\right) + q_{1-\alpha;g,N-g}\sqrt{\frac{MS_{\text{Err}}}{n}}\right) \geq 1-\alpha$$

$$\Rightarrow \text{Simultaneous } (1-\alpha_E)100\% \text{ CIs for } \mu_i - \mu_j : \left(\bar{y}_{i\cdot} - \bar{y}_{j\cdot}\right) \pm q_{1-\alpha;g,N-g}\sqrt{\frac{MS_{\text{Err}}}{n}}$$

For unequal samples, Tukey-Kramer Method: $\left(\bar{y}_{i\cdot} - \bar{y}_{j\cdot}\right) \pm \frac{q_{1-\alpha;g,N-g}}{\sqrt{2}} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j}\right)}$

Define: Balanced Case: $HSD \equiv q_{1-\alpha;g,N-g}\sqrt{\frac{MS_{\text{Err}}}{n}}$ Unbalanced: $HSD_{i,j} \equiv \frac{q_{1-\alpha;g,N-g}}{\sqrt{2}} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j}\right)}$

Example: Whole Breast Weight of Broiler Chickens

$$\bar{y}_{1\cdot} = 606.33 \quad \bar{y}_{2\cdot} = 610.67 \quad \bar{y}_{3\cdot} = 566.00 \quad \bar{y}_{4\cdot} = 680.00 \quad n = 60 \quad MS_{\text{Err}} = 8636.5 \quad q(0.05; 4, 236) = 3.659$$

$$HSD = q(0.05; 4, 236) \sqrt{\frac{MS_{\text{Err}}}{n}} = 3.659 \sqrt{\frac{8636.5}{60}} = 43.90$$

Simultaneous 95% CIs for $\mu_i - \mu_j$:

$$\mu_1 - \mu_2 : (606.33 - 610.67) \pm 43.90 \equiv -4.34 \pm 43.90 \equiv (-48.24, 39.56)$$

$$\mu_1 - \mu_3 : (606.33 - 566.00) \pm 43.90 \equiv 40.33 \pm 43.90 \equiv (-3.67, 84.23)$$

$$\mu_1 - \mu_4 : (606.33 - 680.00) \pm 43.90 \equiv -73.67 \pm 43.90 \equiv (-117.57, -29.77)$$

$$\mu_2 - \mu_3 : (610.67 - 566.00) \pm 43.90 \equiv 44.67 \pm 43.90 \equiv (0.77, 88.57)$$

$$\mu_2 - \mu_4 : (610.67 - 680.00) \pm 43.90 \equiv -69.33 \pm 43.90 \equiv (-113.23, -25.43)$$

$$\mu_3 - \mu_4 : (566.00 - 680.00) \pm 43.90 \equiv -114.00 \pm 43.90 \equiv (-157.90, -70.10)$$

The following R code produces Tukey's method for the whole breast weight analysis. The first version is in the base R package, the second version makes use of the **multcomp** package.

R Program:

```
wbw <- read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F,col.names=c("trt","repnum","base","meth","wtg"))
attach(wbw); names(wbw)

# Treatment Ordering: BS, BSM, BC, BCM

trt.f <- factor(trt)

wbw.mod1 <- aov(wtg ~ trt.f)
summary(wbw.mod1)
TukeyHSD(wbw.mod1,"trt.f")

install.packages("multcomp")
require(multcomp)

wbw.glht <- glht(wbw.mod1, linfct = mcp(trt.f="Tukey"))
summary(wbw.glht) # the summary of the tests
confint(wbw.glht)

windows(width=5,height=3,pointsize=10)
plot(wbw.glht)
title(sub="whole Breast Weight Data",adj=0)
mtext("Tukey Honest Significant Differences",side=3,line=0.5)
```

R Output (Version 1):

```
> wbw.mod1 <- aov(wtg ~ trt.f)
> summary(wbw.mod1)
      Df Sum Sq Mean Sq F value    Pr(>F)
trt.f   3  403056   134352   15.56 2.89e-09 ***
Residuals 236 2038207     8636
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> TukeyHSD(wbw.mod1,"trt.f")
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = wtg ~ trt.f)

$trt.f
      diff      lwr      upr      p adj
2-1  4.339667 -39.56149  48.2408213 0.9941188
3-1 -40.329667 -84.23082   3.5714880 0.0843571
4-1  73.669667  29.76851 117.5708213 0.0001228
3-2 -44.669333 -88.57049  -0.7681787 0.0444098
4-2  69.330000  25.42885 113.2311547 0.0003486
4-3 113.999333  70.09818 157.9004880 0.0000000
```

Note that R takes the higher labelled treatment minus the lower labelled treatment.

R Output (Version 2):

```
> wbw.glht <- glht(wbw.mod1, linfct = mcp(trt.f="Tukey"))
> summary(wbw.glht) # the summary of the tests

      Simultaneous Tests for General Linear Hypotheses

Multiple Comparisons of Means: Tukey Contrasts

Fit: aov(formula = wtg ~ trt.f)

Linear Hypotheses:
      Estimate Std. Error t value Pr(>|t|)
2 - 1 == 0      4.34      16.97   0.256  0.9941
3 - 1 == 0     -40.33      16.97  -2.377  0.0842 .
4 - 1 == 0      73.67      16.97   4.342 <0.001 ***
3 - 2 == 0     -44.67      16.97  -2.633  0.0443 *
4 - 2 == 0      69.33      16.97   4.086 <0.001 ***
4 - 3 == 0     114.00      16.97   6.719 <0.001 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)

> confint(wbw.glht)

      Simultaneous Confidence Intervals

Multiple Comparisons of Means: Tukey Contrasts

Fit: aov(formula = wtg ~ trt.f)

Quantile = 2.5874
95% family-wise confidence level

Linear Hypotheses:
      Estimate lwr      upr
2 - 1 == 0   4.3397 -39.5613  48.2406
3 - 1 == 0  -40.3297 -84.2306   3.5713
4 - 1 == 0   73.6697  29.7687 117.5706
3 - 2 == 0  -44.6693 -88.5703  -0.7684
4 - 2 == 0   69.3300  25.4290 113.2310
4 - 3 == 0  113.9993  70.0984 157.9003
```

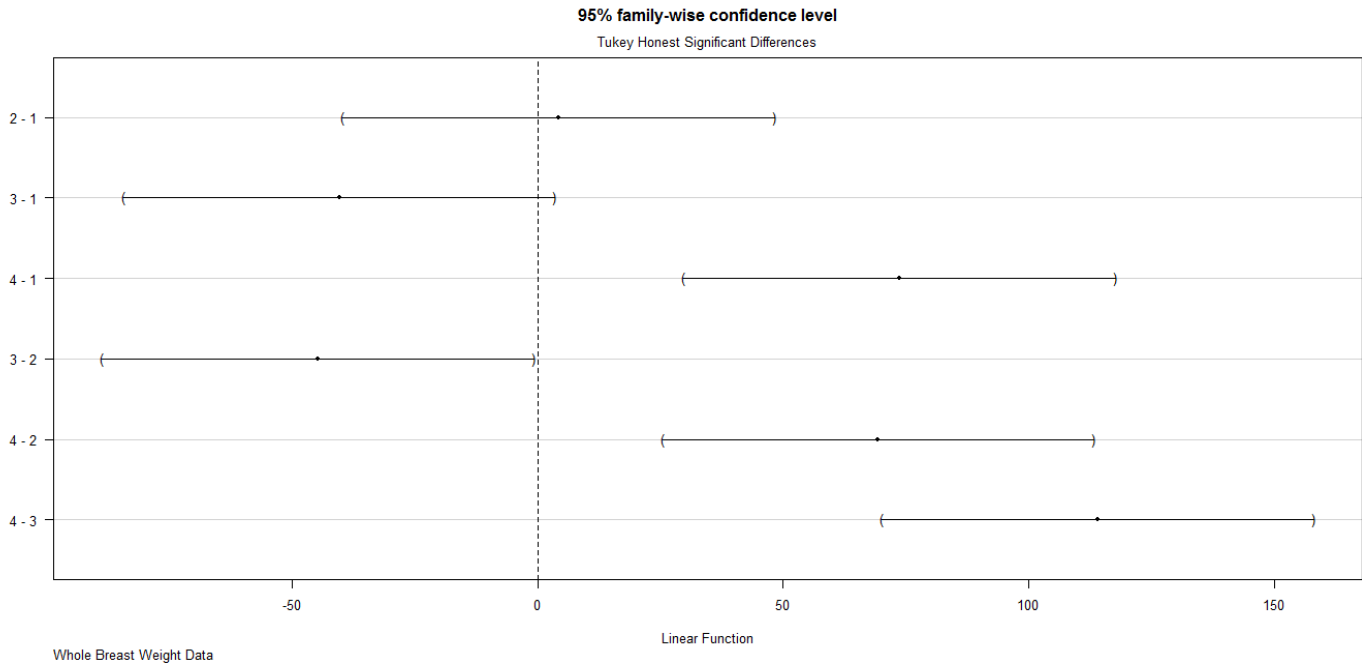
Note the form that R uses for computing *HSD* :

$$HSD = \frac{q_{1-\alpha;g,N-g}}{\sqrt{2}} \hat{SE} \{ \bar{Y}_{i\cdot} - \bar{Y}_{j\cdot} \}$$

$$\text{Quantile: } \frac{q_{.95;4,236}}{\sqrt{2}} = \frac{3.659}{\sqrt{2}} = 2.587$$

$$\text{Standard Error: } \sqrt{\frac{2MS_{\text{Err}}}{n}} = \sqrt{\frac{2(8636.5)}{60}} = 16.967$$

$$HSD = 2.587(16.967) = 43.894$$



3.3. Bonferroni's Method for All Pairwise Comparisons

This method is very general, and conservative, and can be used in any testing/estimation settings where we have S parameters and/or contrasts of interest. In the case of all possible pairwise comparisons among treatment means, we have the following tests and simultaneous confidence interval methods, based on the Bonferroni inequality:

$$S = \frac{g(g-1)}{2} \quad B_{ij} = t_{1-\alpha_E/(2S), N-g} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j} \right)}$$

Reject $H_{0(i,j)} = \mu_i - \mu_j = 0$ if $|\bar{y}_{i\cdot} - \bar{y}_{j\cdot}| \geq B_{ij}$

Simultaneous $(1-\alpha_E)100\%$ CIs for $\mu_i - \mu_j$: $(\bar{y}_{i\cdot} - \bar{y}_{j\cdot}) \pm B_{ij}$

The critical values will be higher than Tukey's HSD and the simultaneous confidence intervals will be wider. The usefulness of the Bonferroni is its generality to any testing situation.

Example: Whole Breast Weight of Broiler Chickens

$$\bar{y}_{1\bullet} = 606.33 \quad \bar{y}_{2\bullet} = 610.67 \quad \bar{y}_{3\bullet} = 566.00 \quad \bar{y}_{4\bullet} = 680.00 \quad n = 60 \quad MS_{\text{Err}} = 8636.5 \quad t_{1-.05/(2(6)),236} = 2.661$$

$$B_{i,j} = t_{1-.05/(2(6)),236} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j} \right)} = 2.661 \sqrt{8636.5 \left(\frac{2}{60} \right)} = 45.15$$

Simultaneous 95% CIs for $\mu_i - \mu_j$:

$$\mu_1 - \mu_2 : (606.33 - 610.67) \pm 45.15 \equiv -4.34 \pm 45.15 \equiv (-49.49, 40.84)$$

$$\mu_1 - \mu_3 : (606.33 - 566.00) \pm 45.15 \equiv 40.33 \pm 45.15 \equiv (-4.82, 85.48)$$

$$\mu_1 - \mu_4 : (606.33 - 680.00) \pm 45.15 \equiv -73.67 \pm 45.15 \equiv (-118.82, -28.52)$$

$$\mu_2 - \mu_3 : (610.67 - 566.00) \pm 45.15 \equiv 44.67 \pm 45.15 \equiv (-0.48, 89.82)$$

$$\mu_2 - \mu_4 : (610.67 - 680.00) \pm 45.15 \equiv -69.33 \pm 45.15 \equiv (-114.48, -24.18)$$

$$\mu_3 - \mu_4 : (566.00 - 680.00) \pm 45.15 \equiv -114.00 \pm 45.15 \equiv (-159.15, -68.85)$$

3.4. Protected Least Significant Difference (LSD) Test

For this test, the F-test for equal means is conducted. If the test does not reject the null hypothesis, stop and conclude that all means are equal. If the test does reject, then make all comparisons based on the t-distribution with no adjustment for multiple tests. This method controls the experiment-wise error rate in the weak sense (under the hypothesis that all means are equal). The LSD method is conducted as follows:

$$LSD_{ij} = t_{1-\alpha_E/2; N-g} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j} \right)}$$

$$\text{Reject } H_{0(i,j)} = \mu_i - \mu_j = 0 \quad \text{if} \quad \left| \bar{y}_{i\bullet} - \bar{y}_{j\bullet} \right| \geq LSD_{ij}$$

Example: Whole Breast Weight of Broiler Chickens

$$\bar{Y}_{1\bullet} = 606.33 \quad \bar{Y}_{2\bullet} = 610.67 \quad \bar{Y}_{3\bullet} = 566.00 \quad \bar{Y}_{4\bullet} = 680.00 \quad n = 60 \quad MS_{\text{Err}} = 8636.5 \quad t_{1-.05/2,236} = 1.970$$

$$LSD_{i,j} = t_{1-.05/2,236} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j} \right)} = 1.970 \sqrt{8636.5 \left(\frac{2}{60} \right)} = 33.43$$

Conclude: $\mu_1 > \mu_3$ $\mu_2 > \mu_3$ $\mu_4 > \mu_3$ $\mu_4 > \mu_1$ $\mu_4 > \mu_2$

3.5. Student-Newman-Keuls (SNK) Multiple Range Test

This method is a multiple range test that controls the False Discovery rate (the expected fraction of false rejections out of the total number of rejections). It makes use of the studentized range distribution, and has different critical values depending on the number of means within the range.

The procedure begins with ordering the means from lowest to highest: $\bar{Y}_{(1)} \leq \bar{Y}_{(2)} \leq \dots \leq \bar{Y}_{(g-1)} \leq \bar{Y}_{(g)}$.

Start with the longest range (length g), comparing the largest and smallest means, based on Tukey's HSD. If those are not significantly different, stop and conclude no means are significantly different. Otherwise, adjust the critical value to take into account that we are comparing means of range length $g-1$ (the first versus second largest, and the second versus largest). Continue until neighboring means (range length 2 are compared). Once a given range is determined to be non-significant, do not consider "sub-ranges" of the range. The critical values for the different ranges are given below. As with Tukey's HSD, the method can be used with unequal sample sizes, rendering the error rates as approximate.

Range of length $k = i - j + 1$: Conclude $\mu_{(i)} - \mu_{(j)} \neq 0$ if $\bar{y}_{(i)} - \bar{y}_{(j)} \geq q_{\alpha_E; k, v} \sqrt{\frac{MS_{\text{Err}}}{n}}$ $i > j$

For unequal sample sizes: $\bar{y}_{(i)} - \bar{y}_{(j)} \geq \frac{q_{\alpha_E; k, v}}{\sqrt{2}} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_{(i)}} + \frac{1}{n_{(j)}} \right)}$ $i > j$

Example: Whole Breast Weight of Broiler Chickens

$\bar{y}_{1\bullet} = 606.33$ $\bar{y}_{2\bullet} = 610.67$ $\bar{y}_{3\bullet} = 566.00$ $\bar{y}_{4\bullet} = 680.00$ $n = 60$ $MS_{\text{Err}} = 8636.5$

$\bar{y}_{(1)} = 566.00$ $\bar{y}_{(2)} = 606.33$ $\bar{y}_{(3)} = 610.67$ $\bar{y}_{(4)} = 680.00$

$k = 4$: $q_{.05; 4, 236} = 3.659$ $SNK_{1,4} = 3.659 \sqrt{\frac{8636.5}{60}} = 43.90$ $\bar{y}_{(4)} - \bar{y}_{(1)} = 680.00 - 566.00 = 114.00$

$k = 3$: $q_{.05; 3, 236} = 3.336$ $SNK_{1,3} = SNK_{2,4} = 3.336 \sqrt{\frac{8636.5}{60}} = 40.02$

$\bar{y}_{(3)} - \bar{y}_{(1)} = 610.67 - 566.00 = 44.67$ $\bar{y}_{(4)} - \bar{y}_{(2)} = 680.00 - 606.33 = 73.67$

$k = 2$: $q_{.05; 2, 236} = 2.786$ $SNK_{1,2} = SNK_{2,3} = SNK_{3,4} = 2.786 \sqrt{\frac{8636.5}{60}} = 33.43$

$\bar{y}_{(2)} - \bar{y}_{(1)} = 40.33$ $\bar{y}_{(3)} - \bar{y}_{(2)} = 4.34$ $\bar{y}_{(4)} - \bar{y}_{(3)} = 69.33$

Conclude (In terms of original subscripts): $\mu_1 > \mu_3$ $\mu_2 > \mu_3$ $\mu_4 > \mu_3$ $\mu_4 > \mu_1$ $\mu_4 > \mu_2$

Note that the critical value for the full range of treatments ($k = g$) corresponds to Tukey's HSD, and the critical values for neighboring treatments ($k = 2$) are the LSD. If we had found ordered treatments 2 and 4 not significantly different, we would not have compared ordered treatments 2 and 3 or 3 and 4.

3.6. Duncan's Multiple Range Test

This method is widely used, although probably not widely understood. It concerns protection levels against finding false positive rejections, as in the strong experiment-wise error rate. The purpose of the method is to increase power for finding differences as the number of means in a given range increases, presuming that the further 2 groups are apart, the more likely it is that they are different. For a range of k means, we have:

Error rate: $1 - (1 - \alpha_E)^{k-1}$ $k = 2 \Rightarrow 1 - (1 - \alpha_E)^{2-1} = \alpha_E$
 $k = 3 \Rightarrow 1 - (1 - \alpha_E)^{3-1} = 1 - (1 + \alpha_E^2 - 2\alpha_E) = \alpha_E (2 - \alpha_E) \approx 2\alpha_E$

This method is similar to the SNK method, except the SNK method keeps the error rate constant at α_E at each range length. Thus, Duncan's method is more powerful at finding true differences at a cost of increased false rejections. Special tables are needed for Duncan's method, however the **qtukey** function can be used in R to obtain the critical values with the various error rates for various ranges.

Range of length $k = i - j + 1$: Conclude $\mu_{(i)} - \mu_{(j)} \neq 0$ if $\bar{y}_{(i)} - \bar{y}_{(j)} \geq q_{1-\alpha_E^*;k,v} \sqrt{\frac{MS_{Err}}{n}}$ $i > j$
 For unequal sample sizes: $\bar{y}_{(i)} - \bar{y}_{(j)} \geq \frac{q_{1-\alpha_E^*;k,v}}{\sqrt{2}} \sqrt{MS_{Err} \left(\frac{1}{n_{(i)}} + \frac{1}{n_{(j)}} \right)}$ $i > j$

Example: Whole Breast Weight of Broiler Chickens

$\bar{y}_{1\bullet} = 606.33$ $\bar{y}_{2\bullet} = 610.67$ $\bar{y}_{3\bullet} = 566.00$ $\bar{y}_{4\bullet} = 680.00$ $n = 60$ $MS_{Err} = 8636.5$
 $\bar{y}_{(1)} = 566.00$ $\bar{y}_{(2)} = 606.33$ $\bar{y}_{(3)} = 610.67$ $\bar{y}_{(4)} = 680.00$
 $k = 4$: $\alpha_E^* = 1 - (1 - .05)^{4-1} = .143$ $q_{.857;4,236} = 3.031$ $D_{1,4} = 3.031 \sqrt{\frac{8636.5}{60}} = 36.36$
 $\bar{y}_{(4)} - \bar{y}_{(1)} = 680.00 - 566.00 = 114.00$
 $k = 3$: $\alpha_E^* = 1 - (1 - .05)^{3-1} = .098$ $q_{.902;3,236} = 2.933$ $D_{1,3} = D_{2,4} = 2.933 \sqrt{\frac{8636.5}{60}} = 35.19$
 $\bar{y}_{(3)} - \bar{y}_{(1)} = 610.67 - 566.00 = 44.67$ $\bar{y}_{(4)} - \bar{y}_{(2)} = 680.00 - 606.33 = 73.67$
 $k = 2$: $q_{.95;2,236} = 2.786$ $D_{1,2} = D_{2,3} = D_{3,4} = 2.786 \sqrt{\frac{8636.5}{60}} = 33.43$
 $\bar{y}_{(2)} - \bar{y}_{(1)} = 40.33$ $\bar{y}_{(3)} - \bar{y}_{(2)} = 4.34$ $\bar{y}_{(4)} - \bar{y}_{(3)} = 69.33$
 Conclude (In terms of original subscripts): $\mu_1 > \mu_3$ $\mu_2 > \mu_3$ $\mu_4 > \mu_3$ $\mu_4 > \mu_1$ $\mu_4 > \mu_2$

We obtain the same conclusions as for the SNK method. Note however the critical values for $k=3$ and $k=4$ were lower for Duncan's method than the SNK method. They are the same for $k=2$, since both have the same error rate.

Duncan's and Student-Newman-Keuls tests can be programmed directly in R making use of the **qtukey** command to obtain critical values of the Studentized Range Distribution. The **agricolae** package has functions to conduct the tests.

R Program:

```
wbw <- read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F,col.names=c("trt","repnum","base","meth","wtg"))
attach(wbw); names(wbw)

# Treatment Ordering: BS, BSM, BC, BCM

trt.f <- factor(trt)
wbw.mod1 <- aov(wtg ~ trt.f)
summary(wbw.mod1)

### Duncan's and SNK Test

install.packages("agricolae")
require(agricolae)
duncan.test(wbw.mod1,"trt.f",main="Whole Breast Weight",console=TRUE)
SNK.test(wbw.mod1,"trt.f",main="Whole Breast Weight",console=TRUE)
```

R Output:

```
> wbw.mod1 <- aov(wtg ~ trt.f)
> summary(wbw.mod1)
      Df Sum Sq Mean Sq F value    Pr(>F)
trt.f   3 403056  134352  15.56 2.89e-09 ***
Residuals 236 2038207    8636
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> duncan.test(wbw.mod1,"trt.f",main="Whole Breast Weight",console=TRUE)

Study: whole Breast weight

Duncan's new multiple range test
for wtg

Mean Square Error: 8636.469

trt.f, means

      wtg      std  r   Min   Max
1 606.3300  54.17975 60 491.08 724.69
2 610.6697  53.68048 60 491.35 736.35
3 566.0003 102.40992 60 301.85 799.07
4 679.9997 135.05940 60 349.95 920.66

alpha: 0.05 ; Df Error: 236

Critical Range
      2      3      4
33.42631 35.18704 36.36233

Means with the same letter are not significantly different.

Groups, Treatments and means
a      4      680
b      2      610.7
b      1      606.3
c      3      566
```

R Program (Continued):

```
> SNK.test(wbw.mod1,"trt.f",main="Whole Breast Weight",console=TRUE)
Study: Whole Breast Weight
Student Newman Keuls Test
for wtg
Mean Square Error: 8636.469
trt.f, means
      wtg      std  r   Min   Max
1 606.3300 54.17975 60 491.08 724.69
2 610.6697 53.68048 60 491.35 736.35
3 566.0003 102.40992 60 301.85 799.07
4 679.9997 135.05940 60 349.95 920.66
alpha: 0.05 ; Df Error: 236
Critical Range
      2      3      4
33.42631 40.01854 43.90115
Means with the same letter are not significantly different.
Groups, Treatments and means
a      4      680
b      2      610.7
b      1      606.3
c      3      566
>
```

3.7. Dunnett's Method for Comparing Treatments with Control or Best Treatment

Dunnett's method was first developed to compare $g-1$ treatment conditions with a pre-determined control treatment. The method has also been developed to determine which of the $g-1$ remaining treatments are not significantly different from the "best" observed treatment. The test makes use of a special table that is indexed by $g-1$, the number of simultaneous tests, the error degrees of freedom ($\nu = N-g$), the error rate, and whether the tests are 2-sided or 1-sided. Assume that the control treatment is labelled as treatment 1.

Consider the 2-sided case:

$$\text{Conclude } \mu_i - \mu_1 \neq 0 \text{ if } \left| \bar{y}_{i\cdot} - \bar{y}_{1\cdot} \right| \geq d_{1-\alpha_E; g-1, N-g}^{2-s} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_1} \right)} \quad i = 2, \dots, g$$
$$\text{Simultaneous 95\% CIs: } \left(\bar{y}_{i\cdot} - \bar{y}_{1\cdot} \right) \pm d_{1-\alpha_E; g-1, N-g}^{2-s} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_1} \right)} \quad i = 2, \dots, g$$

For the 1-sided case:

$$\text{Conclude } \mu_i - \mu_1 > 0 \text{ if } \bar{y}_{i\bullet} - \bar{y}_{1\bullet} \geq d_{1-\alpha_E; g-1, N-g}^{1-s} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_1} \right)} \quad i = 2, \dots, g$$

$$\text{Conclude } \mu_i - \mu_1 < 0 \text{ if } \bar{y}_{i\bullet} - \bar{y}_{1\bullet} \leq -d_{1-\alpha_E; g-1, N-g}^{1-s} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_1} \right)} \quad i = 2, \dots, g$$

For the multiple comparisons with the best treatment method, we would like to choose the subset of treatments that contains the best treatment with probability $1-\alpha_E$. There are 2 possible cases, High values are considered best, or Low values are considered best.

High Scores are Good:

$$\text{Treatment } i \text{ is in best subset if: } \bar{y}_{i\bullet} \geq \bar{y}_{j\bullet} - d_{\alpha_E; g-1, N-g}^{1-s} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j} \right)} \quad \forall j \neq i$$

Low Scores are Good:

$$\text{Treatment } i \text{ is in best subset if: } \bar{y}_{i\bullet} \leq \bar{y}_{j\bullet} + d_{\alpha_E; g-1, N-g}^{1-s} \sqrt{MS_{\text{Err}} \left(\frac{1}{n_i} + \frac{1}{n_j} \right)} \quad \forall j \neq i$$

Any treatment that lies within some critical difference of the “best” observed treatment is in the best subset.

Example: Theophylline Release Under Packaging and Humidity Conditions

An experiment was conducted to determine effects of relative humidity and packaging on the amount of theophylline released from tablets (Sanchez, *et al* (1992)). The researchers measured $n = 6$ tablets from each of $g = 5$ conditions: Control (Zero Years), 3 Years with packaging at 54% RH, 3 Years without packaging at 54% RH, 3 Years with packaging at 90% RH, and 3 Years without packaging at 90% RH. The experiment was conducted for 6 formulations, this example corresponds to B-175.

ANOVA						
Source	df	SS	MS	F	F(.05)	P-value
Trtreatments	4	579.65	144.91	7.292	2.759	0.0005
Error	25	496.79	19.87			
Total	29	1076.43				
		Trt1	Trt2	Trt3	Trt4	Trt5
	Mean	96.4	91.7	87.1	93.3	84.1
	SD	5.84	5.1	3.67	2.19	4.58
	n	6	6	6	6	6

If we wish to do 1-sided tests, to determine whether the mean amount released is lower for the delayed conditions than the control, then we have the following:

$$d_{.95;5-1,30-5}^{1-s} = 2.28 \quad \hat{SE}\{\bar{Y}_{i\cdot} - \bar{Y}_{1\cdot}\} = \sqrt{19.87\left(\frac{1}{6} + \frac{1}{6}\right)} = 2.57$$

\Rightarrow Conclude $\mu_i < \mu_1$ if $\bar{y}_{i\cdot} - \bar{y}_{1\cdot} \leq -2.28(2.57) = -5.86$

$$\bar{y}_{2\cdot} - \bar{y}_{1\cdot} = -4.7 \quad \bar{y}_{3\cdot} - \bar{y}_{1\cdot} = -9.3 \quad \bar{y}_{4\cdot} - \bar{y}_{1\cdot} = -3.1 \quad \bar{y}_{5\cdot} - \bar{y}_{1\cdot} = -12.3$$

We conclude the 2 unpackaged means are significantly less than the control.

R Program:

```
tp1 <-
read.csv("http://www.stat.ufl.edu/~winner/data/teoph_package_b175.csv",
         header=T)
attach(tp1); names(tp1)

theoph.trt <- factor(theoph.trt)

require(multcomp)

tp1.mod1 <- aov(theoph ~ theoph.trt)
summary(tp1.mod1)

tp1.Dunnett <- glht(tp1.mod1, linfct=mcp(theoph.trt="Dunnett"),
                    alternative="less")
summary(tp1.Dunnett)
confint(tp1.Dunnett)

windows(width=5,height=3,pointsize=10)
plot(tp1.Dunnett,sub="Theophylline package Data")
mtext("Dunnet's Method",side=3,line=0.5)
```

R Output:

```
> tp1.Dunnett <- glht(tp1.mod1, linfct=mcp(theoph.trt="Dunnett"),
alternative="less")
> summary(tp1.Dunnett)

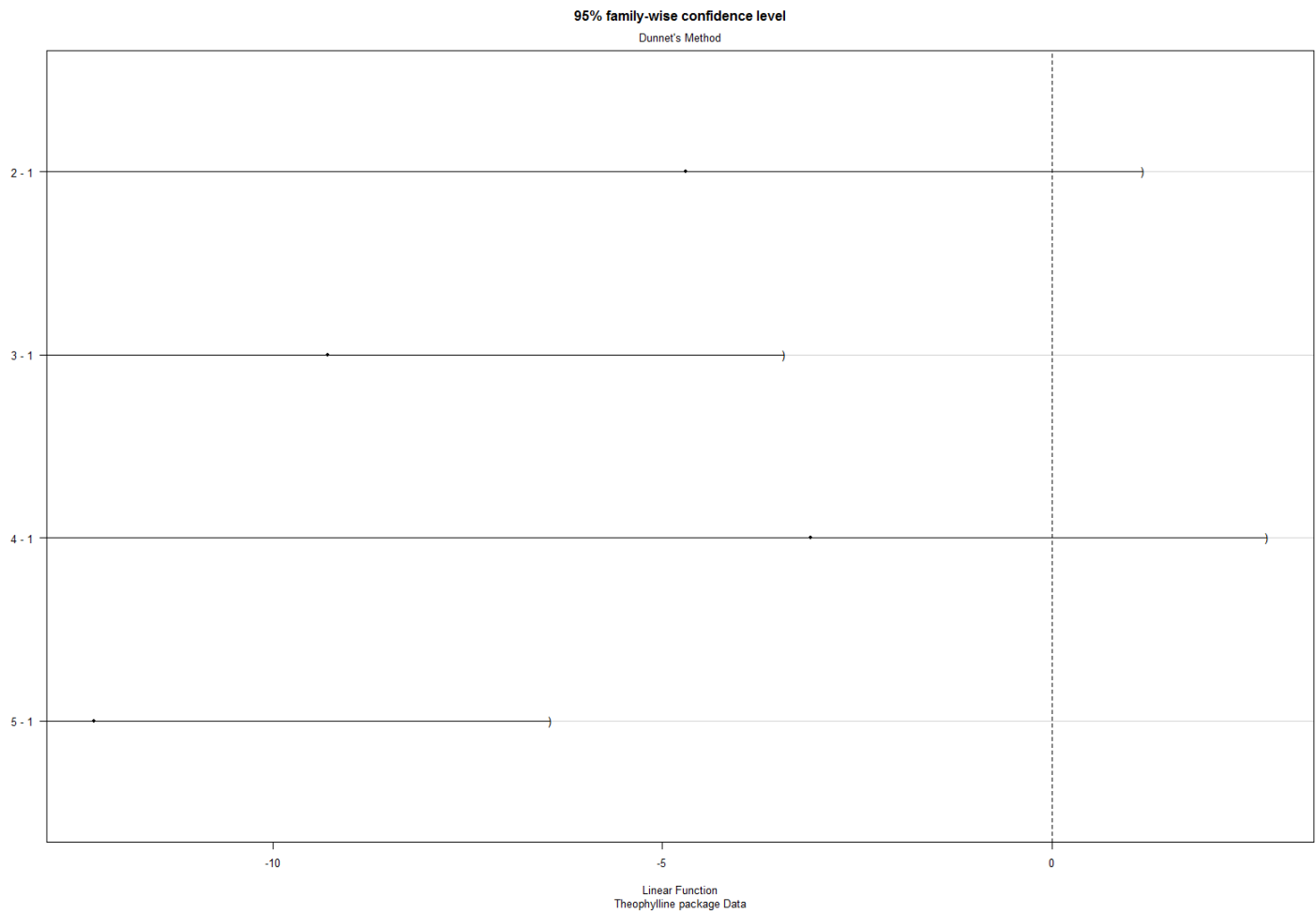
      Simultaneous Tests for General Linear Hypotheses
Multiple Comparisons of Means: Dunnett Contrasts
Fit: aov(formula = theoph ~ theoph.trt)

Linear Hypotheses:
      Estimate Std. Error t value Pr(<t)
2 - 1 >= 0    -4.700      2.574  -1.826 0.11565
3 - 1 >= 0    -9.300      2.574  -3.614 0.00245 **
4 - 1 >= 0    -3.100      2.574  -1.204 0.29664
5 - 1 >= 0   -12.300      2.574  -4.779 < 0.001 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)

> confint(tp1.Dunnett)
      Simultaneous Confidence Intervals
Multiple Comparisons of Means: Dunnett Contrasts
Fit: aov(formula = theoph ~ theoph.trt)

Quantile = 2.2735
95% family-wise confidence level

Linear Hypotheses:
      Estimate lwr      upr
2 - 1 >= 0   -4.7000   -Inf    1.1512
3 - 1 >= 0   -9.3000   -Inf   -3.4488
4 - 1 >= 0   -3.1000   -Inf    2.7513
5 - 1 >= 0  -12.3000   -Inf   -6.4488
```



Data Sources:

M.I. Aksu, H. Imik, M. Karoglu (2007). "Influence of Dietary Sorghum (*Sorghum vulgare*) and Corn Supplemented with Methionine on Cut-Up Pieces Weights of Broiler Carcass and Quality Properties of Breast and Drumsticks Meat," *Food Science and Technology International*, Vol. 13, #5, pp. 361-367.

E. Sanchez, C.M. Evora, M. Llabres (1992). "Effect of Humidity and Packaging on the Long-Term Aging of Commercial Sustained-Release Theophylline Tablets," *International Journal of Pharmaceutics*, Vol. 83, pp. 59-63.

Chapter 4 – Model Diagnostics

Ordinary least squares estimators can be obtained regardless of the distributions of the error terms. The distribution of the resulting estimators does depend on the error distributions. The assumptions that lead to the t-tests and F-tests for estimators and contrasts are for the following model:

$$Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad i = 1, \dots, g; \quad j = 1, \dots, n_i \quad \varepsilon_{ij} \sim NID(0, \sigma^2)$$

- Errors are normally distributed.
- Errors have constant variance.
- Errors are independent.

Some violations of assumptions are more problematic than others. In this chapter, we will cover graphical methods and statistical tests for assessing whether the data are problematic. In many cases, by transforming the response variable, we can meet the assumptions for the transformed variable. Before we continue, we first fit the ANOVA model in cell means form, and obtain the **residuals** which can be thought of as estimates of the true error terms.

$$Y_{ij} = \mu_i + \varepsilon_{ij} = \hat{Y}_{ij} + e_{ij} \quad \hat{Y}_{ij} = \bar{Y}_{i\cdot} \quad e_{ij} = Y_{ij} - \hat{Y}_{ij} = Y_{ij} - \bar{Y}_{i\cdot}$$

$$E\{\varepsilon_{ij}\} = 0 \quad V\{\varepsilon_{ij}\} = \sigma^2 \quad E\{e_{ij}\} = E\{Y_{ij} - \bar{Y}_{i\cdot}\} = \mu_i - \mu_i = 0$$

$$V\{e_{ij}\} = V\{Y_{ij} - \bar{Y}_{i\cdot}\} = V\{Y_{ij}\} + V\{\bar{Y}_{i\cdot}\} - 2\text{COV}\{Y_{ij}, \bar{Y}_{i\cdot}\} = \sigma^2 + \frac{\sigma^2}{n_i} - 2\frac{\sigma^2}{n_i} = \sigma^2 - \frac{\sigma^2}{n_i} = \sigma^2 \left(1 - \frac{1}{n_i}\right)$$

In matrix form: $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{P}\mathbf{Y}$ $\mathbf{P} =$

$$\begin{bmatrix} \frac{1}{n_1} \mathbf{J}_{n_1 \times n_1} & \mathbf{0}_{n_1 \times n_2} & \cdots & \mathbf{0}_{n_1 \times n_g} \\ \mathbf{0}_{n_2 \times n_1} & \frac{1}{n_2} \mathbf{J}_{n_2 \times n_2} & \cdots & \mathbf{0}_{n_2 \times n_g} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g \times n_1} & \mathbf{0}_{n_g \times n_2} & \cdots & \frac{1}{n_g} \mathbf{J}_{n_g \times n_g} \end{bmatrix}$$

$$\Rightarrow V\{e_{ij}\} = \sigma^2 \left(1 - \frac{1}{n_i}\right) = \sigma^2 (1 - P_{ij}) \quad P_{ij} \text{ is the diagonal element of } \mathbf{P}, \text{ corresponding to } Y_{ij}$$

4.1. Normality of Error Terms

First, we can check for **outliers**, observations that fall further from their treatment means than would be expected if observations were normally distributed. First, we compute the **studentized residuals**, which under the normality assumption follow a t-distribution with $N-g-1$ degrees of freedom. They are computed as follows.

Standardized Residual (aka) Internally Studentized Residual:
$$e_{ij}^* = \frac{e_{ij}}{\sqrt{MS_{\text{Err}}(1 - P_{ij})}}$$

Studentized Residual (aka) Externally Studentized Residual:
$$e_{ij}^{**} = e_{ij}^* \left[\frac{N - g - 1}{N - g - (e_{ij}^*)^2} \right] = \frac{e_{ij}}{\sqrt{MS_{\text{Err}(ij)}(1 - P_{ij})}}$$

$MS_{\text{Err}(ij)}$ is the Mean Square Error if Y_{ij} had been excluded from the analysis

Conclude Y_{ij} is an outlier if $|e_{ij}^{**}| \geq t_{1 - \frac{\alpha}{2N}; N - g - 1}$ Bonferroni adjustment for multiple tests

If an outlier is detected, it should be investigated. Is it a data entry/recording error? Does it have some characteristic that is not included in the model? Is it a subject who did not understand the instructions of the experiment? Studentized residuals are standard output from statistical computing packages.

Graphical Methods include **histograms** when the overall sample size is large, and **normal probability plots**. A histogram should be mound shaped like a normal distribution. A normal probability plot plots the ordered residuals or studentized residuals versus their expected values under normality. The process involves the following steps:

- Order the residuals or studentized residuals from smallest (large and negative) to largest (large and positive).
- Transform the rank of the ordered residual to a quantile: $q^*(i) = (i - 0.375) / (N - 0.25)$
- Transform the quantiles to points along the standard normal cumulative distribution function: $z(q^*)$. These are the expected values of the studentized residuals under normality.
- Plot the residuals or studentized residuals (y-axis) versus their expected values under normality (x-axis).
- The points will follow an approximate straight-line (Southwest-Northeast) if errors are normally distributed.

These are very straightforward to compute in spreadsheets, and are easily obtained from statistical software packages.

One formal statistical test is the **Shapiro-Wilk test**. It makes use of the expected values of the measurements under normality, as well as the Variance-Covariance matrix of the order statistics. This test can be used on any data, not just residuals from a linear model. The null hypothesis is that the measurements are normally distributed (from a common distribution), and a p-value is reported. Small p-values provide evidence against the hypothesis of normality.

Example: Inoculation of Entozoic Amoebae

A study was conducted to compare $g = 5$ inoculation treatments for yield in amoeba (Griffin and McCarten (1949). The treatments were: (1) Control (none), (2) heat @ 70C for 10 minutes, (3) addition of 10% formalin, (4) heat followed by formalin, and (5) formalin followed by heat. There were $n = 10$ replicates per treatment, and Yield ($\times 10^{-4}$) was the response.

R Program:

```
amoeba <- read.table("http://www.stat.ufl.edu/~winner/data/entozamoeba.dat",
  header=F,col.names=c("inoc.trt","inoc.yld"))
attach(amoeba)

inoc.trt <- factor(inoc.trt)

inoc.mod1 <- aov(inoc.yld ~ inoc.trt)
summary(inoc.mod1)
student_e <- rstudent(inoc.mod1)

summary(student_e)
qqnorm(student_e); qqline(student_e)
shapiro.test(student_e)

qt(1-.05/(2*50),50-5-1)
```

R Output:

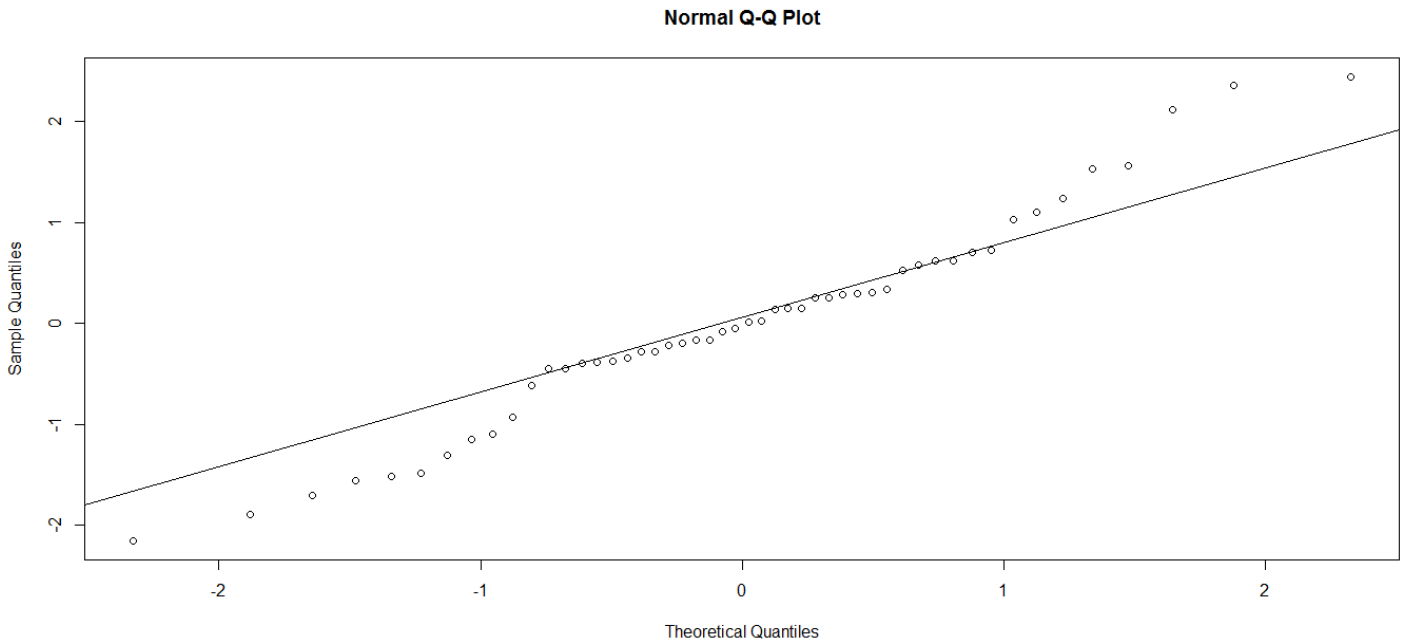
```
> inoc.mod1 <- aov(inoc.yld ~ inoc.trt)
> summary(inoc.mod1)
      Df Sum Sq Mean Sq F value Pr(>F)
inoc.trt  4 19666    4916   5.044 0.00191 **
Residuals 45 43858     975
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> student_e <- rstudent(inoc.mod1)
>
> summary(student_e)
      Min.      1st Qu.      Median      Mean      3rd Qu.      Max.
-2.155000 -0.438300 -0.015020  0.002314  0.561200  2.444000
> qqnorm(student_e); qqline(student_e)
> shapiro.test(student_e)

      Shapiro-Wilk normality test

data:  student_e
W = 0.9741, p-value = 0.3356

>
> qt(1-.05/(2*50),50-5-1)
[1] 3.525801
>
```

We observe that there are significant differences among the inoculation treatments ($p = .0019$). None of the studentized residuals are larger in absolute value than we would expect under normality (larger than 3.5258). The Shapiro-Wilk test does not reject the null hypothesis of normally distributed errors ($p = .3356$). Below, we provide a normal probability plot of the studentized residuals. While some of the extreme residuals fall below and above the line, the departure is not overly dramatic.



When errors are not normally distributed, if sample sizes are reasonably large and variances are homogeneous, tests and confidence intervals tend to work as advertised. Transformations can often be made to obtain approximate normality. The **Box-Cox** transformation is widely used in practice. It can often also make variances more equal, as well.

Box-Cox Transformations

Procedure to choose a transformation on Y (not X) with goal of choosing a power of Y that meets the model assumptions.

- Automatically selects a transformation from power family with goal of obtaining: normality and constant variance (not always successful, but widely used)
- Goal: Fit the ANOVA model for various power transformations on Y , and select a transformation producing minimum SSE (maximum likelihood)
- Procedure: over a range of λ from, say -2 to +2, obtain the ANOVA based on the power transformation of Y (assuming all $Y_i > 0$, although adding a constant won't affect shape or spread of Y distribution).
- When the power (λ) is 0, this implies a logarithmic transformation.

$$W_i = \begin{cases} K_1 (Y_i^\lambda - 1) & \lambda \neq 0 \\ K_2 \ln(Y_i) & \lambda = 0 \end{cases} \quad K_2 = \left(\prod_{i=1}^n Y_i \right)^{1/n} \quad K_1 = \frac{1}{\lambda K_2^{\lambda-1}}$$

Example: Inoculation of Entozoic Amoebae

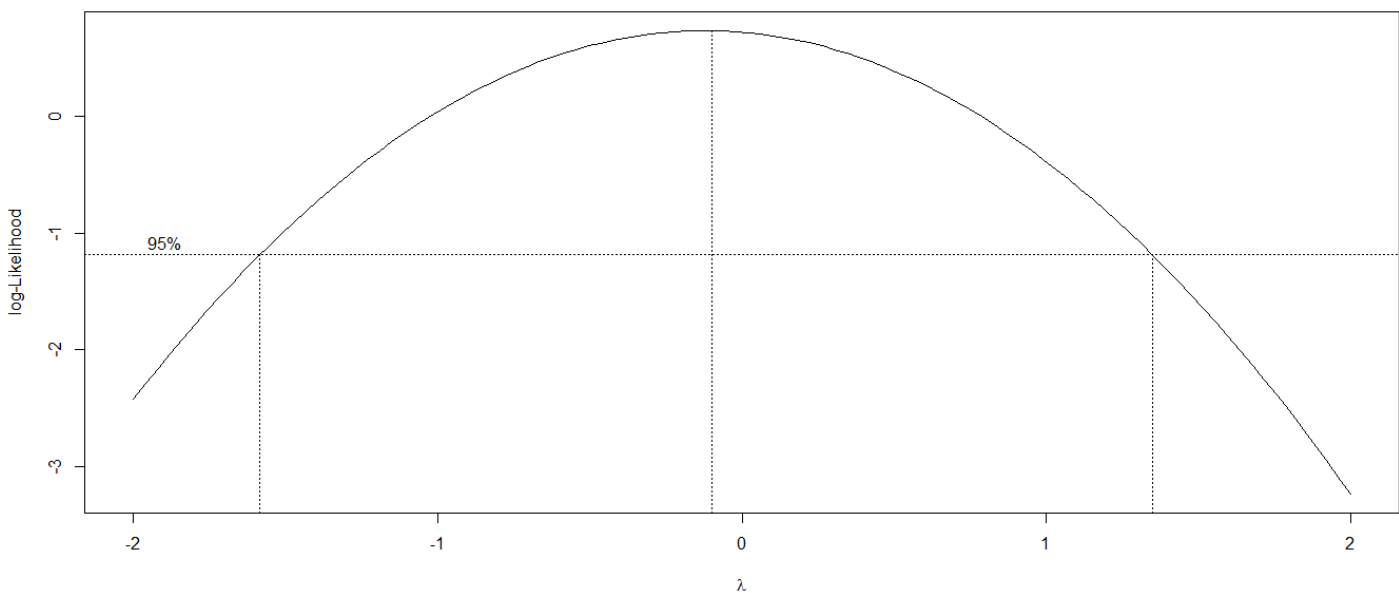
While the data for the amoeba example show no evidence of non-normality, we will run the method here for illustration purposes.

R Program:

```
amoeba <- read.table("http://www.stat.ufl.edu/~winner/data/entozamoeba.dat",
  header=F,col.names=c("inoc.trt","inoc.yld"))
attach(amoeba)

inoc.trt <- factor(inoc.trt)
inoc.mod1 <- aov(inoc.yld ~ inoc.trt)

library(MASS)
boxcox(inoc.mod1, plotit=T)
```



While the log-likelihood is maximized close to $\lambda = 0$ (logarithmic transformation), the curve is fairly flat with $\lambda = 1$ falling within the 95% confidence interval. When in doubt, do not transform data, as interpretations are easiest in the original units.

Another option is a rank-based (non-parametric) test, the **Kruskal-Wallis Test**. This test is robust to outliers which can impact group means and variances. The test involves ranking the observations from smallest (1) to largest (N) across treatments, adjusting for ties by taking the average rank that measurements would have received had they not been tied. Rank sums for each treatment are obtained (T_i), and the test is conducted as follows. Note that the Rank sums will add up to $1+2+\dots+N = N(N+1)/2$. The test is whether the g population medians are equal.

$$T.S.: H = \frac{12}{N(N+1)} \sum_{i=1}^g \frac{T_i^2}{n_i} - 3(N+1)$$

$$R.R.: H \geq \chi_{1-\alpha, g-1}^2 \quad \text{P-value: } P(\chi^2 \geq H)$$

An adjustment is made when there are many ties (discrete data):

$$H' = \frac{H}{1 - \frac{\sum_j (t_j^3 - t_j)}{N^3 - N}} \quad t_j \equiv \text{number of observations in the } j^{\text{th}} \text{ group of tied ranks}$$

Post-hoc comparisons can be made based on simultaneous confidence intervals based on mean ranks. When the Kruskal-Wallis test fails to be significant, no comparisons should be made.

$$\left(\bar{T}_{i\cdot} - \bar{T}_{i'\cdot} \right) \pm z_{1-\alpha/2c} \sqrt{\frac{N(N+1)}{12} \left(\frac{1}{n_i} + \frac{1}{n_{i'}} \right)} \quad \bar{T}_{i\cdot} = \frac{T_{i\cdot}}{n_i} \quad c = \binom{g}{2} = \frac{g(g-1)}{2}$$

Example: Inoculation of Entozoic Amoebae

We first conduct the test in EXCEL, and then provide R program and output.

j	Y Trt1	Y Trt2	Y Trt3	Y Trt4	Y Trt5		Rank Trt1	Rank Trt2	Rank Trt3	Rank Trt4	Rank Trt5	
1	265	204	191	221	259		45	24	17	33	44	
2	292	234	207	205	206		50	39	28	25	26.5	
3	268	197	218	178	179		46	21	32	8	9	
4	251	176	201	167	199		43	7	23	4	22	
5	245	240	192	224	180		41	40	19	36	10	
6	192	190	192	225	146		19	15.5	19	37	1	
7	228	171	214	171	182		38	5.5	30.5	5.5	11.5	
8	291	190	206	214	147		49	15.5	26.5	30.5	2	
9	185	222	185	283	182		13.5	34	13.5	48	11.5	
10	247	211	163	277	223		42	29	3	47	35	
												Sum
						T_i	386.5	230.5	211.5	274	172.5	1275
						n_i	10	10	10	10	10	50
						(T_i)^2/n_i	14938.23	5313.025	4473.225	7507.6	2975.625	35207.7
						H		X^2(.95,4)	P-value			
							12.6833	9.4877	0.0129			

For the post-hoc comparisons, we have:

$$C = \frac{5(5-1)}{2} = 10 \quad z_{1-(0.05/2(10))} = 2.807 \quad \sqrt{\frac{N(N+1)}{12} \left(\frac{1}{n_i} + \frac{1}{n_{i'}} \right)} = \sqrt{\frac{50(50+1)}{12} \left(\frac{1}{10} + \frac{1}{10} \right)} = 6.519$$

$$z_{1-(0.05/2(10))} \sqrt{\frac{N(N+1)}{12} \left(\frac{1}{n_i} + \frac{1}{n_{i'}} \right)} = 2.807(6.519) = 18.30$$

Mean Rank: 17.25 21.15 23.05 27.40 38.65

Treatment 5 3 2 4 1

R Program for Kruskal-Wallis Test:

```
amoeba <- read.table("http://www.stat.ufl.edu/~winner/data/entozamoeba.dat",
  header=F,col.names=c("inoc.trt","inoc.yld"))
attach(amoeba)

inoc.trt <- factor(inoc.trt)
kruskal.test(inoc.yld ~ inoc.trt)
```

R Output for Kruskal-Wallis Test:

```
> kruskal.test((inoc.yld ~ inoc.trt)
+ > kruskal.test(inoc.yld ~ inoc.trt)
      kruskal-wallis rank sum test
data:  inoc.yld by inoc.trt
kruskal-wallis chi-squared = 12.6894, df = 4, p-value = 0.0129
```

4.2. Constant Error Variance

A plot of residuals versus treatment or fitted values should demonstrate consistent amounts of variation within each treatment group. When some group(s) show much more (less) spread than other group(s), the assumption of equal (homogeneous) variances may not hold. In general, this is more problematic than non-normality of variance in terms of performances of tests and confidence intervals. One special case is when the standard deviation is a power function of the mean.

There are many tests for homogeneity of variances among the treatments. Here we will describe 3 tests. The modified Levene test is robust to non-normality, Hartley's and Bartlett's are not. Hartley's test is restricted to balanced data (equal sample sizes among treatments) and makes use of a special table of critical values. We describe the 3 tests below.

$$H_0 : \sigma_1^2 = \sigma_2^2 = \dots = \sigma_g^2 \quad \text{Sample Variances: } s_1^2, s_2^2, \dots, s_g^2 \quad MS_{\text{Err}} = \frac{\sum_{i=1}^g (n_i - 1) s_i^2}{N - g}$$

Modified Levene Test:

$$z_{ij} = \left| y_{ij} - \tilde{y}_i \right| \quad i = 1, \dots, g; j = 1, \dots, n_i \quad \tilde{y}_i = \text{median}(y_{i1}, \dots, y_{in_i}) \quad i = 1, \dots, g$$

$$\bar{z}_{i\bullet} = \frac{\sum_{j=1}^{n_i} z_{ij}}{n_i} \quad \bar{z}_{\bullet\bullet} = \frac{\sum_{i=1}^g \sum_{j=1}^{n_i} z_{ij}}{N} \quad TS : F_L = \frac{\left[\frac{\sum_{i=1}^g n_i (\bar{z}_{i\bullet} - \bar{z}_{\bullet\bullet})^2}{g-1} \right]}{\left[\frac{\sum_{i=1}^g \sum_{j=1}^{n_i} (z_{ij} - \bar{z}_{i\bullet})^2}{N-g} \right]} \quad RR : F_L \geq F_{1-\alpha; g-1, N-g}$$

Bartlett's Test:

$$TS : B = \frac{1}{C} \left[(N-g) \ln(MS_{\text{Err}}) - \sum_{i=1}^g (n_i - 1) \ln(s_i^2) \right] \quad C = 1 + \frac{1}{3(g-1)} \left[\left(\sum_{i=1}^g \frac{1}{n_i - 1} \right) - \left(\frac{1}{N-g} \right) \right]$$

$$RR : B \geq \chi_{1-\alpha; g-1}^2$$

Hartley's Test:

$$TS : F_{\text{MAX}} = \frac{\max(s_1^2, \dots, s_g^2)}{\min(s_1^2, \dots, s_g^2)} \quad RR : F_{\text{MAX}} \geq F_{1-\alpha; g, n-1}^{\text{Hartley}}$$

Example: Inoculation of Entozoic Amoebae

We apply these methods to the Amoebae data. First, we conduct tests in EXCEL, and then give an R Program and output for Levene's and Bartlett's tests.

j	Y Trt1	Y Trt2	Y Trt3	Y Trt4	Y Trt5		Z Trt1	Z Trt2	Z Trt3	Z Trt4	Z Trt5
1	265	204	191	221	259		16	3.5	5.5	3.5	77
2	292	234	207	205	206		43	33.5	10.5	12.5	24
3	268	197	218	178	179		19	3.5	21.5	39.5	3
4	251	176	201	167	199		2	24.5	4.5	50.5	17
5	245	240	192	224	180		4	39.5	4.5	6.5	2
6	192	190	192	225	146		57	10.5	4.5	7.5	36
7	228	171	214	171	182		21	29.5	17.5	46.5	0
8	291	190	206	214	147		42	10.5	9.5	3.5	35
9	185	222	185	283	182		64	21.5	11.5	65.5	0
10	247	211	163	277	223		2	10.5	33.5	59.5	41
Mean	246.4	203.5	196.9	216.5	190.3	Mean	27.0	18.7	12.3	29.5	23.5
Median	249.0	200.5	196.5	217.5	182.0	SSErr	4750.0	1473.6	801.6	5680.0	5486.5
SD	36.47	23.29	16.03	39.96	33.86	SSTrt	230.40	122.50	980.10	532.90	16.90

Levene's Test:

	Sum	MeanSq	F_Levene	F(.95;4,45)	P-value
SSErr	18191.70	404.26	1.1643	2.5787	0.3392
SSTrt	1882.80	470.70			

Bartlett's Test:

Trt	1	2	3	4	5	Overall
df	9	9	9	9	9	45
Variance	1330.27	542.28	256.99	1596.94	1146.68	974.63
df*ln(var)	64.74	56.66	49.94	66.38	63.40	309.69
1/df	0.1111	0.1111	0.1111	0.1111	0.1111	0.0222
C	B	$\chi^2(.95,4)$	P-value			
1.0444	8.2024	9.4877	0.0844			

Hartley's Test:

$$F_{MAX} = \frac{1596.94}{256.99} = 6.21 \quad F_{1-\alpha;g,n-1}^{\text{Hartley}} = F_{.95;5,10-1}^{\text{Hartley}} = 7.11$$

R Program:

```
amoeba <- read.table("http://www.stat.ufl.edu/~winner/data/entozamoeba.dat",
  header=F,col.names=c("inoc.trt","inoc.yld"))
attach(amoeba)

inoc.trt <- factor(inoc.trt)
install.packages("lawstat")
library(lawstat)
levene.test(inoc.yld, inoc.trt, "median")
bartlett.test(inoc.yld ~ inoc.trt)  ### Does not need lawstat package
```

R Output:

```
> levene.test(inoc.yld, inoc.trt, "median")
      modified robust Brown-Forsythe Levene-type test based on the absolute
      deviations from the median
data:  inoc.yld
Test Statistic = 1.1643, p-value = 0.3392
> bartlett.test(inoc.yld ~ inoc.trt)
      Bartlett test of homogeneity of variances
data:  inoc.yld by inoc.trt
Bartlett's K-squared = 8.2024, df = 4, p-value = 0.08444
```

When the error variances are not constant, there are various methods used in practice to adjust estimates and tests. Here are a few possibilities.

- Determine whether the variance (or standard deviation) is functionally related to the mean, and if so, estimate any parameters in the function, and transform the data accordingly (Bartlett's method).
- Make an adjustment to the F-ratio and degrees of freedom for an approximate test that takes into account the non-constant variances among the treatments (Welch's Test).
- Perform estimated weighted least squares (EWLS), with weights being the reciprocal of the variance within the treatments (higher variance leads to smaller weight, and vice versa).
- Obtain the F-statistic for the original data based on (EWLS), followed by a parametric bootstrap. Means and variances are obtained from normal and chi-square distributions under the null hypothesis of equal means. F-ratios are computed for each sample, and obtain an approximate P-value for the original data.

Bartlett's Method

- Usual Assumption in ANOVA and Regression is that the variance of each observation is the same.
- Problem: In many cases, the variance is not constant, but is related to the mean.
 - Poisson Data (Counts of events): $E\{Y\} = V\{Y\} = \mu$
 - Binomial Data (and Percentages): $E\{Y\} = n\pi \quad V\{Y\} = n\pi(1-\pi)$
 - General Case: $E\{Y\} = \mu \quad V\{Y\} = \Omega(\mu)$
 - Power relationship: $V\{Y\} = \sigma^2 = \alpha^2 \mu^{2\beta}$

$$\sigma = \alpha \mu^\beta \Rightarrow \ln(\sigma) = \ln(\alpha) + \beta \ln(\mu) = \alpha^* + \beta \mu^*$$

Transformation to stabilize variance:

- $V\{Y\} = \sigma^2 = \Omega(\mu)$. Then let:

$$f(\mu) = \int \frac{1}{[\Omega(\mu)]^{1/2}} d\mu \Rightarrow V[f(Y)] \approx \text{constant}$$

This results from a Taylor Series expansion:

$$\begin{aligned} f(Y) &\approx f(\mu) + (Y - \mu) f'(\mu) \\ \Rightarrow [f(Y) - f(\mu)]^2 &\approx (Y - \mu)^2 [f'(\mu)]^2 \\ \Rightarrow V(f(Y)) &\approx \Omega(\mu) \left(\frac{1}{(\Omega(\mu))^{1/2}} \right)^2 = 1 \end{aligned}$$

Special Cases:

Case 1: $\beta \neq 1$:

$$f(\mu) = \int \frac{1}{[\Omega(\mu)]^{1/2}} d\mu = \int \frac{1}{\alpha \mu^\beta} d\mu = \frac{1}{\alpha} \left(\frac{\mu^{-\beta+1}}{-\beta+1} \right) = c \mu^{1-\beta}$$

Case 2: $\beta = 1$

$$f(\mu) = \int \frac{1}{[\Omega(\mu)]^{1/2}} d\mu = \int \frac{1}{\alpha \mu} d\mu = \frac{1}{\alpha} \ln(\mu)$$

Estimating β from sample data:

- For each group in an ANOVA (or similar X levels in Regression), obtain the sample mean and standard deviation
- Fit a simple linear regression, relating the log of the standard deviation to the log of the mean
- The regression coefficient of the log of the mean is an estimate of β

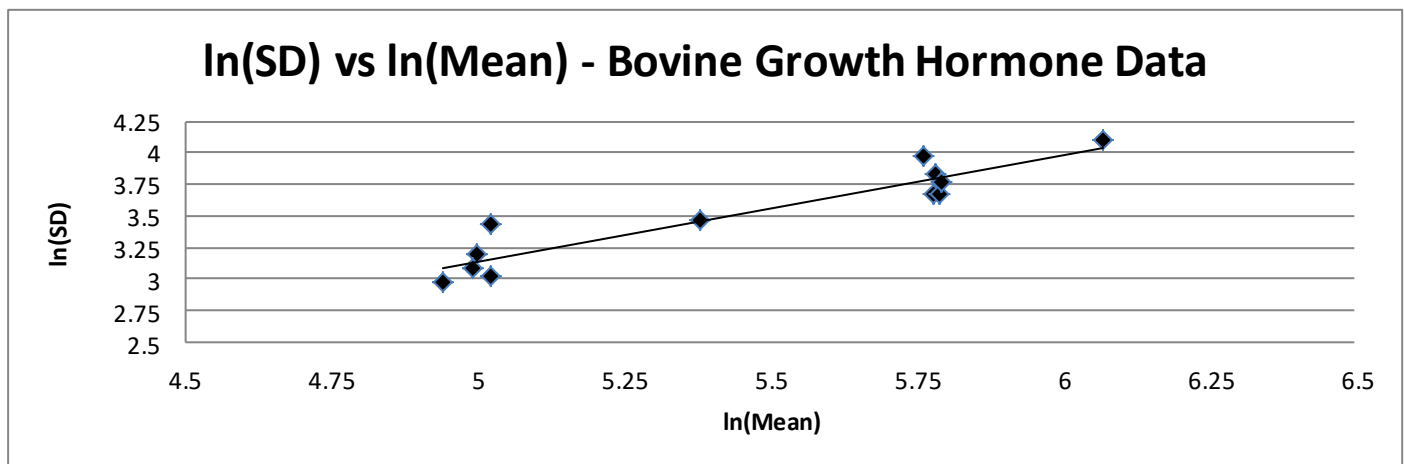
Example: Weight Gain in Rats Receiving Bovine Growth Hormone

An experiment was conducted in rats to measure weight gain in rats receiving bovine growth hormone. There were a total of $g = 12$ treatments (combinations of gender and dose). There were $n_i = 5$ rats per treatment, so that $N = 5(12) = 60$.

The following table gives the means, standard deviations, $\ln(\text{means})$, and $\ln(\text{SDs})$ for the 12 treatments:

	Trt1	Trt2	Trt3	Trt4	Trt5	Trt6	Trt7	Trt8	Trt9	Trt10	Trt11	Trt12
Mean	324	432	327	318	325	328	148	217	140	152	147	152
SD	39.2	60.3	39.1	53.0	46.3	43.0	24.4	32.3	19.6	31.0	22.0	20.5
$\ln(\text{Mean})$	5.7807	6.0684	5.7900	5.7621	5.7838	5.7930	4.9972	5.3799	4.9416	5.0239	4.9904	5.0239
$\ln(\text{SD})$	3.6687	4.0993	3.6661	3.9703	3.8351	3.7612	3.1946	3.4751	2.9755	3.4340	3.0910	3.0204

A plot of $\ln(\text{SD})$ versus $\ln(\text{Mean})$, and regression output are given below:



	Coefficient	Standard Err	t Stat	P-value	Lower 95%	Upper 95%
Intercept	-1.05531	0.537262	-1.96424	0.077887	-2.2524	0.141785
$\ln(\text{Mean})$	0.839598	0.098405	8.532042	6.67E-06	0.620337	1.058859

The estimated slope is 0.84, with 95% Confidence Interval: (0.62, 1.06). Since 1 is within the confidence interval, and close to the point estimate, the logarithmic transformation should approximately stabilize the variance.

R Program for Untransformed and Transformed Weight Gain:

```
bgh1 <- read.table("http://www.stat.ufl.edu/~winner/data/bgh1.dat", header=F,
  col.names = c("gender", "bgh.dose", "wtgain"))
attach(bgh1)

bgh.trt <- 10*gender + bgh.dose
bgh.trt <- factor(bgh.trt)

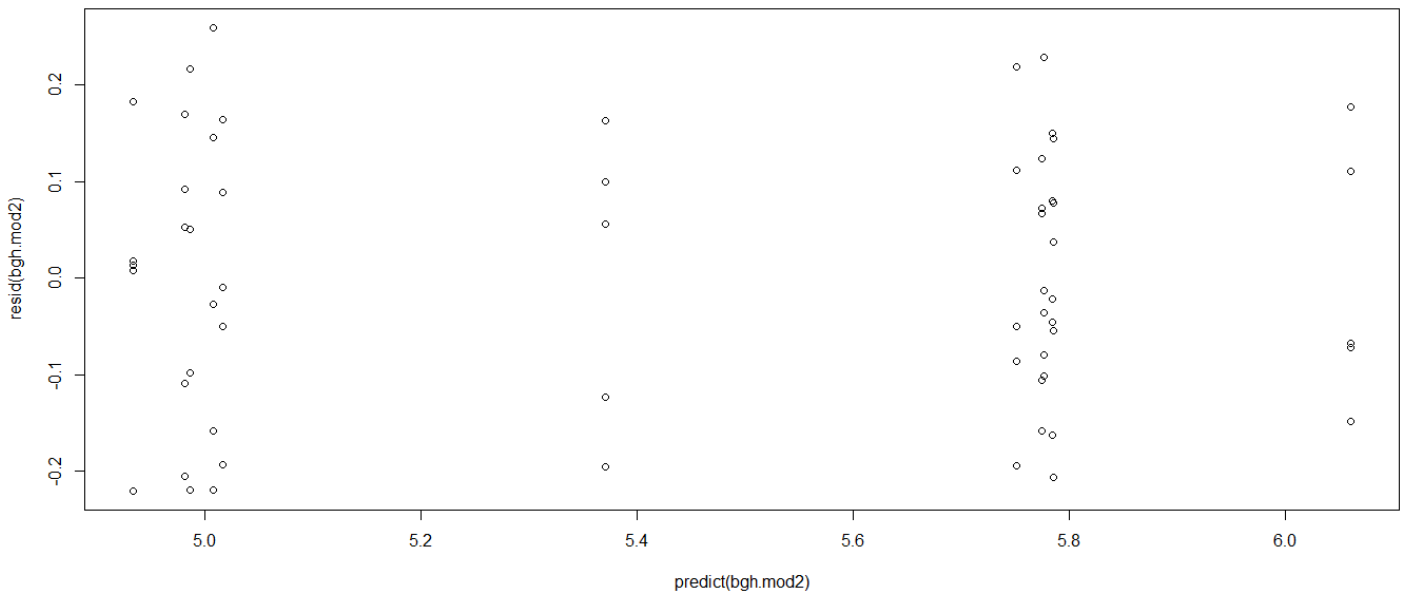
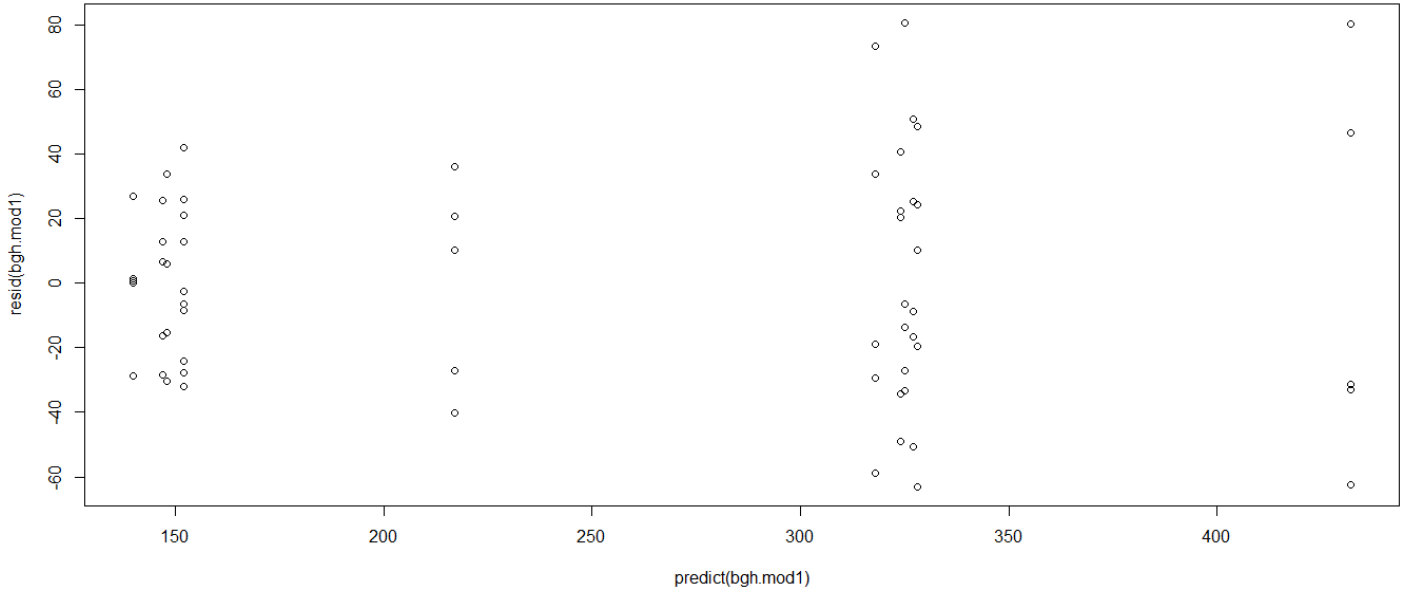
bgh.mod1 <- aov(wtgain ~ bgh.trt)
summary(bgh.mod1)
plot(predict(bgh.mod1), resid(bgh.mod1))

bgh.mod2 <- aov(log(wtgain) ~ bgh.trt)
summary(bgh.mod2)
plot(predict(bgh.mod2), resid(bgh.mod2))
```

R Text Output:

```
> bgh.mod1 <- aov(wtgain ~ bgh.trt)
> summary(bgh.mod1)
      Df Sum Sq Mean Sq F value Pr(>F)
bgh.trt  11 571318   51938   35.84 <2e-16 ***
Residuals  48  69564    1449
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> plot(predict(bgh.mod1), resid(bgh.mod1))
>
> bgh.mod2 <- aov(log(wtgain) ~ bgh.trt)
> summary(bgh.mod2)
      Df Sum Sq Mean Sq F value Pr(>F)
bgh.trt  11  9.947  0.9043   40.76 <2e-16 ***
Residuals  48  1.065  0.0222
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> plot(predict(bgh.mod2), resid(bgh.mod2))
```

Below we have the residual plots for the untransformed and transformed weight gains. The first plot clearly displays variance increasing with the mean. The second plot shows that the variance has been stabilized. Note that these data have been simulated to preserve the treatment means and standard deviations, and is not the raw data that the authors used.



Welch's Test

Welch's test was developed as a means of adjusting a weighted F-statistic and its corresponding degrees of freedom, so that the new F-statistic is distributed approximately F_{g-1, v^*} . The procedure is conducted as follows.

$$w_i = \frac{1}{V\{\bar{Y}_{i\bullet}\}} = \frac{n_i}{s_i^2} \quad w_{\bullet} = \sum_{i=1}^g w_i \quad F^* = \frac{1}{g-1} \left[\sum_{i=1}^g w_i y_{i\bullet}^2 - \frac{\left(\sum_{i=1}^g w_i \bar{Y}_{i\bullet} \right)^2}{w_{\bullet}} \right]$$

$$C_W = \sum_{i=1}^g \left[\frac{1}{n_i - 1} \left(1 - \frac{w_i}{w_{\bullet}} \right)^2 \right] \quad m_W = \left[1 + \frac{2(g-2)}{g^2-1} C_W \right]^{-1} \quad \nu_W = \left[\frac{3}{g^2-1} C_W \right]^{-1} \Rightarrow F_W = m_W F^* \stackrel{\text{approx}}{\sim} F_{g-1, \nu_W}$$

Example: Whole Breast Weight Broiler Chickens Weight

Diet (i)	n	Mean	SD	Var	w_i	w*Ybar	w*Ybar^2	w_i/w_•	C_W
BS(1)	60	606.33	54.18	2935.47	0.02044	12.39317	7514.349	0.406581	0.005969
BSM(2)	60	610.67	53.68	2881.54	0.020822	12.71548	7764.963	0.41419	0.005816
BC(3)	60	566.00	102.41	10487.81	0.005721	3.238046	1832.734	0.113799	0.013311
BC(4)	60	680.00	135.06	18241.20	0.003289	2.236695	1520.952	0.065429	0.014804
Sum					0.050272	30.58339	18633	1.0000	0.0399

$$F^* = \frac{1}{4-1} \left[18633 - \frac{(30.5834)^2}{.050272} \right] = 9.1092$$

$$C_W = \sum_{i=1}^g \left[\frac{1}{60-1} \left(1 - \frac{w_i}{w_{\bullet}} \right)^2 \right] = 0.0399$$

$$m_W = \left[1 + \frac{2(4-2)}{4^2-1} (0.0399) \right]^{-1} = 0.9895 \quad \nu_W = \left[\frac{3}{4^2-1} (0.0399) \right]^{-1} = 125.3$$

$$\Rightarrow F_W = 0.9895(9.1092) = 9.0136 \stackrel{\text{approx}}{\sim} F_{3,125.3} \quad F_{.95,3,125} = 2.677 \quad P(F_{3,125} \geq 9.0136) = .0000$$

R Program:

```
wbw <-
read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F, col.names=c("trt", "repnum", "base", "meth", "wtg"))
attach(wbw); names(wbw)

# Treatment Ordering: BS, BSM, BC, BCM

trt.f <- factor(trt)

oneway.test(wtg ~ trt.f, var.equal=T)
oneway.test(wtg ~ trt.f, var.equal=F)

bartlett.test(wtg ~ trt.f)
```

R Output:

```

> oneway.test(wtg ~ trt.f, var.equal=T)

One-way analysis of means

data: wtg and trt.f
F = 15.5563, num df = 3, denom df = 236, p-value = 2.887e-09

> oneway.test(wtg ~ trt.f, var.equal=F)

One-way analysis of means (not assuming equal variances)

data: wtg and trt.f
F = 9.0181, num df = 3.000, denom df = 125.314, p-value = 1.879e-05

>
> bartlett.test(wtg ~ trt.f)

Bartlett test of homogeneity of variances

data: wtg by trt.f
Bartlett's K-squared = 72.3473, df = 3, p-value = 1.341e-15

```

Estimated Weighted Least Squares

When we know the variances for the different treatments, we can run a weighted least squares (WLS) analysis, which is more efficient than ordinary least squares. We can run the analysis as follows.

$$\begin{aligned}
 Y_{ij} &= \mu + \alpha_i + \varepsilon_{ij} = \mu_i + \varepsilon_{ij} \quad i=1, \dots, g; j=1, \dots, n_i \quad \varepsilon_{ij} \sim N(0, \sigma_i^2) \quad \text{independent} \quad \mathbf{Y}_i = \begin{bmatrix} Y_{i1} \\ Y_{i2} \\ \vdots \\ Y_{in_i} \end{bmatrix} \quad V\{\mathbf{Y}_i\} = \sigma_i^2 \mathbf{I}_{n_i} \\
 \mathbf{Y} &= \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \\ \vdots \\ \mathbf{Y}_g \end{bmatrix} \quad \mathbf{V}_Y = \begin{bmatrix} \sigma_1^2 \mathbf{I}_{n_1 \times n_1} & \mathbf{0}_{n_1 \times n_2} & \cdots & \mathbf{0}_{n_1 \times n_g} \\ \mathbf{0}_{n_2 \times n_1} & \sigma_2^2 \mathbf{I}_{n_2 \times n_2} & \cdots & \mathbf{0}_{n_2 \times n_g} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g \times n_1} & \mathbf{0}_{n_g \times n_2} & \cdots & \sigma_g^2 \mathbf{I}_{n_g \times n_g} \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} \mathbf{1}_{n_1} & \mathbf{0}_{n_1} & \cdots & \mathbf{0}_{n_1} \\ \mathbf{0}_{n_2} & \mathbf{1}_{n_2} & \cdots & \mathbf{0}_{n_2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g} & \mathbf{0}_{n_g} & \cdots & \mathbf{1}_{n_g} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_g \end{bmatrix} \\
 \mathbf{X}_0 &= \begin{bmatrix} \mathbf{1}_{n_1} \\ \mathbf{1}_{n_2} \\ \vdots \\ \mathbf{1}_{n_g} \end{bmatrix} \quad \boldsymbol{\beta}_0 = [\mu] \quad \mathbf{Y}^* = \mathbf{V}_Y^{-1/2} \mathbf{Y} \quad \mathbf{X}^* = \mathbf{V}_Y^{-1/2} \mathbf{X} \quad \mathbf{X}_0^* = \mathbf{V}_Y^{-1/2} \mathbf{X}_0 \quad \mathbf{P}^* = \mathbf{X}^* (\mathbf{X}^{*'} \mathbf{X}^*)^{-1} \mathbf{X}^{*'} \quad \mathbf{P}_0^* = \mathbf{X}_0^* (\mathbf{X}_0^{*'} \mathbf{X}_0^*)^{-1} \mathbf{X}_0^{*'} \\
 SS_{\text{Trt}}^W &= \mathbf{Y}^{*'} (\mathbf{P}^* - \mathbf{P}_0^*) \mathbf{Y}^* \quad SS_{\text{Err}}^W = \mathbf{Y}^{*'} (\mathbf{I} - \mathbf{P}^*) \mathbf{Y}^* \quad F^W = \frac{\left[\frac{SS_{\text{Trt}}^W}{g-1} \right]}{\left[\frac{SS_{\text{Err}}^W}{N-g} \right]} \sim F_{g-1, N-g}
 \end{aligned}$$

In practice, the variances will be unknown (although there are occasions where they may be known up to a multiplicative constant, as when data are means of known numbers of observations). We can use **Estimated Weighted Least Squares (EWLS)**, replacing the unknown group population variances with their sample variances.

$$\begin{aligned}
& Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} = \mu_i + \varepsilon_{ij} \quad i = 1, \dots, g; j = 1, \dots, n_i \quad \varepsilon_{ij} \sim N(0, \sigma_i^2) \quad \text{independent} \quad \mathbf{Y}_i = \begin{bmatrix} Y_{i1} \\ Y_{i2} \\ \vdots \\ Y_{in_i} \end{bmatrix} \quad \hat{V}\{\mathbf{Y}_i\} = s_i^2 \mathbf{I}_{n_i} \\
\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \\ \vdots \\ \mathbf{Y}_g \end{bmatrix} \quad \hat{\mathbf{V}}_{\mathbf{Y}} = \begin{bmatrix} s_1^2 \mathbf{I}_{n_1 \times n_1} & \mathbf{0}_{n_1 \times n_2} & \cdots & \mathbf{0}_{n_1 \times n_g} \\ \mathbf{0}_{n_2 \times n_1} & s_2^2 \mathbf{I}_{n_2 \times n_2} & \cdots & \mathbf{0}_{n_2 \times n_g} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g \times n_1} & \mathbf{0}_{n_g \times n_2} & \cdots & s_g^2 \mathbf{I}_{n_g \times n_g} \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} \mathbf{1}_{n_1} & \mathbf{0}_{n_1} & \cdots & \mathbf{0}_{n_1} \\ \mathbf{0}_{n_2} & \mathbf{1}_{n_2} & \cdots & \mathbf{0}_{n_2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g} & \mathbf{0}_{n_g} & \cdots & \mathbf{1}_{n_g} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_g \end{bmatrix} \\
\mathbf{X}_0 = \begin{bmatrix} \mathbf{1}_{n_1} \\ \mathbf{1}_{n_2} \\ \vdots \\ \mathbf{1}_{n_g} \end{bmatrix} \quad \boldsymbol{\beta}_0 = [\mu] \quad \mathbf{Y}^{**} = \left(\hat{\mathbf{V}}_{\mathbf{Y}} \right)^{-1/2} \mathbf{Y} \quad \mathbf{X}^{**} = \left(\hat{\mathbf{V}}_{\mathbf{Y}} \right)^{-1/2} \mathbf{X} \quad \mathbf{X}_0^{**} = \left(\hat{\mathbf{V}}_{\mathbf{Y}} \right)^{-1/2} \mathbf{X}_0 \quad \mathbf{P}^{**} = \mathbf{X}^{**} (\mathbf{X}^{**}{}^T \mathbf{X}^{**})^{-1} \mathbf{X}^{**}{}^T \quad \mathbf{P}_0^{**} = \mathbf{X}_0^{**} (\mathbf{X}_0^{**}{}^T \mathbf{X}_0^{**})^{-1} \mathbf{X}_0^{**}{}^T \\
SS_{\text{Trt}}^{EW} = \mathbf{Y}^{**}{}^T (\mathbf{P}^{**} - \mathbf{P}_0^{**}) \mathbf{Y}^{**} \quad SS_{\text{Err}}^{EW} = \mathbf{Y}^{**}{}^T (\mathbf{I} - \mathbf{P}^{**}) \mathbf{Y}^{**} \quad TS : F^{EW} = \frac{\frac{SS_{\text{Trt}}^{EW}}{g-1}}{\frac{SS_{\text{Err}}^{EW}}{N-g}} \approx \sim F_{g-1, N-g}
\end{aligned}$$

Note that the forms of \mathbf{P}^* , \mathbf{P}^{**} , \mathbf{P}_0^* , and \mathbf{P}_0^{**} for this model are as follow.

$$\begin{aligned}
\mathbf{P}^* = \mathbf{P}^{**} &= \begin{bmatrix} \frac{1}{n_1} \mathbf{J}_{n_1 \times n_1} & \mathbf{0}_{n_1 \times n_2} & \cdots & \mathbf{0}_{n_1 \times n_g} \\ \mathbf{0}_{n_2 \times n_1} & \frac{1}{n_2} \mathbf{J}_{n_2 \times n_2} & \cdots & \mathbf{0}_{n_2 \times n_g} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_g \times n_1} & \mathbf{0}_{n_g \times n_2} & \cdots & \frac{1}{n_g} \mathbf{J}_{n_g \times n_g} \end{bmatrix} \\
\mathbf{P}_0^* &= \left(\sum_{i=1}^g \frac{n_i}{\sigma_i^2} \right)^{-1} \begin{bmatrix} \frac{1}{\sigma_1^2} \mathbf{J}_{n_1 \times n_1} & \frac{1}{\sigma_1 \sigma_2} \mathbf{J}_{n_1 \times n_2} & \cdots & \frac{1}{\sigma_1 \sigma_g} \mathbf{J}_{n_1 \times n_g} \\ \frac{1}{\sigma_1 \sigma_2} \mathbf{J}_{n_2 \times n_1} & \frac{1}{\sigma_2^2} \mathbf{J}_{n_2 \times n_2} & \cdots & \frac{1}{\sigma_2 \sigma_g} \mathbf{J}_{n_2 \times n_g} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sigma_1 \sigma_g} \mathbf{J}_{n_g \times n_1} & \frac{1}{\sigma_2 \sigma_g} \mathbf{J}_{n_g \times n_2} & \cdots & \frac{1}{\sigma_g^2} \mathbf{J}_{n_g \times n_g} \end{bmatrix} \\
\mathbf{P}_0^{**} &= \left(\sum_{i=1}^g \frac{n_i}{S_i^2} \right)^{-1} \begin{bmatrix} \frac{1}{S_1^2} \mathbf{J}_{n_1 \times n_1} & \frac{1}{S_1 S_2} \mathbf{J}_{n_1 \times n_2} & \cdots & \frac{1}{S_1 S_g} \mathbf{J}_{n_1 \times n_g} \\ \frac{1}{S_1 S_2} \mathbf{J}_{n_2 \times n_1} & \frac{1}{S_2^2} \mathbf{J}_{n_2 \times n_2} & \cdots & \frac{1}{S_2 S_g} \mathbf{J}_{n_2 \times n_g} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{S_1 S_g} \mathbf{J}_{n_g \times n_1} & \frac{1}{S_2 S_g} \mathbf{J}_{n_g \times n_2} & \cdots & \frac{1}{S_g^2} \mathbf{J}_{n_g \times n_g} \end{bmatrix}
\end{aligned}$$

A scalar form of the model involves conducting a general linear test, based on (weighted) Error sums of squares under the null and alternative hypotheses.

$$H_0: \mu_1 = \dots = \mu_g = \mu \quad \hat{\mu}_W = \frac{\sum_{i=1}^g \sum_{j=1}^{n_i} w_{ij} y_{ij}}{\sum_{i=1}^g \sum_{j=1}^{n_i} w_{ij}} \quad w_{ij} = \frac{1}{s_i^2} \Rightarrow \hat{\mu}_W = \frac{\sum_{i=1}^g \sum_{j=1}^{n_i} \frac{1}{s_i^2} y_{ij}}{\sum_{i=1}^g \sum_{j=1}^{n_i} \frac{1}{s_i^2}} = \frac{\sum_{i=1}^g \frac{y_{i\cdot}}{s_i^2}}{\sum_{i=1}^g \frac{n_i}{s_i^2}} \quad \hat{\mu}_{iW} = \frac{\sum_{j=1}^{n_i} \frac{1}{s_i^2} y_{ij}}{\sum_{j=1}^{n_i} \frac{1}{s_i^2}} = \bar{y}_{i\cdot}$$

$$SSE_C^W = \sum_{i=1}^g \sum_{j=1}^{n_i} w_{ij} \left(y_{ij} - \hat{\mu}_{iW} \right)^2 \quad df_C = N - g \quad SSE_R^W = \sum_{i=1}^g \sum_{j=1}^{n_i} w_{ij} \left(y_{ij} - \hat{\mu}_W \right)^2 \quad df_R = N - 1$$

$$TS: F_W = \frac{\left[\frac{SSE_R^W - SSE_C^W}{df_R - df_E} \right]}{\left[\frac{SSE_C^W}{df_E} \right]} = \frac{\left[\frac{SSE_R^W - SSE_C^W}{g - 1} \right]}{\left[\frac{SSE_C^W}{N - g} \right]} \quad RR: F_W \geq F_{1-\alpha; g-1, N-g}$$

Example: Whole Breast Weight Broiler Chickens Weight

We analyze the whole breast weight example in R, first in matrix form, then in scalar form, then with the **aov** function with the **weight** statement. First, we give the summary statistics for the $g = 4$ treatments:

Diet (i)	n	Mean	SD	Var	1/SD	1/Var
BS(1)	60	606.33	54.18	2935.47	0.01845700	0.00034066
BSM(2)	60	610.67	53.68	2881.54	0.01862891	0.00034704
BC(3)	60	566.00	102.41	10487.81	0.00976467	0.00009535
BC(4)	60	680.00	135.06	18241.20	0.00740412	0.00005482

R Program: Matrix Form

```
wbw <-
read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F,col.names=c("trt","repnum","base","meth","wtg"))
attach(wbw); names(wbw)

trt.f <- factor(trt)

#### Matrix form

wbw.mean <- as.vector(tapply(wtg,trt.f,mean))
wbw.sd <- as.vector(tapply(wtg,trt.f,sd))
wbw.n <- as.vector(tapply(wtg,trt.f,length))

w.matrix <- as.matrix(diag(rep(1/wbw.sd,wbw.n)),ncol=sum(wbw.n))

x1 <- rep(c(1,0,0,0),wbw.n)
x2 <- rep(c(0,1,0,0),wbw.n)
x3 <- rep(c(0,0,1,0),wbw.n)
x4 <- rep(c(0,0,0,1),wbw.n)
X <- as.matrix(cbind(x1,x2,x3,x4))

X0 <- as.matrix(rep(1,sum(wbw.n)),ncol=1)

Y <- as.matrix(wtg,ncol=1)
```

continued

```
X.star <- W.matrix %**% X
X0.star <- W.matrix %**% X0
Y.star <- W.matrix %**% Y

P.star <- X.star %**% solve(t(X.star) %**% X.star) %**% t(X.star)
P0.star <- X0.star %**% solve(t(X0.star) %**% X0.star) %**% t(X0.star)
I.N <- as.matrix(diag(sum(wbw.n)))

(SS.Trt <- t(Y.star) %**% (P.star - P0.star) %**% Y.star)
(SS.Err <- t(Y.star) %**% (I.N - P.star) %**% Y.star)

g <- ncol(X); N <- sum(wbw.n)

(F_W1 <- (SS.Trt/(g-1))/(SS.Err/(N-g)))

(F.alpha <- qf(.95,g-1,N-g))

(P.F_W1 <- 1-pf(F_W1,g-1,N-g))
```

R Output: Matrix Form

```
> (SS.Trt <- t(Y.star) %**% (P.star - P0.star) %**% Y.star)
      [,1]
[1,] 27.34203
> (SS.Err <- t(Y.star) %**% (I.N - P.star) %**% Y.star)
      [,1]
[1,] 236
>
> g <- ncol(X); N <- sum(wbw.n)
>
> (F_W1 <- (SS.Trt/(g-1))/(SS.Err/(N-g)))
      [,1]
[1,] 9.11401
>
> (F.alpha <- qf(.95,g-1,N-g))
[1] 2.642851
>
> (P.F_W1 <- 1-pf(F_W1,g-1,N-g))
      [,1]
[1,] 9.888664e-06
>
```

Note that the F-statistic is still highly significant, but not nearly as large as the ordinary least squares case ($F_{OLS}=15.36$). Note that Welch's test makes a (very small) adjustment to this F-statistic and adjusts the denominator degrees of freedom. This method (EWLS) can be used in a wide range of modeling situations, while Welch's test is specific to the 1-Way Analysis of Variance.

R Program: Scalar form

```
wbw <- read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F,col.names=c("trt","repnum","base","meth","wtg"))
attach(wbw); names(wbw)

trt.f <- factor(trt)

### Scalar Form

wbw.mean <- as.vector(tapply(wtg,trt.f,mean))
wbw.n <- as.vector(tapply(wtg,trt.f,length))
wbw.var <- as.vector(tapply(wtg,trt.f,var))
wt.vec <- rep(1/wbw.var,wbw.n)
N <- sum(wbw.n)
g <- length(wbw.n)

(muhat_w <- sum(wt.vec*wtg)/sum(wt.vec))
(muhat_iw <- wbw.mean)

muhat_w.vec <- rep(muhat_w,N)
muhat_iw.vec <- rep(muhat_iw,wbw.n)

(SSE.C <- sum(wt.vec*(wtg-muhat_iw.vec)^2))
(df.C <- N-g)

(SSE.R <- sum(wt.vec*(wtg-muhat_w.vec)^2))
(df.R <- N-1)

(F_w2 <- ((SSE.R-SSE.C)/(df.R-df.C))/(SSE.C/df.C))
(F.alpha <- qf(.95,df.R-df.C,df.C))

(P.F_w2 <- 1-pf(F_w2,df.R-df.C,df.C))
```

R Output: Scalar form

```
> ### Scalar Form
>
> (muhat_w <- sum(wt.vec*wtg)/sum(wt.vec))
[1] 608.3581
> (muhat_iw <- wbw.mean)
[1] 606.3300 610.6697 566.0003 679.9997
>
>
> (SSE.C <- sum(wt.vec*(wtg-muhat_iw.vec)^2))
[1] 236
> (df.C <- N-g)
[1] 236
>
> (SSE.R <- sum(wt.vec*(wtg-muhat_w.vec)^2))
[1] 263.342
> (df.R <- N-1)
[1] 239
>
> (F_w2 <- ((SSE.R-SSE.C)/(df.R-df.C))/(SSE.C/df.C))
[1] 9.11401
> (F.alpha <- qf(.95,df.R-df.C,df.C))
[1] 2.642851
>
> (P.F_w2 <- 1-pf(F_w2,df.R-df.C,df.C))
[1] 9.888664e-06
```

R Program: aov Function

```
wbw <- read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F,col.names=c("trt","repnum","base","meth","wtg"))
attach(wbw); names(wbw)

trt.f <- factor(trt)

wbw.var <- as.vector(tapply(wtg,trt.f,var))
wbw.n <- as.vector(tapply(wtg,trt.f,length))
wt.vec <- rep(1/wbw.var,wbw.n)

### aov function

wbw.modw <- aov(wtg ~ trt.f, weight=wt.vec)
anova(wbw.modw)
```

R Output: aov Function

```
> wbw.modw <- aov(wtg ~ trt.f, weight=wt.vec)
> anova(wbw.modw)
Analysis of Variance Table

Response: wtg
      Df Sum Sq Mean Sq F value    Pr(>F)
trt.f   3  27.342    9.114   9.114 9.889e-06 ***
Residuals 236 236.000    1.000
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
>
```

Parametric Bootstrap

Sample means and variances can be obtained from normal and chi-square distributions and used to compute F-statistics under the null hypothesis of equality of means (which can be arbitrarily set to 0). The algorithm is run as follows.

$$\text{Compute: } F_{EWLS} = \frac{1}{g-1} \left[\sum_{i=1}^g \frac{n_i}{s_i^2} y_i^2 - \frac{\left(\sum_{i=1}^g \frac{n_i}{s_i^2} y_i \right)^2}{\sum_{i=1}^g \frac{n_i}{s_i^2}} \right]$$

Generate $Z_1, \dots, Z_g \sim NID(0,1)$ and independent $X_i \sim \chi_{n_i-1}^2 \quad i=1, \dots, g$

$$\text{Transform: } \bar{Y}_{PBi} = \sqrt{\frac{s_i^2}{n_i}} Z_i \quad i=1, \dots, g \quad s_{PBi}^2 = \frac{s_i^2}{n_i-1} X_i \quad i=1, \dots, g$$
$$\text{Compute: } F_{PB} = \frac{1}{g-1} \left[\sum_{i=1}^g \frac{n_i}{s_{PBi}^2} \bar{Y}_{PBi}^2 - \frac{\left(\sum_{i=1}^g \frac{n_i}{s_{PBi}^2} \bar{Y}_{PBi} \right)^2}{\sum_{i=1}^g \frac{n_i}{s_{PBi}^2}} \right]$$

Repeat for M resamples \Rightarrow P-value is the proportion of resampled values of F_{PB} that exceed F_{EWLS}

R Program:

```
wbw <- read.table("http://www.stat.ufl.edu/~winner/data/whole_breast_weight.dat",
header=F,col.names=c("trt","repnum","base","meth","wtg"))
attach(wbw); names(wbw)

trt.f <- factor(trt)

wbw.mean <- as.vector(tapply(wtg,trt.f,mean))
wbw.var <- as.vector(tapply(wtg,trt.f,var))
wbw.n <- as.vector(tapply(wtg,trt.f,length))
g <- length(wbw.n)

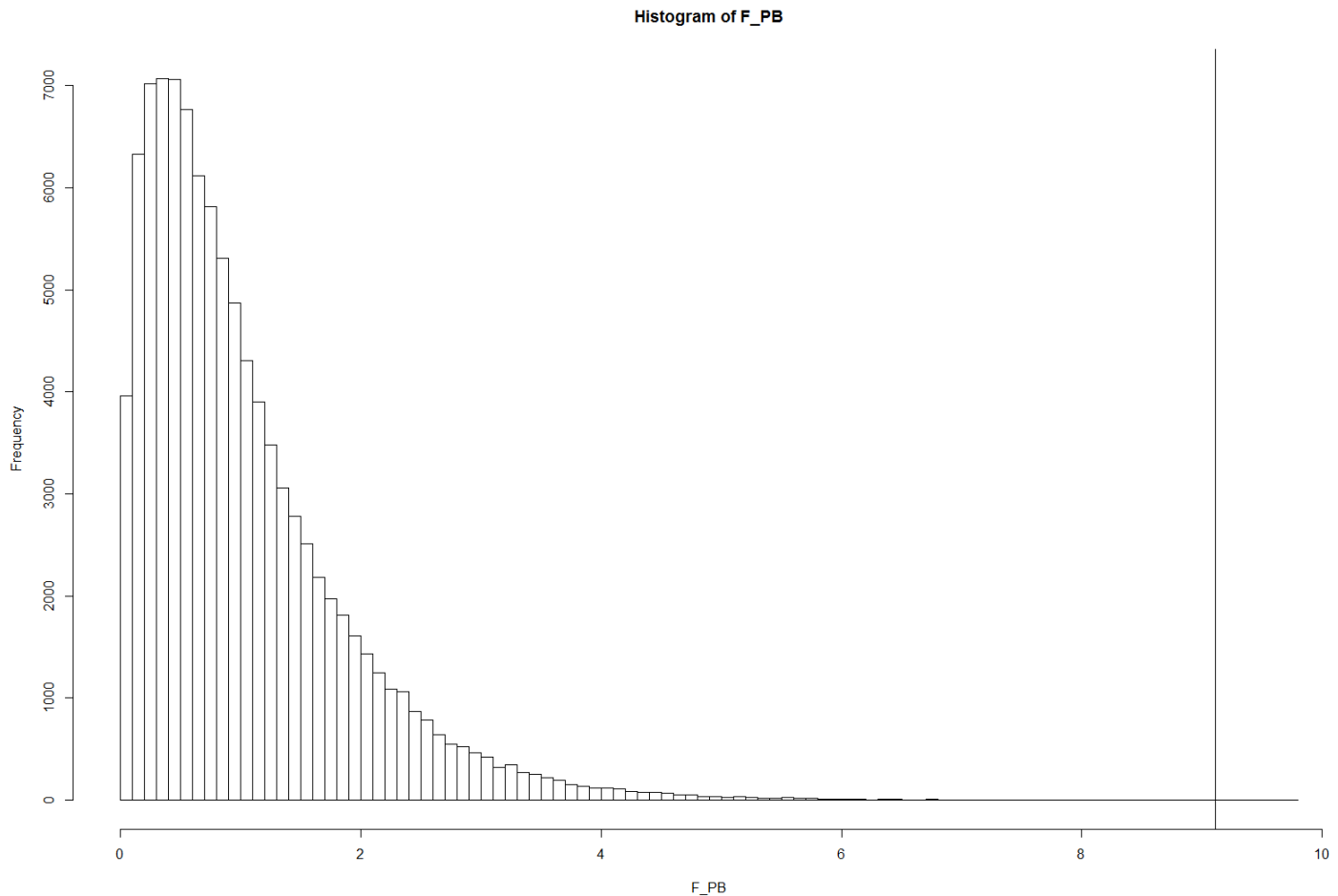
(F_EWLS <- (1/(g-1))*(sum((wbw.n/wbw.var)*wbw.mean^2) -
(sum((wbw.n/wbw.var)*wbw.mean))^2 / sum(wbw.n/wbw.var)))

M.sim <- 100000
set.seed(34567)
F_PB <- numeric(M.sim)

for (i in 1:M.sim) {
Z_PB <- rnorm(g)
X2_PB <- rchisq(g,(wbw.n-1))
Ybar_PB <- sqrt(wbw.var/wbw.n)*Z_PB
s2_PB <- (wbw.var/(wbw.n-1))*X2_PB
F_PB[i] <- (1/(g-1))*(sum((wbw.n/s2_PB)*Ybar_PB^2) -
(sum((wbw.n/s2_PB)*Ybar_PB))^2 / sum(wbw.n/s2_PB))
}

sum(F_PB >= F_EWLS)/M.sim
hist(F_PB,breaks=100)
abline(v=F_EWLS)
```

In 100000 resamples, 1 generated an F-statistic as large or larger than the observed value of 9.11401. This leads to a P-value of .00001. Below is a histogram of the generated F-statistics, with a vertical line at the observed F.



Data Sources:

A.M. Griffin and W.G. McCarten (1949). "Some Methods for the Quantitative Study of Entozoic Amoebae in Cultures," *The Journal of Parasitology*, Vol.35, #2, pp193-198.

J.C. Juskevich and C.G. Guyer (1990). "Bovine Growth Hormone: Human Food Safety Evaluation," *Science*, Vol.249, #4971, pp875-884.

M.I. Aksu, H. Imik, M. Karoglu (2007). "Influence of Dietary Sorghum(*Sorghum vulgare*) and Corn Supplemented with Methionine on Cut-Up Pieces Weights of Broiler Carcass and Quality Properties of Breast and Drumsticks Meat," *Food Science and Technology International*, Vol. 13, #5, pp. 361-367.

Chapter 5 – Factorial Designs (Fixed Effects Models)

In many applications, researchers are interested in the effects of more than one factor on the response variable. In particular, they may be interested in the **main effects** of the various factors, as well as possible **interaction effects** among the factors. Main effects are considered to be effects for the individual factors, averaged across levels of the other factor(s). Interaction effects are effects that occur when specific levels of each factor are matched, and the mean is impacted by their simultaneous presence. In this chapter, we assume all levels of interest of each factor are included in the model (**fixed effects**).

5.1. Additive Model: Factor A @ a Levels Factor B @ b Levels, n Replicates/Treatment N=abn

$$Y_{ijk} = \mu_{ij} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n \quad \varepsilon_{ijk} \sim NID(0, \sigma^2)$$

Factor B

Mean Structure: Factor A	$\begin{matrix} \mu_{11} & \mu_{12} & \cdots & \mu_{1b} \\ \mu_{21} & \mu_{22} & \cdots & \mu_{2b} \\ \vdots & \vdots & \cdots & \vdots \\ \mu_{a1} & \mu_{a2} & \cdots & \mu_{ab} \end{matrix}$	$\begin{matrix} \bar{\mu}_{1\bullet} \\ \bar{\mu}_{2\bullet} \\ \vdots \\ \bar{\mu}_{a\bullet} \\ \bar{\mu}_{\bullet 1} \quad \bar{\mu}_{\bullet 2} \quad \cdots \quad \bar{\mu}_{\bullet b} \quad \mu \end{matrix}$
--------------------------	--	--

$$\mu_{ij} = \mu + \alpha_i + \beta_j \quad \alpha_i = \bar{\mu}_{i\bullet} - \mu \quad \beta_j = \bar{\mu}_{\bullet j} - \mu \quad \sum_{i=1}^a \alpha_i = \sum_{j=1}^b \beta_j = 0$$

$$\Rightarrow \mu_{ij} = \mu + (\bar{\mu}_{i\bullet} - \mu) + (\bar{\mu}_{\bullet j} - \mu) = \bar{\mu}_{i\bullet} + \bar{\mu}_{\bullet j} - \mu$$

Ordinary least squares estimators are obtained as follows.

$$Q = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n \varepsilon_{ijk}^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - (\mu + \alpha_i + \beta_j))^2$$

$$\frac{\partial Q}{\partial \mu} = -2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - (\mu + \alpha_i + \beta_j)) = -2 \left[\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk} - abn\mu - bn \sum_{i=1}^a \alpha_i - an \sum_{j=1}^b \beta_j \right] = -2 \left[\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk} - abn\mu \right]$$

Setting the derivative to 0, and solving for $\hat{\mu}$: $\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk} - abn \hat{\mu} = 0 \Rightarrow \hat{\mu} = \frac{Y_{\dots}}{abn} = \bar{Y}_{\dots}$

$$\frac{\partial Q}{\partial \alpha_i} = -2 \sum_{j=1}^b \sum_{k=1}^n (Y_{i,jk} - (\mu + \alpha_i + \beta_j)) = -2 \left[\sum_{j=1}^b \sum_{k=1}^n Y_{i,jk} - bn\mu - bn\alpha_i - n \sum_{j=1}^b \beta_j \right] = -2 \left[\sum_{j=1}^b \sum_{k=1}^n Y_{i,jk} - bn\mu - bn\alpha_i \right]$$

Setting the derivative to 0, and solving for $\hat{\alpha}_i$: $\sum_{j=1}^b \sum_{k=1}^n Y_{i,jk} - bn \hat{\mu} - bn \hat{\alpha}_i = 0 \Rightarrow \hat{\alpha}_i = \frac{Y_{i\bullet\bullet}}{bn} - \hat{\mu} = \bar{Y}_{i\bullet\bullet} - \bar{Y}_{\dots}$

By direct analogy: $\hat{\beta}_j = \frac{Y_{\bullet j\bullet}}{an} - \hat{\mu} = \bar{Y}_{\bullet j\bullet} - \bar{Y}_{\dots}$

The means and variances of the OLS estimators are derived below.

$$\begin{aligned}
 E\left\{\hat{\mu}\right\} &= E\left\{\bar{Y}\dots\right\} = E\left\{\frac{1}{abn} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{abn} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\mu + \alpha_i + \beta_j) = \frac{1}{abn} \left[abn\mu + bn \sum_{i=1}^a \alpha_i + an \sum_{j=1}^b \beta_j \right] = \mu \\
 V\left\{\hat{\mu}\right\} &= V\left\{\bar{Y}\dots\right\} = V\left\{\frac{1}{abn} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{(abn)^2} abn\sigma^2 = \frac{\sigma^2}{abn} \\
 E\left\{\hat{\alpha}_i\right\} &= E\left\{\bar{Y}_{i\dots} - \bar{Y}\dots\right\} = E\left\{\frac{1}{bn} \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}\right\} - \mu = \frac{1}{bn} \sum_{j=1}^b (\mu + \alpha_i + \beta_j) - \mu = \frac{1}{bn} \left[bn\mu + bn\alpha_i + n \sum_{j=1}^b \beta_j \right] - \mu = \\
 &\mu + \alpha_i - \mu = \alpha_i \quad \text{By direct analogy: } E\left\{\hat{\beta}_j\right\} = \beta_j \\
 \text{COV}\left\{\bar{Y}_{i\dots}, \bar{Y}\dots\right\} &= \text{COV}\left\{\bar{Y}_{i\dots}, \frac{1}{a} \sum_{i=1}^a \bar{Y}_{i\dots}\right\} = \frac{1}{a} V\left\{\bar{Y}_{i\dots}\right\} = \frac{\sigma^2}{abn} \\
 V\left\{\hat{\alpha}_i\right\} &= V\left\{\bar{Y}_{i\dots} - \bar{Y}\dots\right\} = V\left\{\bar{Y}_{i\dots}\right\} + V\left\{\bar{Y}\dots\right\} - 2\text{COV}\left\{\bar{Y}_{i\dots}, \bar{Y}\dots\right\} = \frac{\sigma^2}{bn} + \frac{\sigma^2}{abn} - 2\frac{\sigma^2}{abn} = \frac{\sigma^2}{bn} - \frac{\sigma^2}{abn} = \frac{\sigma^2}{bn} \left(1 - \frac{1}{a}\right) \\
 V\left\{\hat{\beta}_j\right\} &= \frac{\sigma^2}{an} \left(1 - \frac{1}{b}\right)
 \end{aligned}$$

The Analysis of Variance has sources of variation for Factor A, Factor B, and Error, and is obtained below.

$$\begin{aligned}
 \text{Total (Corrected) Sum of Squares: } SS_{\text{Total}} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - \bar{Y}\dots)^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2 - N\bar{Y}\dots^2 \quad df_{\text{Total}} = N - 1 \\
 \text{Factor A Sum of Squares: } SS_A &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\bar{Y}_{i\dots} - \bar{Y}\dots)^2 = bn \sum_{i=1}^a (\bar{Y}_{i\dots} - \bar{Y}\dots)^2 = bn \sum_{i=1}^a \bar{Y}_{i\dots}^2 - N\bar{Y}\dots^2 \quad df_A = a - 1 \\
 \text{Factor B Sum of Squares: } SS_B &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\bar{Y}_{\cdot j\cdot} - \bar{Y}\dots)^2 = an \sum_{j=1}^b (\bar{Y}_{\cdot j\cdot} - \bar{Y}\dots)^2 = an \sum_{j=1}^b \bar{Y}_{\cdot j\cdot}^2 - N\bar{Y}\dots^2 \quad df_B = b - 1 \\
 \text{Error Sum of Squares: } SS_{\text{Err}} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - \bar{Y}_{i\dots} - \bar{Y}_{\cdot j\cdot} + \bar{Y}\dots)^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2 - bn \sum_{i=1}^a \bar{Y}_{i\dots}^2 - an \sum_{j=1}^b \bar{Y}_{\cdot j\cdot}^2 + N\bar{Y}\dots^2 \\
 \text{Error Sum of Squares: } SS_{\text{Err}} &= SS_{\text{Total}} - SS_A - SS_B \quad df_{\text{Error}} = (N - 1) - (a - 1) - (b - 1) = N - a - b + 1
 \end{aligned}$$

The expected sums of squares and mean squares are obtained as follows.

$$\begin{aligned}
E\{Y_{ijk}\} &= \mu + \alpha_i + \beta_j & V\{Y_{ijk}\} &= \sigma^2 \Rightarrow E\{Y_{ijk}^2\} = \sigma^2 + (\mu + \alpha_i + \beta_j)^2 = \sigma^2 + \mu^2 + \alpha_i^2 + \beta_j^2 + 2(\mu\alpha_i + \mu\beta_j + \alpha_i\beta_j) \\
E\{\bar{Y}_{ij\cdot}\} &= \mu + \alpha_i + \beta_j & V\{\bar{Y}_{ij\cdot}\} &= \frac{\sigma^2}{n} \Rightarrow E\{\bar{Y}_{ij\cdot}^2\} = \frac{\sigma^2}{n} + (\mu + \alpha_i + \beta_j)^2 = \frac{\sigma^2}{n} + \mu^2 + \alpha_i^2 + \beta_j^2 + 2(\mu\alpha_i + \mu\beta_j + \alpha_i\beta_j) \\
E\{\bar{Y}_{i\cdot\cdot}\} &= \mu + \alpha_i & V\{\bar{Y}_{i\cdot\cdot}\} &= \frac{\sigma^2}{bn} \Rightarrow E\{\bar{Y}_{i\cdot\cdot}^2\} = \frac{\sigma^2}{bn} + (\mu + \alpha_i)^2 = \frac{\sigma^2}{bn} + \mu^2 + \alpha_i^2 + 2\mu\alpha_i \\
E\{\bar{Y}_{\cdot j\cdot}\} &= \mu + \beta_j & V\{\bar{Y}_{\cdot j\cdot}\} &= \frac{\sigma^2}{an} \Rightarrow E\{\bar{Y}_{\cdot j\cdot}^2\} = \frac{\sigma^2}{an} + (\mu + \beta_j)^2 = \frac{\sigma^2}{an} + \mu^2 + \beta_j^2 + 2\mu\beta_j \\
E\{\bar{Y}_{\dots}\} &= \mu & V\{\bar{Y}_{\dots}\} &= \frac{\sigma^2}{abn} \Rightarrow E\{\bar{Y}_{\dots}^2\} = \frac{\sigma^2}{abn} + \mu^2
\end{aligned}$$

$$\begin{aligned}
E\{SS_A\} &= \left[bn \sum_{i=1}^a \left(\frac{\sigma^2}{bn} + \mu^2 + \alpha_i^2 + 2\mu\alpha_i \right) \right] - \left[abn \left(\frac{\sigma^2}{abn} + \mu^2 \right) \right] = \sigma^2(a-1) + bn \sum_{i=1}^a \alpha_i^2 \\
\Rightarrow E\{MS_A\} &= \sigma^2 + \frac{bn \sum_{i=1}^a \alpha_i^2}{a-1} \\
E\{SS_B\} &= \left[an \sum_{j=1}^b \left(\frac{\sigma^2}{an} + \mu^2 + \beta_j^2 + 2\mu\beta_j \right) \right] - \left[abn \left(\frac{\sigma^2}{abn} + \mu^2 \right) \right] = \sigma^2(b-1) + an \sum_{j=1}^b \beta_j^2 \\
\Rightarrow E\{MS_B\} &= \sigma^2 + \frac{an \sum_{j=1}^b \beta_j^2}{b-1} \\
E\{SS_{Err}\} &= \\
&= \left[\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\sigma^2 + \mu^2 + \alpha_i^2 + \beta_j^2 + 2(\mu\alpha_i + \mu\beta_j + \alpha_i\beta_j)) \right] - \left[bn \sum_{i=1}^a \left(\frac{\sigma^2}{bn} + \mu^2 + \alpha_i^2 + 2\mu\alpha_i \right) \right] \\
&\quad - \left[an \sum_{j=1}^b \left(\frac{\sigma^2}{an} + \mu^2 + \beta_j^2 + 2\mu\beta_j \right) \right] + \left[abn \left(\frac{\sigma^2}{abn} + \mu^2 \right) \right] = \sigma^2(abn - a - b + 1) = \sigma^2(N - a - b + 1) \\
\Rightarrow E\{MS_{Err}\} &= \sigma^2
\end{aligned}$$

Testing for Main Effects for Factors A and B:

$$\begin{aligned}
H_0^A : \alpha_1 = \dots = \alpha_a = 0 & \quad \text{Test Statistic: } F_A = \frac{MS_A}{MS_{Err}} \stackrel{H_0^A}{\sim} F_{a-1, N-a-b+1} \\
H_0^B : \beta_1 = \dots = \beta_b = 0 & \quad \text{Test Statistic: } F_B = \frac{MS_B}{MS_{Err}} \stackrel{H_0^B}{\sim} F_{b-1, N-a-b+1}
\end{aligned}$$

Example: Reading Times for 3 E-Reader Devices at 4 Illumination Levels

A study was conducted as a Completely Randomized Design with a total of $N = 60$ subjects randomized to one of 12 combinations of $a = 3$ E-Reader devices and $b = 4$ illumination levels (200, 500, 1000, 1500) (Chang, *et al* (2013)). The response was the time to complete reading a book passage, in 100s of seconds. The means and standard deviations are given below. There were $n = 5$ subjects per treatment.

Dev\Illum Mean	1	2	3	4	Mean	Dev/Illum SD	1	2	3	4
1	14.62	13.86	10.94	10.69	12.53	1	2.620	2.522	2.817	2.854
2	12.50	10.97	9.14	8.68	10.32	2	2.975	2.587	2.981	2.981
3	12.08	11.02	9.04	8.41	10.14	3	2.534	2.628	2.773	2.759
Mean	13.07	11.95	9.71	9.26	11.00					

The model fit is: $Y_{ijk} = \mu + \alpha_i + \beta_j + \varepsilon_{ijk} \quad i = 1, 2, 3; j = 1, 2, 3, 4; k = 1, \dots, 5 \quad \varepsilon_{ijk} \sim NID(0, \sigma^2)$

The parameter estimates are computed below.

$$\begin{aligned} \hat{\mu} &= 11.00 & \hat{\alpha}_1 &= 12.53 - 11.00 = 1.53 & \hat{\alpha}_2 &= 10.32 - 11.00 = -0.68 & \hat{\alpha}_3 &= 10.14 - 11.00 = -0.86 \\ \hat{\beta}_1 &= 13.07 - 11.00 = 2.07 & \hat{\beta}_2 &= 11.95 - 11.00 = 0.95 & \hat{\beta}_3 &= 9.71 - 11.00 = -1.29 & \hat{\beta}_4 &= 9.26 - 11.00 = -1.74 \end{aligned}$$

We compute the sums of squares for E-readers and Illumination Levels and the F-tests for main effects:

$$\begin{aligned} SS_{\text{Total}} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - \bar{Y} \dots)^2 = 585.98 \\ SS_A &= bn \sum_{i=1}^a (\bar{Y}_{i..} - \bar{Y} \dots)^2 = bn \sum_{i=1}^a (\hat{\alpha}_i)^2 = 4(5) [(1.53)^2 + (-0.68)^2 + (-0.86)^2] = 70.86 \\ MS_A &= \frac{SS_A}{a-1} = \frac{70.86}{3-1} = 35.43 \\ SS_B &= an \sum_{j=1}^b (\bar{Y}_{.j} - \bar{Y} \dots)^2 = an \sum_{j=1}^b (\hat{\beta}_j)^2 = 3(5) [(2.07)^2 + (0.95)^2 + (-1.29)^2 + (-1.74)^2] = 148.19 \\ MS_B &= \frac{SS_B}{b-1} = \frac{148.19}{4-1} = 49.40 \\ SS_{\text{Err}} &= 585.98 - 70.86 - 148.19 = 366.93 \quad df_{\text{Err}} = N - a - b + 1 = 60 - 3 - 4 + 1 = 54 \quad MS_{\text{Err}} = \frac{366.93}{54} = 6.795 \\ H_0^A : \alpha_1 = \alpha_2 = \alpha_3 = 0 & \quad TS_A : F_A = \frac{MS_A}{MS_{\text{Error}}} = \frac{35.43}{6.795} = 5.21 \\ RR_A : F_A \geq F_{.95; a-1, N-a-b+1} &= F_{.95; 2, 54} = 3.168 \quad P(F_{2, 54} \geq 5.21) = .0085 \\ H_0^B : \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0 & \quad TS_B : F_B = \frac{MS_B}{MS_{\text{Err}}} = \frac{49.40}{6.795} = 7.27 \\ RR_B : F_B \geq F_{.95; b-1, N-a-b+1} &= F_{.95; 3, 54} = 2.776 \quad P(F_{3, 54} \geq 7.27) = .0004 \end{aligned}$$

For the additive model, we can make post-hoc comparisons among levels of Factors A and B, respectively. When the interaction is significant, we would make comparisons within levels of the other factor(s), these are often referred to as “slices.” Here we use Tukey’s method to compare all pairs of E-readers, and to compare all pairs of Illumination levels.

$$\text{Factor A: } HSD_{i,j}^A = q_{\alpha;a,N-a-b+1} \sqrt{\frac{MS_{\text{Err}}}{bn}} \quad \text{Factor B: } HSD_{i,j}^B = q_{\alpha;b,N-a-b+1} \sqrt{\frac{MS_{\text{Err}}}{an}}$$

$$a = 3 \quad b = 4 \quad n = 5 \quad q_{.05;3,54} = 3.408 \quad q_{.05;4,54} = 3.749 \quad MS_{\text{Error}} = 6.795$$

$$\text{Factor A: } HSD_{i,j}^A = 3.408 \sqrt{\frac{6.795}{4(5)}} = 1.99 \quad \text{Factor B: } HSD_{i,j}^B = 3.749 \sqrt{\frac{6.795}{3(5)}} = 2.52$$

$$\text{E-Readers: } \bar{y}_{1..} = 12.53 \quad \bar{y}_{2..} = 10.32 \quad \bar{y}_{3..} = 10.14$$

$$\text{Illumination Levels: } \bar{y}_{\cdot 1.} = 13.07 \quad \bar{y}_{\cdot 2.} = 11.95 \quad \bar{y}_{\cdot 3.} = 9.71 \quad \bar{y}_{\cdot 4.} = 9.26$$

E-Readers: Device3 Device2 Device1 Illumination: 1500 1000 500 200

R Program

```
eread <-
read.table("http://www.stat.ufl.edu/~winner/data/ereader1.dat", header=F,
           col.names=c("device", "illum", "readtime"))
attach(eread)

readtime <- readtime/100
device <- factor(device)
illum <- factor(illum)

eread.mod1 <- aov(readtime ~ device + illum)
anova(eread.mod1)

TukeyHSD(eread.mod1, "device")
TukeyHSD(eread.mod1, "illum")

interaction.plot(device, illum, readtime)
```

R Output

```
> erezad.mod1 <- aov(readtime ~ device + illum)
> anova(erezad.mod1)
Analysis of Variance Table

Response: readtime
      Df Sum Sq Mean Sq F value    Pr(>F)
device  2   70.70   35.348    5.1987 0.0086140 **
illum   3  148.11   49.369    7.2606 0.0003531 ***
Residuals 54  367.17    6.800

---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
> TukeyHSD(erezad.mod1,"device")
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = readtime ~ device + illum)

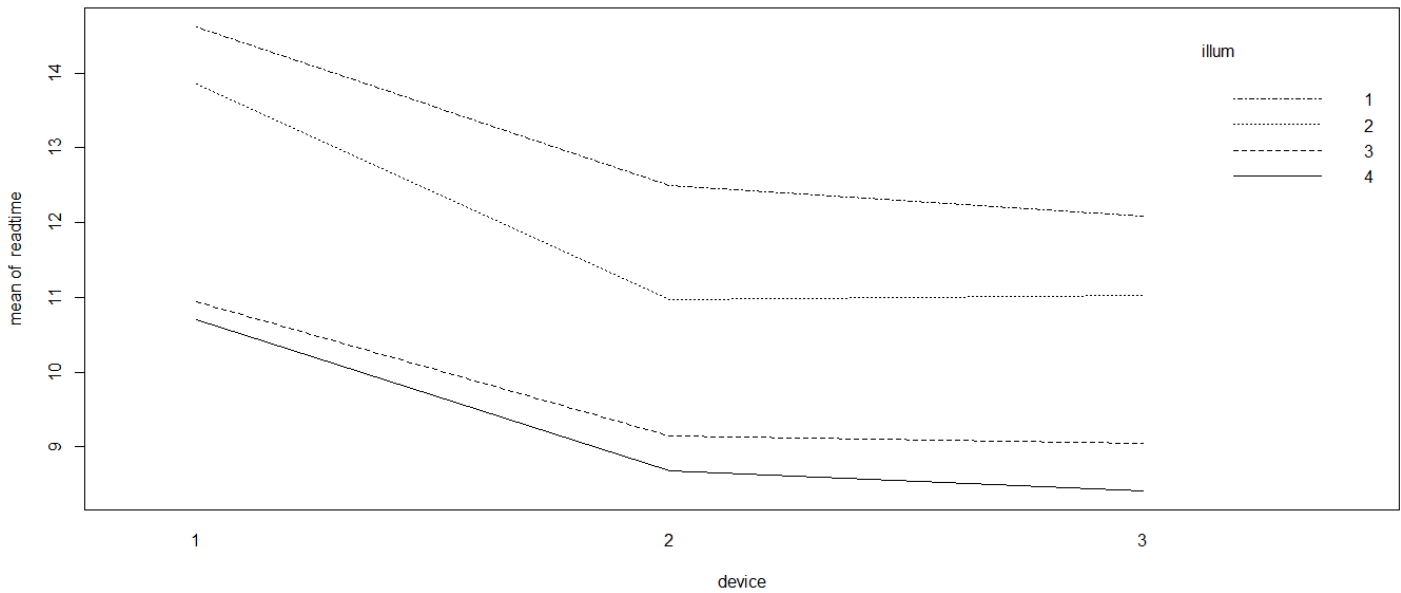
$device
      diff      lwr      upr    p adj
2-1 -2.206260 -4.193515 -0.219005 0.0262395
3-1 -2.388265 -4.375520 -0.401010 0.0148045
3-2 -0.182005 -2.169260  1.805250 0.9735138

> TukeyHSD(erezad.mod1,"illum")
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = readtime ~ device + illum)

$illum
      diff      lwr      upr    p adj
2-1 -1.119987 -3.644038  1.4040644 0.6442676
3-1 -3.361987 -5.886038 -0.8379356 0.0046176
4-1 -3.806987 -6.331038 -1.2829356 0.0010910
3-2 -2.242000 -4.766051  0.2820510 0.0984819
4-2 -2.687000 -5.211051 -0.1629490 0.0327612
4-3 -0.445000 -2.969051  2.0790510 0.9658741
```

If there is no interaction, then when the population means are plotted versus one factor, with separate lines for levels of the other factor, the lines will be parallel. This is due to the additivity of effects. When we plot the sample means, they will not be exactly parallel due to sampling variation, even if there is no interaction in the population model. Below is an **interaction plot** of reading time versus device, with separate lines for each illumination level. There is certainly no evidence of an interaction between device and illumination level.



As with the 1-Way model, we often have distinct contrasts of interest, and we would like to partition the various sums of squares into a set of orthogonal contrasts. In the case of the E-Reader experiment, Device 1 was small, while Devices 2 and 3 were of larger (and comparable) sizes. Thus, we may want to contrast Device 1 with Devices 2 and 3, and also contrast Device 2 with Device 3. The illumination levels are numeric (though not equally spaced, with levels (200, 500, 1000, 1500)). We may wish to partition the Illumination sum of squares into linear, quadratic, and cubic polynomials. We make use of the **orpol** function in **SAS Proc IML** to obtain the coefficients for the Illumination Level Contrasts.

Device	1 vs (2&3)	2 vs 3		Illum	Linear	Quadratic	Cubic
1 (Small)	2	0		200	-0.60609	0.50745	-0.35377
2 (Large)	-1	1		500	-0.30305	-0.34163	0.73583
3 (Large)	-1	-1		1000	0.20203	-0.63610	-0.55188
				1500	0.70711	0.47028	0.16981

The contrasts, estimated contrasts, Sums of Squares, and F-tests are given here. We see that the significant contrasts are Device 1 versus Devices 2 and 3, and the Linear effect of Illumination.

$$C_{A1} = \sum_{i=1}^a w_i^{A1} \bar{\mu}_{i\bullet} = 2\bar{\mu}_{1\bullet} - \bar{\mu}_{2\bullet} - \bar{\mu}_{3\bullet} \quad \hat{C}_{A1} = 2\bar{y}_{1\bullet} - \bar{y}_{2\bullet} - \bar{y}_{3\bullet} = 2(12.53) - 10.32 - 10.14 = 4.60$$

$$SSC_{A1} = bn \frac{(\hat{C}_{A1})^2}{\sum_{i=1}^a (w_i^{A1})^2} = 4(5) \frac{(4.60)^2}{4+1+1} = 70.53$$

$$C_{A2} = \sum_{i=1}^a w_i^{A2} \bar{\mu}_{i\bullet} = \bar{\mu}_{2\bullet} - \bar{\mu}_{3\bullet} \quad \hat{C}_{A2} = \bar{y}_{2\bullet} - \bar{y}_{3\bullet} = 10.32 - 10.14 = 0.18 \quad SSC_{A2} = bn \frac{(\hat{C}_{A2})^2}{\sum_{i=1}^a (w_i^{A2})^2} = 4(5) \frac{(0.18)^2}{0+1+1} = 0.324$$

$$C_{B1} = \sum_{j=1}^b w_j^{B1} \bar{\mu}_{\bullet j} = -0.60609\bar{\mu}_{\bullet 1} - 0.30305\bar{\mu}_{\bullet 2} + 0.20203\bar{\mu}_{\bullet 3} + 0.70711\bar{\mu}_{\bullet 4} \quad \sum_{j=1}^b (w_j^{B1})^2 = 1$$

$$\hat{C}_{B1} = -.60609(13.07) - .30305(11.95) + .20203(9.71) + .70711(9.26) = -3.0335 \quad SSC_{B1} = 3(5) \frac{(-3.0335)^2}{1} = 138.03$$

$$C_{B2} = \sum_{j=1}^b w_j^{B2} \bar{\mu}_{\bullet j} = .50745\bar{\mu}_{\bullet 1} - .34163\bar{\mu}_{\bullet 2} - .63610\bar{\mu}_{\bullet 3} + .47028\bar{\mu}_{\bullet 4} \quad \sum_{j=1}^b (w_j^{B2})^2 = 1$$

$$\hat{C}_{B2} = .50745(13.07) - .34163(11.95) - .63610(9.71) + .47028(9.26) = 0.7281 \quad SSC_{B2} = 3(5) \frac{(0.7281)^2}{1} = 7.95$$

$$C_{B3} = \sum_{j=1}^b w_j^{B3} \bar{\mu}_{\bullet j} = -.35377\bar{\mu}_{\bullet 1} + .73583\bar{\mu}_{\bullet 2} - .55188\bar{\mu}_{\bullet 3} + .16981\bar{\mu}_{\bullet 4} \quad \sum_{j=1}^b (w_j^{B3})^2 = 1$$

$$\hat{C}_{B3} = -.35377(13.07) + .73583(11.95) - .55188(9.71) + .16981(9.26) = 0.3832 \quad SSC_{B3} = 3(5) \frac{(0.3832)^2}{1} = 2.203$$

$$F_{.95;1,54} = 4.020 \quad F_{A1} = \frac{SSC_{A1}}{MS_{Err}} = \frac{70.53}{6.795} = 10.380 \quad F_{A2} = \frac{SSC_{A2}}{MS_{Err}} = \frac{0.324}{6.795} = 0.048$$

$$F_{B1} = \frac{SSC_{B1}}{MS_{Err}} = \frac{138.03}{6.795} = 20.313 \quad F_{B2} = \frac{SSC_{B2}}{MS_{Err}} = \frac{7.95}{6.795} = 1.170 \quad F_{B3} = \frac{SSC_{B3}}{MS_{Err}} = \frac{2.203}{6.795} = 0.324$$

The R Program is given here. Note that R conducts the t-tests, where the t-statistics are the signed square roots of the F-statistics given above.

R Program

```

eread <-
read.table("http://www.stat.ufl.edu/~winner/data/ereader1.dat", header=F,
           col.names=c("device", "illum", "readtime"))
attach(eread)

readtime <- readtime/100

device <- factor(device)
illum <- factor(illum)

contrasts(device) <- cbind(c(2, -1, -1), c(0, 1, -1))
contrasts(illum) <- cbind(c(-.60609, -.30305, .20203, .70711),
                          c(.50745, -.34163, -.63610, .47028), c(-.35377, .73583, -.55188, .16981))

eread.mod2 <- aov(readtime ~ device + illum)
anova(eread.mod2)
summary.lm(eread.mod2)

```

R Output

```
> contrasts(device) <- cbind(c(2,-1,-1),c(0,1,-1))
> contrasts(illum) <- cbind(c(-.60609,-.30305,.20203,.70711),
+   c(.50745,-.34163,-.63610,.47028),c(-.35377,.73583,-.55188,.16981))
>
>  eread.mod2 <- aov(readtime ~ device + illum)
>  anova(eread.mod2)
Analysis of Variance Table

Response: readtime
      Df Sum Sq Mean Sq F value    Pr(>F)
device  2  70.70   35.348   5.1987 0.0086140 **
illum   3 148.11   49.369   7.2606 0.0003531 ***
Residuals 54 367.17    6.800
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary.lm(eread.mod2)

Call:
aov(formula = readtime ~ device + illum)

Residuals:
    Min       1Q   Median       3Q      Max
-5.0727 -1.9774 -0.1943  1.9634  4.6411

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  10.9968     0.3366  32.666 < 2e-16 ***
device1       0.7658     0.2380   3.217  0.00219 **
device2       0.0910     0.4123   0.221  0.82614
illum1      -3.0318     0.6733  -4.503 3.62e-05 ***
illum2       0.7308     0.6733   1.085  0.28253
illum3       0.3848     0.6733   0.572  0.57000
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.608 on 54 degrees of freedom
Multiple R-squared:  0.3734,    Adjusted R-squared:  0.3154
F-statistic: 6.436 on 5 and 54 DF,  p-value: 9.296e-05
```

It should be noted that in R, the default contrast is the **contr.treatment** option. In this case, when the **summary.lm(model)** is run, the following parameters are being estimated.

```
Intercept:  $\mu + \alpha_1 + \beta_1$   Ai:  $\alpha_i - \alpha_1$    $i = 2, \dots, a$   Bj:  $\beta_j - \beta_1$    $r = 2, \dots, b$ 
```

R Program

```
eread <-
read.table("http://www.stat.ufl.edu/~winner/data/ereader1.dat",header=F,
           col.names=c("device","illum","readtime"))
attach(eread)

readtime <- readtime/100

device <- factor(device)
illum <- factor(illum)

eread.mod1 <- aov(readtime ~ device + illum)
anova(eread.mod1)
summary.lm(eread.mod1)
```


R Output

```
> ereal.mod1 <- aov(readtime ~ device + illum)
> anova(ereal.mod1)
Analysis of Variance Table

Response: readtime
      Df Sum Sq Mean Sq F value    Pr(>F)
device  2  70.70  35.348   5.1987 0.0086140 **
illum   3 148.11  49.369   7.2606 0.0003531 ***
Residuals 54 367.17   6.800
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary.lm(ereal.mod1)

Call:
aov(formula = readtime ~ device + illum)

Residuals:
    Min       1Q   Median       3Q      Max
-5.0727 -1.9774 -0.1943  1.9634  4.6411

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  14.6005     0.8246  17.706 < 2e-16 ***
device2      -2.2063     0.8246  -2.676 0.009854 **
device3      -2.3883     0.8246  -2.896 0.005442 **
illum2       -1.1200     0.9522  -1.176 0.244650
illum3       -3.3620     0.9522  -3.531 0.000856 ***
illum4       -3.8070     0.9522  -3.998 0.000195 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.608 on 54 degrees of freedom
Multiple R-squared:  0.3734,    Adjusted R-squared:  0.3154
F-statistic: 6.436 on 5 and 54 DF,  p-value: 9.296e-05
```

To obtain the estimates under the model with effects summing to 0 for factors A and B (as we have fit above), use the **contr.sum** option.

R Program

```
ereal <- read.table("http://www.stat.ufl.edu/~winner/data/ereader1.dat",header=F,
  col.names=c("device","illum","readtime"))
attach(ereal)

readtime <- readtime/100

device <- factor(device)
illum <- factor(illum)

options(contrasts=c("contr.sum","contr.poly"))

ereal.mod3 <- aov(readtime ~ device + illum)
anova(ereal.mod3)
summary.lm(ereal.mod3)
```

R Output

```
> eread.mod3 <- aov(readtime ~ device + illum)
> anova(eread.mod3)
Analysis of Variance Table

Response: readtime
      Df Sum Sq Mean Sq F value    Pr(>F)
device  2  70.70  35.348   5.1987 0.0086140 **
illum   3 148.11  49.369   7.2606 0.0003531 ***
Residuals 54 367.17   6.800
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary.lm(eread.mod3)

Call:
aov(formula = readtime ~ device + illum)

Residuals:
    Min       1Q   Median       3Q      Max
-5.0727 -1.9774 -0.1943  1.9634  4.6411

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  10.9967     0.3366   32.666 < 2e-16 ***
device1       1.5315     0.4761    3.217 0.002191 **
device2      -0.6748     0.4761   -1.417 0.162136
illum1        2.0722     0.5831    3.554 0.000797 ***
illum2        0.9523     0.5831    1.633 0.108254
illum3       -1.2897     0.5831   -2.212 0.031219 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.608 on 54 degrees of freedom
Multiple R-squared:  0.3734,    Adjusted R-squared:  0.3154
F-statistic: 6.436 on 5 and 54 DF,  p-value: 9.296e-05
```

Matrix Approach

In the matrix form of the model, with the restrictions $\sum_{i=1}^a \alpha_i = \sum_{j=1}^b \beta_j = 0$ the \mathbf{X} matrix will have one column for the mean, $a-1$ columns for factor A, and $b-1$ columns for factor B. The vector $\boldsymbol{\beta}$ will have an overall mean (μ), $a-1$ terms ($\alpha_1, \dots, \alpha_{a-1}$) and $b-1$ terms ($\beta_1, \dots, \beta_{b-1}$).

Assuming the data are ordered across the levels of A and B, the matrices will be of the following forms, using the E-reader experiment as a model ($a=3$, $b=4$, $n_{ij}=5$).

$$\mathbf{Y} = \begin{bmatrix} Y_{11} \\ Y_{12} \\ Y_{13} \\ Y_{14} \\ Y_{21} \\ Y_{22} \\ Y_{23} \\ Y_{24} \\ Y_{31} \\ Y_{32} \\ Y_{33} \\ Y_{34} \end{bmatrix} \quad \mathbf{Y}_{ij} = \begin{bmatrix} Y_{ij1} \\ \vdots \\ Y_{ijn_{ij}} \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} \mathbf{1}_{n11} & \mathbf{1}_{n11} & \mathbf{0}_{n11} & \mathbf{1}_{n11} & \mathbf{0}_{n11} & \mathbf{0}_{n11} \\ \mathbf{1}_{n12} & \mathbf{1}_{n12} & \mathbf{0}_{n12} & \mathbf{0}_{n12} & \mathbf{1}_{n12} & \mathbf{0}_{n12} \\ \mathbf{1}_{n13} & \mathbf{1}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{1}_{n13} \\ \mathbf{1}_{n14} & \mathbf{1}_{n14} & \mathbf{0}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} \\ \mathbf{1}_{n21} & \mathbf{0}_{n21} & \mathbf{1}_{n21} & \mathbf{1}_{n21} & \mathbf{0}_{n21} & \mathbf{0}_{n21} \\ \mathbf{1}_{n22} & \mathbf{0}_{n22} & \mathbf{1}_{n22} & \mathbf{0}_{n22} & \mathbf{1}_{n22} & \mathbf{0}_{n22} \\ \mathbf{1}_{n23} & \mathbf{0}_{n23} & \mathbf{1}_{n23} & \mathbf{0}_{n23} & \mathbf{0}_{n23} & \mathbf{1}_{n23} \\ \mathbf{1}_{n24} & \mathbf{0}_{n24} & \mathbf{1}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} \\ \mathbf{1}_{n31} & -\mathbf{1}_{n31} & -\mathbf{1}_{n31} & \mathbf{1}_{n31} & \mathbf{0}_{n31} & \mathbf{0}_{n31} \\ \mathbf{1}_{n32} & -\mathbf{1}_{n32} & -\mathbf{1}_{n32} & \mathbf{0}_{n32} & \mathbf{1}_{n32} & \mathbf{0}_{n32} \\ \mathbf{1}_{n33} & -\mathbf{1}_{n33} & -\mathbf{1}_{n33} & \mathbf{0}_{n33} & \mathbf{0}_{n33} & \mathbf{1}_{n33} \\ \mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$$

The following portion of an EXCEL worksheet gives $\mathbf{X}'\mathbf{X}$, $\mathbf{X}'\mathbf{Y}$, $(\mathbf{X}'\mathbf{X})^{-1}$, OLS estimates, analysis of variance, standard errors and tests. Note that the estimates, standard errors and t-statistics match those from R for the **contr.sum** option.

X'X							X'Y			
60	0	0	0	0	0	0	659.8048			
0	40	20	0	0	0	0	47.7653			
0	20	40	0	0	0	0	3.6401			
0	0	0	30	15	15		57.1048			
0	0	0	15	30	15		40.3050			
0	0	0	15	15	30		6.6750			
INV(X'X)							Beta-hat	SE{Beta}	t	P-value
0.0167	0.0000	0.0000	0.0000	0.0000	0.0000		10.9967	0.3366	32.6663	0.0000
0.0000	0.0333	-0.0167	0.0000	0.0000	0.0000		1.5315	0.4761	3.2169	0.0022
0.0000	-0.0167	0.0333	0.0000	0.0000	0.0000		-0.6748	0.4761	-1.4173	0.1621
0.0000	0.0000	0.0000	0.0500	-0.0167	-0.0167		2.0722	0.5831	3.5540	0.0008
0.0000	0.0000	0.0000	-0.0167	0.0500	-0.0167		0.9523	0.5831	1.6332	0.1083
0.0000	0.0000	0.0000	-0.0167	-0.0167	0.0500		-1.2897	0.5831	-2.2120	0.0312
Y'Y	Y'PY	Y'(1/n)JY	SSErr	dfErr	MSErr	SSReg	dfReg	MSReg	F_obs	F(.05)
7841.6840	7474.5094	7255.7062	367.1746	54	6.7995	218.8032	5	43.7606	6.4358	2.3861

5.2. Interaction Model: Factor A @ a Levels Factor B @ b Levels, n Replicates/Treatment N=abn

$$Y_{ijk} = \mu_{ij} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n \quad \varepsilon_{ijk} \sim NID(0, \sigma^2)$$

Factor B

Mean Structure: Factor A

$$\mu_{ij} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} \quad \alpha_i = \bar{\mu}_{i\cdot} - \mu \quad \beta_j = \bar{\mu}_{\cdot j} - \mu \quad (\alpha\beta)_{ij} = \mu_{ij} - \bar{\mu}_{i\cdot} - \bar{\mu}_{\cdot j} + \mu$$

$$\sum_{i=1}^a \alpha_i = \sum_{j=1}^b \beta_j = \sum_{i=1}^a (\alpha\beta)_{ij} = \sum_{j=1}^b (\alpha\beta)_{ij} = 0$$

$$\Rightarrow \mu_{ij} = \mu + (\bar{\mu}_{i\cdot} - \mu) + (\bar{\mu}_{\cdot j} - \mu) + (\mu_{ij} - \bar{\mu}_{i\cdot} - \bar{\mu}_{\cdot j} + \mu)$$

Ordinary least squares estimators for the interaction terms are obtained as follows:

$$Q = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n \varepsilon_{ijk}^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n \left(Y_{ijk} - (\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij}) \right)^2$$

$$\frac{\partial Q}{\partial (\alpha\beta)_{i'j'}} = -2 \sum_{k=1}^n \left(Y_{i'j'k} - (\mu + \alpha_{i'} + \beta_{j'} + (\alpha\beta)_{i'j'}) \right) = -2 \left[\sum_{k=1}^n Y_{i'j'k} - n\mu - n\alpha_{i'} - n\beta_{j'} - n(\alpha\beta)_{i'j'} \right]$$

$$\text{Setting the derivative to 0, and solving for } (\hat{\alpha}\hat{\beta})_{i'j'}: \sum_{k=1}^n Y_{i'j'k} - n\hat{\mu} - n\hat{\alpha}_{i'} - n\hat{\beta}_{j'} - n(\hat{\alpha}\hat{\beta})_{i'j'} = 0$$

$$\Rightarrow \left(\hat{\alpha}\hat{\beta} \right)_{i'j'} = \frac{Y_{i'j'\cdot}}{n} - \hat{\mu} - \hat{\alpha}_{i'} - \hat{\beta}_{j'} = \bar{Y}_{i'j'\cdot} - \bar{Y}\dots - (\bar{Y}_{i'\cdot\cdot} - \bar{Y}\dots) - (\bar{Y}_{\cdot j'\cdot} - \bar{Y}\dots) = \bar{Y}_{i'j'\cdot} - \bar{Y}_{i'\cdot\cdot} - \bar{Y}_{\cdot j'\cdot} + \bar{Y}\dots$$

The means and variances of the OLS estimators for interaction effects are derived below.

$$\begin{aligned} \text{COV}\{Y_{ijk}, \bar{Y}_{ij\cdot}\} &= \frac{\sigma^2}{n} & \text{COV}\{\bar{Y}_{ij\cdot}, \bar{Y}_{i\cdot\cdot}\} &= \frac{\sigma^2}{bn} & \text{COV}\{\bar{Y}_{ij\cdot}, \bar{Y}_{\cdot j\cdot}\} &= \frac{\sigma^2}{an} & \text{COV}\{\bar{Y}_{ij\cdot}, \bar{Y}_{\cdot\cdot\cdot}\} &= \frac{\sigma^2}{abn} & \text{COV}\{\bar{Y}_{i\cdot\cdot}, \bar{Y}_{\cdot j\cdot}\} &= \frac{\sigma^2}{abn} \\ E\left\{\left(\hat{\alpha}\beta\right)_{ij}\right\} &= V\left\{\bar{Y}_{ij\cdot} - \bar{Y}_{i\cdot\cdot} - \bar{Y}_{\cdot j\cdot} + \bar{Y}_{\cdot\cdot\cdot}\right\} = \mu_{ij} - \bar{\mu}_{i\cdot} - \bar{\mu}_{\cdot j} + \mu \\ V\left\{\left(\hat{\alpha}\beta\right)_{ij}\right\} &= V\left\{\bar{Y}_{ij\cdot} - \bar{Y}_{i\cdot\cdot} - \bar{Y}_{\cdot j\cdot} + \bar{Y}_{\cdot\cdot\cdot}\right\} = V\left\{\bar{Y}_{ij\cdot}\right\} + V\left\{\bar{Y}_{i\cdot\cdot}\right\} + V\left\{\bar{Y}_{\cdot j\cdot}\right\} + V\left\{\bar{Y}_{\cdot\cdot\cdot}\right\} \\ &\quad - 2\text{COV}\left\{\bar{Y}_{ij\cdot}, \bar{Y}_{i\cdot\cdot}\right\} - 2\text{COV}\left\{\bar{Y}_{ij\cdot}, \bar{Y}_{\cdot j\cdot}\right\} + 2\text{COV}\left\{\bar{Y}_{i\cdot\cdot}, \bar{Y}_{\cdot\cdot\cdot}\right\} + 2\text{COV}\left\{\bar{Y}_{\cdot j\cdot}, \bar{Y}_{\cdot\cdot\cdot}\right\} - 2\text{COV}\left\{\bar{Y}_{i\cdot\cdot}, \bar{Y}_{\cdot j\cdot}\right\} - 2\text{COV}\left\{\bar{Y}_{\cdot j\cdot}, \bar{Y}_{\cdot\cdot\cdot}\right\} \\ &= \frac{\sigma^2}{n} + \frac{\sigma^2}{bn} + \frac{\sigma^2}{an} + \frac{\sigma^2}{abn} - 2\frac{\sigma^2}{bn} - 2\frac{\sigma^2}{an} + 2\frac{\sigma^2}{abn} + 2\frac{\sigma^2}{abn} - 2\frac{\sigma^2}{abn} - 2\frac{\sigma^2}{abn} = \\ &= \frac{\sigma^2}{abn} [ab + a + b + 1 - 2a - 2b + 2 + 2 - 2 - 2] = \frac{\sigma^2}{abn} [ab - a - b + 1] = \frac{\sigma^2}{abn} (a-1)(b-1) \end{aligned}$$

The Analysis of Variance has sources of variation for Factors A, B, AB interaction, and Error, and is obtained below for Interaction and Error. Factors A and B are the same as before.

$$\begin{aligned} \text{AB Interaction Sum of Squares: } SS_{AB} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n \left(\bar{Y}_{ij\cdot} - \bar{Y}_{i\cdot\cdot} - \bar{Y}_{\cdot j\cdot} - \bar{Y}_{\cdot\cdot\cdot} \right)^2 = \\ &= n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij\cdot}^2 - bn \sum_{i=1}^a \bar{Y}_{i\cdot\cdot}^2 - an \sum_{j=1}^b \bar{Y}_{\cdot j\cdot}^2 + N \bar{Y}_{\cdot\cdot\cdot}^2 \quad df_{AB} = (a-1)(b-1) \\ \text{Error Sum of Squares: } SS_{\text{Err}} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n \left(Y_{ijk} - \bar{Y}_{ij\cdot} \right)^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2 - n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij\cdot}^2 \quad df_{\text{Error}} = ab(n-1) = N - ab \end{aligned}$$

The expected sums of squares and mean squares are obtained as follows.

$$\begin{aligned} E\{Y_{ijk}\} &= \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} & V\{Y_{ijk}\} &= \sigma^2 \Rightarrow E\{Y_{ijk}^2\} = \sigma^2 + \left(\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} \right)^2 = \\ &= \sigma^2 + \mu^2 + \alpha_i^2 + \beta_j^2 + (\alpha\beta)_{ij}^2 + 2\left(\mu\alpha_i + \mu\beta_j + \mu(\alpha\beta)_{ij} + \alpha_i\beta_j + \alpha_i(\alpha\beta)_{ij} + \beta_j(\alpha\beta)_{ij} \right) \\ E\{\bar{Y}_{ij\cdot}\} &= \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} & V\{\bar{Y}_{ij\cdot}\} &= \frac{\sigma^2}{n} \Rightarrow E\{\bar{Y}_{ij\cdot}^2\} = \frac{\sigma^2}{n} + \left(\mu + \alpha_i + \beta_j \right)^2 = \\ &= \frac{\sigma^2}{n} + \mu^2 + \alpha_i^2 + \beta_j^2 + (\alpha\beta)_{ij}^2 + 2\left(\mu\alpha_i + \mu\beta_j + \mu(\alpha\beta)_{ij} + \alpha_i\beta_j + \alpha_i(\alpha\beta)_{ij} + \beta_j(\alpha\beta)_{ij} \right) \\ E\{\bar{Y}_{i\cdot\cdot}\} &= \mu + \alpha_i & V\{\bar{Y}_{i\cdot\cdot}\} &= \frac{\sigma^2}{bn} \Rightarrow E\{\bar{Y}_{i\cdot\cdot}^2\} = \frac{\sigma^2}{bn} + (\mu + \alpha_i)^2 = \frac{\sigma^2}{bn} + \mu^2 + \alpha_i^2 + 2\mu\alpha_i \\ E\{\bar{Y}_{\cdot j\cdot}\} &= \mu + \beta_j & V\{\bar{Y}_{\cdot j\cdot}\} &= \frac{\sigma^2}{an} \Rightarrow E\{\bar{Y}_{\cdot j\cdot}^2\} = \frac{\sigma^2}{an} + (\mu + \beta_j)^2 = \frac{\sigma^2}{an} + \mu^2 + \beta_j^2 + 2\mu\beta_j \\ E\{\bar{Y}_{\cdot\cdot\cdot}\} &= \mu & V\{\bar{Y}_{\cdot\cdot\cdot}\} &= \frac{\sigma^2}{abn} \Rightarrow E\{\bar{Y}_{\cdot\cdot\cdot}^2\} = \frac{\sigma^2}{abn} + \mu^2 \end{aligned}$$

$$\begin{aligned}
E\{SS_{AB}\} &= n \sum_{i=1}^a \sum_{j=1}^b \left(\frac{\sigma^2}{n} + \mu^2 + \alpha_i^2 + \beta_j^2 + (\alpha\beta)_{ij}^2 + 2(\mu\alpha_i + \mu\beta_j + \mu(\alpha\beta)_{ij} + \alpha_i\beta_j + \alpha_i(\alpha\beta)_{ij} + \beta_j(\alpha\beta)_{ij}) \right) \\
&\quad - \left[bn \sum_{i=1}^a \left(\frac{\sigma^2}{bn} + \mu^2 + \alpha_i^2 + 2\mu\alpha_i \right) \right] - \left[an \sum_{j=1}^b \left(\frac{\sigma^2}{an} + \mu^2 + \beta_j^2 + 2\mu\beta_j \right) \right] + \left[abn \left(\frac{\sigma^2}{abn} + \mu^2 \right) \right] = \\
&= \sigma^2(ab - a - b + 1) + n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2 = \sigma^2(a-1)(b-1) + n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2 \\
\Rightarrow E\{MS_{AB}\} &= \sigma^2 + \frac{n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2}{(a-1)(b-1)}
\end{aligned}$$

$$\begin{aligned}
E\{SS_{Err}\} &= \\
&= \left[\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n \left(\sigma^2 + \mu^2 + \alpha_i^2 + \beta_j^2 + (\alpha\beta)_{ij}^2 + 2(\mu\alpha_i + \mu\beta_j + \mu(\alpha\beta)_{ij} + \alpha_i\beta_j + \alpha_i(\alpha\beta)_{ij} + \beta_j(\alpha\beta)_{ij}) \right) \right] \\
&\quad - \left[n \sum_{i=1}^a \sum_{j=1}^b \left(\frac{\sigma^2}{n} + \mu^2 + \alpha_i^2 + \beta_j^2 + (\alpha\beta)_{ij}^2 + 2(\mu\alpha_i + \mu\beta_j + \mu(\alpha\beta)_{ij} + \alpha_i\beta_j + \alpha_i(\alpha\beta)_{ij} + \beta_j(\alpha\beta)_{ij}) \right) \right] \\
&= \sigma^2(abn - ab) = \sigma^2 ab(n-1) \Rightarrow E\{MS_{Err}\} = \sigma^2
\end{aligned}$$

Testing for Main Effects for Factors A and B and Interaction AB:

$$H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad \text{Test Statistic: } F_A = \frac{MS_A}{MS_{Err}} \stackrel{H_0^A}{\sim} F_{a-1, ab(n-1)}$$

$$H_0^B : \beta_1 = \dots = \beta_b = 0 \quad \text{Test Statistic: } F_B = \frac{MS_B}{MS_{Err}} \stackrel{H_0^B}{\sim} F_{b-1, ab(n-1)}$$

$$H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{ab} = 0 \quad \text{Test Statistic: } F_{AB} = \frac{MS_{AB}}{MS_{Err}} \stackrel{H_0^{AB}}{\sim} F_{(a-1)(b-1), ab(n-1)}$$

Note that in R, the default for the estimates based on the **cont.treatment** option are the following.

$$\begin{aligned}
\text{Intercept: } &\mu + \alpha_1 + \beta_1 + (\alpha\beta)_{11} \quad \text{Ai: } \alpha_i - \alpha_1 + (\alpha\beta)_{i1} - (\alpha\beta)_{11} \quad i = 2, \dots, a \\
\text{Bj: } &\beta_j - \beta_1 + (\alpha\beta)_{1j} - (\alpha\beta)_{11} \quad j = 2, \dots, b \quad \text{ABij: } (\alpha\beta)_{ij} - (\alpha\beta)_{i1} - (\alpha\beta)_{1j} + (\alpha\beta)_{11} \quad i = 2, \dots, a; j = 2, \dots, b
\end{aligned}$$

When using the **contr.sum** option, the estimates are:

$$\begin{aligned}
\text{Intercept: } &\mu \quad \text{Ai: } \alpha_i \quad i = 1, \dots, a-1 \quad \text{Bj: } \beta_j \quad j = 1, \dots, b-1 \quad \text{ABij: } (\alpha\beta)_{ij} \quad i = 1, \dots, a-1; j = 1, \dots, b-1 \\
\text{This implies: } &\alpha_a = -\sum_{i=1}^{a-1} \alpha_i \quad \beta_b = -\sum_{j=1}^{b-1} \beta_j \quad (\alpha\beta)_{aj} = -\sum_{i=1}^{a-1} (\alpha\beta)_{ij} \quad j = 1, \dots, b \quad (\alpha\beta)_{ib} = -\sum_{j=1}^{b-1} (\alpha\beta)_{ij} \quad i = 1, \dots, a
\end{aligned}$$

Example: Reading Times for 3 E-Reader Devices at 4 Illumination Levels

The following EXCEL spreadsheet gives the cell and marginal means (top portion) and estimated main effect and interaction effects for the E-Reader experiment.

Dev\Illum Means	1	2	3	4	Mean	Dev/Illum SD	1	2	3	4	Sum((n-1)SD^2)
1	14.62	13.86	10.94	10.69	12.53	1	2.620	2.522	2.817	2.854	117.232
2	12.50	10.97	9.14	8.68	10.32	2	2.975	2.587	2.981	2.981	133.288
3	12.08	11.02	9.04	8.41	10.14	3	2.534	2.628	2.773	2.759	114.510
Mean	13.07	11.95	9.71	9.26	11.00						365.030

Dev\Illum Effects	1	2	3	4	Mean
1	0.02	0.38	-0.30	-0.10	1.53
2	0.11	-0.31	0.11	0.09	-0.67
3	-0.13	-0.07	0.19	0.01	-0.86
Mean	2.07	0.95	-1.29	-1.73	11.00

We obtain the sums of squares and the Analysis of Variance for the interaction model as follows. Note that SS_A and SS_B and their degrees of freedom are unchanged from the additive model. We are partitioning SS_{Err} and its degrees of freedom into SS_{AB} and a “new” SS_{Err} and their degrees of freedom.

$$SS_A = 4(5) \left[(1.53)^2 + (-0.67)^2 + (-0.86)^2 \right] = 70.59 \quad df_A = 3 - 1 = 2 \quad MS_A = 35.30$$

$$SS_B = (3)(5) \left[(2.07)^2 + (0.95)^2 + (-1.29)^2 + (-1.73)^2 \right] = 147.67 \quad df_B = 4 - 1 = 3 \quad MS_B = 49.22$$

$$SS_{AB} = 5 \left[(0.02)^2 + \dots + (0.01)^2 \right] = 2.15 \quad df_{AB} = (3-1)(4-1) = 6 \quad MS_{AB} = 0.36$$

$$SS_{Err} = (5-1) \left[2.620^2 + \dots + 2.759^2 \right] = 365.03 \quad df_{Err} = 3(4)(5-1) = 48 \quad MS_{Err} = 7.60$$

Test for Interaction Effects: $H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{ab} = 0 \quad H_A^{AB} : \text{Not all } (\alpha\beta)_{ij} = 0$

Test Stat: $F_{AB} = \frac{MS_{AB}}{MS_{Err}} = 0.05 \quad \text{Rejection Region: } F_{AB} \geq F_{.95;6,48} = 2.295 \quad \text{P-Value: } P(F_{6,48} \geq F_{AB}) = .9994$

Test for Factor A Main Effects: $H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad H_A^A : \text{Not all } \alpha_i = 0$

Test Stat: $F_A = \frac{MS_A}{MS_{Err}} = 4.62 \quad \text{Rejection Region: } F_A \geq F_{.95;2,48} = 3.191 \quad \text{P-Value: } P(F_{2,48} \geq F_A) = .0146$

Test for Factor B Main Effects: $H_0^B : \beta_1 = \dots = \beta_b = 0 \quad H_A^B : \text{Not all } \beta_j = 0$

Test Statistic: $F_B = \frac{MS_B}{MS_{Err}} = 6.48 \quad \text{Rejection Region: } F_B \geq F_{.95;3,48} = 2.798 \quad \text{P-Value: } P(F_{3,48} \geq F_B) = .0009$

Thus, there is no evidence of any interaction between factors A and B, while both have significant main effects (recall the analysis and interaction plot in the case of an additive model). Below is R code for running this analysis. The first uses the default parameter estimates (**contr.treatment**). The second uses the parameter estimates when effects sum to zero (**contr.sum**). Note that R is using many more decimal places than the EXCEL spreadsheet (which began with means rounded to 2 decimal places).

R Program

```
eread <-
read.table("http://www.stat.ufl.edu/~winner/data/ereader1.dat",header=F,
           col.names=c("device","illum","readtime"))
attach(eread)

readtime <- readtime/100

device <- factor(device)
illum <- factor(illum)

eread.mod1 <- aov(readtime ~ device + illum + device:illum)
anova(eread.mod1)
summary.lm(eread.mod1)

options(contrasts=c("contr.sum","contr.poly"))

eread.mod2 <- aov(readtime ~ device + illum + device:illum)
# anova(eread.mod2)
summary.lm(eread.mod2)
```

R Output

```
> eread.mod1 <- aov(readtime ~ device + illum + device:illum)
> anova(eread.mod1)
Analysis of Variance Table

Response: readtime
      Df Sum Sq Mean Sq F value    Pr(>F)
device    2  70.70   35.348   4.6483 0.0142790 *
illum     3 148.11   49.369   6.4920 0.0008906 ***
device:illum 6   2.15    0.359   0.0472 0.9995253
Residuals 48 365.02    7.605
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary.lm(eread.mod1)

Call: aov(formula = readtime ~ device + illum + device:illum)

Coefficients:
(Intercept)      14.6216  Std. Error 1.2333  t value 11.856  Pr(>|t|) 7.22e-16 ***
device2         -2.1197    1.7441  -1.215   0.2302
device3         -2.5381    1.7441  -1.455   0.1521
illum2          -0.7620    1.7441  -0.437   0.6641
illum3          -3.6846    1.7441  -2.113   0.0399 *
illum4          -3.9267    1.7441  -2.251   0.0290 *
device2:illum2  -0.7740    2.4665  -0.314   0.7550
device3:illum2  -0.3001    2.4665  -0.122   0.9037
device2:illum3   0.3228    2.4665   0.131   0.8964
device3:illum3   0.6451    2.4665   0.262   0.7948
device2:illum4   0.1049    2.4665   0.043   0.9663
device3:illum4   0.2542    2.4665   0.103   0.9184

Residual standard error: 2.758 on 48 degrees of freedom
Multiple R-squared:  0.3771,    Adjusted R-squared:  0.2343
F-statistic: 2.641 on 11 and 48 DF,  p-value: 0.01001
```

Continued below


```

> ereal.mod2 <- aov(readtime ~ device + illum + device:illum)
> # anova(ereal.mod2)
> summary.lm(ereal.mod2)

Call:
aov(formula = readtime ~ device + illum + device:illum)

Residuals:
    Min       1Q   Median       3Q      Max
-4.9741 -1.8720 -0.2066  2.0688  4.6353

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  10.99675    0.35601   30.889 < 2e-16 ***
device1       1.53151    0.50347    3.042  0.00380 **
device2      -0.67475    0.50347   -1.340  0.18649
illum1        2.07224    0.61663    3.361  0.00153 **
illum2        0.95225    0.61663    1.544  0.12909
illum3       -1.28975    0.61663   -2.092  0.04179 *
device1:illum1  0.02108    0.87204    0.024  0.98081
device2:illum1  0.10765    0.87204    0.123  0.90227
device1:illum2  0.37909    0.87204    0.435  0.66572
device2:illum2 -0.30831    0.87204   -0.354  0.72523
device1:illum3 -0.30157    0.87204   -0.346  0.73099
device2:illum3  0.10781    0.87204    0.124  0.90212
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.758 on 48 degrees of freedom
Multiple R-squared:  0.3771,    Adjusted R-squared:  0.2343
F-statistic: 2.641 on 11 and 48 DF,  p-value: 0.01001

```

In the additive model, we partitioned sums of squares for factors A and B into orthogonal contrasts that were of interest among the treatment levels. For the devices (factor A), we compared the small device (Device 1) with the larger (Devices 2 and 3), as well as a comparison between the two larger devices. For the illumination levels (factor B), we partitioned the sum of squares into orthogonal polynomial contrasts: linear, quadratic, and cubic.

For the interaction model, we can test whether (for instance) the polynomial contrasts are the same for small and large devices (contrast 1) and whether they are the same for the large devices (contrast 2). We can also consider it as whether the small versus large device contrast and large versus large device contrasts are the same for each illumination level. These interaction contrasts are obtained by multiplying each of the $a-1$ orthogonal contrasts for Factor A by each of the $b-1$ orthogonal contrasts for Factor B. Note that we have created $(a-1)(b-1)$ orthogonal contrasts, corresponding to the interaction degrees of freedom. Below is an EXCEL spreadsheet to visualize the process for the E-Reader experiment.

The spreadsheet includes all contrast estimates, sums of squares, and F-statistics, as well as the partitioning of SS_A , SS_B , and SS_{AB} . Note, that for each F-test the critical value is $F_{.95;1,48} = 4.043$.

Dev (i)	illum (j)	Ybar	SD	n	Dev1vs2&C1	Dev2vs3C2	IlllumLinC3	IlllumQuadC4	IlllumCubC5	C1*C3C6	C2*C3C7	C1*C4C8	C2*C4C9	C1*C5C10	C2*C5C11		
1	200	14.6216	2.62	5	2	0	-0.60609	0.50745	-0.35377	-1.21218	0.00000	1.01489	0.00000	-0.70753	0.00000		
1	500	13.8596	2.522	5	2	0	-0.30305	-0.34163	0.73583	-0.60609	0.00000	-0.68327	0.00000	1.47167	0.00000		
1	1000	10.9369	2.817	5	2	0	0.20203	-0.63610	-0.55188	0.40406	0.00000	-1.27219	0.00000	-1.10375	0.00000		
1	1500	10.6949	2.854	5	2	0	0.70711	0.47028	0.16981	1.41421	0.00000	0.94056	0.00000	0.33962	0.00000		
2	200	12.5019	2.975	5	-1	1	-0.60609	0.50745	-0.35377	0.60609	-0.60609	-0.50745	0.50745	0.35377	-0.35377		
2	500	10.966	2.587	5	-1	1	-0.30305	-0.34163	0.73583	0.30305	-0.30305	0.34163	-0.34163	-0.73583	0.73583		
2	1000	9.1401	2.981	5	-1	1	0.20203	-0.63610	-0.55188	-0.20203	0.20203	0.63610	-0.63610	0.55188	-0.55188		
2	1500	8.6801	2.981	5	-1	1	0.70711	0.47028	0.16981	-0.70711	0.70711	-0.47028	0.47028	-0.16981	0.16981		
3	200	12.0835	2.534	5	-1	-1	-0.60609	0.50745	-0.35377	0.60609	0.60609	-0.50745	-0.50745	0.35377	0.35377		
3	500	11.0215	2.628	5	-1	-1	-0.30305	-0.34163	0.73583	0.30305	0.30305	0.34163	0.34163	-0.73583	-0.73583		
3	1000	9.044	2.773	5	-1	-1	0.20203	-0.63610	-0.55188	-0.20203	-0.20203	0.63610	0.63610	0.55188	0.55188		
3	1500	8.411	2.759	5	-1	-1	0.70711	0.47028	0.16981	-0.70711	-0.70711	-0.47028	-0.47028	-0.16981	-0.16981		
					Contrast		18.3779	0.7281	-9.0954	2.1924	1.1545	-0.7750	-0.0271	0.0800	0.2967	1.2635	-0.1962
					Sum(W^2)		24	8	3.00000	3.00000	3.00000	6.00000	2.00000	6.00000	2.00000	6.00000	2.00000
					SSC		70.3640	0.3313	137.8761	8.0111	2.2214	0.5005	0.0018	0.0053	0.2201	1.3304	0.0962
					F_C		9.2526	0.0436	18.1302	1.0534	0.2921	0.0658	0.0002	0.0007	0.0289	0.1749	0.0127
					P-value		0.0038	0.8355	0.0001	0.3099	0.5914	0.7986	0.9877	0.9790	0.8656	0.6776	0.9109
					SSA		70.6953			SSB		148.1087				SSAB	2.1543

R Program

```

eread <- read.table("http://www.stat.ufl.edu/~winner/data/ereader1.dat",header=F,
  col.names=c("device","illum","readtime"))
attach(eread)

readtime <- readtime/100

device <- factor(device)
illum <- factor(illum)

contrasts(device) <- cbind(c(2,-1,-1),c(0,1,-1))
contrasts(illum) <- cbind(c(-.60609,-.30305,.20203,.70711),
  c(.50745,-.34163,-.63610,.47028),c(-.35377,.73583,-.55188,.16981))

eread.mod3 <- aov(readtime ~ device + illum + device:illum)
anova(eread.mod3)
summary.lm(eread.mod3)

```

R Output (summary.lm portion)

```

> summary.lm(eread.mod3)

Call:
aov(formula = readtime ~ device + illum + device:illum)

Residuals:
    Min       1Q   Median       3Q      Max
-4.9741 -1.8720 -0.2066  2.0688  4.6353

Coefficients:
(Intercept)      10.99675      0.35601      30.889      < 2e-16 ***
device1          0.76575       0.25174       3.042       0.0038 **
device2          0.09100       0.43602       0.209       0.8356
illum1          -3.03175       0.71202      -4.258      9.54e-05 ***
illum2           0.73082       0.71202       1.026       0.3098
illum3           0.38480       0.71202       0.540       0.5914
device1:illum1  -0.12916       0.50347      -0.257       0.7986
device2:illum1  -0.01353       0.87204      -0.016       0.9877
device1:illum2  0.01332       0.50347       0.026       0.9790
device2:illum2  0.14836       0.87204       0.170       0.8656
device1:illum3  0.21059       0.50347       0.418       0.6776
device2:illum3 -0.09809       0.87204      -0.112       0.9109

```

5.3. Tukey's 1-Degree of Freedom Test for Non-Additivity (ODOFNA) with 1 Replicate per Cell

With $n = 1$ replicate per cell, there is no means to distinguish between error and interaction ($df_{\text{Err}} = ab(n-1)=0$). In this case, Tukey devised a test, placing a particular type of structure on the form of the interaction.

$$Y_{ij} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ij} \quad i = 1, \dots, a; j = 1, \dots, b \quad \varepsilon_{ij} \sim NID(0, \sigma^2) \quad (\alpha\beta)_{ij} = \gamma\alpha_i\beta_j$$

This sets the form of the interaction effect as a multiple of the corresponding main effects. The procedure involves first estimating the main effects $\{\alpha_i\}$ and $\{\beta_j\}$, then fitting a regression model to estimate γ . The residuals are then obtained from that fitted model, and an F-statistic is computed from the residual sum of squares and the remainder of the interaction sum of squares.

- Fit the additive Model and estimate μ , α_i and β_j

$$\hat{\mu} = \bar{Y}_{..} \quad \hat{\alpha}_i = \bar{Y}_{i.} - \bar{Y}_{..} \quad \hat{\beta}_j = \bar{Y}_{.j} - \bar{Y}_{..}$$

- Fit the interaction model with $(\alpha\beta)_{ij} = \gamma\alpha_i\beta_j$

$$Y_{ij} = \mu + \alpha_i + \beta_j + \gamma\alpha_i\beta_j + \varepsilon_{ij}$$

$$\hat{Y}_{ij} = \hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}\hat{\alpha}_i\hat{\beta}_j + e_{ij}$$

- Use Least Squares to estimate γ

$$Q = \sum_{i=1}^a \sum_{j=1}^b e_{ij}^2 = \sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} - \hat{\mu} - \hat{\alpha}_i - \hat{\beta}_j - \hat{\gamma}\hat{\alpha}_i\hat{\beta}_j \right)^2$$

$$\frac{\partial Q}{\partial \gamma} = 2 \sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} - \hat{\mu} - \hat{\alpha}_i - \hat{\beta}_j - \hat{\gamma}\hat{\alpha}_i\hat{\beta}_j \right) \left(-\hat{\alpha}_i\hat{\beta}_j \right)$$

$$= -2 \left[\sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} \hat{\alpha}_i \hat{\beta}_j \right) - \hat{\mu} \sum_{i=1}^a \hat{\alpha}_i \sum_{j=1}^b \hat{\beta}_j - \sum_{i=1}^a \hat{\alpha}_i^2 \sum_{j=1}^b \hat{\beta}_j - \sum_{i=1}^a \hat{\alpha}_i \sum_{j=1}^b \hat{\beta}_j^2 - \gamma \sum_{i=1}^a \hat{\alpha}_i^2 \sum_{j=1}^b \hat{\beta}_j^2 \right]$$

$$= -2 \left[\sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} \hat{\alpha}_i \hat{\beta}_j \right) - 0 - 0 - 0 - \gamma \sum_{i=1}^a \hat{\alpha}_i^2 \sum_{j=1}^b \hat{\beta}_j^2 \right]$$

$$\text{Setting } \frac{\partial Q}{\partial \gamma} = 0 \Rightarrow 0 = \left[\sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} \hat{\alpha}_i \hat{\beta}_j \right) - \gamma \sum_{i=1}^a \hat{\alpha}_i^2 \sum_{j=1}^b \hat{\beta}_j^2 \right] \Rightarrow \hat{\gamma} = \frac{\sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} \hat{\alpha}_i \hat{\beta}_j \right)}{\sum_{i=1}^a \hat{\alpha}_i^2 \sum_{j=1}^b \hat{\beta}_j^2}$$

$$\Rightarrow \hat{\gamma} = \frac{\sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} (\bar{Y}_{i.} - \bar{Y}_{..}) (\bar{Y}_{.j} - \bar{Y}_{..}) \right)}{\sum_{i=1}^a (\bar{Y}_{i.} - \bar{Y}_{..})^2 \sum_{j=1}^b (\bar{Y}_{.j} - \bar{Y}_{..})^2}$$

- Obtain the Sum of Squares for Interaction and Remainder.

$$\begin{aligned}
 SS_{AB^*} &= \sum_{i=1}^a \sum_{j=1}^b \hat{\alpha} \hat{\beta}_{ij}^2 = \sum_{i=1}^a \sum_{j=1}^b \gamma \left(\hat{\alpha}_i \right)^2 \left(\hat{\beta}_j \right)^2 = \gamma \sum_{i=1}^a \left(\hat{\alpha}_i \right)^2 \sum_{j=1}^b \left(\hat{\beta}_j \right)^2 \\
 &= \frac{\left[\sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot}) (\bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot}) \right) \right]^2}{\sum_{i=1}^a (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 \sum_{j=1}^b (\bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot})^2} \sum_{i=1}^a (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 \sum_{j=1}^b (\bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot})^2 \\
 &= \frac{\left[\sum_{i=1}^a \sum_{j=1}^b \left(Y_{ij} (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot}) (\bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot}) \right) \right]^2}{\sum_{i=1}^a (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 \sum_{j=1}^b (\bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot})^2}
 \end{aligned}$$

"Remainder" SS: $SS_{REM^*} = SS_{Total} - SS_A - SS_B - SS_{AB^*}$

- Conduct the F-test of $H_0: \gamma = 0$ (No interactions of the form $(\alpha\beta)_{ij} = \gamma\alpha_i\beta_j$).

Under $H_0: \gamma = 0$ (No interactions exist of the form $\gamma\alpha_i\beta_j$)

$$SS_{AB^*} \sim \chi_1^2 \quad SS_{REM^*} \sim \chi_{(a-1)(b-1)-1}^2 \quad SS_{AB^*} \perp SS_{REM^*}$$

$$\Rightarrow F^* = \frac{(SS_{AB^*}/1)}{(SS_{REM^*}/[(a-1)(b-1)-1])} \sim F_{1,(a-1)(b-1)-1}$$

Example: 8 U.S. Business Indices over 18 Years

A study was conducted of 18 years (Factor A: 1948-1965) and 8 U.S. business indices (Factor B: Dow Jones Industrial Average (DJIA), Standard & Poor (POOR), New York Stock Exchange (NYSE), Gross National Product (GNP), Consumer Price Index (CPI), Forbes, Business Week (BWEEK), and Money Magazine (MONEY) (Smith (1969))). There is one "replicate" per combination of year and index.

$$\begin{aligned}
 SS_{TOTAL} &= \sum_{i=1}^{18} \sum_{j=1}^8 (y_{ij} - \bar{y}_{\cdot\cdot})^2 = 1.7899 & SS_A &= 8 \sum_{i=1}^{18} (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot})^2 = 0.6534 & SS_B &= 18 \sum_{j=1}^8 (\bar{y}_{\cdot j} - \bar{y}_{\cdot\cdot})^2 = 0.2060 \\
 SS_{AB} &= \sum_{i=1}^{18} \sum_{j=1}^8 (y_{ij} - \bar{y}_{i\cdot} - \bar{y}_{\cdot j} + \bar{y}_{\cdot\cdot})^2 = 0.9305 & df_{Total} &= 18(8) - 1 = 143 & df_A &= 18 - 1 = 17 & df_B &= 8 - 1 = 7 & df_{AB} &= 17(7) = 119
 \end{aligned}$$

Year\Index	DJIA	POOR	NYSE	GNP	CPI	FRB	BWEEK	MONEY	Ybar_i•	alpha_i
1965	1.103	1.099	1.095	1.086	1.017	1.083	1.093	1.048	1.078	0.010
1964	1.145	1.131	1.143	1.066	1.013	1.064	1.073	1.043	1.085	0.017
1963	1.169	1.201	1.180	1.050	1.012	1.051	1.060	1.038	1.095	0.027
1962	0.890	0.872	0.880	1.072	1.012	1.078	1.018	1.013	0.979	-0.088
1961	1.207	1.231	1.240	1.032	1.011	1.099	1.154	1.031	1.126	0.058
1960	0.896	0.953	0.976	1.041	1.016	1.029	0.917	0.924	0.969	-0.099
1959	1.184	1.094	1.097	1.086	1.008	1.127	1.073	1.006	1.084	0.017
1958	1.425	1.376	1.366	1.044	1.028	0.930	1.099	1.038	1.163	0.095
1957	0.833	0.856	0.866	1.056	1.035	1.008	0.906	0.993	0.944	-0.124
1956	1.000	1.034	1.026	1.055	1.015	1.034	1.011	1.012	1.023	-0.044
1955	1.231	1.301	1.222	1.095	0.997	1.126	1.125	1.020	1.140	0.072
1954	1.393	1.497	1.426	0.994	1.004	0.940	1.074	1.029	1.170	0.102
1953	0.965	0.925	0.938	1.053	1.008	1.083	0.952	1.010	0.992	-0.076
1952	1.074	1.109	1.065	1.055	1.022	1.037	1.141	1.038	1.068	0.000
1951	1.174	1.178	1.132	1.156	1.080	1.085	1.012	1.055	1.109	0.041
1950	1.179	1.247	1.211	1.102	1.009	1.157	1.213	1.057	1.147	0.079
1949	1.114	1.091	1.102	0.996	0.990	0.945	0.995	0.994	1.028	-0.039
1948	0.972	0.996	0.972	1.110	1.077	1.041	1.019	0.985	1.022	-0.046
Ybar_•j	1.109	1.122	1.108	1.064	1.020	1.051	1.052	1.019	1.068	
beta_j	0.041	0.054	0.040	-0.004	-0.048	-0.017	-0.016	-0.049	0.000	

The following “matrix” gives $y_{ij} (\bar{y}_{i\bullet} - \bar{y}_{\bullet\bullet})(\bar{y}_{\bullet j} - \bar{y}_{\bullet\bullet}) \quad i=1,\dots,18; j=1,\dots,8$

Year\Index	DJIA	POOR	NYSE	GNP	CPI	FRB	BWEEK	MONEY
1965	0.0004555	0.0006006	0.0004417	-0.0000443	-0.0004972	-0.0001858	-0.0001764	-0.0005242
1964	0.0007874	0.0010294	0.0007678	-0.0000724	-0.0008248	-0.0003040	-0.0002884	-0.0008688
1963	0.0012975	0.0017643	0.0012794	-0.0001151	-0.0013299	-0.0004847	-0.0004599	-0.0013955
1962	-0.0032051	-0.0041561	-0.0030955	0.0003814	0.0043148	0.0016129	0.0014330	0.0044186
1961	0.0028381	0.0038309	0.0028480	-0.0002397	-0.0028145	-0.0010736	-0.0010607	-0.0029363
1960	-0.0036051	-0.0050748	-0.0038358	0.0004138	0.0048398	0.0017201	0.0014422	0.0045030
1959	0.0007961	0.0009736	0.0007205	-0.0000721	-0.0008025	-0.0003148	-0.0002820	-0.0008193
1958	0.0055329	0.0070710	0.0051808	-0.0004004	-0.0047256	-0.0015002	-0.0016680	-0.0048816
1957	-0.0041949	-0.0057053	-0.0042599	0.0005254	0.0061709	0.0021090	0.0017835	0.0060570
1956	-0.0018104	-0.0024775	-0.0018143	0.0001887	0.0021755	0.0007777	0.0007154	0.0022191
1955	0.0035960	0.0050299	0.0034868	-0.0003160	-0.0034481	-0.0013665	-0.0012846	-0.0036090
1954	0.0057701	0.0082068	0.0057697	-0.0004067	-0.0049237	-0.0016177	-0.0017390	-0.0051627
1953	-0.0029891	-0.0037921	-0.0028381	0.0003222	0.0036966	0.0013937	0.0011527	0.0037893
1952	-0.0000100	-0.0000137	-0.0000097	0.0000010	0.0000113	0.0000040	0.0000042	0.0000117
1951	0.0019661	0.0026110	0.0018518	-0.0001912	-0.0021413	-0.0007549	-0.0006625	-0.0021400
1950	0.0037920	0.0053081	0.0038045	-0.0003501	-0.0038421	-0.0015460	-0.0015250	-0.0041177
1949	-0.0017900	-0.0023202	-0.0017297	0.0001581	0.0018834	0.0006309	0.0006250	0.0019346
1948	-0.0018339	-0.0024870	-0.0017913	0.0002069	0.0024057	0.0008160	0.0007515	0.0022509
						SUM		0.0221122

$$\sum_{i=1}^{18} \sum_{j=1}^8 y_{ij} (\bar{y}_{i\bullet} - \bar{y}_{\bullet\bullet})(\bar{y}_{\bullet j} - \bar{y}_{\bullet\bullet}) = .0221122 \quad \sum_{i=1}^{18} (\bar{y}_{i\bullet} - \bar{y}_{\bullet\bullet})^2 = 0.081676 \quad \sum_{j=1}^8 (\bar{y}_{\bullet j} - \bar{y}_{\bullet\bullet})^2 = 0.0114466$$

$$\Rightarrow \hat{\gamma} = \frac{0.0221122}{(0.081676)(0.0114466)} = 23.6517$$

$$SS_{AB}^* = \frac{(0.0221122)^2}{(0.0816757)(0.0114466)} = 0.5230 \Rightarrow SS_{Rem}^* = SS_{AB} - SS_{AB}^* = 0.9305 - 0.5230 = 0.4075 \quad df_{Rem}^* = 119 - 1 = 118$$

$$H_0: \gamma = 0 \quad H_A: \gamma \neq 0 \quad TS: F_{obs} = \frac{[0.5230/1]}{[0.4075/118]} = 151.445 \quad RR: F_{obs} \geq F_{.95;1,118} = 3.921$$

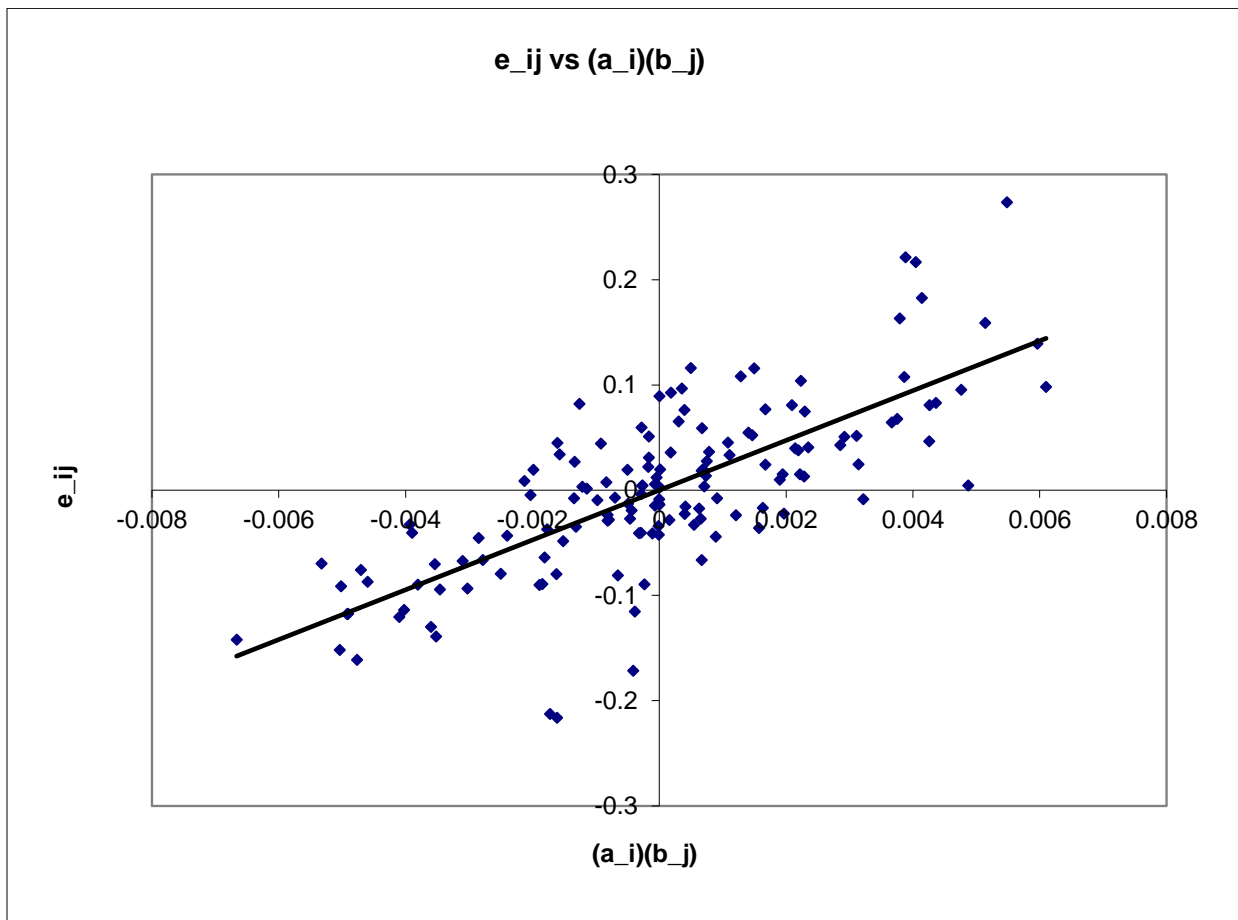
There is strong evidence that there is an interaction of this form between Year and Index. Note the residual from the additive model, in terms of the interaction model terms are as follow:

$$Y_{ij} = \hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma} \hat{\alpha}_i \hat{\beta}_j + e_{ij}$$

Additive Model : $\hat{Y} = \hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j \Rightarrow$ Additive Residual = $\hat{\gamma} \hat{\alpha}_i \hat{\beta}_j + e_{ij}$

If the Interaction model is appropriate, Additive residuals should be linearly related to $\hat{\alpha}_i \hat{\beta}_j$
 (Regression through origin)

Note that the slope of this regression through the origin is $\hat{\gamma}$



Tukey's ODOFNA can be computed from the R package **additivityTests**. The data must first be constructed into a matrix with a rows and b columns. This can be done with the **matrix** command in the following R program. Note that in the original data set, the 18 years for index 1 are entered first, followed by the 18 years for index 2, and so on. The **byrow=F** option informs R of this, and the **ncol=8** option informs R that the matrix will have 8 columns.

R Program:

```
biz <- read.table("http://www.stat.ufl.edu/~winner/data/jb42.dat", header=F,
  col.names=c("index", "year", "Y"))
attach(biz)
# install.packages("additivityTests")
library(additivityTests)
(Y.mat <- matrix(Y, byrow=F, ncol=8))
tukey.test(Y.mat)
```

R Output:

```
> (Y.mat <- matrix(Y, byrow=F, ncol=8))
  [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,] 1.103 1.099 1.095 1.086 1.017 1.083 1.093 1.048
[2,] 1.145 1.131 1.143 1.066 1.013 1.064 1.073 1.043
[3,] 1.169 1.201 1.180 1.050 1.012 1.051 1.060 1.038
[4,] 0.890 0.872 0.880 1.072 1.012 1.078 1.018 1.013
[5,] 1.207 1.231 1.240 1.032 1.011 1.099 1.154 1.031
[6,] 0.896 0.953 0.976 1.041 1.016 1.029 0.917 0.924
[7,] 1.184 1.094 1.097 1.086 1.008 1.127 1.073 1.006
[8,] 1.425 1.376 1.366 1.044 1.028 0.930 1.099 1.038
[9,] 0.833 0.856 0.866 1.056 1.035 1.008 0.906 0.993
[10,] 1.000 1.034 1.026 1.055 1.015 1.034 1.011 1.012
[11,] 1.231 1.301 1.222 1.095 0.997 1.126 1.125 1.020
[12,] 1.393 1.497 1.426 0.994 1.004 0.940 1.074 1.029
[13,] 0.965 0.925 0.938 1.053 1.008 1.083 0.952 1.010
[14,] 1.074 1.109 1.065 1.055 1.022 1.037 1.141 1.038
[15,] 1.174 1.178 1.132 1.156 1.080 1.085 1.012 1.055
[16,] 1.179 1.247 1.211 1.102 1.009 1.157 1.213 1.057
[17,] 1.114 1.091 1.102 0.996 0.990 0.945 0.995 0.994
[18,] 0.972 0.996 0.972 1.110 1.077 1.041 1.019 0.985
> tukey.test(Y.mat)

Tukey test on 5% alpha-level:

Test statistic: 151.5
Critical value: 3.921
The additivity hypothesis was rejected.
```

5.4. 2-Factor ANOVA with Unequal Cell Sample Sizes

As was shown previously, with respect to the matrix form of the ANOVA model, we can have distinct sample sizes among the ab cells. This makes sums of squares computations invalid, but we can fit the model in matrix form, and use general linear tests to test for interactions and main effects. Note that the sequential (aka Type I) and the partial (aka Type III) sums of squares will not be the same for unbalanced data (they are the same for balanced data). The \mathbf{X} matrix and $\boldsymbol{\beta}$ vector are constructed under the restrictions.

$$\sum_{i=1}^a \alpha_i = \sum_{j=1}^b \beta_j = \sum_{i=1}^a (\alpha\beta)_{ij} = \sum_{j=1}^b (\alpha\beta)_{ij} = 0$$

We construct the columns of \mathbf{X} and the rows of $\boldsymbol{\beta}$ for the mean, factor A, and factor B as we did for the additive model previously. The columns of \mathbf{X} for the interaction effects are obtained by pairwise multiplication of the columns of \mathbf{X} representing factors A and B. There are $(a-1)(b-1)$ of these. Going back to the case with $a=3, b=4$, and general n_{ij} , we have:

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_{11} \\ \mathbf{Y}_{12} \\ \mathbf{Y}_{13} \\ \mathbf{Y}_{14} \\ \mathbf{Y}_{21} \\ \mathbf{Y}_{22} \\ \mathbf{Y}_{23} \\ \mathbf{Y}_{24} \\ \mathbf{Y}_{31} \\ \mathbf{Y}_{32} \\ \mathbf{Y}_{33} \\ \mathbf{Y}_{34} \end{bmatrix} \quad \mathbf{Y}_{ij} = \begin{bmatrix} Y_{ij1} \\ \vdots \\ Y_{ijn_j} \end{bmatrix}$$

$$\mathbf{X}_1 = \begin{bmatrix} \mathbf{1}_{n11} & \mathbf{1}_{n11} & \mathbf{0}_{n11} & \mathbf{1}_{n11} & \mathbf{0}_{n11} & \mathbf{0}_{n11} & \mathbf{1}_{n11} & \mathbf{0}_{n11} & \mathbf{0}_{n11} & \mathbf{0}_{n11} & \mathbf{0}_{n11} & \mathbf{0}_{n11} \\ \mathbf{1}_{n12} & \mathbf{1}_{n12} & \mathbf{0}_{n12} & \mathbf{0}_{n12} & \mathbf{1}_{n12} & \mathbf{0}_{n12} & \mathbf{0}_{n12} & \mathbf{1}_{n12} & \mathbf{0}_{n12} & \mathbf{0}_{n12} & \mathbf{0}_{n12} & \mathbf{0}_{n12} \\ \mathbf{1}_{n13} & \mathbf{1}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{1}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{1}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} \\ \mathbf{1}_{n14} & \mathbf{1}_{n14} & \mathbf{0}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} & \mathbf{0}_{n14} & \mathbf{0}_{n14} & \mathbf{0}_{n14} \\ \mathbf{1}_{n21} & \mathbf{0}_{n21} & \mathbf{1}_{n21} & \mathbf{1}_{n21} & \mathbf{0}_{n21} & \mathbf{0}_{n21} & \mathbf{0}_{n21} & \mathbf{0}_{n21} & \mathbf{0}_{n21} & \mathbf{1}_{n21} & \mathbf{0}_{n21} & \mathbf{0}_{n21} \\ \mathbf{1}_{n22} & \mathbf{0}_{n22} & \mathbf{1}_{n22} & \mathbf{0}_{n22} & \mathbf{1}_{n22} & \mathbf{0}_{n22} & \mathbf{0}_{n22} & \mathbf{0}_{n22} & \mathbf{0}_{n22} & \mathbf{0}_{n22} & \mathbf{1}_{n22} & \mathbf{0}_{n22} \\ \mathbf{1}_{n23} & \mathbf{0}_{n23} & \mathbf{1}_{n23} & \mathbf{0}_{n23} & \mathbf{0}_{n23} & \mathbf{1}_{n23} & \mathbf{0}_{n23} & \mathbf{0}_{n23} & \mathbf{0}_{n23} & \mathbf{0}_{n23} & \mathbf{0}_{n23} & \mathbf{1}_{n23} \\ \mathbf{1}_{n24} & \mathbf{0}_{n24} & \mathbf{1}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} & \mathbf{0}_{n24} & \mathbf{0}_{n24} & \mathbf{0}_{n24} & \mathbf{0}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} \\ \mathbf{1}_{n31} & -\mathbf{1}_{n31} & -\mathbf{1}_{n31} & \mathbf{1}_{n31} & \mathbf{0}_{n31} & \mathbf{0}_{n31} & -\mathbf{1}_{n31} & \mathbf{0}_{n31} & \mathbf{0}_{n31} & -\mathbf{1}_{n31} & \mathbf{0}_{n31} & \mathbf{0}_{n31} \\ \mathbf{1}_{n32} & -\mathbf{1}_{n32} & -\mathbf{1}_{n32} & \mathbf{0}_{n32} & \mathbf{1}_{n32} & \mathbf{0}_{n32} & \mathbf{0}_{n32} & -\mathbf{1}_{n32} & \mathbf{0}_{n32} & \mathbf{0}_{n32} & -\mathbf{1}_{n32} & \mathbf{0}_{n32} \\ \mathbf{1}_{n33} & -\mathbf{1}_{n33} & -\mathbf{1}_{n33} & \mathbf{0}_{n33} & \mathbf{0}_{n33} & \mathbf{1}_{n33} & \mathbf{0}_{n33} & \mathbf{0}_{n33} & -\mathbf{1}_{n33} & \mathbf{0}_{n33} & \mathbf{0}_{n33} & -\mathbf{1}_{n33} \\ \mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & \mathbf{1}_{n34} & \mathbf{1}_{n34} & \mathbf{1}_{n34} & \mathbf{1}_{n34} & \mathbf{1}_{n34} & \mathbf{1}_{n34} \end{bmatrix} \quad \boldsymbol{\beta}_1 = \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ (\alpha\beta)_{11} \\ (\alpha\beta)_{12} \\ (\alpha\beta)_{13} \\ (\alpha\beta)_{21} \\ (\alpha\beta)_{22} \\ (\alpha\beta)_{23} \end{bmatrix}$$

The error sum of squares is obtained for this (complete) model as follows.

$$SS_{\text{Err1}} = \mathbf{Y}'(\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1' \mathbf{X}_1)^{-1} \mathbf{X}_1') \mathbf{Y} \quad df_{\text{Err1}} = N - 1 - (a-1) - (b-1) - (a-1)(b-1) = N - ab$$

Next, we create a reduced model, which removes the columns of \mathbf{X}_1 and the rows of $\boldsymbol{\beta}_1$ corresponding to the $(a-1)(b-1)$ $(\alpha\beta)_{ij}$ terms.

$$\mathbf{X}_2 = \begin{bmatrix} \mathbf{1}_{n11} & \mathbf{1}_{n11} & \mathbf{0}_{n11} & \mathbf{1}_{n11} & \mathbf{0}_{n11} & \mathbf{0}_{n11} \\ \mathbf{1}_{n12} & \mathbf{1}_{n12} & \mathbf{0}_{n12} & \mathbf{0}_{n12} & \mathbf{1}_{n12} & \mathbf{0}_{n12} \\ \mathbf{1}_{n13} & \mathbf{1}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{0}_{n13} & \mathbf{1}_{n13} \\ \mathbf{1}_{n14} & \mathbf{1}_{n14} & \mathbf{0}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} & -\mathbf{1}_{n14} \\ \mathbf{1}_{n21} & \mathbf{0}_{n21} & \mathbf{1}_{n21} & \mathbf{1}_{n21} & \mathbf{0}_{n21} & \mathbf{0}_{n21} \\ \mathbf{1}_{n22} & \mathbf{0}_{n22} & \mathbf{1}_{n22} & \mathbf{0}_{n22} & \mathbf{1}_{n22} & \mathbf{0}_{n22} \\ \mathbf{1}_{n23} & \mathbf{0}_{n23} & \mathbf{1}_{n23} & \mathbf{0}_{n23} & \mathbf{0}_{n23} & \mathbf{1}_{n23} \\ \mathbf{1}_{n24} & \mathbf{0}_{n24} & \mathbf{1}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} & -\mathbf{1}_{n24} \\ \mathbf{1}_{n31} & -\mathbf{1}_{n31} & -\mathbf{1}_{n31} & \mathbf{1}_{n31} & \mathbf{0}_{n31} & \mathbf{0}_{n31} \\ \mathbf{1}_{n32} & -\mathbf{1}_{n32} & -\mathbf{1}_{n32} & \mathbf{0}_{n32} & \mathbf{1}_{n32} & \mathbf{0}_{n32} \\ \mathbf{1}_{n33} & -\mathbf{1}_{n33} & -\mathbf{1}_{n33} & \mathbf{0}_{n33} & \mathbf{0}_{n33} & \mathbf{1}_{n33} \\ \mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} & -\mathbf{1}_{n34} \end{bmatrix} \quad \boldsymbol{\beta}_2 = \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$$

The error sum of squares is obtained for this (reduced) model as follows:

$$SS_{\text{Err2}} = \mathbf{Y}'(\mathbf{I} - \mathbf{X}_2(\mathbf{X}_2' \mathbf{X}_2)^{-1} \mathbf{X}_2') \mathbf{Y} \quad df_{\text{Err2}} = N - 1 - (a - 1) - (b - 1) = N - a - b + 1$$

Next, we create a reduced model, which removes the columns of \mathbf{X}_1 and the rows of $\boldsymbol{\beta}_1$ corresponding to the $(a-1) \alpha_i$ terms.

The error sum of squares is obtained for this (reduced) model as follows:

$$SS_{\text{Err3}} = \mathbf{Y}'(\mathbf{I} - \mathbf{X}_3(\mathbf{X}_3' \mathbf{X}_3)^{-1} \mathbf{X}_3') \mathbf{Y} \quad df_{\text{Err3}} = N - 1 - (b - 1) - (a - 1)(b - 1) = N + a - ab - 1$$

Next, we create a reduced model, which removes the columns of \mathbf{X}_1 and the rows of $\boldsymbol{\beta}_1$ corresponding to the $(b-1) \beta_j$ terms.

The error sum of squares is obtained for this (reduced) model as follows:

$$SS_{\text{Err4}} = \mathbf{Y}'(\mathbf{I} - \mathbf{X}_4(\mathbf{X}_4' \mathbf{X}_4)^{-1} \mathbf{X}_4') \mathbf{Y} \quad df_{\text{Err4}} = N - 1 - (a - 1) - (a - 1)(b - 1) = N + b - ab - 1$$

Now we can test for interaction and main effects, controlling for all other effects. Note that these error sums of squares can be obtained from any regression package, with the corresponding “X” variables included.

$$\begin{aligned}
H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{ab} = 0 \quad TS : F_{AB} &= \frac{\left[\frac{SS_{Err2} - SS_{Err1}}{df_{Err2} - df_{Err1}} \right]}{\left[\frac{SS_{Err1}}{df_{Err1}} \right]} = \frac{\left[\frac{SS_{Err2} - SS_{Err1}}{(a-1)(b-1)} \right]}{\left[\frac{SS_{Err1}}{N-ab} \right]} \quad RR : F_{AB} \geq F_{1-\alpha; (a-1)(b-1), N-ab} \\
H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad TS : F_A &= \frac{\left[\frac{SS_{Err3} - SS_{Err1}}{df_{Err3} - df_{Err1}} \right]}{\left[\frac{SS_{Err1}}{df_{Err1}} \right]} = \frac{\left[\frac{SS_{Err3} - SS_{Err1}}{a-1} \right]}{\left[\frac{SS_{Err1}}{N-ab} \right]} \quad RR : F_A \geq F_{1-\alpha; a-1, N-ab} \\
H_0^B : \beta_1 = \dots = \beta_b = 0 \quad TS : F_B &= \frac{\left[\frac{SS_{Err4} - SS_{Err1}}{df_{Err4} - df_{Err1}} \right]}{\left[\frac{SS_{Err1}}{df_{Err1}} \right]} = \frac{\left[\frac{SS_{Err4} - SS_{Err1}}{b-1} \right]}{\left[\frac{SS_{Err1}}{N-ab} \right]} \quad RR : F_B \geq F_{1-\alpha; b-1, N-ab}
\end{aligned}$$

Example: Deflection of Makiwara Punching Boards

An experiment was conducted to measure deflection of boards used in karate (Smith, *et al* (2010)). There were $a = 4$ wood types (cherry, ash, fir, and oak) and $b = 2$ board types (stacked and tapered). It appears that the original plan was $n = 45$ boards per treatment, but some loss must have occurred during the experiment. The following table gives the sample sizes among the $ab = 4(2) = 8$ treatments. There were a total of $N = 336$ measurements.

Wood\Board	Stacked(j=1)	Tapered(j=2)
Cherry(i=1)	41	45
Ash(i=2)	36	45
Fir(i=3)	34	45
Oak(i=4)	45	45

The first two and the last two rows of the \mathbf{X} matrix are given below (first 2 cases have $i=1, j=1$; last 2 cases have $i=4, j=2$). The first column (X0) corresponds to the mean μ . The next $4-1 = 3$ columns (X1, X2, X3) correspond to $\alpha_1, \alpha_2, \alpha_3$. The next $2-1 = 1$ column corresponds to β_1 . The final $(4-1)(2-1) = 3$ columns correspond to $(\alpha\beta)_{11}, (\alpha\beta)_{21}, (\alpha\beta)_{31}$.

X0 (Mean)	X1	X2	X3	X4	X1X4	X2X4	X3X4
1	1	0	0	1	1	0	0
1	1	0	0	1	1	0	0
...
1	-1	-1	-1	-1	1	1	1
1	-1	-1	-1	-1	1	1	1

The partial Analysis of Variance Tables for the 4 regression models are given below.

ANOVA	Model 1		ANOVA	Model 2	
	<i>df</i>	<i>SS</i>		<i>df</i>	<i>SS</i>
Regression	7	162873	Regression	4	161431
Residual	328	1036027	Residual	331	1037469
Total	335	1198900	Total	335	1198900

ANOVA	Model 3		ANOVA		
	<i>df</i>	<i>SS</i>		<i>df</i>	<i>SS</i>
Regression	4	117667	Regression	6	47657
Residual	331	1081233	Residual	329	1151243
Total	335	1198900	Total	335	1198900

$$H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{42} = 0 \quad TS : F_{AB} = \frac{\left[\frac{1037469 - 1036027}{331 - 328} \right]}{\left[\frac{1036027}{328} \right]} = 0.1522 \quad RR : F_{AB} \geq F_{.95;3,328} = 2.632$$

$$H_0^A : \alpha_1 = \dots = \alpha_4 = 0 \quad TS : F_A = \frac{\left[\frac{1081233 - 1036027}{331 - 328} \right]}{\left[\frac{1036027}{328} \right]} = 4.771 \quad RR : F_A \geq F_{.95;3,328} = 2.632$$

$$H_0^B : \beta_1 = \beta_2 = 0 \quad TS : F_B = \frac{\left[\frac{1151243 - 1036027}{329 - 328} \right]}{\left[\frac{1036027}{328} \right]} = 36.477 \quad RR : F_B \geq F_{.95;1,328} = 3.870$$

Thus, there is no evidence of an interaction, and there are main effects for both wood type and board type.

Tukey's HSD is computed for each pair of wood types. $H_{ij} = \frac{q_{.95;4,328}}{\sqrt{2}} \sqrt{MS_{\text{Err1}} \left(\frac{1}{n_{i\cdot}} + \frac{1}{n_{\cdot j}} \right)}$

Comparing	q(.95,4,df)	3.652	MSE	3158.619					
Woods	Ybar_i	Ybar_j	n_i	n_j	Diff	SE(Diff)	H_ij		SiG Diff?
1 vs 2	97.1	89.3	86	81	7.7	8.70	22.47		No
1 vs 3	97.1	71.8	86	79	25.3	8.76	22.62		Yes
1 vs 4	97.1	70.0	86	90	27.1	8.47	21.89		Yes
2 vs 3	89.3	71.8	81	79	17.5	8.89	22.95		No
2 vs 4	89.3	70.0	81	90	19.3	8.61	22.23		No
3 vs 4	71.8	70.0	79	90	1.8	8.66	22.38		No

The means for the two board types and a 95% CI for $\beta_1 - \beta_2$ are given below.

$$\begin{aligned} \bar{y}_{.1} = 101.92 \quad \bar{y}_{.2} = 64.75 &\Rightarrow (101.92 - 64.75) \pm 1.967 \sqrt{3158.619 \left(\frac{1}{156} + \frac{1}{180} \right)} \\ \equiv 37.17 \pm 12.09 &\equiv (25.08, 49.26) \end{aligned}$$

Based on the confidence interval (and the F-test), we conclude that the stacked boards have significantly higher deflection scores than the tapered boards.

R Program:

```
karate <- read.csv("http://www.stat.ufl.edu/~winner/data/karate_board.csv",
                  header=T)

attach(karate)
names(karate)

kb.mod1 <- lm(Deflect ~ X1 + X2 + X3 + X4 + X1X4 + X2X4 + X3X4)
anova(kb.mod1)

kb.mod2 <- lm(Deflect ~ X1 + X2 + X3 + X4)
anova(kb.mod2)

kb.mod3 <- lm(Deflect ~ X4 + X1X4 + X2X4 + X3X4)
anova(kb.mod3)

kb.mod4 <- lm(Deflect ~ X1 + X2 + X3 + X1X4 + X2X4 + X3X4)
anova(kb.mod4)

anova(kb.mod2, kb.mod1)
anova(kb.mod3, kb.mod1)
anova(kb.mod4, kb.mod1)

kb.mod5 <- aov(Deflect ~ factor(Wood) + factor(Bdtype))
anova(kb.mod5)
drop1(kb.mod5)
TukeyHSD(kb.mod5)

options(contrasts=c("contr.sum", "contr.poly"))

kb.mod6 <- aov(Deflect ~ factor(Wood)*factor(Bdtype))
anova(kb.mod6)

library(car)

Anova(kb.mod6, type="III")
```

R Output:

```
> kb.mod1 <- lm(Deflect ~ X1 + X2 + X3 + X4 + X1X4 + X2X4 + X3X4)
> anova(kb.mod1)
Analysis of Variance Table

Response: Deflect
      Df Sum Sq Mean Sq F value    Pr(>F)
X1      1  32085   32085  10.1578 0.001575 **
X2      1   1696    1696   0.5371 0.464181
X3      1  11307   11307   3.5798 0.059365 .
X4      1 116342  116342  36.8329 3.552e-09 ***
X1X4    1     0         0  0.0001 0.994156
X2X4    1   1360    1360   0.4306 0.512132
X3X4    1     81     81   0.0256 0.872927
Residuals 328 1036035    3159
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
> kb.mod2 <- lm(Deflect ~ X1 + X2 + X3 + X4)
> anova(kb.mod2)
Analysis of Variance Table

Response: Deflect
      Df Sum Sq Mean Sq F value    Pr(>F)
X1      1  32085   32085  10.2365 0.00151 **
X2      1   1696    1696   0.5412 0.46245
X3      1  11307   11307   3.6076 0.05839 .
X4      1 116342  116342  37.1181 3.088e-09 ***
Residuals 331 1037476    3134
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
> kb.mod3 <- lm(Deflect ~ X4 + X1X4 + X2X4 + X3X4)
> anova(kb.mod3)
Analysis of Variance Table

Response: Deflect
      Df Sum Sq Mean Sq F value    Pr(>F)
X4      1 115483  115483  35.3528 6.985e-09 ***
X1X4    1     23     23   0.0072 0.9325
X2X4    1   1652    1652   0.5057 0.4775
X3X4    1     509     509   0.1558 0.6933
Residuals 331 1081239    3267
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
> kb.mod4 <- lm(Deflect ~ X1 + X2 + X3 + X1X4 + X2X4 + X3X4)
> anova(kb.mod4)
Analysis of Variance Table

Response: Deflect
      Df Sum Sq Mean Sq F value    Pr(>F)
X1      1  32085   32085   9.1691 0.002656 **
X2      1   1696    1696   0.4848 0.486758
X3      1  11307   11307   3.2314 0.073156 .
X1X4    1     40     40   0.0114 0.915111
X2X4    1   2504    2504   0.7156 0.398205
X3X4    1     23     23   0.0065 0.935872
Residuals 329 1151251    3499
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Continued

```

> anova(kb.mod2,kb.mod1)
Analysis of Variance Table

Model 1: Deflect ~ X1 + X2 + X3 + X4
Model 2: Deflect ~ X1 + X2 + X3 + X4 + X1X4 + X2X4 + X3X4
  Res.Df    RSS Df Sum of Sq    F Pr(>F)
1      331 1037476
2      328 1036035  3    1441.4 0.1521 0.9283
> anova(kb.mod3,kb.mod1)
Analysis of Variance Table

Model 1: Deflect ~ X4 + X1X4 + X2X4 + X3X4
Model 2: Deflect ~ X1 + X2 + X3 + X4 + X1X4 + X2X4 + X3X4
  Res.Df    RSS Df Sum of Sq    F  Pr(>F)
1      331 1081239
2      328 1036035  3     45205 4.7705 0.002866 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> anova(kb.mod4,kb.mod1)
Analysis of Variance Table

Model 1: Deflect ~ X1 + X2 + X3 + X1X4 + X2X4 + X3X4
Model 2: Deflect ~ X1 + X2 + X3 + X4 + X1X4 + X2X4 + X3X4
  Res.Df    RSS Df Sum of Sq    F  Pr(>F)
1      329 1151251
2      328 1036035  1    115217 36.477 4.187e-09 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
> kb.mod5 <- aov(Deflect ~ factor(wood) + factor(Bdtype))
> anova(kb.mod5)
Analysis of Variance Table

Response: Deflect
      Df Sum Sq Mean Sq F value    Pr(>F)
factor(wood)  3  45089   15030  4.7951 0.002769 **
factor(Bdtype) 1 116342  116342 37.1181 3.088e-09 ***
Residuals    331 1037476    3134
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> drop1(kb.mod5)
Single term deletions

Model:
Deflect ~ factor(wood) + factor(Bdtype)
      Df Sum of Sq    RSS    AIC
<none>                 1037476 2709.8
factor(wood)           3    45948 1083424 2718.4
factor(Bdtype)         1   116342 1153818 2743.5
> TukeyHSD(kb.mod5)
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = Deflect ~ factor(wood) + factor(Bdtype))

$`factor(wood)`
      diff       lwr       upr     p adj
2-1 -7.736325 -30.11939  14.646739 0.8087781
3-1 -25.284472 -47.81297 -2.755974 0.0207927
4-1 -27.069424 -48.86854 -5.270307 0.0080047
3-2 -17.548147 -40.40713  5.310840 0.1967711
4-2 -19.333099 -41.47359  2.807396 0.1109786
4-3  -1.784952 -24.07246 20.502560 0.9968674

$`factor(Bdtype)`
      diff       lwr       upr     p adj
2-1 -37.25515 -49.30233 -25.20798      0

```

Continued

```

> options(contrasts=c("contr.sum","contr.poly"))
>
> kb.mod6 <- aov(Deflect ~ factor(wood)*factor(Bdtype))
> anova(kb.mod6)
Analysis of Variance Table

Response: Deflect
              Df Sum Sq Mean Sq F value    Pr(>F)
factor(wood)   3  45089   15030  4.7582 0.002913 **
factor(Bdtype) 1 116342  116342 36.8329 3.552e-09 ***
factor(wood):factor(Bdtype) 3   1441    480  0.1521 0.928296
Residuals     328 1036035   3159
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> library(car)
>
> Anova(kb.mod6,type="III")
Anova Table (Type III tests)

Response: Deflect
              Sum Sq Df F value    Pr(>F)
(Intercept) 2308824  1 730.9544 < 2.2e-16 ***
factor(wood)  45205  3  4.7705  0.002866 **
factor(Bdtype) 115217  1 36.4766 4.187e-09 ***
factor(wood):factor(Bdtype) 1441  3  0.1521 0.928296
Residuals     1036035 328
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>

```

5.5. Power and Sample Size Calculations (Balanced Data)

Power to detect particular configurations of the $\{\alpha_i\}$, $\{\beta_j\}$, and $\{(\alpha\beta)_{ij}\}$ for particular sample sizes, and sample sizes needed to obtain particular power levels are often needed. These methods generalize what was done for the 1-Way ANOVA in Chapter 2. Recall that software packages make use of 2Ω in their probability, quantile, and density functions.

$$\begin{aligned}
 \text{Factor A Main Effects: } \Omega_A &= \frac{bn \sum_{i=1}^a \alpha_i^2}{2\sigma^2} & \text{Factor B Main Effects: } \Omega_B &= \frac{an \sum_{j=1}^b \beta_j^2}{2\sigma^2} \\
 \text{Interaction Main Effects: } \Omega_{AB} &= \frac{n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2}{2\sigma^2}
 \end{aligned}$$

Example: Reading Times for 3 E-Reader Devices at 4 Illumination Levels

Using the OLS estimates of the effects and experimental error variance as inputs for the non-centrality parameters, we have (recall there were $n = 5$ subjects per treatment, and $s^2 = MS_{\text{Err}} = 7.60$):

Device\Illum	1	2	3	4	Dev ME
1	0.02	0.38	-0.3	-0.1	1.53
2	0.11	-0.31	0.11	0.09	-0.68
3	-0.13	-0.07	0.19	0.01	-0.86
Illum ME	2.07	0.95	-1.29	-1.76	0
	sum(a^2)	sum(b^2)	sum(ab^2)		
	3.5429	9.9491	0.4312		

$$\text{Factor A Main Effects: } \Omega_A = \frac{bn \sum_{i=1}^a \alpha_i^2}{2\sigma^2} = \frac{4(5)(3.54)}{2(7.60)} = 4.66 \Rightarrow 2\Omega_A = 9.32$$
$$\text{Factor B Main Effects: } \Omega_B = \frac{an \sum_{j=1}^b \beta_j^2}{2\sigma^2} = \frac{3(5)(9.95)}{2(7.60)} = 9.82 \Rightarrow 2\Omega_B = 19.64$$
$$\text{Interaction Main Effects: } \Omega_{AB} = \frac{n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2}{2\sigma^2} = \frac{5(0.43)}{2(7.60)} = 0.14 \Rightarrow 2\Omega_{AB} = 0.28$$

Now in R, we can obtain the power of detecting these effects, based on the observed sample sizes. We could also determine what sample sizes are needed to detect these effects with a given power. First we obtain the critical F value for each test, then we find the probability of falling above the critical value in the non-central F distribution.

$$\text{Factor A: } F_{.95;2,48} = 3.191 \quad \text{Factor B: } F_{.95;3,48} = 2.798 \quad \text{Factor AB: } F_{.95;6,48} = 2.295$$

R Program

```
a <- 3; b <- 4; n <- 5
(power.a <- 1-pf(qf(.95,a-1,a*b*(n-1)),a-1,a*b*(n-1),9.32))
(power.b <- 1-pf(qf(.95,b-1,a*b*(n-1)),b-1,a*b*(n-1),19.64))
(power.ab <- 1-pf(qf(.95,(a-1)*(b-1),a*b*(n-1)),(a-1)*(b-1),a*b*(n-1),0.28))
```


R Output

```
> a <- 3; b <- 4; n <- 5
>
> (power.a <- 1-pf(qf(.95,a-1,a*b*(n-1)),a-1,a*b*(n-1),9.32))
[1] 0.7582581
>
> (power.b <- 1-pf(qf(.95,b-1,a*b*(n-1)),b-1,a*b*(n-1),19.64))
[1] 0.9599262
>
> (power.ab <- 1-pf(qf(.95,(a-1)*(b-1),a*b*(n-1)),(a-1)*(b-1),a*b*(n-1),0.28))
[1] 0.05981329
>
```

The power to detect the observed main effects, based on the actual sample sizes are 0.76 for Device, and 0.96 for Illumination level. Recall that the interaction effects were very small, leading to very small power (0.06) to detect those small levels. We could run a power calculation to see what sample size would be needed to detect these interaction effects with power = 0.80. For these levels of interaction effects, we would need a virtually infinite sample per treatment to meet this power requirement. An R program is given below to determine the sample size needed to meet a given power requirement for a given level of 2Ω .

R Program & Output

```
a <- 3; b <- 4; n <- 5
dpower <- .70; ab.2omega <- 12

while (power.ab <= dpower) {
  n <- n+1
  power.ab <- 1-pf(qf(.95, (a-1)*(b-1), a*b*(n-1)), (a-1)*(b-1), a*b*(n-1), ab.2omega)
}

print(cbind(n, power.ab))

> print(cbind(n, power.ab))
      n power.ab
[1,]  8 0.7002233
```

5.6. Higher Order Models

When we have 3 or more factors, the terms get more complicated, but there is a clear pattern that arises in the interaction effect estimates and sums of squares. The 3-factor model is given below.

$$Y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + \varepsilon_{ijkl} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c \quad l = 1, \dots, n$$
$$\varepsilon_{ijkl} \sim NID(0, \sigma^2) \quad \sum_{i=1}^a \alpha_i = \sum_{i=1}^a (\alpha\beta)_{ij} = \sum_{j=1}^b (\alpha\beta)_{ij} = \sum_{i=1}^a (\alpha\beta\gamma)_{ijk} = \sum_{j=1}^b (\alpha\beta\gamma)_{ijk} = \sum_{k=1}^c (\alpha\beta\gamma)_{ijk} = 0$$

Identical summations occur for the other main effects and 2-factor interactions. Below, we give the typical least squares estimates and sum of squares for each level of main effects and interactions.

$$\hat{\alpha}_i = \bar{Y}_{i\dots\dots} - \bar{Y}_{\dots\dots} \quad (\hat{\alpha}\beta)_{ij} = \bar{Y}_{ij\dots} - \bar{Y}_{i\dots\dots} - \bar{Y}_{\cdot j\dots} + \bar{Y}_{\dots\dots} \quad (\hat{\alpha}\beta\gamma)_{ijk} = \bar{Y}_{ijk\dots} - \bar{Y}_{ij\dots} - \bar{Y}_{i\dots k\dots} - \bar{Y}_{\cdot jk\dots} + \bar{Y}_{i\dots\dots} + \bar{Y}_{\cdot j\dots} + \bar{Y}_{\dots k\dots} - \bar{Y}_{\dots\dots}$$

$$SS_A = bcn \sum_{i=1}^a (\bar{Y}_{i\dots\dots} - \bar{Y}_{\dots\dots})^2 = bcn \sum_{i=1}^a (\hat{\alpha}_i)^2 \quad df_A = a - 1$$

$$SS_{AB} = cn \sum_{i=1}^a \sum_{j=1}^b (\bar{Y}_{ij\dots} - \bar{Y}_{i\dots\dots} - \bar{Y}_{\cdot j\dots} + \bar{Y}_{\dots\dots})^2 = cn \sum_{i=1}^a \sum_{j=1}^b ((\hat{\alpha}\beta)_{ij})^2 \quad df_{AB} = (a-1)(b-1)$$

$$SS_{ABC} = n \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c (\bar{Y}_{ijk\dots} - \bar{Y}_{ij\dots} - \bar{Y}_{i\dots k\dots} - \bar{Y}_{\cdot jk\dots} + \bar{Y}_{i\dots\dots} + \bar{Y}_{\cdot j\dots} + \bar{Y}_{\dots k\dots} - \bar{Y}_{\dots\dots})^2 = n \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c ((\hat{\alpha}\beta\gamma)_{ijk})^2$$

$$df_{ABC} = (a-1)(b-1)(c-1)$$

$$SS_{Err} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^n (Y_{ijkl} - \bar{Y}_{ijk\dots})^2 \quad df_{Err} = abc(n-1)$$

$$SS_{Tot} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^n (Y_{ijkl} - \bar{Y}_{\dots\dots})^2 \quad df_{Tot} = abc n - 1$$

Note that the estimates (and sums of squares) for main effects and interactions start with the mean with all subscripts in the term of interest, then one subscript is replaced with a “dot” and that mean is multiplied by -1. This is done for each subscript, one-at-a-time. Then two subscripts are replaced with “dots”, and that mean is multiplied by $(-1)^2 = 1$. This is done for each pair of subscripts. Then 3 subscripts are replaced with “dots” and that mean is multiplied by $(-1)^3 = -1$. The pattern continues for as many levels as needed.

The analysis of variance for the 3-factor model is given below.

Source	df	SS	MS	F	P-value
A	$a - 1$	SS_A	$MS_A = \frac{SS_A}{a - 1}$	$F_A = \frac{MS_A}{MS_{Err}}$	$P(F_{a-1, abc(n-1)} \geq F_A)$
B	$b - 1$	SS_B	$MS_B = \frac{SS_B}{b - 1}$	$F_B = \frac{MS_B}{MS_{Err}}$	$P(F_{b-1, abc(n-1)} \geq F_B)$
C	$c - 1$	SS_C	$MS_C = \frac{SS_C}{c - 1}$	$F_C = \frac{MS_C}{MS_{Err}}$	$P(F_{c-1, abc(n-1)} \geq F_C)$
AB	$(a - 1)(b - 1)$	SS_{AB}	$MS_{AB} = \frac{SS_{AB}}{(a - 1)(b - 1)}$	$F_{AB} = \frac{MS_{AB}}{MS_{Err}}$	$P(F_{(a-1)(b-1), abc(n-1)} \geq F_{AB})$
AC	$(a - 1)(c - 1)$	SS_{AC}	$MS_{AC} = \frac{SS_{AC}}{(a - 1)(c - 1)}$	$F_{AC} = \frac{MS_{AC}}{MS_{Err}}$	$P(F_{(a-1)(c-1), abc(n-1)} \geq F_{AC})$
BC	$(b - 1)(c - 1)$	SS_{BC}	$MS_{BC} = \frac{SS_{BC}}{(b - 1)(c - 1)}$	$F_{BC} = \frac{MS_{BC}}{MS_{Err}}$	$P(F_{(b-1)(c-1), abc(n-1)} \geq F_{BC})$
ABC	$(a - 1)(b - 1)(c - 1)$	SS_{ABC}	$MS_{ABC} = \frac{SS_{ABC}}{(a - 1)(b - 1)(c - 1)}$	$F_{ABC} = \frac{MS_{ABC}}{MS_{Err}}$	$P(F_{(a-1)(b-1)(c-1), abc(n-1)} \geq F_{ABC})$

Example: Beer Foam Half-Life by Laboratory, Carborundrum Source, and Brand

An experiment was conducted to compare half-life of beer foam across levels of 3 factors: **Lab** (5 levels), **Carborundrum Source** (2 Levels: distributed directly from manufacturer, store bought), and **Brand** (5 Levels) (Hudson (1968)). For the purposes of this analysis, we presume these are the only labs and brands of interest (we will explore them as random effects in later chapters). There were $n = 4$ replicates per treatment, so $N = 5(2)(5)(4) = 200$. Treatment and marginal means are given below.

CARBOR1	BRAND1	BRAND2	BRAND3	BRAND4	BRAND5	LC_i1	
LAB1	98.75	101.00	76.50	130.00	48.25	90.90	
LAB2	92.00	97.00	91.75	132.75	58.25	94.35	
LAB3	90.75	81.00	97.00	138.25	53.75	92.15	
LAB4	97.00	78.75	94.50	140.25	52.75	92.65	
LAB5	90.00	85.75	72.50	100.75	47.75	79.35	
BC_1k	93.70	88.70	86.45	128.40	52.15	89.88	C_1
CARBOR2	BRAND1	BRAND2	BRAND3	BRAND4	BRAND5	LC_i2	
LAB1	93.75	88.25	81.25	134.25	49.00	89.30	
LAB2	96.50	110.50	98.25	142.00	62.00	101.85	
LAB3	97.50	78.50	90.00	135.75	51.25	90.60	
LAB4	97.50	76.00	92.50	138.25	51.00	91.05	
LAB5	92.25	68.00	73.75	101.00	51.00	77.20	
BC_2k	95.50	84.25	87.15	130.25	52.85	90.00	C_2
LB_ik	BRAND1	BRAND2	BRAND3	BRAND4	BRAND5	L_j	
LAB1	96.25	94.63	78.88	132.13	48.63	90.10	
LAB2	94.25	103.75	95.00	137.38	60.13	98.10	
LAB3	94.13	79.75	93.50	137.00	52.50	91.38	
LAB4	97.25	77.38	93.50	139.25	51.88	91.85	
LAB5	91.13	76.88	73.13	100.88	49.38	78.28	
B_k	94.60	86.48	86.80	129.33	52.50	89.94	AllMean

Letting Lab be factor A, Carborundrum be factor B, and Brand be factor C (that is the order they are entered in dataset). We estimate some of the main effect and interaction effects below.

$$\hat{\alpha}_1 = \bar{y}_{1\dots} - \bar{y}_{\dots} = 90.10 - 89.94 = 0.16$$

$$\hat{(\alpha\beta)}_{11} = \bar{y}_{11\dots} - \bar{y}_{1\dots} - \bar{y}_{\cdot 1\dots} + \bar{y}_{\dots} = 90.90 - 90.10 - 89.88 + 89.94 = 0.86$$

$$\hat{(\alpha\beta\gamma)}_{111} = \bar{y}_{111\dots} - \bar{y}_{11\dots} - \bar{y}_{1\cdot 1\dots} - \bar{y}_{\cdot 11\dots} + \bar{y}_{1\dots} + \bar{y}_{\cdot 1\dots} + \bar{y}_{\dots 1\dots} - \bar{y}_{\dots} =$$

$$= 98.75 - 90.90 - 96.25 - 93.70 + 90.10 + 89.88 + 94.60 - 89.94 = 2.54$$

The main effect and interaction estimates, analysis of variance and F-tests are given in the following spreadsheets.

CARBOR1	BRAND1	BRAND2	BRAND3	BRAND4	BRAND5	LC_i1	
LAB1	2.54	3.29	-2.89	-2.06	-0.89	0.86	
LAB2	2.34	-5.29	0.79	-0.01	2.16	-3.69	
LAB3	-3.31	-1.81	3.01	1.34	0.76	0.84	
LAB4	-0.21	-1.71	0.49	1.06	0.36	0.86	
LAB5	-1.36	5.51	-1.41	-0.34	-2.41	1.13	
BC_1k	-0.84	2.29	-0.29	-0.86	-0.29	-0.06	C_1
CARBOR2	BRAND1	BRAND2	BRAND3	BRAND4	BRAND5	LC_i2	
LAB1	-2.54	-3.29	2.89	2.06	0.88	-0.86	
LAB2	-2.34	5.29	-0.79	0.01	-2.16	3.69	
LAB3	3.31	1.81	-3.02	-1.34	-0.76	-0.84	
LAB4	0.21	1.71	-0.49	-1.07	-0.37	-0.86	
LAB5	1.36	-5.51	1.41	0.34	2.41	-1.14	
BC_2k	0.84	-2.29	0.29	0.87	0.29	0.06	C_2
LB_ik	BRAND1	BRAND2	BRAND3	BRAND4	BRAND5	L_i	
LAB1	1.49	7.99	-8.08	2.64	-4.04	0.16	
LAB2	-8.51	9.12	0.04	-0.11	-0.53	8.16	
LAB3	-1.91	-8.16	5.27	6.24	-1.44	1.44	
LAB4	0.74	-11.01	4.79	8.02	-2.54	1.91	
LAB5	8.19	2.07	-2.01	-16.79	8.54	-11.67	
B_k	4.66	-3.47	-3.14	39.39	-37.44	0.00	AllMean

Source	df	SS	MS	F	F(.05)	P-value
Laboratory	4	8335.63	2083.91	55.630	2.432	0.0000
Carborundrum	1	0.72	0.72	0.019	3.904	0.8899
Brand	4	119860.53	29965.13	799.923	2.432	0.0000
LC	4	683.23	170.81	4.560	2.432	0.0017
LB	16	8758.87	547.43	14.614	1.711	0.0000
CB	4	273.73	68.43	1.827	2.432	0.1266
LCB	16	1117.57	69.85	1.865	1.711	0.0279
Error	150	5619.00	37.46			
Total	199	144649.28				

There are clear Lab, Brand, and Lab/Brand effects. There is also a Lab/Carborundrum interaction, and some evidence of a 3-way interaction.

R Program

```
beer <- read.table("http://www.stat.ufl.edu/~winner/data/beerhead_half-life.dat",
  header=F, col.names=c("lab", "carbor", "brand", "foamtime"))
attach(beer)

lab <- factor(lab); carbor <- factor(carbor); brand <- factor(brand)

options(contrasts=c("contr.sum", "contr.poly"))

beer.mod1 <- aov(foamtime ~ lab*carbor*brand)
anova(beer.mod1)
summary.lm(beer.mod1)

par(mfrow=c(1,2))
interaction.plot(lab[carbor==1], brand[carbor==1], foamtime[carbor==1])
interaction.plot(lab[carbor==2], brand[carbor==2], foamtime[carbor==2])
```

R Output

```
> beer.mod1 <- aov(foamtime ~ lab*carbor*brand)
> anova(beer.mod1)
Analysis of Variance Table

Response: foamtime

```

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
lab	4	8336	2083.9	55.6302	< 2.2e-16	***
carbor	1	1	0.7	0.0192	0.889922	
brand	4	119861	29965.1	799.9235	< 2.2e-16	***
lab:carbor	4	683	170.8	4.5597	0.001671	**
lab:brand	16	8759	547.4	14.6137	< 2.2e-16	***
carbor:brand	4	274	68.4	1.8268	0.126574	
lab:carbor:brand	16	1118	69.8	1.8646	0.027935	*
Residuals	150	5619	37.5			

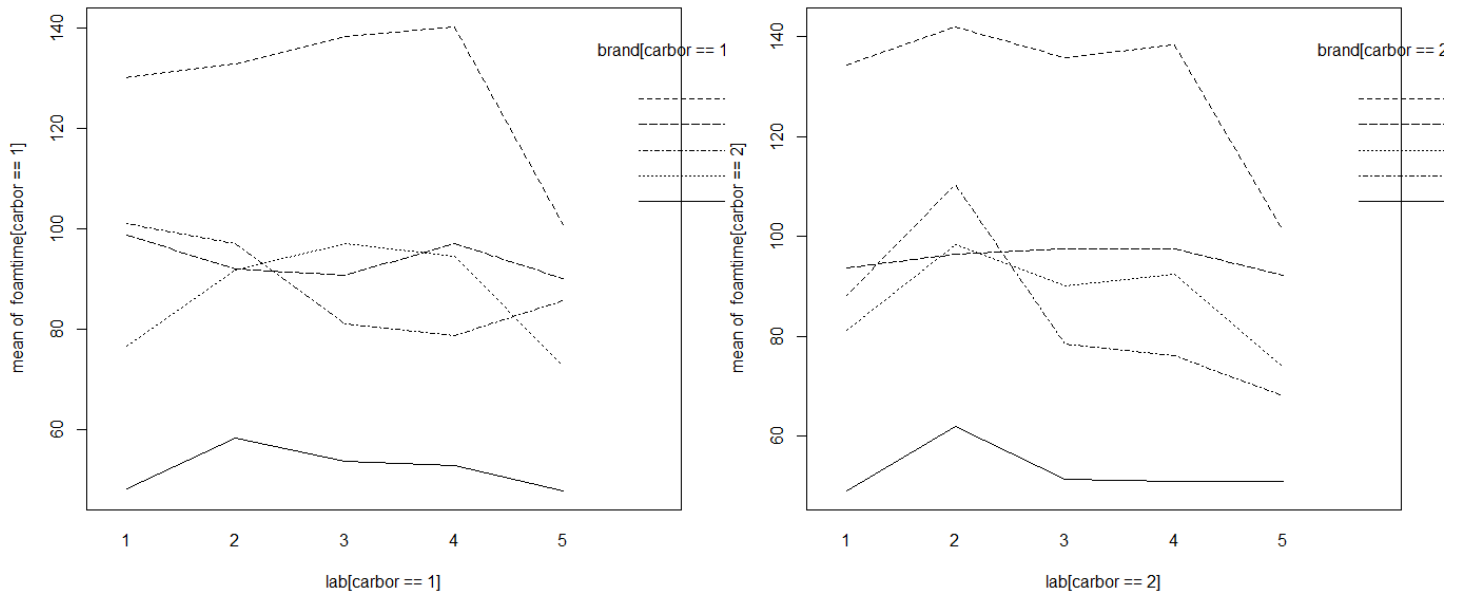
```

aov(formula = foamtime ~ lab * carbor * brand)

Coefficients:
(Intercept)      89.9400  Std. Error 0.4328  t value 207.818  Pr(>|t|) < 2e-16 ***
lab1              0.1600  Std. Error 0.8656  t value  0.185  0.853596
lab2              8.1600  Std. Error 0.8656  t value  9.427  < 2e-16 ***
lab3             1.4350  Std. Error 0.8656  t value  1.658  0.099432 .
lab4             1.9100  Std. Error 0.8656  t value  2.207  0.028858 *
carbor1          -0.0600  Std. Error 0.4328  t value -0.139  0.889922
brand1           4.6600  Std. Error 0.8656  t value  5.384  2.76e-07 ***
brand2          -3.4650  Std. Error 0.8656  t value -4.003  9.80e-05 ***
brand3          -3.1400  Std. Error 0.8656  t value -3.628  0.000391 ***
brand4          39.3850  Std. Error 0.8656  t value 45.502  < 2e-16 ***
lab1:carbor1     0.8600  Std. Error 0.8656  t value  0.994  0.322031
lab2:carbor1    -3.6900  Std. Error 0.8656  t value -4.263  3.55e-05 ***
lab3:carbor1     0.8350  Std. Error 0.8656  t value  0.965  0.336253
lab4:carbor1     0.8600  Std. Error 0.8656  t value  0.994  0.322031
lab1:brand1      1.4900  Std. Error 1.7311  t value  0.861  0.390771
lab2:brand1     -8.5100  Std. Error 1.7311  t value -4.916  2.29e-06 ***
lab3:brand1     -1.9100  Std. Error 1.7311  t value -1.103  0.271652
lab4:brand1      0.7400  Std. Error 1.7311  t value  0.427  0.669652
lab1:brand2      7.9900  Std. Error 1.7311  t value  4.615  8.36e-06 ***
lab2:brand2      9.1150  Std. Error 1.7311  t value  5.265  4.77e-07 ***
lab3:brand2     -8.1600  Std. Error 1.7311  t value -4.714  5.51e-06 ***
lab4:brand2    -11.0100  Std. Error 1.7311  t value -6.360  2.31e-09 ***
lab1:brand3     -8.0850  Std. Error 1.7311  t value -4.670  6.63e-06 ***
lab2:brand3      0.0400  Std. Error 1.7311  t value  0.023  0.981596
lab3:brand3      5.2650  Std. Error 1.7311  t value  3.041  0.002780 **
lab4:brand3      4.7900  Std. Error 1.7311  t value  2.767  0.006370 **
lab1:brand4      2.6400  Std. Error 1.7311  t value  1.525  0.129360
lab2:brand4     -0.1100  Std. Error 1.7311  t value -0.064  0.949419
lab3:brand4      6.2400  Std. Error 1.7311  t value  3.605  0.000425 ***
lab4:brand4      8.0150  Std. Error 1.7311  t value  4.630  7.86e-06 ***
carbor1:brand1  -0.8400  Std. Error 0.8656  t value -0.970  0.333376
carbor1:brand2   2.2850  Std. Error 0.8656  t value  2.640  0.009170 **
carbor1:brand3  -0.2900  Std. Error 0.8656  t value -0.335  0.738062
carbor1:brand4  -0.8650  Std. Error 0.8656  t value -0.999  0.319235
lab1:carbor1:brand1  2.5400  Std. Error 1.7311  t value  1.467  0.144401
lab2:carbor1:brand1  2.3400  Std. Error 1.7311  t value  1.352  0.178499
lab3:carbor1:brand1 -3.3100  Std. Error 1.7311  t value -1.912  0.057776 .
lab4:carbor1:brand1 -0.2100  Std. Error 1.7311  t value -0.121  0.903609
lab1:carbor1:brand2  3.2900  Std. Error 1.7311  t value  1.900  0.059287 .
lab2:carbor1:brand2 -5.2850  Std. Error 1.7311  t value -3.053  0.002682 **
lab3:carbor1:brand2 -1.8100  Std. Error 1.7311  t value -1.046  0.297445
lab4:carbor1:brand2 -1.7100  Std. Error 1.7311  t value -0.988  0.324843
lab1:carbor1:brand3 -2.8850  Std. Error 1.7311  t value -1.667  0.097692 .
lab2:carbor1:brand3  0.7900  Std. Error 1.7311  t value  0.456  0.648798
lab3:carbor1:brand3  3.0150  Std. Error 1.7311  t value  1.742  0.083621 .
lab4:carbor1:brand3  0.4900  Std. Error 1.7311  t value  0.283  0.777527
lab1:carbor1:brand4 -2.0600  Std. Error 1.7311  t value -1.190  0.235936
lab2:carbor1:brand4 -0.0100  Std. Error 1.7311  t value -0.006  0.995399
lab3:carbor1:brand4  1.3400  Std. Error 1.7311  t value  0.774  0.440112
lab4:carbor1:brand4  1.0650  Std. Error 1.7311  t value  0.615  0.539351
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 6.12 on 150 degrees of freedom
Multiple R-squared:  0.9612,    Adjusted R-squared:  0.9485
F-statistic: 75.74 on 49 and 150 DF,  p-value: < 2.2e-16
```

Side-by-side Lab/Brand interaction plots (separate by Caborundrum) show the 3-Way interaction does not appear to be very large.



Data Sources:

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K.V. Smith (1969). "Stock Price and Economic Indexes For Generating Efficient Portfolios," *The Journal of Business*, Vol. 42, #3, pp. 332-336.

P.K. Smith, T. Niiler, and P.W. McCullough (2010). "Evaluating Makiwara Punching Board Performance," *Journal of Asian Martial Arts*, Vol 19, #2, pp. 34-45.

J.R. Hudson (1968). "Institute of Brewing: Analysis Committee Measurement of Head-Retention in Bottled Beer," *Journal of the Institute of Brewing*, Vol. 74, Issue 3, pp. 275-285.

Chapter 6 – Designs with Random Effects

So far, we have assumed all levels of interest for a factor are included in a model. In these cases, the treatment means and effects are fixed parameters that are to be estimated, and inferences are made concerning their numeric values. In other situations, the levels of the factor are considered a sample from a population of such levels. Different experimental “runs” could involve different levels being included in the model. In these studies, interest is in the different sources of variation. First, we consider the 1-Way Random effects model. Then, we consider multi-factor random and then mixed models.

6.1. 1-Way Random Effects Model

In this model, there are two sources of variation: among factor levels and within factor levels. Intuitively, we take a sample of the factor levels from a population of levels, then take multiple measurements on the sampled levels. The model can be written as below, where ρ_I is called the **intraclass correlation coefficient**.

$$\begin{aligned}
 & Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad i=1, \dots, g; j=1, \dots, n_i \quad \alpha_i \sim NID(0, \sigma_\alpha^2) \quad \varepsilon_{ij} \sim NID(0, \sigma^2) \quad \{\alpha_i\} \perp \{\varepsilon_{ij}\} \\
 \Rightarrow & E\{Y_{ij}\} = E\{\mu + \alpha_i + \varepsilon_{ij}\} = \mu + 0 + 0 = \mu \quad V\{Y_{ij}\} = V\{\mu + \alpha_i + \varepsilon_{ij}\} = 0 + \sigma_\alpha^2 + \sigma^2 = \sigma_\alpha^2 + \sigma^2 \\
 \Rightarrow & COV\{Y_{ij}, Y_{ij'}\} = COV\{\mu + \alpha_i + \varepsilon_{ij}, \mu + \alpha_i + \varepsilon_{ij'}\} = V\{\alpha_i\} = \sigma_\alpha^2 \quad j \neq j' \\
 \Rightarrow & COV\{Y_{ij}, Y_{i'j'}\} = \begin{cases} \sigma_\alpha^2 + \sigma^2 & i=i', j=j' \\ \sigma_\alpha^2 & i=i', j \neq j' \\ 0 & i \neq i', \forall j, j' \end{cases} \quad CORR\{Y_{ij}, Y_{ij'}\} = \rho_I = \frac{COV\{Y_{ij}, Y_{ij'}\}}{\sqrt{V\{Y_{ij}\}V\{Y_{ij'}\}}} = \frac{\sigma_\alpha^2}{\sigma_\alpha^2 + \sigma^2} \quad j \neq j'
 \end{aligned}$$

The primary difference between the fixed and random effects models are that for the fixed effects model, observations from the same treatment are independent, while for the random effects model, observations from the same treatment are correlated. The sums of squares for treatments and error are computed as in the fixed effects model, however the expected mean squares differ.

$$\begin{aligned}
 & E\{Y_{ij}\} = \mu \quad V\{Y_{ij}\} = \sigma_\alpha^2 + \sigma^2 \\
 & E\{\bar{Y}_{i\cdot}\} = \mu \\
 & V\{\bar{Y}_{i\cdot}\} = \frac{1}{n_i} \left[\sum_{j=1}^{n_i} V\{Y_{ij}\} + 2 \sum_{j=1}^{n_i-1} \sum_{j'=j+1}^{n_i} COV\{Y_{ij}, Y_{ij'}\} \right] = \frac{1}{n_i} \left[n_i(\sigma_\alpha^2 + \sigma^2) + 2 \frac{n_i(n_i-1)}{2} \sigma_\alpha^2 \right] = \sigma_\alpha^2 + \frac{\sigma^2}{n_i} \\
 & E\{\bar{Y}_{\cdot\cdot}\} = \mu \quad V\{\bar{Y}_{\cdot\cdot}\} = V\left\{ \frac{1}{N} \sum_{i=1}^g n_i \bar{Y}_{i\cdot} \right\} = \frac{1}{N^2} \sum_{i=1}^g n_i^2 \left(\sigma_\alpha^2 + \frac{\sigma^2}{n_i} \right) = \frac{1}{N^2} \sum_{i=1}^g (n_i^2 \sigma_\alpha^2 + n_i \sigma^2) = \frac{\sigma_\alpha^2 \sum_{i=1}^g n_i^2}{N^2} + \frac{\sigma^2}{N} \\
 & E\{Y_{ij}^2\} = \mu^2 + \sigma_\alpha^2 + \sigma^2 \quad E\{\bar{Y}_{i\cdot}^2\} = \mu^2 + \sigma_\alpha^2 + \frac{\sigma^2}{n_i} \quad E\{\bar{Y}_{\cdot\cdot}^2\} = \mu^2 + \frac{\sigma_\alpha^2 \sum_{i=1}^g n_i^2}{N^2} + \frac{\sigma^2}{N}
 \end{aligned}$$

$$E\{Y_{ij}^2\} = \mu^2 + \sigma_\alpha^2 + \sigma^2 \quad E\{\bar{Y}_{i\cdot}^2\} = \mu^2 + \sigma_\alpha^2 + \frac{\sigma^2}{n_i} \quad E\{\bar{Y}_{\cdot\cdot}^2\} = \mu^2 + \frac{\sigma_\alpha^2 \sum_{i=1}^g n_i^2}{N^2} + \frac{\sigma^2}{N}$$

$$SS_{\text{Trr}} = \sum_{i=1}^g n_i (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 = \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2 - N \bar{Y}_{\cdot\cdot}^2 \quad SS_{\text{Err}} = \sum_{i=1}^g \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})^2 = \sum_{i=1}^g \sum_{j=1}^{n_i} Y_{ij}^2 - \sum_{i=1}^g n_i \bar{Y}_{i\cdot}^2$$

$$\Rightarrow E\{SS_{\text{Trr}}\} = [N\mu^2 + N\sigma_\alpha^2 + g\sigma^2] - \left[N\mu^2 + \frac{\sigma_\alpha^2 \sum_{i=1}^g n_i^2}{N} + \sigma^2 \right] = \sigma_\alpha^2 \left(N - \frac{\sum_{i=1}^g n_i^2}{N} \right) + (g-1)\sigma^2$$

$$\Rightarrow E\{MS_{\text{Trr}}\} = \sigma_\alpha^2 \left(\frac{N^2 - \sum_{i=1}^g n_i^2}{N(g-1)} \right) + \sigma^2 \quad \text{NOTE: } n_1 = \dots = n_g = n \Rightarrow \frac{N^2 - \sum_{i=1}^g n_i^2}{N(g-1)} = \frac{N^2 - Nn}{N(g-1)} = \frac{n(g-1)}{(g-1)} = n$$

$$\Rightarrow E\{SS_{\text{Err}}\} = [N\mu^2 + N\sigma_\alpha^2 + N\sigma^2] - [N\mu^2 + N\sigma_\alpha^2 + g\sigma^2] = (N-g)\sigma^2 \Rightarrow E\{MS_{\text{Err}}\} = \sigma^2$$

Inferences Concerning μ , σ_α^2 , σ^2 , ρ_I

In this section, we will work under the assumption of balanced data, which makes all computations much more tractable. Direct use of statistical software packages should be used for unbalanced cases.

First, we consider the population mean, μ . Note the following results from above.

$$E\{\bar{Y}_{\cdot\cdot}\} = \mu \quad V\{\bar{Y}_{\cdot\cdot}\} = V\left\{ \frac{1}{N} \sum_{i=1}^g n \bar{Y}_{i\cdot} \right\} = \frac{n^2}{N^2} \sum_{i=1}^g \left(\sigma_\alpha^2 + \frac{\sigma^2}{n} \right) = \frac{1}{g^2} \left[g\sigma_\alpha^2 + g \frac{\sigma^2}{n} \right] = \frac{\sigma_\alpha^2}{g} + \frac{\sigma^2}{N} = \frac{n\sigma_\alpha^2 + \sigma^2}{N}$$

$$\bar{Y}_{\cdot\cdot} \sim N\left(\mu, \frac{n\sigma_\alpha^2 + \sigma^2}{N} \right) \Rightarrow Z = \frac{\bar{Y}_{\cdot\cdot} - \mu}{\sqrt{\frac{n\sigma_\alpha^2 + \sigma^2}{N}}} \sim N(0,1)$$

$$E\{MS_{\text{Trr}}\} = \sigma_\alpha^2 \left(\frac{N^2 - \sum_{i=1}^g n_i^2}{N(g-1)} \right) + \sigma^2 = n\sigma_\alpha^2 + \sigma^2 \Rightarrow E\left\{ \frac{MS_{\text{Trr}}}{N} \right\} = \frac{n\sigma_\alpha^2 + \sigma^2}{N} = V\{\bar{Y}_{\cdot\cdot}\}$$

$$W = \frac{df_{\text{Trr}} MS_{\text{Trr}}}{n\sigma_\alpha^2 + \sigma^2} \sim \chi_{df_{\text{Trr}}}^2 \equiv \chi_{g-1}^2 \quad \bar{Y}_{\cdot\cdot} \perp MS_{\text{Trr}} \Rightarrow T = \frac{Z}{\sqrt{W/df_{\text{Trr}}}} = \frac{\bar{Y}_{\cdot\cdot} - \mu}{\sqrt{\frac{MS_{\text{Trr}}}{N}}} \sim t_{df_{\text{Trr}}} \equiv t_{g-1}$$

$$\Rightarrow (1-\alpha)100\% \text{ CI for } \mu: \bar{y}_{\cdot\cdot} \pm t_{1-\alpha/2; g-1} \sqrt{\frac{MS_{\text{Trr}}}{N}}$$

Next, we consider the variance component corresponding to the random treatment effect, σ_α^2 . First consider a test of the form $H_0: \sigma_\alpha^2 = 0$.

$$\begin{aligned}
 W_1 &= \frac{df_{\text{Trt}} MS_{\text{Trt}}}{n\sigma_\alpha^2 + \sigma^2} \sim \chi_{df_{\text{Trt}}}^2 \equiv \chi_{g-1}^2 & W_2 &= \frac{df_{\text{Err}} MS_{\text{Err}}}{\sigma^2} \sim \chi_{df_{\text{Err}}}^2 \equiv \chi_{N-g}^2 & MS_{\text{Trt}} &\perp MS_{\text{Err}} \\
 \Rightarrow F &= \frac{W_1/df_{\text{Trt}}}{W_2/df_{\text{Err}}} = \frac{\left[\frac{MS_{\text{Trt}}}{n\sigma_\alpha^2 + \sigma^2} \right]}{\left[\frac{MS_{\text{Err}}}{\sigma^2} \right]} \sim F_{g-1, N-g} & \text{Under } H_0: \sigma_\alpha^2 = 0 & F_A &= \frac{MS_{\text{TRT}}}{MS_{\text{ERR}}} \sim F_{g-1, N-g} \\
 H_0: \sigma_\alpha^2 = 0 & H_A: \sigma_\alpha^2 > 0 & TS: F_A &= \frac{MS_{\text{Trt}}}{MS_{\text{Err}}} & RR: F_A &\geq F_{g-1, N-g} & \text{P-value: } P(F_{g-1, N-g} \geq F_A)
 \end{aligned}$$

To obtain an unbiased (but possibly negative) estimate of the random treatment effect, σ_α^2 , we make use of a linear function of the expected mean squares for Treatment and Error. Note that a multiple of this linear function will not be distributed as a chi-square random variable, but we can make use of **Satterthwaite's approximation** to obtain its approximate degrees of freedom. Suppose we have a particular variance component, or function of variance components we wish to estimate: σ_*^2 , and we have a linear function of mean squares, W^* , that unbiasedly estimates it. The approximation is obtained as follows.

$$\begin{aligned}
 X &\sim \chi_\nu^2 \Rightarrow E\{X\} = \nu & V\{X\} &= 2\nu \\
 \frac{df_i MS_i}{E\{MS_i\}} &\sim \chi_{df_i}^2 \Rightarrow E\left\{ \frac{df_i MS_i}{E\{MS_i\}} \right\} = df_i \\
 V\left\{ \frac{df_i MS_i}{E\{MS_i\}} \right\} &= \left(\frac{df_i}{E\{MS_i\}} \right)^2 V\{MS_i\} = 2df_i \Rightarrow V\{MS_i\} = \frac{2(E\{MS_i\})^2}{df_i} \\
 W^* &= \sum_{i=1}^k g_i MS_i & E\{W^*\} &= \sigma_*^2 & V\{W^*\} &= V\left\{ \sum_{i=1}^k g_i MS_i \right\} = \sum_{i=1}^k g_i^2 V\{MS_i\} = 2 \sum_{i=1}^k g_i^2 \frac{(E\{MS_i\})^2}{df_i} \\
 X^* &= \frac{df_* W^*}{\sigma_*^2} \text{ approx} \sim \chi_{df_*}^2 \\
 E\{X^*\} &= E\left\{ \frac{df_* W^*}{\sigma_*^2} \right\} = \frac{df_*}{\sigma_*^2} E\{W^*\} = df_* \\
 V\{X^*\} &= V\left\{ \frac{df_* W^*}{\sigma_*^2} \right\} = \left(\frac{df_*}{\sigma_*^2} \right)^2 V\{W^*\} \approx 2df_* \Rightarrow V\{W^*\} \approx \frac{2\sigma_*^4}{df_*} \approx \frac{2(W^*)^2}{df_*} \\
 \Rightarrow df_* &\approx \frac{2(W^*)^2}{V\{W^*\}} \approx \frac{2(W^*)^2}{2 \sum_{i=1}^k g_i^2 \frac{(E\{MS_i\})^2}{df_i}} \approx \frac{\left(\sum_{i=1}^k g_i MS_i \right)^2}{\sum_{i=1}^k \frac{(g_i MS_i)^2}{df_i}}
 \end{aligned}$$

Applying this approximation to estimating the random treatment effect, σ_α^2 .

$$\begin{aligned}
 E\{MS_{\text{Trt}}\} &= n\sigma_\alpha^2 + \sigma^2 & E\{MS_{\text{Err}}\} &= \sigma^2 & \Rightarrow & E\left\{\frac{MS_{\text{Trt}} - MS_{\text{Err}}}{n}\right\} = \sigma_\alpha^2 \\
 \Rightarrow \hat{\sigma}_\alpha^2 &= \frac{MS_{\text{Trt}} - MS_{\text{Err}}}{n} \\
 \Rightarrow MS_1 &= MS_{\text{Trt}} & MS_2 &= MS_{\text{Err}} & g_1 &= \frac{1}{n} & g_2 &= -\frac{1}{n} \\
 df_\alpha &\approx \frac{\left(\frac{MS_{\text{Trt}} - MS_{\text{Err}}}{n}\right)^2}{\left(\frac{\left(\frac{MS_{\text{Trt}}}{n}\right)^2}{g-1} + \frac{\left(\frac{-MS_{\text{Err}}}{n}\right)^2}{N-g}\right)} \\
 \Rightarrow \text{Approximate } (1-\alpha)100\% \text{ CI for } \sigma_\alpha^2 &: \left[\frac{\hat{df}_\alpha \hat{\sigma}_\alpha^2}{\chi_{df_\alpha, 1-\alpha/2}^2}, \frac{\hat{df}_\alpha \hat{\sigma}_\alpha^2}{\chi_{df_\alpha, \alpha/2}^2} \right]
 \end{aligned}$$

Note that negative estimates are possible (and likely if $\sigma_\alpha^2 \approx 0$). There are several options, including:

- Setting variance component to 0 (although it makes estimator biased).
- Removing that source of variation from the model.
- Using another estimation method, such as maximum likelihood.
- Leaving term as negative in other computations.

Estimation of the within treatment error variance is straightforward, and exactly the same for the fixed and random effects models.

$$\begin{aligned}
 \frac{df_{\text{Err}} MS_{\text{Err}}}{\sigma^2} &\sim \chi_{df_{\text{Err}}}^2 \equiv \chi_{N-g}^2 & \Rightarrow & P\left(\chi_{df_{\text{Err}}, \alpha/2}^2 \leq \frac{df_{\text{Err}} MS_{\text{Err}}}{\sigma^2} \leq \chi_{df_{\text{Err}}, 1-\alpha/2}^2\right) = 1-\alpha \\
 \Rightarrow (1-\alpha)100\% \text{ CI for } \sigma^2 &: \left[\frac{df_{\text{Err}} MS_{\text{Err}}}{\chi_{df_{\text{Err}}, 1-\alpha/2}^2}, \frac{df_{\text{Err}} MS_{\text{Err}}}{\chi_{df_{\text{Err}}, \alpha/2}^2} \right] \equiv \left[\frac{SS_{\text{Err}}}{\chi_{N-g, 1-\alpha/2}^2}, \frac{SS_{\text{Err}}}{\chi_{N-g, \alpha/2}^2} \right]
 \end{aligned}$$

To obtain a confidence interval for the intraclass correlation coefficient, we make use of the sampling distributions of the mean squares for treatments and error, and some algebraic manipulations.

$$W_1 = \frac{df_{\text{Trt}} MS_{\text{Trt}}}{n\sigma_\alpha^2 + \sigma^2} \sim \chi_{df_{\text{Trt}}}^2 \equiv \chi_{g-1}^2 \quad W_2 = \frac{df_{\text{Err}} MS_{\text{Err}}}{\sigma^2} \sim \chi_{df_{\text{Err}}}^2 \equiv \chi_{N-g}^2 \quad MS_{\text{Trt}} \perp MS_{\text{Err}}$$

$$\Rightarrow F = \frac{W_1/df_{\text{Trt}}}{W_2/df_{\text{Err}}} = \frac{\left[\frac{MS_{\text{Trt}}}{n\sigma_\alpha^2 + \sigma^2} \right]}{\left[\frac{MS_{\text{Err}}}{\sigma^2} \right]} \sim F_{g-1, N-g} \quad \text{Defining: } F^* = \frac{MS_{\text{Trt}}}{MS_{\text{Err}}}$$

$$\Rightarrow 1 - \alpha = P\left(F_{\alpha/2; g-1, N-g} \leq F^* \left(\frac{\sigma^2}{n\sigma_\alpha^2 + \sigma^2} \right) \leq F_{1-\alpha/2; g-1, N-g} \right) =$$

$$P\left(\left(\frac{1}{n} \right) \left(\frac{F^*}{F_{\alpha/2; g-1, N-g}} - 1 \right) \geq \frac{\sigma_\alpha^2}{\sigma^2} \geq \left(\frac{1}{n} \right) \left(\frac{F^*}{F_{1-\alpha/2; g-1, N-g}} - 1 \right) \right) =$$

$$= P\left(n \left(\frac{F^*}{F_{\alpha/2; g-1, N-g}} - 1 \right)^{-1} \leq \frac{\sigma^2}{\sigma_\alpha^2} \leq n \left(\frac{F^*}{F_{1-\alpha/2; g-1, N-g}} - 1 \right)^{-1} \right) =$$

$$= P\left(n \left(\frac{F^*}{F_{\alpha/2; g-1, N-g}} - 1 \right)^{-1} + 1 \leq \frac{\sigma^2}{\sigma_\alpha^2} + \frac{\sigma_\alpha^2}{\sigma_\alpha^2} \leq n \left(\frac{F^*}{F_{1-\alpha/2; g-1, N-g}} - 1 \right)^{-1} + 1 \right) =$$

$$= P\left(\left(n \left(\frac{F^*}{F_{\alpha/2; g-1, N-g}} - 1 \right)^{-1} + 1 \right)^{-1} \geq \frac{\sigma_\alpha^2}{\sigma_\alpha^2 + \sigma^2} = \rho_I \geq \left(n \left(\frac{F^*}{F_{1-\alpha/2; g-1, N-g}} - 1 \right)^{-1} + 1 \right)^{-1} \right)$$

$$\Rightarrow (1 - \alpha) 100\% \text{ CI for } \frac{\sigma_\alpha^2}{\sigma_\alpha^2 + \sigma^2} = \rho_I : \left[\left(n \left(\frac{F^*}{F_{1-\alpha/2; g-1, N-g}} - 1 \right)^{-1} + 1 \right)^{-1}, \left(n \left(\frac{F^*}{F_{\alpha/2; g-1, N-g}} - 1 \right)^{-1} + 1 \right)^{-1} \right]$$

Example: Alpha acids in Bales of 10 Varieties of Beer

A study was conducted to measure variation of alpha acids in a sample of $g = 10$ varieties of beer (Meilgard, (1960)). Samples of $n = 10$ bales were selected from each variety, and measurements of alpha acids were obtained from each bale. Note there are a total of $N = ng = 10(10) = 100$ measurements. Summary computations are given here. The overall mean is 579.61.

	Variety	Variety	Variety	Variety	Variety	Variety	Variety	Variety	Variety	Variety
	1	2	3	4	5	6	7	8	9	10
n	10	10	10	10	10	10	10	10	10	10
mean	709.9	523.9	659.9	463.5	844.8	590.2	411.8	510.9	537.3	543.9
SD	25.74	37.90	10.06	15.02	15.14	32.39	48.93	9.94	24.71	9.59

$$SS_{\text{Trt}} = 10 \left[(709.9 - 579.61)^2 + \dots + (543.9 - 579.61)^2 \right] = 1463916 \quad df_{\text{Trt}} = g - 1 = 10 - 1 = 9$$

$$SS_{\text{Err}} = (10 - 1) \left[25.74^2 + \dots + 9.59^2 \right] = 62101.9 \quad df_{\text{Err}} = g(n - 1) = 10(10 - 1) = 90$$

The Estimated mean, Analysis of Variance, F-test, variance component and intraclass correlation coefficient estimates are as follow.

$$\bar{y}_{..} = 579.61 \quad SE\{\bar{Y}_{..}\} = \sqrt{\frac{MS_{Trit}}{ng}} = \sqrt{\frac{162657.3}{10(10)}} = 40.33 \quad t_{1-.05/2; g-1} = t_{.975; 9} = 2.262$$

$$\Rightarrow 95\% \text{ CI for } \mu: 579.61 \pm 2.262(40.33) \equiv 579.61 \pm 91.23 \equiv [488.38, 670.84]$$

$$H_0: \sigma_\alpha^2 = 0 \quad H_A: \sigma_\alpha^2 > 0 \quad TS: F^* = \frac{MS_{Trit}}{MS_{Err}} = \frac{1463916/9}{62101.9/90} = \frac{162657.3}{690.02} = 235.73 \quad RR: F^* \geq F_{.95; 9, 90} = 1.986$$

$$\hat{\sigma}^2 = MS_{Err} = 690.02 \quad \chi_{.025, 90}^2 = 65.65 \quad \chi_{.975, 90}^2 = 118.14$$

$$95\% \text{ CI for } \sigma^2: \left[\frac{62101.9}{118.14}, \frac{62101.9}{65.65} \right] \equiv [525.68, 946.00] \quad 95\% \text{ CI for } \sigma: [22.93, 30.76]$$

$$\hat{\sigma}_\alpha^2 = \frac{MS_{Trit} - MS_{Err}}{n} = \frac{162657.3 - 690.02}{10} = 16196.73 \quad df_\alpha = \frac{(16196.73)^2}{\left(\frac{\left(\frac{162657.3}{10} \right)^2}{9} + \frac{\left(\frac{-690.02}{10} \right)^2}{90} \right)} = 8.92 \approx 9$$

$$\chi_{.025, 9}^2 = 2.22 \quad \chi_{.975, 9}^2 = 21.03$$

$$\text{Approximate } 95\% \text{ CI for } \sigma_\alpha^2: \left[\frac{9(16196.73)}{21.03}, \frac{9(16196.73)}{2.22} \right] \equiv [7662.95, 53981.31]$$

$$95\% \text{ CI for } \sigma_\alpha: [87.54, 232.34]$$

$$F_{.025; 9, 90} = 0.293 \quad F_{.975; 9, 90} = 2.259 \quad F^* = 235.73$$

$$95\% \text{ CI for } \rho_I = \frac{\sigma_\alpha^2}{\sigma_\alpha^2 + \sigma^2}: \left[\left(10 \left(\frac{235.73}{2.259} - 1 \right)^{-1} + 1 \right)^{-1}, \left(10 \left(\frac{235.73}{0.293} - 1 \right)^{-1} + 1 \right)^{-1} \right] \equiv [.9118, .9877]$$

R Program

```
hops <- read.table("http://www.stat.ufl.edu/~winner/data/hop_alphaacid.dat",
  header=F, col.names=c("variety", "rep.id", "alpha.acid"))
attach(hops)

variety <- factor(variety)

hops.mod1 <- aov(alpha.acid ~ variety)
summary(hops.mod1)

library(nlme)

hops.mod2 <- lme(fixed=alpha.acid~1, random=~1|variety)
summary(hops.mod2)

library(lme4)

hops.mod3 <- lmer(alpha.acid~1+(1|variety))
summary(hops.mod3)
confint(hops.mod3)
```

R Output

```
> hops.mod1 <- aov(alpha.acid ~ variety)
> summary(hops.mod1)
      Df Sum Sq Mean Sq F value Pr(>F)
variety  9 1463916  162657   235.7 <2e-16 ***
Residuals 90   62102    690
---
s.mod2 <- lme(fixed=alpha.acid~1,random=~1|variety)
> summary(hops.mod2)
Linear mixed-effects model fit by REML
Data: NULL
      AIC      BIC    logLik
 987.8546 995.64 -490.9273

Random effects:
Formula: ~1 | variety
(Intercept) Residual
StdDev:    127.2664 26.26825

Fixed effects: alpha.acid ~ 1
      Value Std.Error DF t-value p-value
(Intercept) 579.61   40.3308 90 14.3714    0

s.mod3 <- lmer(alpha.acid~1+(1|variety))
> summary(hops.mod3)
Linear mixed model fit by REML ['lmerMod']
Formula: alpha.acid ~ 1 + (1 | variety)

REML criterion at convergence: 981.9

Scaled residuals:
      Min       1Q   Median       3Q      Max
-2.63193 -0.46012  0.00626  0.56199  3.06408

Random effects:
Groups   Name      Variance Std.Dev.
variety (Intercept) 16197    127.27
Residual          690     26.27
Number of obs: 100, groups: variety, 10

Fixed effects:
      Estimate Std. Error t value
(Intercept)  579.61    40.33   14.37
> confint(hops.mod3)
Computing profile confidence intervals ...
      2.5 %    97.5 %
.sig01    82.11084 201.87602
.sigma    22.85233  30.62824
(Intercept) 496.80650 662.41350
```

Note that the **lmer** package in R uses different formulas for the confidence intervals than we have used here, giving slightly different intervals than we obtained based on Satterthwaite's approximation.

6.2. Distributional Properties and Power Computations – Matrix Form

Distribution of the response vector \mathbf{Y} is given below.

$$E\{Y_{ij}\} = \mu \quad \text{COV}\{Y_{ij}, Y_{i'j'}\} = \begin{cases} \sigma_\alpha^2 + \sigma^2 & i = i', j = j' \\ \sigma_\alpha^2 & i = i', j \neq j' \\ 0 & i \neq i', \forall j, j' \end{cases} \quad \mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_g \end{bmatrix} \quad \mathbf{Y}_i = \begin{bmatrix} Y_{i1} \\ Y_{i2} \\ \vdots \\ Y_{in} \end{bmatrix}$$

$$E\{\mathbf{Y}\} = \mu \begin{bmatrix} \mathbf{1}_n \\ \mathbf{1}_n \\ \vdots \\ \mathbf{1}_n \end{bmatrix} \quad V\{\mathbf{Y}\} = \mathbf{V} = \sigma^2 \begin{bmatrix} \mathbf{I}_n & \mathbf{0}_n & \cdots & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{I}_n & \cdots & \mathbf{0}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_n & \mathbf{0}_n & \cdots & \mathbf{I}_n \end{bmatrix} + \sigma_\alpha^2 \begin{bmatrix} \mathbf{J}_n & \mathbf{0}_n & \cdots & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{J}_n & \cdots & \mathbf{0}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_n & \mathbf{0}_n & \cdots & \mathbf{J}_n \end{bmatrix}$$

Treatment Sum of Squares (SS_{Trt})

$$SS_{\text{Trt}} = \sum_{i=1}^g \sum_{j=1}^n (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 = \mathbf{Y}' \left(\frac{1}{n} \begin{bmatrix} \mathbf{J}_n & \mathbf{0}_n & \cdots & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{J}_n & \cdots & \mathbf{0}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_n & \mathbf{0}_n & \cdots & \mathbf{J}_n \end{bmatrix} - \frac{1}{gn} \begin{bmatrix} \mathbf{J}_n & \mathbf{J}_n & \cdots & \mathbf{J}_n \\ \mathbf{J}_n & \mathbf{J}_n & \cdots & \mathbf{J}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{J}_n & \mathbf{J}_n & \cdots & \mathbf{J}_n \end{bmatrix} \right) \mathbf{Y}$$

Distribution of $\frac{SS_{\text{Trt}}}{\sigma^2 + n\sigma_\alpha^2}$

$$\mathbf{Y} \sim N(\boldsymbol{\mu}, \mathbf{V})$$

$$\frac{SS_{\text{Trt}}}{\sigma^2 + n\sigma_\alpha^2} = \mathbf{Y}' \mathbf{A} \mathbf{Y}$$

(Demonstration for $g = 3, n = 6, \sigma^2 = 64, \sigma_\alpha^2 = 16$ on EXCEL Spreadsheet below):

$$\mathbf{A} \mathbf{V} \mathbf{A} \mathbf{V} = \mathbf{A} \mathbf{V}$$

$$\text{trace}(\mathbf{A} \mathbf{V}) = 2 = g - 1$$

$$\boldsymbol{\mu}' \mathbf{A} \boldsymbol{\mu} = 0 \quad (\text{Columns of } \mathbf{A} \text{ sum to } 0)$$

$$\Rightarrow \frac{SS_{\text{Trt}}}{\sigma^2 + n\sigma_\alpha^2} \sim \chi_{g-1}^2$$

Distribution of $\frac{SS_{\text{Err}}}{\sigma^2}$

$$\mathbf{Y} \sim N(\boldsymbol{\mu}, \mathbf{V})$$

$$\frac{SS_{\text{Err}}}{\sigma^2} = \mathbf{Y}'\mathbf{B}\mathbf{Y}$$

(Demonstration for $g = 3, n = 6$ on EXCEL Spreadsheet below):

$$\mathbf{BVBV} = \mathbf{B}\mathbf{V}$$

$$\text{trace}(\mathbf{B}\mathbf{V}) = 15 = ng - g$$

$$\boldsymbol{\mu}'\mathbf{B}\boldsymbol{\mu} = 0 \quad (\text{Columns of } \mathbf{B} \text{ sum to } 0)$$

$$\Rightarrow \frac{SS_{\text{Err}}}{\sigma^2} \sim \chi_{ng-g}^2 \equiv \chi_{N-g}^2$$

BV																	
0.833	-0.167	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	0.833	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	-0.167	0.833	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	-0.167	-0.167	0.833	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	-0.167	-0.167	-0.167	0.833	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	-0.167	-0.167	-0.167	-0.167	0.833	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.833	-0.167	-0.167	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	0.833	-0.167	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	0.833	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	0.833	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	-0.167	0.833	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.833	-0.167	-0.167	-0.167	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	0.833	-0.167	-0.167	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	0.833	-0.167	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	0.833	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	-0.167	0.833

BVBV																	
0.833	-0.167	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	0.833	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	-0.167	0.833	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	-0.167	-0.167	0.833	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-0.167	-0.167	-0.167	-0.167	0.833	-0.167	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.833	-0.167	-0.167	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	0.833	-0.167	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	0.833	-0.167	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	0.833	-0.167	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	-0.167	0.833	-0.167	-0.167	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.833	-0.167	-0.167	-0.167	-0.167	-0.167	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	0.833	-0.167	-0.167	-0.167	-0.167	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	0.833	-0.167	-0.167	-0.167	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	0.833	-0.167	-0.167	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	0.833	-0.167
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.167	-0.167	-0.167	-0.167	0.833

Continue cycling n until desired power is obtained:

n	$s^2/(s^2+ns_a^2)$	F(.05)	F(s^*/s^{**})	1-B
2	0.6667	9.552	6.368	0.0832
3	0.5714	5.143	2.939	0.1289
4	0.5000	4.256	2.128	0.1751
5	0.4444	3.885	1.727	0.2192
...
14	0.2222	3.238	0.720	0.4933
15	0.2105	3.220	0.678	0.5132
...
39	0.0930	3.076	0.286	0.7517
...
49	0.0755	3.059	0.231	0.7941
50	0.0741	3.058	0.226	0.7976
51	0.0727	3.056	0.222	0.8010

Note that these are very high sample sizes, due to a very low intraclass correlation coefficient. For higher values of ρ_I , the sample sizes will be smaller. For this case, $\rho_I = \frac{\sigma_\alpha^2}{\sigma_\alpha^2 + \sigma^2} = \frac{16}{16 + 64} = \frac{16}{80} = 0.20$. When the variances are reversed, $\sigma_\alpha^2 = 64$ $\sigma^2 = 16$ $\rho_I = 0.80$ $1 - \beta = 0.8334$ when $n = 5$.

R Program

```
s2a <- 16
s2 <- 64
g <- 3
alpha <- 0.05
n_max <- 30

n_power <- matrix(rep(0, 5*(n_max-1)), ncol=5)

trtdf <- g-1
for (n in 2:n_max) {
  errdf <- g*(n-1)
  f_alpha <- qf(1-alpha, trtdf, errdf)
  power <- 1-pf((s2/(s2+n*s2a))*f_alpha, trtdf, errdf)
  n_power[n-1,] <- cbind(n, trtdf, errdf, f_alpha, power)
}

power.names <- c("n", "trtdf", "errdf", "f_0.05", "power")
colnames(n_power) <- power.names

n_power
```

Note that for these settings, n_{\max} would have to be increased for power to reach 0.80.

6.3. 2-Way and Higher Order Random Effects Model

When there are 2 or more factors, the Analysis of Variance is obtained as in the Fixed Effects models. However the expected mean squares change due to the effects being random variables, as opposed to fixed constants. Consider the 2-Way Random Effects model.

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk} \quad i=1, \dots, a; \quad j=1, \dots, b; \quad k=1, \dots, n \quad N = abn$$

$$\alpha_i \sim NID(0, \sigma_\alpha^2) \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \quad \{\alpha_i\} \perp \{\beta_j\} \perp \{(\alpha\beta)_{ij}\} \perp \{\varepsilon_{ijk}\}$$

$$E\{Y_{ijk}\} = E\{\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk}\} = \mu + 0 + 0 + 0 + 0 = \mu$$

$$V\{Y_{ijk}\} = V\{\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk}\} = 0 + \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 = \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2$$

$$\text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 & i=i', j=j', k=k' \\ \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 & i=i', j=j', k \neq k' \\ \sigma_\alpha^2 & i=i', j \neq j', \forall k, k' \\ \sigma_\beta^2 & i \neq i', j=j', \forall k, k' \\ 0 & i \neq i', j \neq j', \forall k, k' \end{cases}$$

Analysis of Variance:

$$SS_A = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\bar{Y}_{i..} - \bar{Y}...) ^2 = bn \sum_{i=1}^a \bar{Y}_{i..}^2 - abn \bar{Y}...^2 \quad df_A = a-1$$

$$SS_B = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\bar{Y}_{.j.} - \bar{Y}...) ^2 = an \sum_{j=1}^b \bar{Y}_{.j.}^2 - abn \bar{Y}...^2 \quad df_B = b-1$$

$$SS_{AB} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\bar{Y}_{ij.} - \bar{Y}_{i..} - \bar{Y}_{.j.} + \bar{Y}...) ^2 = n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2 - bn \sum_{i=1}^a \bar{Y}_{i..}^2 - an \sum_{j=1}^b \bar{Y}_{.j.}^2 + abn \bar{Y}...^2 \quad df_{AB} = (a-1)(b-1)$$

$$SS_{\text{Err}} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - \bar{Y}_{ij.}) ^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2 - n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2 \quad df_{\text{Err}} = ab(n-1)$$

The expected mean squares are derived below.

$$E\{Y_{ijk}\} = E\{\bar{Y}_{ij.}\} = E\{\bar{Y}_{i..}\} = E\{\bar{Y}_{.j.}\} = E\{\bar{Y}...\} = \mu$$

$$V\{Y_{ij.}\} = V\left\{\sum_{k=1}^n Y_{ijk}\right\} = \sum_{k=1}^n V\{Y_{ijk}\} + 2 \sum_{k=1}^{n-1} \sum_{k'=k+1}^n \text{COV}\{Y_{ijk}, Y_{ij'k'}\} = n(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + 2 \binom{n}{2} (\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2)$$

$$= n(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + n(n-1)(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2) = n^2 \sigma_\alpha^2 + n^2 \sigma_\beta^2 + n^2 \sigma_{\alpha\beta}^2 + n\sigma^2$$

$$V\{\bar{Y}_{ij.}\} = V\left\{\frac{1}{n} \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{n^2} V\{Y_{ij.}\} = \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n} \Rightarrow E\{\bar{Y}_{ij.}^2\} = \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n} + \mu^2$$

$$V\{Y_{i..}\} = V\left\{\sum_{j=1}^b \sum_{k=1}^n Y_{ijk}\right\} = \sum_{j=1}^b \sum_{k=1}^n V\{Y_{ijk}\} + 2 \sum_{j=1}^b \sum_{k=1}^{n-1} \sum_{k'=k+1}^n \text{COV}\{Y_{ijk}, Y_{ij'k'}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^n \sum_{k'=1}^n \text{COV}\{Y_{ijk}, Y_{ij'k'}\}$$

$$bn(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + bn(n-1)(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2) + b(b-1)n^2 \sigma_\alpha^2 = b^2 n^2 \sigma_\alpha^2 + bn^2(\sigma_\beta^2 + \sigma_{\alpha\beta}^2) + bn\sigma^2$$

$$V\{\bar{Y}_{i..}\} = \frac{1}{b^2 n^2} V\{Y_{i..}\} = \sigma_\alpha^2 + \frac{\sigma_\beta^2 + \sigma_{\alpha\beta}^2}{b} + \frac{\sigma^2}{bn} \Rightarrow E\{\bar{Y}_{i..}^2\} = \sigma_\alpha^2 + \frac{\sigma_\beta^2 + \sigma_{\alpha\beta}^2}{b} + \frac{\sigma^2}{bn} + \mu^2$$

By direct analogy: $E\{\bar{Y}_{.j.}^2\} = \sigma_\beta^2 + \frac{\sigma_\alpha^2 + \sigma_{\alpha\beta}^2}{a} + \frac{\sigma^2}{an} + \mu^2$

$$\begin{aligned}
V\{Y_{\dots}\} &= abn(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + abn(n-1)(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2) + ab(b-1)n^2\sigma_\alpha^2 + a(a-1)bn^2\sigma_\beta^2 + 0 \\
&= ab^2n^2\sigma_\alpha^2 + a^2bn^2\sigma_\beta^2 + abn^2\sigma_{\alpha\beta}^2 + abn\sigma^2 \Rightarrow V\{\bar{Y}_{\dots}\} = \frac{\sigma_\alpha^2}{a} + \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma^2}{abn} \\
\Rightarrow E\{\bar{Y}_{\dots}^2\} &= \frac{\sigma_\alpha^2}{a} + \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma^2}{abn} + \mu^2
\end{aligned}$$

$$1) E\left\{\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2\right\} = abn(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 + \mu^2) = abn\sigma_\alpha^2 + abn\sigma_\beta^2 + abn\sigma_{\alpha\beta}^2 + abn\sigma^2 + abn\mu^2$$

$$2) E\left\{n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij\cdot}^2\right\} = abn\left(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n} + \mu^2\right) = abn\sigma_\alpha^2 + abn\sigma_\beta^2 + abn\sigma_{\alpha\beta}^2 + ab\sigma^2 + abn\mu^2$$

$$3) E\left\{bn \sum_{i=1}^a \bar{Y}_{i\cdot\cdot}^2\right\} = abn\left(\sigma_\alpha^2 + \frac{\sigma_\beta^2 + \sigma_{\alpha\beta}^2}{b} + \frac{\sigma^2}{bn} + \mu^2\right) = abn\sigma_\alpha^2 + an\sigma_\beta^2 + an\sigma_{\alpha\beta}^2 + a\sigma^2 + abn\mu^2$$

$$4) E\left\{an \sum_{j=1}^b \bar{Y}_{\cdot j\cdot}^2\right\} = abn\left(\sigma_\beta^2 + \frac{\sigma_\alpha^2 + \sigma_{\alpha\beta}^2}{a} + \frac{\sigma^2}{an} + \mu^2\right) = bn\sigma_\alpha^2 + abn\sigma_\beta^2 + bn\sigma_{\alpha\beta}^2 + b\sigma^2 + abn\mu^2$$

$$5) E\left\{abn \bar{Y}_{\dots}^2\right\} = abn\left(\frac{\sigma_\alpha^2}{a} + \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \sigma^2 + \mu^2\right) = bn\sigma_\alpha^2 + an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2 + abn\mu^2$$

Analysis of Variance:

$$E\{SS_A\} = E\left\{bn \sum_{i=1}^a \bar{Y}_{i\cdot\cdot}^2\right\} - E\left\{abn \bar{Y}_{\dots}^2\right\} = (a-1)bn\sigma_\alpha^2 + (a-1)n\sigma_{\alpha\beta}^2 + (a-1)\sigma^2$$

$$df_A = a-1 \Rightarrow E\{MS_A\} = bn\sigma_\alpha^2 + n\sigma_{\alpha\beta}^2 + \sigma^2$$

$$E\{SS_B\} = E\left\{an \sum_{j=1}^b \bar{Y}_{\cdot j\cdot}^2\right\} - E\left\{abn \bar{Y}_{\dots}^2\right\} = a(b-1)n\sigma_\beta^2 + (b-1)n\sigma_{\alpha\beta}^2 + (b-1)\sigma^2$$

$$df_B = b-1 \Rightarrow E\{MS_B\} = an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2$$

$$E\{SS_{AB}\} = E\left\{n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij\cdot}^2\right\} - E\left\{bn \sum_{i=1}^a \bar{Y}_{i\cdot\cdot}^2\right\} - E\left\{an \sum_{j=1}^b \bar{Y}_{\cdot j\cdot}^2\right\} + E\left\{abn \bar{Y}_{\dots}^2\right\} =$$

$$= (a-1)(b-1)n\sigma_{\alpha\beta}^2 + (a-1)(b-1)\sigma^2$$

$$df_{AB} = (a-1)(b-1) \Rightarrow E\{MS_{AB}\} = n\sigma_{\alpha\beta}^2 + \sigma^2$$

$$E\{SS_{Err}\} = E\left\{\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2\right\} - E\left\{n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij\cdot}^2\right\} = ab(n-1)\sigma^2 \quad df_{Err} = ab(n-1) \Rightarrow E\{MS_{Err}\} = \sigma^2$$

$$V\{\bar{Y}_{\dots}\} = \frac{\sigma_\alpha^2}{a} + \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma^2}{abn} = \frac{1}{abn} E\{MS_A + MS_B - MS_{AB}\} \Rightarrow \hat{SE}\{\bar{Y}_{\dots}\} = \sqrt{\frac{MS_A + MS_B - MS_{AB}}{abn}}$$

Note that unlike for the Fixed Effects model, the expected mean squares for the main effects in the Random Effects model depend on interactions that contain the main effects. This leads to the following methods for estimating and testing variance components that make use of Satterthwaite's approximation, as well as estimating the population mean.

$$E\{MS_{\text{Err}}\} = \sigma^2 \Rightarrow \hat{\sigma}^2 = MS_{\text{Err}}$$

$$E\{MS_{AB}\} = \sigma^2 + n\sigma_{\alpha\beta}^2 \Rightarrow \hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{AB} - MS_{\text{Err}}}{n}$$

$$E\{MS_A\} = \sigma^2 + n\sigma_{\alpha\beta}^2 + bn\sigma_\alpha^2 \Rightarrow \hat{\sigma}_\alpha^2 = \frac{MS_A - MS_{AB}}{bn}$$

$$E\{MS_B\} = \sigma^2 + n\sigma_{\alpha\beta}^2 + an\sigma_\beta^2 \Rightarrow \hat{\sigma}_\beta^2 = \frac{MS_B - MS_{AB}}{an}$$

Satterthwaite Approximation for Degrees of Freedom: $df_* = \frac{\left(\sum_{i=1}^k g_i MS_i\right)^2}{\sum_{i=1}^k \frac{(g_i MS_i)^2}{df_i}}$ where $\hat{\sigma}_*^2 = \sum_{i=1}^k g_i MS_i$

Approximate $(1-\alpha)100\%$ CI for σ_*^2 : $\left[\frac{df_* \hat{\sigma}_*^2}{\chi_{1-\alpha/2; df}^2}, \frac{df_* \hat{\sigma}_*^2}{\chi_{\alpha/2; df}^2} \right]$

$H_0^{AB} : \sigma_{\alpha\beta}^2 = 0$ $H_A^{AB} : \sigma_{\alpha\beta}^2 > 0$ Test Stat: $F_{AB} = \frac{MS_{AB}}{MS_{\text{Err}}}$ Rejection Region: $F_{AB} \geq F_{1-\alpha; (a-1)(b-1), ab(n-1)}$

$H_0^A : \sigma_\alpha^2 = 0$ $H_A^A : \sigma_\alpha^2 > 0$ Test Stat: $F_A = \frac{MS_A}{MS_{AB}}$ Rejection Region: $F_A \geq F_{1-\alpha; a-1, (a-1)(b-1)}$

$H_0^B : \sigma_\beta^2 = 0$ $H_A^B : \sigma_\beta^2 > 0$ Test Stat: $F_B = \frac{MS_B}{MS_{AB}}$ Rejection Region: $F_B \geq F_{1-\alpha; b-1, (a-1)(b-1)}$

Approximate $(1-\alpha)100\%$ CI for μ : $\bar{Y} \dots \pm t_{1-\alpha/2; df_\mu} \sqrt{\frac{MS_A + MS_B - MS_{AB}}{abn}}$

Example: Repeatability and Reproducibility of Drill Hole Measurements

An experiment was conducted with a sample of $a = 10$ drilled wood holes being measured by a sample of $b = 3$ operators on each of $n = 3$ replicates (Li and Al-Refaie (2008)). Note that each operator used the same measuring instrument, and the holes were measured in random orders within the separate replicates. In the Gage Repeatability and Reproducibility model, the error variance (same hole, same operator) represents the **repeatability** variance. The sum of the operator and hole by operator variance components represents the **reproducibility** variance. The hole variance component is the “**product**” variance (as these studies are often using manufactured products as factor A). The model is as follows.

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk} \quad i = 1, \dots, 10; j = 1, 2, 3; k = 1, 2, 3$$

$$\alpha_i \sim NID(0, \sigma_\alpha^2) \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \quad \{\alpha_i\} \perp \{\beta_j\} \perp \{(\alpha\beta)_{ij}\} \perp \{\varepsilon_{ijk}\}$$

$$\sigma_{\text{Total}}^2 = \sigma_y^2 = \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 \quad \sigma_{\text{Product}}^2 = \sigma_\alpha^2 \quad \sigma_{\text{Reproducibility}}^2 = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 \quad \sigma_{\text{Repeatability}}^2 = \sigma^2$$

$$\sigma_{\text{Gage}}^2 = \sigma_{\text{Reproducibility}}^2 + \sigma_{\text{Repeatability}}^2$$

Data are in millimeters, and have been multiplied by 10 to make numbers easier to work with, as many of the mean squares and variances are very small in the original units. The ANOVA table is given below.

Source	df	SS	MS	F	F(.05)	P
Drill Hole (A)	9	25.9721	2.8858	25.8058	2.4563	0.0000
Operator (B)	2	0.7716	0.3858	3.4498	3.5546	0.0539
A*B	18	2.0129	0.1118	1.6746	1.7784	0.0703
Error	60	4.0067	0.0668			
Total	89	32.7632	0.3681			

The tests for the variance components are as follow:

$$H_0^{AB} : \sigma_{\alpha\beta}^2 = 0 \quad H_A^{AB} : \sigma_{\alpha\beta}^2 > 0 \quad TS : F_{AB} = \frac{MS_{AB}}{MS_{\text{Err}}} = \frac{0.1118}{0.0668} = 1.6746 \quad RR : F_{AB} \geq F_{.95;18,60} = 1.7784$$

$$H_0^A : \sigma_\alpha^2 = 0 \quad H_A^A : \sigma_\alpha^2 > 0 \quad TS : F_A = \frac{MS_A}{MS_{AB}} = \frac{2.8858}{0.1118} = 25.8058 \quad RR : F_A \geq F_{.95;9,18} = 2.4563$$

$$H_0^B : \sigma_\beta^2 = 0 \quad H_A^B : \sigma_\beta^2 > 0 \quad TS : F_B = \frac{MS_B}{MS_{AB}} = \frac{0.3858}{0.1118} = 3.4498 \quad RR : F_B \geq F_{.95;2,18} = 3.5546$$

The operator (B) and Hole x Operator (AB) variance components are not significant at the 0.05 significance level, but both have p-values below 0.10. Next, estimate the variance components and Gage R&R variances.

$$E\{MS_{Err}\} = \sigma^2 \Rightarrow \hat{\sigma}^2 = \sigma_{\text{Repeatability}}^2 = MS_{Err} = 0.06678$$

$$E\{MS_{AB}\} = \sigma^2 + n\sigma_{\alpha\beta}^2 \Rightarrow \hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{AB} - MS_{Err}}{n} = \frac{0.11183 - 0.06678}{3} = 0.01502$$

$$E\{MS_B\} = \sigma^2 + n\sigma_{\alpha\beta}^2 + an\sigma_{\beta}^2 \Rightarrow \hat{\sigma}_{\beta}^2 = \frac{MS_B - MS_{AB}}{an} = \frac{0.38578 - 0.11183}{10(3)} = 0.00913$$

$$E\{MS_A\} = \sigma^2 + n\sigma_{\alpha\beta}^2 + bn\sigma_{\alpha}^2 \Rightarrow \hat{\sigma}_{\alpha}^2 = \frac{MS_A - MS_{AB}}{bn} = \frac{2.88579 - 0.11183}{3(3)} = 0.30822$$

$$\hat{\sigma}_{\text{Reproducibility}}^2 = \hat{\sigma}_{\beta}^2 + \hat{\sigma}_{\alpha\beta}^2 = 0.00913 + 0.01502 = 0.02415$$

$$\hat{\sigma}_{\text{Gage}}^2 = \hat{\sigma}_{\text{Reproducibility}}^2 + \hat{\sigma}_{\text{Repeatability}}^2 = 0.02415 + 0.06678 = 0.09093$$

We next obtain a confidence interval for the repeatability (error) variance, and approximate confidence intervals for the remaining variance components and the mean, based on Satterthwaite's approximation.

$$MS_{Err} = 0.06678 \quad df_{Err} = 10(3)(3-1) = 60 \quad \chi_{.025;60}^2 = 40.482 \quad \chi_{.975;60}^2 = 83.298$$

$$\Rightarrow 95\% \text{ CI for } \sigma^2 = \sigma_{\text{Repeatability}}^2 :$$

$$\left[\frac{df_{Err} MS_{Err}}{\chi_{.975;60}^2}, \frac{df_{Err} MS_{Err}}{\chi_{.025;60}^2} \right] \equiv \left[\frac{60(0.06678)}{83.298}, \frac{60(0.06678)}{40.482} \right] \equiv [0.0481, 0.0990]$$

$$95\% \text{ CI for } \sigma = \sigma_{\text{Repeatability}} : [0.2193, .3146]$$

$$\hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{AB} - MS_{Err}}{n} = \frac{0.11183 - 0.06678}{3} = 0.01502 \Rightarrow df_{\alpha\beta} = \frac{(0.01502)^2}{\left(\frac{\left(\frac{0.11183}{3}\right)^2}{18} + \frac{\left(\frac{-0.06678}{3}\right)^2}{60} \right)} = 2.64$$

$$\chi_{.025;2.64}^2 = 0.143 \quad \chi_{.975;2.64}^2 = 8.665 \Rightarrow$$

$$\text{Approx. 95\% CI for } \sigma_{\alpha\beta}^2 \equiv \left[\frac{2.64(0.01502)}{8.665}, \frac{2.64(0.01502)}{0.143} \right] \equiv [0.00458, 0.27729] \quad \sigma_{\alpha\beta} : [0.06768, 0.52658]$$

$$\hat{\sigma}_\beta^2 = \frac{MS_B - MS_{AB}}{an} = \frac{0.38578 - 0.11183}{10(3)} = 0.00913 \Rightarrow \hat{df}_\beta = \frac{(0.00913)^2}{\left(\frac{\left(\frac{0.38578}{30}\right)^2}{2} + \frac{\left(\frac{-0.11183}{30}\right)^2}{18} \right)} = 1.00$$

$$\chi_{0.025;1}^2 = 0.00098 \quad \chi_{0.975;1}^2 = 5.024 \Rightarrow$$

$$\text{Approx. 95\% CI for } \sigma_\beta^2 \equiv \left[\frac{1.00(0.00913)}{5.024}, \frac{1.00(0.00913)}{0.00098} \right] \equiv [0.00182, 9.316] \quad \sigma_\beta : [0.04263, 3.052]$$

$$\hat{\sigma}_\alpha^2 = \frac{MS_A - MS_{AB}}{bn} = \frac{2.88579 - 0.11183}{3(3)} = 0.30822 \Rightarrow \hat{df}_\alpha = \frac{(0.30822)^2}{\left(\frac{\left(\frac{2.88579}{9}\right)^2}{9} + \frac{\left(\frac{-0.11183}{9}\right)^2}{18} \right)} = 8.31$$

$$\chi_{0.025;8.31}^2 = 2.338 \quad \chi_{0.975;8.31}^2 = 17.999 \Rightarrow$$

$$\text{Approx. 95\% CI for } \sigma_\alpha^2 \equiv \left[\frac{8.31(0.30822)}{17.999}, \frac{8.31(0.30822)}{2.338} \right] \equiv [0.14230, 1.0955] \quad \sigma_\alpha : [0.37723, 1.0467]$$

$$\hat{V}\left\{\hat{\mu}\right\} = \hat{V}\left\{\bar{Y}_{\dots}\right\} = \frac{MS_A + MS_B - MS_{AB}}{abn} = \frac{2.88579 + 0.38578 - 0.11183}{10(3)(3)} = 0.03511 \Rightarrow \hat{V}\left\{\hat{\mu}\right\} = \sqrt{0.03511} = 0.18738$$

$$\Rightarrow \hat{df}_\mu = \frac{(0.03511)^2}{\left(\frac{\left(\frac{2.88579}{90}\right)^2}{9} + \frac{\left(\frac{0.38578}{90}\right)^2}{2} + \frac{\left(\frac{-0.11183}{90}\right)^2}{18} \right)} = 9.98 \quad t_{0.975;9.98} = 2.229$$

$$\text{Approx. 95\% CI for } \mu \equiv 256.1544 \pm 2.229(0.18738) \equiv 256.1544 \pm 0.4177 \equiv [255.7367, 256.5721]$$

R Program

```

gage <- read.csv("http://www.stat.ufl.edu/~winner/data/wood_drill_gage.csv",
  header=T)
attach(gage); names(gage)

Part <- factor(Part)
Operator <- factor(Operator)
Ymeas <- 10*Ymeas

gage.mod1 <- aov(Ymeas ~ Part*Operator)
summary(gage.mod1)

library(lme4)

gage.mod2 <- lmer(Ymeas ~1 + (1|Part) + (1|Operator) + (1|Part:Operator))
summary(gage.mod2)
confint(gage.mod2)

```


R Output

```
> gage.mod1 <- aov(Ymeas ~ Part*Operator)
> summary(gage.mod1)
          Df Sum Sq Mean Sq F value Pr(>F)
Part          9  25.972   2.8858  43.215 < 2e-16 ***
Operator       2   0.772   0.3858   5.777 0.00508 **
Part:Operator  18   2.013   0.1118   1.675 0.07026 .
Residuals     60   4.007   0.0668
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
> library(lme4)
>
> gage.mod2 <- lmer(Ymeas ~1 + (1|Part) + (1|Operator) + (1|Part:Operator))
> summary(gage.mod2)
Linear mixed model fit by REML ['lmerMod']
Formula: Ymeas ~ 1 + (1 | Part) + (1 | Operator) + (1 | Part:Operator)

REML criterion at convergence: 62.9

Scaled residuals:
    Min       1Q   Median       3Q      Max
-1.59675 -0.70766 -0.01723  0.62462  1.90364

Random effects:
Groups             Name                Variance Std.Dev.
Part:Operator      (Intercept) 0.015016 0.12254
Part               (Intercept) 0.308218 0.55517
Operator           (Intercept) 0.009132 0.09556
Residual                   0.066778 0.25841
Number of obs: 90, groups: Part:Operator, 30; Part, 10; Operator, 3

Fixed effects:
              Estimate Std. Error t value
(Intercept) 256.1544    0.1874   1367
> confint(gage.mod2)
Computing profile confidence intervals ...
              2.5 %       97.5 %
.sig01       0.0000000 0.2369451
.sig02       0.3499637 0.8943210
.sig03       0.0000000 0.3731768
.sigma       0.2182646 0.3125672
(Intercept) 255.7714170 256.5374719
>
```

Note that the confidence intervals computed in the **lme4** package are not computed in the same manner as was done above. In particular, for the degrees of freedom associated with the mean, the package appears to be using $df_{\mu} = 30$.

For the 3-Way balanced random effects model, we obtain the following expected mean squares, and tests and estimates for the variance components.

$$Y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + \varepsilon_{ijkl} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c; l = 1, \dots, n$$
$$\alpha_i \sim NID(0, \sigma_{\alpha}^2) \quad \beta_j \sim NID(0, \sigma_{\beta}^2) \quad \gamma_k \sim NID(0, \sigma_{\gamma}^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2) \quad (\alpha\gamma)_{ik} \sim NID(0, \sigma_{\alpha\gamma}^2)$$
$$(\beta\gamma)_{jk} \sim NID(0, \sigma_{\beta\gamma}^2) \quad (\alpha\beta\gamma)_{ijk} \sim NID(0, \sigma_{\alpha\beta\gamma}^2) \quad \varepsilon_{ijkl} \sim NID(0, \sigma^2) \quad \text{All random effects independent}$$

Factor/Interaction	df	Expected Mean Square
A	$a-1$	$\sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + cn\sigma_{\alpha\beta}^2 + bn\sigma_{\alpha\gamma}^2 + bcn\sigma_{\alpha}^2$
B	$b-1$	$\sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + cn\sigma_{\alpha\beta}^2 + an\sigma_{\beta\gamma}^2 + acn\sigma_{\beta}^2$
C	$c-1$	$\sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + bn\sigma_{\alpha\gamma}^2 + an\sigma_{\beta\gamma}^2 + abn\sigma_{\gamma}^2$
AB	$(a-1)(b-1)$	$\sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + cn\sigma_{\alpha\beta}^2$
AC	$(a-1)(c-1)$	$\sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + bn\sigma_{\alpha\gamma}^2$
BC	$(b-1)(c-1)$	$\sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + an\sigma_{\beta\gamma}^2$
ABC	$(a-1)(b-1)(c-1)$	$\sigma^2 + n\sigma_{\alpha\beta\gamma}^2$
Error	$abc(n-1)$	σ^2

$$H_0^{ABC} : \sigma_{\alpha\beta\gamma}^2 = 0 \quad H_A^{ABC} : \sigma_{\alpha\beta\gamma}^2 > 0 \quad TS : F_{ABC} = \frac{MS_{ABC}}{MS_{Err}} \quad RR : F_{ABC} \geq F_{1-\alpha; (a-1)(b-1)(c-1), abc(n-1)} \quad \hat{\sigma}_{\alpha\beta\gamma}^2 = \frac{MS_{ABC} - MS_{Err}}{n}$$

$$H_0^{AB} : \sigma_{\alpha\beta}^2 = 0 \quad H_A^{AB} : \sigma_{\alpha\beta}^2 > 0 \quad TS : F_{AB} = \frac{MS_{AB}}{MS_{ABC}} \quad RR : F_{AB} \geq F_{1-\alpha; (a-1)(b-1), (a-1)(b-1)(c-1)} \quad \hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{AB} - MS_{ABC}}{cn}$$

$$H_0^A : \sigma_{\alpha}^2 = 0 \quad H_A^A : \sigma_{\alpha}^2 > 0 \quad TS : F_A = \frac{MS_A + MS_{ABC}}{MS_{AB} + MS_{AC}} \quad RR : F_A \geq F_{1-\alpha; df1, df2} \quad \hat{\sigma}_{\alpha}^2 = \frac{MS_A - MS_{AB} - MS_{AC} + MS_{ABC}}{bcn}$$

$$V\{\bar{Y} \dots\} = \frac{\sigma_{\alpha}^2}{a} + \frac{\sigma_{\beta}^2}{b} + \frac{\sigma_{\gamma}^2}{c} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_{\alpha\gamma}^2}{ac} + \frac{\sigma_{\beta\gamma}^2}{bc} + \frac{\sigma_{\alpha\beta\gamma}^2}{abc} + \frac{\sigma^2}{abcn}$$

$$\Rightarrow \hat{SE}\{\bar{Y} \dots\} = \sqrt{\frac{MS_A + MS_B + MS_C - MS_{AB} - MS_{AC} - MS_{BC} + MS_{ABC}}{abcn}}$$

There are obvious analogies for the estimates and tests for the remaining main effects and 2-factor interactions.

Example: Reliability in Measuring Inversion of Subtalar Joint with Biometer

A study (Freeman, *et al* (2007)) studied the use of a Phillips Biometer to measure inversion of the subtalar joint in feet. There were 3 factors: (A = Subject, $a = 12$), (B = Tester, $b = 2$), (C = Day, $c = 2$). There were $n = 2$ replicates per treatment. Thus $N = abc n = 96$. Note the study also measured eversion, which is not included here. The Analysis of Variance is given below.

Source	df	SS	MS
Subject	11	1903.5313	173.0483
Tester	1	0.8438	0.8438
Day	1	11.3438	11.3438
SxT	11	114.0313	10.3665
SxD	11	34.0313	3.0938
TxD	1	1.7604	1.7604
SxTxD	11	8.6146	0.7831
Error	48	15.5000	0.3229
Total	95	2089.6563	

Tests and estimates for the variance components are given below.

$$H_0^{STD} : \sigma_{\alpha\beta\gamma}^2 = 0 \quad H_A^{STD} : \sigma_{\alpha\beta\gamma}^2 > 0 \quad TS : F_{STD} = \frac{MS_{STD}}{MS_{Err}} = \frac{0.7831}{0.3229} = 2.4252 \quad RR : F_{STD} \geq F_{.95;11,48} = 1.9946$$

$$\hat{\sigma}_{\alpha\beta\gamma}^2 = \frac{MS_{STD} - MS_{Err}}{n} = \frac{0.7831 - 0.3229}{2} = 0.2301$$

$$H_0^{ST} : \sigma_{\alpha\beta}^2 = 0 \quad H_A^{ST} : \sigma_{\alpha\beta}^2 > 0 \quad TS : F_{ST} = \frac{MS_{ST}}{MS_{STD}} = \frac{10.3665}{0.7831} = 13.237 \quad RR : F_{ST} \geq F_{.95;11,11} = 2.818$$

$$\hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{ST} - MS_{STD}}{cn} = \frac{10.3665 - 0.7831}{2(2)} = 2.3959$$

$$H_0^{SD} : \sigma_{\alpha\gamma}^2 = 0 \quad H_A^{SD} : \sigma_{\alpha\gamma}^2 > 0 \quad TS : F_{SD} = \frac{MS_{SD}}{MS_{STD}} = \frac{3.0938}{0.7831} = 3.9504 \quad RR : F_{SD} \geq F_{.95;11,11} = 2.818$$

$$\hat{\sigma}_{\alpha\gamma}^2 = \frac{MS_{SD} - MS_{STD}}{bn} = \frac{3.0938 - 0.7831}{2(2)} = 0.5777$$

$$H_0^{TD} : \sigma_{\beta\gamma}^2 = 0 \quad H_A^{TD} : \sigma_{\beta\gamma}^2 > 0 \quad TS : F_{TD} = \frac{MS_{TD}}{MS_{STD}} = \frac{1.7604}{0.7831} = 2.2479 \quad RR : F_{TD} \geq F_{.95;1,11} = 4.8443$$

$$\hat{\sigma}_{\beta\gamma}^2 = \frac{MS_{TD} - MS_{STD}}{an} = \frac{1.7604 - 0.7831}{12(2)} = 0.0407$$

$$H_0^S : \sigma_\alpha^2 = 0 \quad H_A^S : \sigma_\alpha^2 > 0 \quad TS : F_S = \frac{MS_S + MS_{STD}}{MS_{ST} + MS_{SD}} = \frac{173.0483 + 0.7831}{10.3665 + 3.0938} = \frac{173.8314}{13.4603} = 12.9144$$

$$df_1 = \frac{(173.8314)^2}{\left(\frac{(173.0483)^2}{11} + \frac{(0.7831)^2}{11} \right)} = 11.10 \quad df_2 = \frac{(13.4603)^2}{\left(\frac{(10.3665)^2}{11} + \frac{(3.0938)^2}{11} \right)} = 17.03 \quad RR : F_S \geq F_{0.95; 11, 10, 17, 0.3} = 2.4079$$

$$\hat{\sigma}_\alpha^2 = \frac{MS_S - MS_{ST} - MS_{SD} + MS_{STD}}{bcn} = \frac{173.0483 - 10.3665 - 3.0938 + 0.7831}{2(2)(2)} = 20.0464$$

$$H_0^T : \sigma_\beta^2 = 0 \quad H_A^T : \sigma_\beta^2 > 0 \quad TS : F_T = \frac{MS_T + MS_{STD}}{MS_{ST} + MS_{TD}} = \frac{0.8438 + 0.7831}{10.3665 + 2.7604} = \frac{1.6269}{13.1269} = 0.1239$$

$$df_1 = \frac{(1.6269)^2}{\left(\frac{(0.8438)^2}{1} + \frac{(0.7831)^2}{11} \right)} = 3.45 \quad df_2 = \frac{(13.1269)^2}{\left(\frac{(10.3665)^2}{11} + \frac{(2.7604)^2}{1} \right)} = 9.91 \quad RR : F_T \geq F_{0.95; 3, 45, 9, 91} = 3.6038$$

$$\hat{\sigma}_\beta^2 = \frac{MS_T - MS_{ST} - MS_{TD} + MS_{STD}}{acn} = \frac{0.8438 - 10.3665 - 2.7604 + 0.7831}{12(2)(2)} = -0.24$$

$$H_0^D : \sigma_\gamma^2 = 0 \quad H_A^D : \sigma_\gamma^2 > 0 \quad TS : F_D = \frac{MS_D + MS_{STD}}{MS_{SD} + MS_{TD}} = \frac{11.3438 + 0.7831}{3.0938 + 2.7604} = \frac{12.1269}{5.8542} = 2.0715$$

$$df_1 = \frac{(12.1269)^2}{\left(\frac{(11.3438)^2}{1} + \frac{(0.7831)^2}{11} \right)} = 1.14 \quad df_2 = \frac{(5.8542)^2}{\left(\frac{(3.0938)^2}{11} + \frac{(2.7604)^2}{1} \right)} = 4.04 \quad RR : F_D \geq F_{0.95; 1, 14, 4, 04} = 7.4919$$

$$\hat{\sigma}_\gamma^2 = \frac{MS_D - MS_{SD} - MS_{TD} + MS_{STD}}{abn} = \frac{11.3438 - 3.0938 - 2.7604 + 0.7831}{12(2)(2)} = 0.1307$$

$$\hat{\sigma}^2 = MS_{Err} = 0.3229$$

$$SE\{\bar{Y} \dots\} = \sqrt{\frac{173.0483 + 0.8438 + 11.3438 - 10.3665 - 3.0938 - 1.7604 + 0.7831}{12(2)(2)(2)}} = 1.3338$$

Note that by far most of the variation is due to between subjects variation.

R Program

```
foot <- read.table("http://www.stat.ufl.edu/~winner/data/biometer_foot.dat",
  header=F, col.names=c("subject", "inv_eve", "tester", "day", "trial_num", "angle"))
attach(foot)

subject_inv <- subject[inv_eve==1]
tester_inv <- tester[inv_eve==1]
day_inv <- day[inv_eve==1]
angle_inv <- angle[inv_eve==1]

subject_inv <- factor(subject_inv)
tester_inv <- factor(tester_inv)
day_inv <- factor(day_inv)

foot.mod1 <- aov(angle_inv ~ subject_inv*tester_inv*day_inv)
anova(foot.mod1)

library(lme4)
foot.mod2 <- lmer(angle_inv ~ 1 + (1|subject_inv) + (1|tester_inv) + (1|day_inv) +
  (1|subject_inv:tester_inv) + (1|subject_inv:day_inv) + (1|tester_inv:day_inv) +
  (1|subject_inv:tester_inv:day_inv))
summary(foot.mod2)
```

R Output

```
> foot.mod1 <- aov(angle_inv ~ subject_inv*tester_inv*day_inv)
> anova(foot.mod1)
Analysis of Variance Table

Response: angle_inv

```

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
subject_inv	11	1903.53	173.048	535.8915	< 2.2e-16	***
tester_inv	1	0.84	0.844	2.6129	0.11255	
day_inv	1	11.34	11.344	35.1290	3.241e-07	***
subject_inv:tester_inv	11	114.03	10.366	32.1026	< 2.2e-16	***
subject_inv:day_inv	11	34.03	3.094	9.5806	7.863e-09	***
tester_inv:day_inv	1	1.76	1.760	5.4516	0.02378	*
subject_inv:tester_inv:day_inv	11	8.61	0.783	2.4252	0.01717	*
Residuals	48	15.50	0.323			

```
Linear mixed model fit by REML ['lmerMod']
Formula:
angle_inv ~ 1 + (1 | subject_inv) + (1 | tester_inv) + (1 | day_inv) +
(1 | subject_inv:tester_inv) + (1 | subject_inv:day_inv) +
(1 | tester_inv:day_inv) + (1 | subject_inv:tester_inv:day_inv)

REML criterion at convergence: 316.5

Scaled residuals:
    Min       1Q   Median       3Q      Max
-1.76446 -0.65678 -0.01183  0.66413  2.06895

Random effects:
Groups                Name                Variance Std.Dev.
subject_inv:tester_inv:day_inv (Intercept) 2.326e-01 4.823e-01
subject_inv:day_inv      (Intercept) 5.764e-01 7.592e-01
subject_inv:tester_inv   (Intercept) 2.208e+00 1.486e+00
subject_inv              (Intercept) 2.014e+01 4.488e+00
tester_inv:day_inv       (Intercept) 3.167e-02 1.780e-01
day_inv                  (Intercept) 1.560e-01 3.950e-01
tester_inv               (Intercept) 9.966e-21 9.983e-11
Residual                 3.229e-01 5.683e-01

Number of obs: 96, groups:
subject_inv:tester_inv:day_inv, 48; subject_inv:day_inv, 24; subject_inv:tester_inv, 24;
subject_inv, 12; tester_inv:day_inv, 4; day_inv, 2; tester_inv, 2

Fixed effects:
              Estimate Std. Error t value
(Intercept)   19.344      1.374    14.08
```

Data Sources:

M. Meilgaard (1960). "Hop Analysis, Cohumulone Factor and the Bitterness of Beer: Review and Critical Evaluation," *Journal of the Institute of Brewing*, Vol. 66, Issue 1, pp. 35-50.

M-H. C. Li and A. Al-Refaie (2008). "Improving Wooden Parts' Quality by Adopting DMAIC Procedure," *Quality and Reliability Engineering International*, Vol. 24, pp. 351-360.

D. Freeman, A. Jaeger, R. Johnson, S. Geletta, K. Cooper, P. Toney (2007). "Reliability Study of the Phillips Biometer for the Measurement of Subtalar Joint Range of Motion," *The Foot*, Vol. 17, pp. 102-110.

Chapter 7 – Designs with Fixed and Random Effects

7.1. 2-Way Mixed Effects Model

Many models contain both fixed and random effects, and are referred to as **Mixed Models**. Thus, some factor(s) will have all levels of interest, while other factor(s) will have a sample from a population of levels in the experiment. Note that interactions between fixed and random factors will be random. There are two ways these interactions can be handled, reflected in the 2-Way mixed model given below. We will label the fixed factor as factor A, and the random factor as factor B.

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n$$

$\mu \equiv$ Overall Population mean

$\alpha_i \equiv$ Effect of i^{th} level of factor A: $\sum_{i=1}^a \alpha_i = 0$

$\beta_j \equiv$ Effect of j^{th} level of Factor B: $\beta_j \sim NID(0, \sigma_\beta^2)$

$(\alpha\beta)_{ij} \equiv$ Interaction Effect of i^{th} level of A and j^{th} level of B: $(\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2)$

$\varepsilon_{ijk} \equiv$ Random Error term: $\varepsilon_{ijk} \sim NID(0, \sigma^2)$

$\{\beta_j\} \perp \{(\alpha\beta)_{ij}\} \perp \{\varepsilon_{ijk}\}$

Note that this is an Unrestricted Model (wrt interaction effect). This is the model fit in SAS and R.

Restricted Model (interaction effects sum to zero over Factor A levels for all Factor B levels):

$$Y_{ijk} = \mu + \alpha_i + \left(\beta_j + \overline{(\alpha\beta)_{\cdot j}}\right) + \left((\alpha\beta)_{ij} - \overline{(\alpha\beta)_{\cdot j}}\right) + \varepsilon_{ijk} = \mu + \alpha_i + \beta_j^* + (\alpha\beta)_{ij}^* + \varepsilon_{ijk}$$

$$\sum_{i=1}^a \alpha\beta_{ij}^* = 0 \quad (\alpha\beta)_{ij}^* \sim N\left(0, \frac{a-1}{a} \sigma_{\alpha\beta}^2\right) \quad \text{COV}\left\{(\alpha\beta)_{ij}^*, (\alpha\beta)_{i'j}^*\right\} = -\frac{1}{a} \sigma_{\alpha\beta}^2 \quad i \neq i'$$

The covariance structure for the unrestricted model is as follows.

$$E\{Y_{ijk}\} = E\left\{\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk}\right\} = \mu + \alpha_i + 0 + 0 + 0 = \mu + \alpha_i$$

$$V\{Y_{ijk}\} = V\left\{\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk}\right\} = 0 + 0 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2$$

$$k \neq k': \text{COV}\{Y_{ijk}, Y_{ijk'}\} = \text{COV}\left\{\beta_j + (\alpha\beta)_{ij} + e_{ijk}, \beta_j + (\alpha\beta)_{ij} + e_{ijk'}\right\} = \sigma_\beta^2 + \sigma_{\alpha\beta}^2$$

$$i \neq i' \quad \forall k, k': \text{COV}\{Y_{ijk}, Y_{i'jk'}\} = \text{COV}\left\{\beta_j + (\alpha\beta)_{ij} + e_{ijk}, \beta_j + (\alpha\beta)_{i'j} + e_{i'jk'}\right\} = \sigma_\beta^2$$

$$j \neq j' \quad \forall i, i', k, k': \text{COV}\{Y_{ijk}, Y_{i'jk'}\} = \text{COV}\left\{\beta_j + (\alpha\beta)_{ij} + e_{ijk}, \beta_{j'} + (\alpha\beta)_{i'j'} + e_{i'jk'}\right\} = 0$$

The Analysis of Variance is computed in the same manner as for fixed and random effects models. The expected mean squares are obtained based on the covariance structure of the data.

$$SS_A = bn \sum_{i=1}^a (\bar{Y}_{i..} - \bar{Y} \dots)^2 = bn \sum_{i=1}^a \bar{Y}_{i..}^2 - abn \bar{Y} \dots^2$$

$$SS_B = an \sum_{j=1}^b (\bar{Y}_{.j.} - \bar{Y} \dots)^2 = an \sum_{j=1}^b \bar{Y}_{.j.}^2 - abn \bar{Y} \dots^2$$

$$SS_{AB} = n \sum_{i=1}^a \sum_{j=1}^b (\bar{Y}_{ij.} - \bar{Y}_{i..} - \bar{Y}_{.j.} + \bar{Y} \dots)^2 = n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2 - bn \sum_{i=1}^a \bar{Y}_{i..}^2 - an \sum_{j=1}^b \bar{Y}_{.j.}^2 + abn \bar{Y} \dots^2$$

$$SS_{Err} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - \bar{Y}_{ij.})^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2 - n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2$$

$$V\{Y\} = E\{(Y - \mu)^2\} = E\{Y^2 + \mu^2 - 2Y\mu\} = E\{Y^2\} + \mu^2 - 2\mu E\{Y\} = E\{Y^2\} - \mu^2 \Rightarrow E\{Y^2\} = V\{Y\} + \mu^2$$

$$E\{Y_{ijk}\} = \mu + \alpha_i \quad V\{Y_{ijk}\} = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 \Rightarrow E\{Y_{ijk}^2\} = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 + (\mu + \alpha_i)^2$$

$$E\{\bar{Y}_{ij.}\} = E\left\{\frac{1}{n} \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{n} n (\mu + \alpha_i) = \mu + \alpha_i$$

$$V\{\bar{Y}_{ij.}\} = V\left\{\frac{1}{n} \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{n^2} \left[\sum_{k=1}^n V\{Y_{ijk}\} + 2 \sum_{k < k'} \text{COV}\{Y_{ijk}, Y_{ijk'}\} \right] = \frac{1}{n^2} \left[n(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + 2 \binom{n}{2} (\sigma_\beta^2 + \sigma_{\alpha\beta}^2) \right] =$$

$$= \frac{1}{n^2} \left[n(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + n(n-1)(\sigma_\beta^2 + \sigma_{\alpha\beta}^2) \right] = \frac{1}{n^2} \left[n^2 \sigma_\beta^2 + n^2 \sigma_{\alpha\beta}^2 + n \sigma^2 \right] \Rightarrow E\{\bar{Y}_{ij.}^2\} = \frac{n\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{n} + (\mu + \alpha_i)^2$$

$$E\{\bar{Y}_{i..}\} = E\left\{\frac{1}{b} \sum_{j=1}^b \bar{Y}_{ij.}\right\} = \frac{1}{b} b (\mu + \alpha_i) = \mu + \alpha_i \quad \text{Note: } \text{COV}\{\bar{Y}_{ij.}, \bar{Y}_{i'j.}\} = \text{COV}\left\{\frac{1}{n} \sum_{k=1}^n Y_{ijk}, \frac{1}{n} \sum_{k=1}^n Y_{i'jk}\right\} = 0$$

$$V\{\bar{Y}_{i..}\} = V\left\{\frac{1}{b} \sum_{j=1}^b \bar{Y}_{ij.}\right\} = \frac{1}{b^2} \left[\sum_{j=1}^b V\{\bar{Y}_{ij.}\} + 2 \sum_{j < j'} \text{COV}\{\bar{Y}_{ij.}, \bar{Y}_{i'j.}\} \right] = \frac{1}{b^2} \left[b \left(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n} \right) + b(b-1)(0) \right]$$

$$= \frac{n\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{bn} \Rightarrow E\{\bar{Y}_{i..}^2\} = \frac{n\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{bn} + (\mu + \alpha_i)^2$$

$$\text{Note: } \text{COV}\{\bar{Y}_{ij.}, \bar{Y}_{i'j.}\} = \text{COV}\left\{\frac{1}{n} \sum_{k=1}^n Y_{ijk}, \frac{1}{n} \sum_{k=1}^n Y_{i'jk}\right\} = \frac{1}{n^2} n^2 \sigma_\beta^2 = \sigma_\beta^2$$

$$E\{\bar{Y}_{.j.}\} = E\left\{\frac{1}{a} \sum_{i=1}^a \bar{Y}_{ij.}\right\} = \frac{1}{a} \sum_{i=1}^a (\mu + \alpha_i) = \frac{1}{a} a\mu + \frac{1}{a} \sum_{i=1}^a \alpha_i = \mu + 0 = \mu$$

$$V\{\bar{Y}_{.j.}\} = V\left\{\frac{1}{a} \sum_{i=1}^a \bar{Y}_{ij.}\right\} = \frac{1}{a^2} \left[\sum_{i=1}^a V\{\bar{Y}_{ij.}\} + 2 \sum_{i < i'} \text{COV}\{\bar{Y}_{ij.}, \bar{Y}_{i'j.}\} \right] =$$

$$= \frac{1}{a^2} \left[a \left(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n} \right) + a(a-1) \sigma_\beta^2 \right] = \frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{an}$$

$$\Rightarrow E\{\bar{Y}_{.j.}^2\} = \frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{an} + \mu^2$$

$$E\{\bar{Y} \dots\} = E\left\{\frac{1}{b} \sum_{j=1}^b \bar{Y}_{.j.}\right\} = \frac{1}{b} b \mu = \mu$$

$$V\{\bar{Y} \dots\} = V\left\{\frac{1}{b} \sum_{j=1}^b \bar{Y}_{.j.}\right\} = \frac{1}{b^2} b \left(\frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{an} \right) = \frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{abn}$$

$$\Rightarrow E\{\bar{Y} \dots^2\} = \frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{abn} + \mu^2$$

$$SS_A = bn \sum_{i=1}^a \bar{Y}_{i..}^2 - abn \bar{Y}_{...}^2$$

$$\Rightarrow E\{SS_A\} = \left[abn \left[\frac{n\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{bn} \right] + bn \sum_{i=1}^a (\mu + \alpha_i)^2 \right] - abn \left[\frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{abn} + \mu^2 \right]$$

$$= \sigma_\beta^2(an - an) + \sigma_{\alpha\beta}^2(an - n) + \sigma^2(a - 1) + bn \left(a\mu^2 + \sum_{i=1}^n \alpha_i^2 + 2\mu \sum_{i=1}^n \alpha_i \right) - abn\mu^2 =$$

$$= (a - 1)\sigma^2 + n(a - 1)\sigma_{\alpha\beta}^2 + bn \sum_{i=1}^n \alpha_i^2 \Rightarrow E\{MS_A\} = E\left\{ \frac{SS_A}{a - 1} \right\} = \sigma^2 + n\sigma_{\alpha\beta}^2 + \frac{bn \sum_{i=1}^n \alpha_i^2}{a - 1}$$

$$SS_B = an \sum_{j=1}^b \bar{Y}_{.j.}^2 - abn \bar{Y}_{...}^2$$

$$\Rightarrow E\{SS_B\} = abn \left[\frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{an} + \mu^2 \right] - abn \left[\frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{abn} + \mu^2 \right]$$

$$= \sigma_\beta^2(abn - an) + \sigma_{\alpha\beta}^2(bn - n) + \sigma^2(b - 1)$$

$$= (b - 1)\sigma^2 + n(b - 1)\sigma_{\alpha\beta}^2 + an(b - 1)\sigma_\beta^2 \Rightarrow E\{MS_B\} = E\left\{ \frac{SS_B}{b - 1} \right\} = \sigma^2 + n\sigma_{\alpha\beta}^2 + an\sigma_\beta^2$$

$$SS_{AB} = n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2 - bn \sum_{i=1}^a \bar{Y}_{i..}^2 - an \sum_{j=1}^b \bar{Y}_{.j.}^2 + abn \bar{Y}_{...}^2$$

$$\Rightarrow E\{SS_{AB}\} =$$

$$\left[abn \frac{n\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{n} + bn \sum_{i=1}^n (\mu + \alpha_i)^2 \right] - \left[abn \left[\frac{n\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{bn} \right] + bn \sum_{i=1}^n (\mu + \alpha_i)^2 \right]$$

$$- abn \left[\frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{an} + \mu^2 \right] + abn \left[\frac{an\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{abn} + \mu^2 \right]$$

$$= \sigma_\beta^2(abn - an - abn + an) + \sigma_{\alpha\beta}^2(abn - an - bn + n) + \sigma^2(ab - a - b + 1)$$

$$+ bn \sum_{i=1}^n (\mu + \alpha_i)^2 - bn \sum_{i=1}^n (\mu + \alpha_i)^2 - abn\mu^2 + abn\mu^2$$

$$= (ab - a - b + 1)\sigma^2 + n(ab - a - b + 1)\sigma_{\alpha\beta}^2 = (a - 1)(b - 1)\sigma^2 + n(a - 1)(b - 1)\sigma_{\alpha\beta}^2$$

$$\Rightarrow E\{MS_{AB}\} = E\left\{ \frac{SS_{AB}}{(a - 1)(b - 1)} \right\} = \sigma^2 + n\sigma_{\alpha\beta}^2$$

$$SS_{Err} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2 - n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2$$

$$\Rightarrow E\{SS_{Err}\} = \left[abn(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + bn \sum_{i=1}^n (\mu + \alpha_i)^2 \right] - \left[abn \frac{n\sigma_\beta^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{n} + bn \sum_{i=1}^n (\mu + \alpha_i)^2 \right]$$

$$= \sigma_\beta^2(abn - abn) + \sigma_{\alpha\beta}^2(abn - abn) + \sigma^2(abn - ab) + bn \sum_{i=1}^n (\mu + \alpha_i)^2 - bn \sum_{i=1}^n (\mu + \alpha_i)^2 = ab(n - 1)\sigma^2$$

$$\Rightarrow E\{MS_{Err}\} = E\left\{ \frac{SS_{Err}}{ab(n - 1)} \right\} = \sigma^2$$

These results lead to the F-tests for factors A and B and for the AB interaction.

$$\begin{aligned}
 H_0 : \sigma_{\alpha\beta}^2 = 0 \quad H_A : \sigma_{\alpha\beta}^2 > 0 \quad TS : F_{AB} &= \frac{MS_{AB}}{MS_{Err}} \quad RR : F_{AB} \geq F_{(a-1)(b-1), ab(n-1)} \\
 H_0 : \sigma_{\beta}^2 = 0 \quad H_A : \sigma_{\beta}^2 > 0 \quad TS : F_B &= \frac{MS_B}{MS_{AB}} \quad RR : F_B \geq F_{(b-1), (a-1)(b-1)} \\
 H_0 : \alpha_1 = \dots = \alpha_a = 0 \quad H_A : \text{Not all } \alpha_i = 0 \quad TS : F_A &= \frac{MS_A}{MS_{AB}} \quad RR : F_A \geq F_{(a-1), (a-1)(b-1)}
 \end{aligned}$$

Estimation of the fixed effects and simple effects is based on the following results.

Estimating the Population Mean:

$$E\{\bar{Y}_{\dots}\} = \mu \quad V\{\bar{Y}_{\dots}\} = \frac{an\sigma_{\beta}^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{abn}$$

$$E\{MS_B\} = an\sigma_{\beta}^2 + n\sigma_{\alpha\beta}^2 + \sigma^2 \Rightarrow \hat{V}\{\bar{Y}_{\dots}\} = \frac{MS_B}{abn}$$

$$\Rightarrow (1-\alpha)100\% \text{ CI for } \mu: \bar{Y}_{\dots} \pm t_{1-\alpha/2, b-1} \sqrt{\frac{MS_B}{abn}}$$

Differences in fixed factor means for a level of the random factor:

Estimator: $\bar{Y}_{ij\cdot} - \bar{Y}_{i'j\cdot}$

$$V\{\bar{Y}_{ij\cdot}\} = \frac{1}{n^2} [n^2\sigma_{\beta}^2 + n^2\sigma_{\alpha\beta}^2 + n\sigma^2] = \sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n} = V\{\bar{Y}_{i'j\cdot}\}$$

$$\text{COV}\{\bar{Y}_{ij\cdot}, \bar{Y}_{i'j\cdot}\} = \text{COV}\left\{\frac{1}{n} \sum_{k=1}^n Y_{ijk}, \frac{1}{n} \sum_{k=1}^n Y_{i'jk}\right\} = \frac{1}{n^2} n^2 \sigma_{\beta}^2 = \sigma_{\beta}^2$$

$$\Rightarrow V\{\bar{Y}_{ij\cdot} - \bar{Y}_{i'j\cdot}\} = V\{\bar{Y}_{ij\cdot}\} + V\{\bar{Y}_{i'j\cdot}\} - 2\text{COV}\{\bar{Y}_{ij\cdot}, \bar{Y}_{i'j\cdot}\} = 2\left[\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n}\right] - 2\sigma_{\beta}^2 = \frac{2(\sigma^2 + n\sigma_{\alpha\beta}^2)}{n}$$

$$E\{MS_{AB}\} = \sigma^2 + n\sigma_{\alpha\beta}^2 \Rightarrow \hat{V}\{\bar{Y}_{ij\cdot} - \bar{Y}_{i'j\cdot}\} = \frac{2MS_{AB}}{n}$$

$$(1-\alpha)100\% \text{ CI for Simple Effect: } (\bar{Y}_{ij\cdot} - \bar{Y}_{i'j\cdot}) \pm t_{\alpha/2, (a-1)(b-1)} \sqrt{\frac{2MS_{AB}}{n}}$$

Estimating the differences in the marginal means for different levels of the fixed factor is shown below.

Differences in Factor A means across levels of Factor B:

Estimator: $\bar{Y}_{i..} - \bar{Y}_{i'..}$

$$V\{\bar{Y}_{i..}\} = \frac{n\sigma_{\beta}^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{bn} = V\{\bar{Y}_{i'..}\}$$

$$\text{COV}\{\bar{Y}_{i..}, \bar{Y}_{i'..}\} = \text{COV}\left\{\frac{1}{b}\sum_{j=1}^b \bar{Y}_{ij\cdot}, \frac{1}{b}\sum_{j=1}^b \bar{Y}_{i'j\cdot}\right\} = \frac{1}{b^2}\left\{\sum_{j=1}^b \text{COV}\{\bar{Y}_{ij\cdot}, \bar{Y}_{i'j\cdot}\} + 2\sum_{j < j'} \text{COV}\{\bar{Y}_{ij\cdot}, \bar{Y}_{i'j'\cdot}\}\right\} =$$

$$\frac{1}{b^2}[b\sigma_{\beta}^2 + b(b-1)0] = \frac{\sigma_{\beta}^2}{b}$$

$$\Rightarrow V\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = V\{\bar{Y}_{i..}\} + V\{\bar{Y}_{i'..}\} - 2\text{COV}\{\bar{Y}_{i..}, \bar{Y}_{i'..}\} = 2\left[\frac{n\sigma_{\beta}^2 + n\sigma_{\alpha\beta}^2 + \sigma^2}{bn}\right] - 2\frac{\sigma_{\beta}^2}{b} = \frac{2(n\sigma^2 + \sigma_{\alpha\beta}^2)}{bn}$$

$$E\{MS_{AB}\} = n\sigma^2 + \sigma_{\alpha\beta}^2 \Rightarrow \hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{2MS_{AB}}{bn}$$

$$(1-\alpha)100\% \text{ CI for Marginal Effect: } (\bar{Y}_{i..} - \bar{Y}_{i'..}) \pm t_{\alpha/2, (a-1)(b-1)} \sqrt{\frac{2MS_{AB}}{bn}}$$

Example: Bowling Scores on 4 Oil Patterns among 15 Elite Female Bowlers

- Women's Professional Bowling Association – Qualifying rounds at Alan Park, Michigan (2009).
- Factors:
 - A: Oil Pattern (Fixed) with $a = 4$ levels:
 - 1=Viper, 2=Chameleon, 3=Scorpion, 4=Shark
 - B: Bowler (Random) with $b = 15$ levels:
 - 1=Diandra Abaty, 2=Shalin Zulkiffi, 3=Liz Johnson, 4=Kelly Kulick, 5=Clara Guerrero, 6=Jennifer Petrick, 7=Wendy MacPherson, 8=Shannon Pluhowski, 9=Stephanie Nation, 10=Tammy Boomershine, 11=Amanda Fagan, 12=Aumi Guerra, 13=Michelle Feldman, 14=Shannon O'Keefe, 15=Jodie Woessner
- Replicates: Each bowler rolled 2 sets of 7 games on each pattern ($Y =$ Total Pins in a game, $n = 14$)

Mean	OilPatt1	OilPatt2	OilPatt3	OilPatt4	SD	OilPatt1	OilPatt2	OilPatt3	OilPatt4
Bowler1	223.29	208.79	195.57	211.00	Bowler1	42.44	22.98	27.27	28.85
Bowler2	211.79	195.71	196.43	191.57	Bowler2	28.77	27.06	24.31	19.77
Bowler3	218.14	208.50	209.64	215.50	Bowler3	24.51	26.23	27.78	14.09
Bowler4	219.43	216.64	212.43	216.21	Bowler4	18.72	21.74	27.52	35.62
Bowler5	210.57	198.43	204.71	219.07	Bowler5	20.77	18.80	28.70	24.82
Bowler6	211.00	203.29	193.07	187.14	Bowler6	30.91	16.90	23.72	30.82
Bowler7	223.36	199.29	194.43	221.07	Bowler7	34.26	30.29	20.24	22.84
Bowler8	209.57	214.21	208.64	201.29	Bowler8	25.17	31.64	20.76	25.94
Bowler9	199.57	198.57	193.29	204.43	Bowler9	27.98	21.67	18.57	26.78
Bowler10	205.86	213.71	198.36	219.29	Bowler10	33.02	20.73	31.23	27.84
Bowler11	202.50	205.29	194.36	207.57	Bowler11	26.88	14.49	21.40	17.67
Bowler12	206.21	182.64	196.14	194.00	Bowler12	31.98	25.80	16.73	26.59
Bowler13	198.50	207.86	210.71	193.86	Bowler13	15.51	22.39	25.88	33.64
Bowler14	212.00	205.86	208.29	220.21	Bowler14	30.03	25.49	22.43	13.01
Bowler15	199.57	209.79	204.86	208.64	Bowler15	27.98	23.93	20.27	13.62

ANOVA							
Source	df	SS	MS	MSError	F*	F(0.05)	P-value
Oil Pattern	3	8785.1	2928.4	819.6	3.573	2.827	0.0217
Bowler	14	29964.7	2140.3	819.6	2.611	1.935	0.0082
OilPattxBowler	42	34423.2	819.6	649.6	1.262	1.400	0.1271
Error	780	506679.0	649.6				
Total	839	579852.0					

Note that the error term for the main effects is the interaction mean square, while the error term for the interaction effects is the error mean square. We fail to reject $H_0^{AB} : \sigma_{\alpha\beta}^2 = 0$, but do reject the null hypotheses for main effects: $H_0^A : \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0$ $H_0^B : \sigma_\beta^2 = 0$. The point estimates for the variance components are given here, followed by estimates of the population mean, simple effects (oil pattern differences within bowlers), and marginal effects.

$$\hat{\sigma}^2 = MS_{\text{Err}} = 649.6 \quad \hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{AB} - MS_{\text{Err}}}{n} = \frac{819.6 - 649.6}{14} = 12.14$$

$$\hat{\sigma}_\beta^2 = \frac{MS_B - MS_{AB}}{an} = \frac{2140.3 - 819.6}{4(14)} = 23.58$$

$$\bar{y}_{\dots} = 205.9 \quad t_{.975,14} = 2.145 \quad MS_B = 2140.3 \quad a = 4 \quad b = 15 \quad n = 14$$

$$SE\{\bar{Y}_{\dots}\} = \sqrt{\frac{MS_B}{abn}} = \sqrt{\frac{2140.3}{4(15)(14)}} = \sqrt{\frac{2140.3}{840}} = \sqrt{2.55} = 1.60$$

$$\Rightarrow (1-\alpha)100\% \text{ CI for } \mu: \bar{y}_{\dots} \pm t_{1-\alpha/2, b-1} \sqrt{\frac{MS_B}{abn}} \equiv 205.9 \pm 2.145(1.60) \quad 205.9 \pm 3.43 \quad (202.47, 209.33)$$

$$(1-\alpha)100\% \text{ CI for Simple Effect: } (\bar{y}_{ij\bullet} - \bar{y}_{i'\bullet}) \pm t_{1-\alpha/2, (a-1)(b-1)} \sqrt{\frac{2MS_{AB}}{n}}$$

$$t_{.975,42} = 2.018 \quad \sqrt{\frac{2MS_{AB}}{n}} = \sqrt{\frac{2(819.6)}{14}} = 10.82 \quad \Rightarrow \quad t_{1-\alpha/2, (a-1)(b-1)} \sqrt{\frac{2MS_{AB}}{n}} = 2.018(10.82) = 21.83$$

$$(1-\alpha)100\% \text{ CI for Marginal Effect: } (\bar{y}_{i\bullet\bullet} - \bar{y}_{i'\bullet\bullet}) \pm t_{1-\alpha/2, (a-1)(b-1)} \sqrt{\frac{2MS_{AB}}{bn}}$$

$$t_{.975,42} = 2.018 \quad \sqrt{\frac{2MS_{AB}}{bn}} = \sqrt{\frac{2(819.6)}{15 \times 14}} = 2.80 \quad \Rightarrow \quad t_{1-\alpha/2, (a-1)(b-1)} \sqrt{\frac{MS_{AB}}{n}} = 2.018(2.80) = 5.65$$

Making use of Tukey's and Bonferroni's methods, we compare all pairs of oil patterns marginally and within bowler 1 below.

Family: All Comparisons among Oil Patterns (Within Bowler and Across Bowlers)

$a = 4$ Oil Patterns $b = 15$ Bowlers $n = 14$ Replicates $MS_{AB} = 819.6$

of Oil Patterns = 4, # Pairs of Oil Patterns = $4(3)/2 = 6$ $df_{AB} = (a-1)(b-1) = 42$

$$\hat{SE}\{\bar{Y}_{ij\cdot} - \bar{Y}_{i'j\cdot}\} = \sqrt{\frac{2MS_{AB}}{n}} = 10.82 \quad \hat{SE}\{\bar{Y}_{i\cdot\cdot} - \bar{Y}_{i'\cdot\cdot}\} = \sqrt{\frac{2MS_A}{bn}} = 2.80$$

Critical Values: Tukey: $q_{.95,4,42} = 3.784$ Bonferroni: $t_{1-.025/6,42} = 2.764$

Comparing Simple (Within Bowler) Means:

Tukey: $\frac{3.784}{\sqrt{2}}(10.82) = 28.95$ Bonferroni: $2.764(10.82) = 29.91$

Comparing Marginal (Across Bowler) Means:

Tukey: $\frac{3.784}{\sqrt{2}}(2.80) = 7.49$ Bonferroni: $2.764(2.80) = 7.74$

Oil Pattern	i	Marginal		
Scorpion	3	201.40		
Chameleon	2	204.57		
Shark	4	207.39		
Viper	1	210.09		
Oil Pattern	i	Bowler 1		
Scorpion	3	195.57		
Chameleon	2	208.79		
Shark	4	211.00		
Viper	1	223.29		

R Program

```
wpba2009 <- read.fwf("http://www.stat.ufl.edu/~winner/data/wpba2009.dat",
width=rep(8,5),
col.names=c("bowler","pattern","set","game","score"))

attach(wpba2009)

bowler <- factor(bowler)
pattern <- factor(pattern)

options(contrasts=c("contr.sum","contr.poly"))

wpba.mod1 <- aov(score ~ bowler + pattern + bowler:pattern)
anova(wpba.mod1)
```

```

library(nlme)
wpba.mod3 <- lme(fixed = score ~ pattern, random = ~1|bowler/pattern)
summary(wpba.mod3)
intervals(wpba.mod3)
anova(wpba.mod3)

library(lmerTest)
wpba.mod4 <- lmer(score~pattern+(1|bowler)+(1|pattern:bowler))
summary(wpba.mod4)
anova(wpba.mod4)
lsmeans(wpba.mod4)
diff lsmeans(wpba.mod4)
confint(wpba.mod4)

```

R Output

```

> wpba.mod1 <- aov(score ~ bowler + pattern + bowler:pattern)
> anova(wpba.mod1)
Analysis of Variance Table

Response: score
          Df Sum Sq Mean Sq F value    Pr(>F)
bowler     14  29965  2140.34   3.2949 3.844e-05 ***
pattern     3   8785  2928.37   4.5080 0.003817 **
bowler:pattern 42 34423   819.60   1.2617 0.127108
Residuals  780 506679   649.59
---
> wpba.mod3 <- lme(fixed = score ~ pattern, random = ~1|bowler/pattern)
> summary(wpba.mod3)
Linear mixed-effects model fit by REML
Data: NULL
      AIC      BIC    logLik
7851.303 7884.403 -3918.652

Random effects:
Formula: ~1 | bowler
(Intercept)
StdDev:    4.856495

Formula: ~1 | pattern %in% bowler
(Intercept) Residual
StdDev:    3.484903 25.48701

Fixed effects: score ~ pattern
              Value Std.Error DF   t-value p-value
(Intercept) 205.86190  1.596276 780 128.96385 0.0000
pattern1     4.22857  1.710901 42   2.47155 0.0176
pattern2    -1.29048  1.710901 42  -0.75427 0.4549
pattern3    -4.46667  1.710901 42  -2.61071 0.0125

> intervals(wpba.mod3)
Approximate 95% confidence intervals

Fixed effects:
      lower      est.      upper
(Intercept) 202.7283989 205.861905 208.995411
pattern1     0.7758329   4.228571   7.681310
pattern2    -4.7432148  -1.290476   2.162262
pattern3    -7.9194052  -4.466667  -1.013928

```

Continued

```

Random Effects:
  Level: bowler
              lower    est.    upper
sd((Intercept)) 2.627534 4.856495 8.976303
  Level: pattern
              lower    est.    upper
sd((Intercept)) 1.221161 3.484903 9.94508

  Within-group standard error:
    lower    est.    upper
24.25312 25.48701 26.78367
> anova(wpba.mod3)
              numDF denDF   F-value p-value
(Intercept)     1   780 16631.675 <.0001
pattern         3    42   3.573  0.0217
>
> library(lmerTest)
> wpba.mod4 <- lmer(score~pattern+(1|bowler)+(1|pattern:bowler))
> summary(wpba.mod4)
Linear mixed model fit by REML t-tests use Satterthwaite approximations to
degrees of freedom [merModLmerTest]
Formula: score ~ pattern + (1 | bowler) + (1 | pattern:bowler)

REML criterion at convergence: 7837.3

Random effects:
  Groups      Name                Variance Std.Dev.
pattern:bowler (Intercept)    12.14     3.485
bowler        (Intercept)    23.58     4.856
Residual                                649.59    25.487
Number of obs: 840, groups: pattern:bowler, 60; bowler, 15

Fixed effects:
              Estimate Std. Error    df t value Pr(>|t|)
(Intercept)  205.862    1.596  14.000 128.966 <2e-16 ***
pattern1     4.229     1.711  42.000  2.472  0.0176 *
pattern2    -1.290     1.711  42.000 -0.754  0.4549
pattern3    -4.467     1.711  42.000 -2.611  0.0125 *
> anova(wpba.mod4)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
              Sum Sq Mean Sq NumDF DenDF F.value Pr(>F)
pattern 6962.8 2320.9 3 42 3.5729 0.02172 *
> lsmeans(wpba.mod4)
Least Squares Means table:
              pattern Estimate Standard Error    DF t-value Lower CI Upper CI p-value
pattern 1 1.0 210.09 2.34 44.9 89.79 205 215 <2e-16 ***
pattern 2 2.0 204.57 2.34 44.9 87.43 200 209 <2e-16 ***
pattern 3 3.0 201.40 2.34 44.9 86.07 197 206 <2e-16 ***
pattern 4 4.0 207.39 2.34 44.9 88.63 203 212 <2e-16 ***

Differences of LSMEANS:
              Estimate Standard Error    DF t-value Lower CI Upper CI p-value
pattern 1 - 2 5.5 2.79 42.0 1.98 -0.119 11.157 0.055 .
pattern 1 - 3 8.7 2.79 42.0 3.11 3.057 14.334 0.003 **
pattern 1 - 4 2.7 2.79 42.0 0.97 -2.938 8.338 0.339
pattern 2 - 3 3.2 2.79 42.0 1.14 -2.462 8.814 0.262
pattern 2 - 4 -2.8 2.79 42.0 -1.01 -8.457 2.819 0.319
pattern 3 - 4 -6.0 2.79 42.0 -2.15 -11.633 -0.357 0.038 * >
confint(wpba.mod4)
Computing profile confidence intervals ...
              2.5 % 97.5 %
.sig01 0.0000000 6.246137
.sig02 1.8529064 8.180054
.sigma 24.2727350 26.806045
(Intercept) 202.6351562 209.088654
pattern1 0.9186156 7.538527
pattern2 -4.6004320 2.019480
pattern3 -7.7766225 -1.156711

```

7.2. Matrix Approach to 2-Way Additive Mixed Model

$$Y_{ijk} = \mu + \alpha_i + \beta_j + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n$$

$$\sum_{i=1}^a \alpha_i = 0 \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \quad \{\beta_j\} \perp \{\varepsilon_{ijk}\}$$

Here μ , $\{\alpha_i\}$ are fixed constants and $\{\beta_j\}$ and $\{\varepsilon_{ijk}\}$ are random variables. For clarity, set $a = 2$, $b = 3$, $n = 2$. In Matrix form, re-write model in terms of: fixed effects, random effects, and error term.

$$\mathbf{Y} = \begin{bmatrix} Y_{111} \\ Y_{112} \\ Y_{121} \\ Y_{122} \\ Y_{131} \\ Y_{132} \\ Y_{211} \\ Y_{212} \\ Y_{221} \\ Y_{222} \\ Y_{231} \\ Y_{232} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \quad \mathbf{u} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} \quad \mathbf{Z} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{111} \\ \varepsilon_{112} \\ \varepsilon_{121} \\ \varepsilon_{122} \\ \varepsilon_{131} \\ \varepsilon_{132} \\ \varepsilon_{211} \\ \varepsilon_{212} \\ \varepsilon_{221} \\ \varepsilon_{222} \\ \varepsilon_{231} \\ \varepsilon_{232} \end{bmatrix}$$

$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\varepsilon}$

$$E\{\mathbf{u}\} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \mathbf{0}_3 \quad V\{\mathbf{u}\} = \sigma_\beta^2 \mathbf{I}_3 = \mathbf{G} \quad E\{\boldsymbol{\varepsilon}\} = \mathbf{0}_{12} \quad V\{\boldsymbol{\varepsilon}\} = \sigma^2 \mathbf{I}_{12} = \mathbf{R}$$

$$\mathbf{u} \sim N(\mathbf{0}, \mathbf{G}) \quad f(\mathbf{u}) = (2\pi)^{-b/2} |\mathbf{G}|^{-1/2} \exp\left\{-\frac{1}{2} \mathbf{u}' \mathbf{G}^{-1} \mathbf{u}\right\}$$

$$E\{\mathbf{Y}\} = \mathbf{X}\boldsymbol{\beta} \quad V\{\mathbf{Y}\} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R} = \mathbf{V}$$

$$\mathbf{Y} \sim N(\mathbf{X}\boldsymbol{\beta}, \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}) \quad f(\mathbf{y}) = (2\pi)^{-N/2} |\mathbf{V}|^{-1/2} \exp\left\{-\frac{1}{2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{V}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})\right\}$$

To obtain a least squares estimator for $\boldsymbol{\beta}$, we can choose the value that maximizes $f(\mathbf{Y})$.

$$\mathbf{Y} \sim N(\mathbf{X}\boldsymbol{\beta}, \mathbf{ZGZ}' + \mathbf{R})$$

$$f(\mathbf{y}) = (2\pi)^{-N/2} |\mathbf{V}|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{V}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})\right\} =$$

$$= (2\pi)^{-N/2} |\mathbf{V}|^{-1/2} \exp\left\{-\frac{1}{2}[\mathbf{y}' \mathbf{V}^{-1} \mathbf{y} + \boldsymbol{\beta}' \mathbf{X}' \mathbf{V}^{-1} \mathbf{X} \boldsymbol{\beta} - 2\mathbf{y}' \mathbf{V}^{-1} \mathbf{X} \boldsymbol{\beta}]\right\}$$

$$\Rightarrow \frac{\partial f(\mathbf{y})}{\partial \boldsymbol{\beta}} = f(\mathbf{y}) \left[-\frac{1}{2} (2\mathbf{X}' \mathbf{V}^{-1} \mathbf{X} \boldsymbol{\beta} - 2\mathbf{X}' \mathbf{V}^{-1} \mathbf{y}) \right]$$

$$\mathbf{X}' \mathbf{V}^{-1} \mathbf{X} \boldsymbol{\beta} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{y} \Rightarrow \frac{\partial f(\mathbf{y})}{\partial \boldsymbol{\beta}} = \mathbf{0} \Rightarrow \hat{\boldsymbol{\beta}} = (\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-} \mathbf{X}' \mathbf{V}^{-1} \mathbf{y}$$

$(\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-}$ is a generalized inverse of $\mathbf{X}' \mathbf{V}^{-1} \mathbf{X}$

$$\Rightarrow \mathbf{X}' \mathbf{V}^{-1} \mathbf{X} (\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-} \mathbf{X}' \mathbf{V}^{-1} \mathbf{X} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{X}$$

By another approach, we can obtain the joint density of \mathbf{Y} and \mathbf{u} , and obtain $f(\mathbf{Y}, \mathbf{u}) = f(\mathbf{u})f(\mathbf{Y}|\mathbf{u})$:

$$\mathbf{Y} | \mathbf{u} \sim N(\mathbf{X}\boldsymbol{\beta} + \mathbf{Zu}, \mathbf{R}) \quad f(\mathbf{y} | \mathbf{u}) = (2\pi)^{-N/2} |\mathbf{R}|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Zu})' \mathbf{R}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Zu})\right\}$$

$$f(\mathbf{y}, \mathbf{u}) = f(\mathbf{u})f(\mathbf{y} | \mathbf{u}) =$$

$$= (2\pi)^{-(N+b)/2} |\mathbf{G}|^{-1/2} |\mathbf{R}|^{-1/2} \exp\left\{-\frac{1}{2}[(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Zu})' \mathbf{R}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Zu}) + \mathbf{u}' \mathbf{G}^{-1} \mathbf{u}]\right\}$$

$$= (2\pi)^{-(N+b)/2} |\mathbf{G}|^{-1/2} |\mathbf{R}|^{-1/2} \times$$

$$\exp\left\{-\frac{1}{2}[\mathbf{y}' \mathbf{R}^{-1} \mathbf{y} + \boldsymbol{\beta}' \mathbf{X}' \mathbf{R}^{-1} \mathbf{X} \boldsymbol{\beta} + \mathbf{u}' \mathbf{Z}' \mathbf{R}^{-1} \mathbf{Z} \mathbf{u} - 2\mathbf{y}' \mathbf{R}^{-1} \mathbf{X} \boldsymbol{\beta} - 2\mathbf{y}' \mathbf{R}^{-1} \mathbf{Z} \mathbf{u} + 2\boldsymbol{\beta}' \mathbf{X}' \mathbf{R}^{-1} \mathbf{Z} \mathbf{u} + \mathbf{u}' \mathbf{G}^{-1} \mathbf{u}]\right\}$$

Then, we can obtain an estimator for $\boldsymbol{\beta}$ and a predictor for \mathbf{u} that maximize this joint density, leading to the **mixed model equations**, providing BLUE for $\mathbf{X}\boldsymbol{\beta}$ and BLUP for \mathbf{u} .

$$f(\mathbf{y}, \mathbf{u}) = (2\pi)^{-(N+b)/2} |\mathbf{G}|^{-1/2} |\mathbf{R}|^{-1/2} \times$$

$$\exp \left\{ -\frac{1}{2} \left[\mathbf{y}'\mathbf{R}^{-1}\mathbf{y} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{R}^{-1}\mathbf{X}\boldsymbol{\beta} + \mathbf{u}'\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{u} - 2\mathbf{y}'\mathbf{R}^{-1}\mathbf{X}\boldsymbol{\beta} - 2\mathbf{y}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{u} + 2\boldsymbol{\beta}'\mathbf{X}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{u} + \mathbf{u}'\mathbf{G}^{-1}\mathbf{u} \right] \right\}$$

$$\Rightarrow \frac{\partial f(\mathbf{y}, \mathbf{u})}{\partial \boldsymbol{\beta}} = f(\mathbf{y}, \mathbf{u}) \left(-\frac{1}{2} \right) \left[2\mathbf{X}'\mathbf{R}^{-1}\mathbf{X}\boldsymbol{\beta} - 2\mathbf{X}'\mathbf{R}^{-1}\mathbf{y} + 2\mathbf{X}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{u} \right]$$

$$\Rightarrow \mathbf{X}'\mathbf{R}^{-1}\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z}\tilde{\mathbf{u}} = \mathbf{X}'\mathbf{R}^{-1}\mathbf{y} \Rightarrow \frac{\partial f(\mathbf{y}, \mathbf{u})}{\partial \boldsymbol{\beta}} = \mathbf{0}$$

$$\Rightarrow \frac{\partial f(\mathbf{y}, \mathbf{u})}{\partial \mathbf{u}} = f(\mathbf{y}, \mathbf{u}) \left(-\frac{1}{2} \right) \left[2\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{u} - 2\mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} + 2\mathbf{Z}'\mathbf{R}^{-1}\mathbf{X}\boldsymbol{\beta} + 2\mathbf{G}^{-1}\mathbf{u} \right]$$

$$\Rightarrow \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}\tilde{\mathbf{u}} + \mathbf{G}^{-1}\tilde{\mathbf{u}} = \mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} \Rightarrow \frac{\partial f(\mathbf{y}, \mathbf{u})}{\partial \mathbf{u}} = \mathbf{0}$$

Mixed Model Equations:

$$\begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1} \end{bmatrix} \begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{y} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} \end{bmatrix} \Rightarrow \begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{y} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} \end{bmatrix}$$

Note that the variance components are unknown and must be estimated.

$$\Rightarrow \begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{X}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{X}} & \hat{\mathbf{X}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{Z}} \\ \hat{\mathbf{Z}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{X}} & \hat{\mathbf{Z}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{Z}} + \hat{\mathbf{G}}^{-1} \end{bmatrix}^{-1} \begin{bmatrix} \hat{\mathbf{X}}'\hat{\mathbf{R}}^{-1}\mathbf{y} \\ \hat{\mathbf{Z}}'\hat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix}$$

$$\hat{\mathbf{V}} \begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{X}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{X}} & \hat{\mathbf{X}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{Z}} \\ \hat{\mathbf{Z}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{X}} & \hat{\mathbf{Z}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{Z}} + \hat{\mathbf{G}}^{-1} \end{bmatrix}^{-1} =$$

$$= \begin{bmatrix} \left(\hat{\mathbf{X}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{X}} \right)^{-1} & -\left(\hat{\mathbf{X}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{X}} \right)^{-1} \hat{\mathbf{X}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{Z}}\hat{\mathbf{G}}^{-1} \\ -\hat{\mathbf{G}}^{-1}\hat{\mathbf{Z}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{X}} \left(\hat{\mathbf{X}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{X}} \right)^{-1} & \left(\hat{\mathbf{Z}}'\hat{\mathbf{R}}^{-1}\hat{\mathbf{Z}} + \hat{\mathbf{G}}^{-1} \right)^{-1} + \hat{\mathbf{G}}^{-1}\hat{\mathbf{Z}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{X}} \left(\hat{\mathbf{X}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{X}} \right)^{-1} \hat{\mathbf{X}}'\hat{\mathbf{V}}^{-1}\hat{\mathbf{Z}}\hat{\mathbf{G}}^{-1} \end{bmatrix}$$

This method generalizes to any number of fixed and random factors and interactions. The number of columns of \mathbf{Z} will be the number of random effects in the model ($b + ab$) in the 2-way mixed model with interaction.

$$\mathbf{Y} = \begin{bmatrix} Y_{111} \\ Y_{112} \\ Y_{121} \\ Y_{122} \\ Y_{131} \\ Y_{132} \\ Y_{211} \\ Y_{212} \\ Y_{221} \\ Y_{222} \\ Y_{231} \\ Y_{232} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \quad \mathbf{u} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ (\alpha\beta)_{11} \\ (\alpha\beta)_{12} \\ (\alpha\beta)_{13} \\ (\alpha\beta)_{21} \\ (\alpha\beta)_{22} \\ (\alpha\beta)_{23} \end{bmatrix} \quad \mathbf{Z} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{111} \\ \varepsilon_{112} \\ \varepsilon_{121} \\ \varepsilon_{122} \\ \varepsilon_{131} \\ \varepsilon_{132} \\ \varepsilon_{211} \\ \varepsilon_{212} \\ \varepsilon_{221} \\ \varepsilon_{222} \\ \varepsilon_{231} \\ \varepsilon_{232} \end{bmatrix}$$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\varepsilon}$$

Two methods of estimating the variance components that are implemented by software packages are **maximum likelihood (ML)** and **restricted maximum likelihood (REML)**. The log likelihood functions for the two methods are (where p is the rank of \mathbf{X}):

$$\text{ML: } l(\mathbf{G}, \mathbf{R}) = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\mathbf{ZGZ}' + \mathbf{R}| - \frac{1}{2} \mathbf{y}' \left(\mathbf{I} - \mathbf{X} \left(\mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \mathbf{X} \right)^{-1} \mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \right)' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \left(\mathbf{I} - \mathbf{X} \left(\mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \mathbf{X} \right)^{-1} \mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \right) \mathbf{y}$$

$$\text{REML: } l_R(\mathbf{G}, \mathbf{R}) = -\frac{n-p}{2} \log(2\pi) - \frac{1}{2} \log |\mathbf{ZGZ}' + \mathbf{R}| - \frac{1}{2} \log \left| \mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \mathbf{X} \right| - \frac{1}{2} \mathbf{y}' \left(\mathbf{I} - \mathbf{X} \left(\mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \mathbf{X} \right)^{-1} \mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \right)' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \left(\mathbf{I} - \mathbf{X} \left(\mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \mathbf{X} \right)^{-1} \mathbf{X}' (\mathbf{ZGZ}' + \mathbf{R})^{-1} \right) \mathbf{y}$$

Restricted maximum likelihood is based on transforming the response variable to have mean $\mathbf{0}$ and estimating variance components after removing fixed effects. Consider the 2-way model described above (with or without the random interaction, with $a = 2$, $b = 3$, $n = 2$). The REML estimator is invariant to the transformation matrix, which is $(N-p) \times N$ where p is the number of fixed parameters (besides μ). In this case, the matrix is $(12-2) \times 12$.

$$\begin{aligned}
E\{\mathbf{Y}\} &= \begin{bmatrix} \mu + \alpha_1 \\ \mu + \alpha_1 \\ \mu + \alpha_1 \\ \mu + \alpha_1 \\ \mu + \alpha_1 \\ \mu + \alpha_2 \\ \mu + \alpha_2 \\ \mu + \alpha_2 \\ \mu + \alpha_2 \\ \mu + \alpha_2 \\ \mu + \alpha_2 \end{bmatrix} & V\{\mathbf{Y}\} = \mathbf{V} = \mathbf{ZGZ}' + \mathbf{R} & \text{Let } \mathbf{T} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \\
\Rightarrow E\{\mathbf{TY}\} = \mathbf{TE}\{\mathbf{Y}\} = \mathbf{0}_{10} & & V\{\mathbf{TY}\} = \mathbf{TVT}' = \mathbf{T}(\mathbf{ZGZ}' + \mathbf{R})\mathbf{T}'
\end{aligned}$$

7.3. Higher Order Mixed Models

Higher order balanced models generalize to a general pattern with respect to error terms for the mean squares. Here we consider three factor models: models with one fixed and two random factors, and models with two fixed and one random factor. The patterns seen below generalize to models with 4 or more factors.

$$\begin{aligned}
\text{A Fixed: } Y_{ijkl} &= \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + \varepsilon_{ijkl} \quad i=1, \dots, a; j=1, \dots, b; k=1, \dots, c; l=1, \dots, n \\
\sum_{i=1}^a \alpha_i &= 0 \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad \gamma_k \sim NID(0, \sigma_\gamma^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2) \quad (\alpha\gamma)_{ik} \sim NID(0, \sigma_{\alpha\gamma}^2) \quad (\beta\gamma)_{jk} \sim NID(0, \sigma_{\beta\gamma}^2) \\
(\alpha\beta\gamma)_{ijk} &\sim NID(0, \sigma_{\alpha\beta\gamma}^2) \quad \varepsilon_{ijkl} \sim NID(0, \sigma^2) \\
\{\beta_j\} &\perp \{\gamma_k\} \perp \{(\alpha\beta)_{ij}\} \perp \{(\alpha\gamma)_{ik}\} \perp \{(\beta\gamma)_{jk}\} \perp \{(\alpha\beta\gamma)_{ijk}\} \perp \{\varepsilon_{ijkl}\}
\end{aligned}$$

$$\begin{aligned}
E\{MS_A\} &= \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + cn\sigma_{\alpha\beta}^2 + bn\sigma_{\alpha\gamma}^2 + \frac{bcn\sum_{i=1}^a \alpha_i^2}{a-1} \Rightarrow F_A = \frac{MS_A + MS_{ABC}}{MS_{AB} + MS_{AC}} \quad \text{or} \quad F_A = \frac{MS_A}{MS_{AB} + MS_{AC} - MS_{ABC}} \\
E\{MS_B\} &= \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + cn\sigma_{\alpha\beta}^2 + an\sigma_{\beta\gamma}^2 + acn\sigma_{\beta}^2 \Rightarrow F_B = \frac{MS_B + MS_{ABC}}{MS_{AB} + MS_{BC}} \quad \text{or} \quad F_B = \frac{MS_B}{MS_{AB} + MS_{BC} - MS_{ABC}} \\
E\{MS_C\} &= \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + bn\sigma_{\alpha\gamma}^2 + an\sigma_{\beta\gamma}^2 + abn\sigma_{\gamma}^2 \Rightarrow F_C = \frac{MS_C + MS_{ABC}}{MS_{AC} + MS_{BC}} \quad \text{or} \quad F_C = \frac{MS_C}{MS_{AC} + MS_{BC} - MS_{ABC}} \\
E\{MS_{AB}\} &= \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + cn\sigma_{\alpha\beta}^2 \Rightarrow F_{AB} = \frac{MS_{AB}}{MS_{ABC}} \\
E\{MS_{AC}\} &= \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + bn\sigma_{\alpha\gamma}^2 \Rightarrow F_{AC} = \frac{MS_{AC}}{MS_{ABC}} \\
E\{MS_{BC}\} &= \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + an\sigma_{\beta\gamma}^2 \Rightarrow F_{BC} = \frac{MS_{BC}}{MS_{ABC}} \\
E\{MS_{ABC}\} &= \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 \Rightarrow F_{ABC} = \frac{MS_{ABC}}{MS_{Err}} \\
E\{MS_{Err}\} &= \sigma^2
\end{aligned}$$

For the case of 2 fixed, and 1 random factors, we have:

$$\begin{aligned}
&\text{A, B Fixed: } Y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + \varepsilon_{ijkl} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c; l = 1, \dots, n \\
&\sum_{i=1}^a \alpha_i = \sum_{j=1}^b \beta_j = \sum_{i=1}^a (\alpha\beta)_{ij} = \sum_{j=1}^b (\alpha\beta)_{ij} = 0 \quad \gamma_k \sim NID(0, \sigma_{\gamma}^2) \quad (\alpha\gamma)_{ik} \sim NID(0, \sigma_{\alpha\gamma}^2) \quad (\beta\gamma)_{jk} \sim NID(0, \sigma_{\beta\gamma}^2) \\
&(\alpha\beta\gamma)_{ijk} \sim NID(0, \sigma_{\alpha\beta\gamma}^2) \quad \varepsilon_{ijkl} \sim NID(0, \sigma^2) \\
&\{\gamma_k\} \perp \{(\alpha\gamma)_{ik}\} \perp \{(\beta\gamma)_{jk}\} \perp \{(\alpha\beta\gamma)_{ijk}\} \perp \{\varepsilon_{ijkl}\}
\end{aligned}$$

$$E\{MS_A\} = \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + bn\sigma_{\alpha\gamma}^2 + \frac{bcn\sum_{i=1}^a \alpha_i^2}{a-1} \Rightarrow F_A = \frac{MS_A}{MS_{AC}}$$

$$E\{MS_B\} = \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + an\sigma_{\beta\gamma}^2 + \frac{acn\sum_{j=1}^b \beta_j^2}{b-1} \Rightarrow F_B = \frac{MS_B}{MS_{BC}}$$

$$E\{MS_C\} = \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + bn\sigma_{\alpha\gamma}^2 + an\sigma_{\beta\gamma}^2 + abn\sigma_{\gamma}^2 \Rightarrow F_C = \frac{MS_C + MS_{ABC}}{MS_{AC} + MS_{BC}} \quad \text{or} \quad F_C = \frac{MS_C}{MS_{AC} + MS_{BC} - MS_{ABC}}$$

$$E\{MS_{AB}\} = \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + \frac{cn\sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2}{(a-1)(b-1)} \Rightarrow F_{AB} = \frac{MS_{AB}}{MS_{ABC}}$$

$$E\{MS_{AC}\} = \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + bn\sigma_{\alpha\gamma}^2 \Rightarrow F_{AC} = \frac{MS_{AC}}{MS_{ABC}}$$

$$E\{MS_{BC}\} = \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 + an\sigma_{\beta\gamma}^2 \Rightarrow F_{BC} = \frac{MS_{BC}}{MS_{ABC}}$$

$$E\{MS_{ABC}\} = \sigma^2 + n\sigma_{\alpha\beta\gamma}^2 \Rightarrow F_{ABC} = \frac{MS_{ABC}}{MS_{Err}}$$

$$E\{MS_{Err}\} = \sigma^2$$

Example: Beer Head Half-Life

An experiment (Hudson (1968)) was conducted with 3 factors: Source of carborundum (from distributor, purchased in store), beer brand (5 brands), and laboratory (5 labs). The response was foam half-life in seconds, and there were $n = 4$ replicates per treatment combination. Here we treat Source of carborundum as a Fixed factor, and Beer Brand and Laboratory as Random factors. The treatment means are given below.

Carbor=Distributed						Carbor=Purchased					
Brand\Laboratory	1	2	3	4	5	Brand\Laboratory	1	2	3	4	5
1	98.75	92	90.75	97	90	1	93.75	96.5	97.5	97.5	92.25
2	101	97	81	78.75	85.75	2	88.25	110.5	78.5	76	68
3	76.5	91.75	97	94.5	72.5	3	81.25	98.25	90	92.5	73.75
4	130	132.75	138.25	140.25	100.75	4	134.25	142	135.75	138.25	101
5	48.25	58.25	53.75	52.75	47.75	5	49	62	51.25	51	51

The Analysis of Variance is given here:

Source	df	SS	MS	F	df1	df2	F(.05)	P-value	Variance
Carborundum	1	0.72	0.72	0.004250	1	3.27	9.235	0.9518	
Brand	4	119860.53	29965.13	54.880	4	14.75	3.069	0.0000	735.48
Laboratory	4	8335.63	2083.91	3.214	4	15.97	3.008	0.0436	35.89
C*B	4	273.73	68.43	0.980	4	16	3.007	0.4461	-0.07
C*L	4	683.23	170.81	2.445	4	16	3.007	0.0888	5.05
B*L	16	8758.87	547.43	7.837	16	16	2.333	0.0001	59.70
C*B*L	16	1117.57	69.85	1.865	16	150	1.711	0.0279	8.10
Error	150	5619.00	37.46						
Total	199	144649.28							

R Program:

```
beer <-
read.table("http://www.stat.ufl.edu/~winner/data/beerhead_half-life.dat",
  header=F,col.names=c("lab","carbor","brand","foamtime"))
attach(beer)

lab <- factor(lab); carbor <- factor(carbor); brand <- factor(brand)

beer.mod1 <- aov(foamtime ~ lab*carbor*brand)
anova(beer.mod1)

library(lmerTest)

beer.mod2 <- lmer(foamtime ~ carbor + (1|brand) + (1|lab) +
  (1|carbor:brand) +
  (1|carbor:lab) + (1|brand:lab) + (1|carbor:brand:lab))
summary(beer.mod2)
anova(beer.mod2)
anova(beer.mod2,ddf="Kenward-Roger")
```

The default denominator degrees of freedom for the fixed effects test is the Satterthwaite approximation, an alternative is the Kenward-Roger method.

R Output: (Note that the F-statistics from the `aov` function use MS_{Err} for the error terms)

```
> beer.mod1 <- aov(foamtime ~ lab*carbor*brand)
> anova(beer.mod1)
Analysis of Variance Table

Response: foamtime
          Df Sum Sq Mean Sq  F value    Pr(>F)
lab         4  8336   2083.9   55.6302 < 2.2e-16 ***
carbor      1     1     0.7    0.0192  0.889922
brand       4 119861 29965.1  799.9235 < 2.2e-16 ***
lab:carbor  4   683   170.8    4.5597  0.001671 **
lab:brand   16  8759   547.4   14.6137 < 2.2e-16 ***
carbor:brand 4   274    68.4    1.8268  0.126574
lab:carbor:brand 16  1118    69.8    1.8646  0.027935 *
Residuals  150  5619    37.5

Linear mixed model fit by REML t-tests use Satterthwaite approximations to
degrees of freedom [merModLmerTest]
Formula: foamtime ~ carbor + (1 | brand) + (1 | lab) + (1 | carbor:brand) +
  (1 | carbor:lab) + (1 | brand:lab) + (1 | carbor:brand:lab)

REML criterion at convergence: 1392.7
Random effects:
Groups          Name          Variance Std.Dev.
carbor:brand:lab (Intercept)    8.026   2.833
brand:lab       (Intercept)   59.733   7.729
carbor:lab      (Intercept)    5.062   2.250
carbor:brand    (Intercept)    0.000   0.000
lab             (Intercept)   35.881   5.990
brand          (Intercept)  735.440  27.119
Residual              37.460   6.120

Number of obs: 200, groups:
carbor:brand:lab, 50; brand:lab, 25; carbor:lab, 10; carbor:brand, 10; lab, 5;
brand, 5

Fixed effects:
              Estimate Std. Error    df t value Pr(>|t|)
(Intercept)   89.880    12.584   4.447  7.142  0.00135 **
carbor2         0.120     1.848   4.000  0.065  0.95135
```

Continued

```

> anova(beer.mod2)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF  F.value Pr(>F)
carbor 0.1579  0.1579     1     4 0.0042153 0.9513

> anova(beer.mod2,ddf="Kenward-Roger")
Loading required package: pbkrtest
Analysis of Variance Table of type 3 with Kenward-Roger
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF  F.value Pr(>F)
carbor 0.1579  0.1579     1 3.3131 0.0042153 0.952

```

Note that both methods give very similar results.

Example: Navigational Techniques of Web Maps

A study of computer-based navigation of web maps had three factors, with one response being task completion time (Wu, *et al* (2011)). Factor A was Navigation Technique (Combined Panning Buttons (CPB), Distributed Panning Buttons (DPB), Enhanced navigator w/ continuous control (ENCC), Grab and Drag (GD)). Factor B was Input Method (Direct Touch (DT), Mouse (M)). Factor C was Subject (36 participants). Each subject was observed once on each of the 8 combinations of Factors A and B, so $n = 1$. In models, such as this, the highest order interaction term and the error term are “undistinguishable.” In this study, Factors A and B are fixed and C is random. This study can also be treated as a Repeated Measures Design with two “within subjects” factors.

Trt	Trt1	Trt2	Trt3	Trt4	Trt5	Trt6	Trt7	Trt8	
Factor_A	A1	A1	A2	A2	A3	A3	A4	A4	
Factor_B	B1	B2	B1	B2	B1	B2	B1	B2	SubjMean
Subject1	163.30	141.23	184.63	127.97	197.05	251.96	132.08	90.58	161.10
Subject2	214.95	112.38	222.46	126.79	54.58	119.24	127.10	50.82	128.54
Subject3	179.73	88.03	183.69	221.24	115.31	145.65	120.18	89.91	142.97
Subject4	164.35	181.68	212.66	125.85	122.03	128.51	91.40	128.94	144.43
Subject5	184.68	144.92	132.57	106.03	156.71	165.00	145.40	133.47	146.10
Subject6	165.21	87.48	119.35	158.34	134.65	107.89	164.91	91.25	128.64
Subject7	171.03	218.02	164.38	175.06	83.26	188.49	124.08	113.43	154.72
Subject8	151.97	148.30	200.06	114.83	43.71	34.78	143.56	112.15	118.67
Subject9	141.27	133.63	190.83	137.32	135.09	133.58	189.17	182.08	155.37
Subject10	146.66	169.38	133.05	224.46	80.78	52.35	191.69	165.22	145.45
Subject11	208.07	110.25	221.84	225.31	90.71	182.57	219.80	159.84	177.30
Subject12	202.50	70.47	230.19	57.34	141.67	82.79	104.17	100.42	123.69
Subject13	221.43	112.14	155.76	110.05	118.50	135.74	175.36	124.65	144.20
Subject14	174.87	111.15	161.20	125.65	163.19	140.89	91.30	55.41	127.96
Subject15	166.08	204.44	159.54	149.55	108.17	107.38	85.44	143.54	140.52
Subject16	177.53	181.48	178.31	91.38	131.60	116.81	162.37	136.37	146.98
Subject17	179.58	202.76	215.61	188.05	110.02	187.60	112.71	200.56	174.61
Subject18	154.37	133.85	188.63	178.62	126.11	111.82	157.39	84.35	141.89
Subject19	243.73	189.98	189.65	137.01	156.90	132.77	202.14	229.90	185.26
Subject20	160.82	136.26	143.35	150.48	119.93	118.32	147.50	181.98	144.83
Subject21	211.94	151.08	190.92	117.70	169.93	101.10	204.37	92.51	154.94
Subject22	178.88	144.35	200.36	122.20	186.91	132.58	152.50	185.77	162.94
Subject23	126.75	182.35	147.85	186.76	127.58	184.29	86.13	114.05	144.47
Subject24	204.81	126.50	142.64	136.08	156.64	128.67	147.29	94.05	142.09
Subject25	152.80	119.68	182.80	127.56	119.07	143.22	99.61	109.20	131.74
Subject26	199.08	159.91	154.04	181.33	110.26	67.74	105.39	144.79	140.32
Subject27	153.48	137.76	185.90	169.92	145.01	90.63	173.21	169.16	153.13
Subject28	164.34	134.61	165.18	164.04	114.98	155.37	141.09	162.04	150.21
Subject29	279.33	207.65	233.47	188.27	136.81	188.10	231.04	179.11	205.47
Subject30	218.29	145.88	169.10	85.59	189.20	103.37	103.26	99.69	139.30
Subject31	213.82	109.13	188.86	183.73	146.53	82.40	181.64	155.26	157.67
Subject32	132.31	176.15	169.81	137.50	64.11	158.56	174.14	172.36	148.12
Subject33	189.12	139.23	182.66	113.12	146.67	110.88	66.90	147.22	136.98
Subject34	225.02	162.85	162.50	126.15	142.59	130.61	104.94	105.90	145.07
Subject35	178.13	95.58	147.25	140.40	153.15	154.66	121.45	73.22	132.98
Subject36	193.50	105.90	210.23	172.75	124.81	127.09	171.96	78.10	148.04
TrtMean	183.16	143.79	178.37	146.79	128.45	130.65	143.13	129.37	147.96

The Analysis of Variance Table is given below.

Source	df	SS	MS	F	df1	df2	F(.05)	P-value	Variance
Navigation Technique	3	66996	22331.84	15.759	3	105	2.691	0.0000	
Input Method	1	30636	30635.76	15.629	1	35	4.121	0.0004	
Subject	35	84008	2400.23	0.979	35	43.82	1.695	0.5212	-6.32
NTxIM	3	18710	6236.76	6.732	3	105	2.691	0.0003	
NTxS	105	148797	1417.12	1.530	105	105	1.381	0.0152	245.31
IMxS	35	68605	1960.13	2.116	35	105	1.535	0.0019	258.41
Error (NTxIMxS)	105	97282	926.50						926.50
Total	287	515034							

R Program (Note that the F-statistics from the `aov` function use MS_{ERR} for the error terms):

```

navmap <-
read.table("http://www.stat.ufl.edu/~winner/data/navtechmap1.dat",
           header=F,col.names=c("navtech","inpmeth","subj","tasktime"))

attach(navmap)
navtech <- factor(navtech)
inpmeth <- factor(inpmeth)
subj <- factor(subj)

navmap.mod1 <- aov(tasktime ~ navtech + inpmeth + subj + navtech:inpmeth
+
  navtech:subj + inpmeth:subj)
anova(navmap.mod1)

library(lmerTest)

navmap.mod2 <- lmer(tasktime ~ navtech + inpmeth + navtech:inpmeth +
  (1|subj) + (1|navtech:subj) + (1|inpmeth:subj))
summary(navmap.mod2)
anova(navmap.mod2)
anova(navmap.mod2, ddf="kenward-Roger")
diff1smeans(navmap.mod2)

```

R Output:

```

> navmap.mod1 <- aov(tasktime ~ navtech + inpmeth + subj + navtech:inpmeth +
+   navtech:subj + inpmeth:subj)
> anova(navmap.mod1)
Analysis of Variance Table

Response: tasktime
      Df Sum Sq Mean Sq F value    Pr(>F)
navtech    3  66996  22331.8  24.1035 6.033e-12 ***
inpmeth    1  30636  30635.8  33.0662 8.840e-08 ***
subj      35  84008   2400.2   2.5906 0.0001025 ***
navtech:inpmeth  3  18710   6236.8   6.7316 0.0003376 ***
navtech:subj 105 148797   1417.1   1.5295 0.0152294 *
inpmeth:subj  35  68605   1960.1   2.1156 0.0018646 **
Residuals 105  97282    926.5

```

Continued

Linear mixed model fit by REML t-tests use Satterthwaite approximations to degrees of freedom [merModLmerTest]
 Formula: tasktime ~ navtech + inpmeth + navtech:inpmeth + (1 | subj) + (1 | navtech:subj) + (1 | inpmeth:subj)

REML criterion at convergence: 2840.2

Scaled residuals:

	Min	1Q	Median	3Q	Max
	-2.14081	-0.60108	0.01166	0.59746	2.75578

Random effects:

Groups	Name	Variance	Std.Dev.
navtech:subj	(Intercept)	243.0	15.59
inpmeth:subj	(Intercept)	253.6	15.92
subj	(Intercept)	0.0	0.00
Residual		927.9	30.46

Number of obs: 288, groups: navtech:subj, 144; inpmeth:subj, 72; subj, 36

Fixed effects:

	Estimate	Std. Error	df	t value	Pr(> t)
(Intercept)	183.159	6.290	250.220	29.117	< 2e-16 ***
navtech2	-4.789	8.065	204.610	-0.594	0.5533
navtech3	-54.709	8.065	204.610	-6.783	1.24e-10 ***
navtech4	-40.029	8.065	204.610	-4.963	1.46e-06 ***
inpmeth2	-39.369	8.102	141.100	-4.859	3.09e-06 ***
navtech2:inpmeth2	7.789	10.154	107.590	0.767	0.4447
navtech3:inpmeth2	41.569	10.154	107.590	4.094	8.23e-05 ***
navtech4:inpmeth2	25.609	10.154	107.590	2.522	0.0131 *

> anova(navmap.mod2)

Analysis of Variance Table of type 3 with Satterthwaite approximation for degrees of freedom

	Sum Sq	Mean Sq	NumDF	DenDF	F.value	Pr(>F)
navtech	43964	14654.6	3	112.449	15.7940	1.228e-08 ***
inpmeth	14636	14635.9	1	54.542	15.7738	0.0002109 ***
navtech:inpmeth	18710	6236.8	3	107.588	6.7216	0.0003360 ***

> anova(navmap.mod2, ddf="Kenward-Roger")

Analysis of Variance Table of type 3 with Kenward-Roger approximation for degrees of freedom

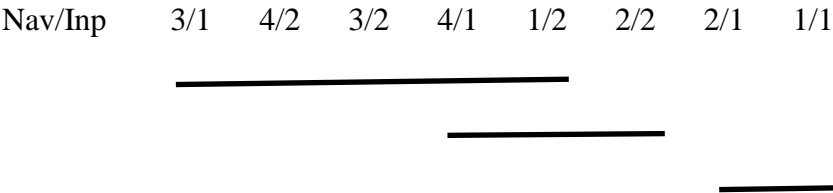
	Sum Sq	Mean Sq	NumDF	DenDF	F.value	Pr(>F)
navtech	43964	14654.6	3	105	15.7940	1.511e-08 ***
inpmeth	14636	14635.9	1	35	15.7738	0.0003389 ***
navtech:inpmeth	18710	6236.8	3	105	6.7216	0.0003416 ***

Note that Navigation techniques and input methods, as well as their interaction are highly significant. Below, based on the **diffsmeans** option, we find the differences in the least squares means for all pairs of the 8 combinations of navigation technique and input method.

navtech:inpmeth	1	1	-	2	1	4.8	8.065	204.6	0.59	-11.113	20.691	0.55
navtech:inpmeth	1	1	-	3	1	54.7	8.065	204.6	6.78	38.807	70.611	<2e-16 ***
navtech:inpmeth	1	1	-	4	1	40.0	8.065	204.6	4.96	24.128	55.931	<2e-16 ***
navtech:inpmeth	1	1	-	1	2	39.4	8.102	141.1	4.86	23.353	55.385	<2e-16 ***
navtech:inpmeth	1	1	-	2	2	36.4	8.896	250.2	4.09	18.849	53.890	1e-04 ***
navtech:inpmeth	1	1	-	3	2	52.5	8.896	250.2	5.90	34.988	70.029	<2e-16 ***
navtech:inpmeth	1	1	-	4	2	53.8	8.896	250.2	6.05	36.269	71.310	<2e-16 ***
navtech:inpmeth	2	1	-	3	1	49.9	8.065	204.6	6.19	34.018	65.822	<2e-16 ***
navtech:inpmeth	2	1	-	4	1	35.2	8.065	204.6	4.37	19.339	51.142	<2e-16 ***
navtech:inpmeth	2	1	-	1	2	34.6	8.896	250.2	3.89	17.060	52.101	1e-04 ***
navtech:inpmeth	2	1	-	2	2	31.6	8.102	141.1	3.90	15.564	47.597	1e-04 ***
navtech:inpmeth	2	1	-	3	2	47.7	8.896	250.2	5.36	30.200	65.240	<2e-16 ***
navtech:inpmeth	2	1	-	4	2	49.0	8.896	250.2	5.51	31.480	66.521	<2e-16 ***

navtech:inpmeth	3	1	-	4	1	-14.7	8.065	204.6	-1.82	-30.581	1.223	0.07	.
navtech:inpmeth	3	1	-	1	2	-15.3	8.896	250.2	-1.72	-32.860	2.181	0.09	.
navtech:inpmeth	3	1	-	2	2	-18.3	8.896	250.2	-2.06	-35.860	-0.819	0.04	*
navtech:inpmeth	3	1	-	3	2	-2.2	8.102	141.1	-0.27	-18.216	13.816	0.79	.
navtech:inpmeth	3	1	-	4	2	-0.9	8.896	250.2	-0.10	-18.439	16.602	0.92	.
navtech:inpmeth	4	1	-	1	2	-0.7	8.896	250.2	-0.07	-18.181	16.860	0.94	.
navtech:inpmeth	4	1	-	2	2	-3.7	8.896	250.2	-0.41	-21.180	13.861	0.68	.
navtech:inpmeth	4	1	-	3	2	12.5	8.896	250.2	1.40	-5.041	30.000	0.16	.
navtech:inpmeth	4	1	-	4	2	13.8	8.102	141.1	1.70	-2.256	29.776	0.09	.
navtech:inpmeth	1	2	-	2	2	-3.0	8.065	204.6	-0.37	-18.902	12.902	0.71	.
navtech:inpmeth	1	2	-	3	2	13.1	8.065	204.6	1.63	-2.762	29.042	0.10	.
navtech:inpmeth	1	2	-	4	2	14.4	8.065	204.6	1.79	-1.481	30.323	0.08	.
navtech:inpmeth	2	2	-	3	2	16.1	8.065	204.6	2.00	0.237	32.041	0.05	*
navtech:inpmeth	2	2	-	4	2	17.4	8.065	204.6	2.16	1.518	33.322	0.03	*
navtech:inpmeth	3	2	-	4	2	1.3	8.065	204.6	0.16	-14.621	17.183	0.87	.

The treatments ordered from lowest to highest mean task times are:



7.4. An Alternative (Restricted) Model for Balanced Data

An alternative model assumes that interactions involving fixed and random effects sum to zero when summed over any fixed effects. This model is appropriate if the interaction effects are correlated over levels of the random effects. The restricted model will not be used if data are unbalanced. Keep in mind that standard software packages fit the unrestricted model. Here we consider the 2-Way Mixed (restricted) model.

$$\begin{aligned}
 Y_{ijk} &= \mu^* + \alpha_i^* + \beta_j^* + (\alpha\beta)_{ij}^* + \varepsilon_{ijk}^* \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n \\
 \varepsilon_{ijk}^* &\sim NID(0, \sigma^2) \quad (\alpha\beta)_{ij}^* \sim N(0, \sigma_{\alpha\beta}^2) \quad \sum_{i=1}^a (\alpha\beta)_{ij}^* = (\alpha\beta)_{\cdot j}^* = 0 \\
 \Rightarrow 0 &= V\{(\alpha\beta)_{\cdot j}^*\} = \sum_{i=1}^a V\{(\alpha\beta)_{ij}^*\} + 2 \binom{a}{2} \text{COV}\{(\alpha\beta)_{ij}^*, (\alpha\beta)_{i'j}^*\} = a\sigma_{\alpha\beta}^2 + a(a-1)\text{COV}\{(\alpha\beta)_{ij}^*, (\alpha\beta)_{i'j}^*\} \\
 \Rightarrow \text{COV}\{(\alpha\beta)_{ij}^*, (\alpha\beta)_{i'j}^*\} &= -\frac{\sigma_{\alpha\beta}^2}{a-1}
 \end{aligned}$$

Note the following relations between the unrestricted and restricted models:

$$\text{Unrestricted: } Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n$$

$$\varepsilon_{ijk} \sim NID(0, \sigma^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2) \quad \{\varepsilon\} \perp \{(\alpha\beta)\}$$

$$\text{Restricted: } Y_{ijk} = \mu^* + \alpha_i^* + \beta_j^* + (\alpha\beta)_{ij}^* + \varepsilon_{ijk}^* \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n$$

$$\varepsilon_{ijk}^* \sim NID(0, \sigma^2) \quad (\alpha\beta)_{ij}^* \sim N(0, \sigma_{\alpha\beta^*}^2) \quad \sum_{i=1}^a (\alpha\beta)_{ij}^* = (\alpha\beta)_{\bullet j}^* = 0 \quad \{\varepsilon\} \perp \{(\alpha\beta)\}$$

$$(\alpha\beta)_{ij}^* = (\alpha\beta)_{ij} - \overline{(\alpha\beta)}_{\bullet j} \Rightarrow \beta_j^* = \beta_j + \overline{(\alpha\beta)}_{\bullet j} \quad \mu^* = \mu \quad \alpha_i^* = \alpha_i$$

$$V\{(\alpha\beta)_{ij}^*\} = \sigma_{\alpha\beta^*}^2 = V\{(\alpha\beta)_{ij}\} + V\{\overline{(\alpha\beta)}_{\bullet j}\} - 2\text{COV}\{(\alpha\beta)_{ij}, \overline{(\alpha\beta)}_{\bullet j}\} = \sigma_{\alpha\beta}^2 + \frac{\sigma_{\alpha\beta}^2}{a} - 2\frac{\sigma_{\alpha\beta}^2}{a} = \frac{(a-1)\sigma_{\alpha\beta}^2}{a} = \sigma_{\alpha\beta^*}^2$$

$$V\{\beta_j^*\} = \sigma_{\beta^*}^2 = V\{\beta_j\} + V\{\overline{(\alpha\beta)}_{\bullet j}\} + 2\text{COV}\{\beta_j, \overline{(\alpha\beta)}_{\bullet j}\} = \sigma_{\beta}^2 + \frac{\sigma_{\alpha\beta}^2}{a} + 0 = \sigma_{\beta}^2 + \frac{\sigma_{\alpha\beta}^2}{a} = \sigma_{\beta^*}^2$$

$$\text{COV}\{(\alpha\beta)_{ij}^*, \beta_j^*\} = \text{COV}\{(\alpha\beta)_{ij} - \overline{(\alpha\beta)}_{\bullet j}, \beta_j + \overline{(\alpha\beta)}_{\bullet j}\} = \text{COV}\{(\alpha\beta)_{ij}, \overline{(\alpha\beta)}_{\bullet j}\} - V\{\overline{(\alpha\beta)}_{\bullet j}\} = \frac{\sigma_{\alpha\beta}^2}{a} - \frac{\sigma_{\alpha\beta}^2}{a} = 0$$

Here we obtain the Expected Mean Squares for the Restricted Model.

$$E\{Y_{ijk}\} = \mu + \alpha_i \quad E\{\overline{Y}_{ij\bullet}\} = \mu + \alpha_i \quad E\{\overline{Y}_{i\bullet\bullet}\} = \mu + \alpha_i \quad E\{\overline{Y}_{\bullet j\bullet}\} = \mu \quad E\{\overline{Y}_{\bullet\bullet\bullet}\} = \mu$$

$$V\{Y_{ijk}\} = V\{\mu^* + \alpha_i^* + \beta_j^* + (\alpha\beta)_{ij}^* + \varepsilon_{ijk}^*\} = \sigma_{\beta^*}^2 + \frac{\sigma_{\alpha\beta}^2}{a} + \frac{(a-1)\sigma_{\alpha\beta}^2}{a} + \sigma^2 =$$

$$= \sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \sigma^2 = \left(\sigma_{\beta}^2 + \frac{\sigma_{\alpha\beta}^2}{a}\right) + \frac{(a-1)\sigma_{\alpha\beta}^2}{a} + \sigma^2 = \sigma_{\beta^*}^2 + \sigma_{\alpha\beta^*}^2 + \sigma^2$$

$$\text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \sigma^2 = \sigma_{\beta^*}^2 + \sigma_{\alpha\beta^*}^2 + \sigma^2 & i = i', j = j', k = k' \\ \sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 = \sigma_{\beta^*}^2 + \sigma_{\alpha\beta^*}^2 & i = i', j = j', k \neq k' \\ \sigma_{\beta}^2 = \sigma_{\beta^*}^2 - \frac{\sigma_{\alpha\beta}^2}{a} & i \neq i', j = j', \forall k, k' \\ 0 & \forall i, i' j \neq j', \forall k, k' \end{cases}$$

$$V\{\overline{Y}_{ij\bullet}\} = \left(\frac{1}{n}\right)^2 [n(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + n(n-1)(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2)] = \sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma^2}{n} =$$

$$= \left(\sigma_{\beta}^2 + \frac{\sigma_{\alpha\beta}^2}{a}\right) + \frac{(a-1)\sigma_{\alpha\beta}^2}{a} + \frac{\sigma^2}{n} = \sigma_{\beta^*}^2 + \sigma_{\alpha\beta^*}^2 + \frac{\sigma^2}{n}$$

$$V\{\overline{Y}_{i\bullet\bullet}\} = \left(\frac{1}{bn}\right)^2 [bn(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + bn(n-1)(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2) + b(b-1)n^2(0)] = \frac{\sigma_{\beta}^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma^2}{bn} =$$

$$= \left(\frac{\sigma_{\beta}^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab}\right) + \frac{(a-1)\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma^2}{bn} = \frac{\sigma_{\beta^*}^2}{b} + \frac{\sigma_{\alpha\beta^*}^2}{b} + \frac{\sigma^2}{bn}$$

$$V\{\overline{Y}_{\bullet j\bullet}\} = \left(\frac{1}{an}\right)^2 [an(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + an(n-1)(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2) + a(a-1)n^2(\sigma_{\beta}^2)] =$$

$$= \sigma_{\beta}^2 + \frac{\sigma_{\alpha\beta}^2}{a} + \frac{\sigma^2}{an} = \left(\sigma_{\beta}^2 + \frac{\sigma_{\alpha\beta}^2}{a}\right) + \frac{\sigma^2}{an} = \sigma_{\beta^*}^2 + \frac{\sigma^2}{an}$$

$$V\{\overline{Y}_{\bullet\bullet\bullet}\} = \left(\frac{1}{abn}\right)^2 [abn(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + abn(n-1)(\sigma_{\beta}^2 + \sigma_{\alpha\beta}^2) + a(a-1)bn^2(\sigma_{\beta}^2) + a^2b(b-1)n^2(0)] =$$

$$= \frac{\sigma_{\beta}^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma^2}{abn} = \left(\frac{\sigma_{\beta}^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab}\right) + \frac{\sigma^2}{abn} = \frac{\sigma_{\beta^*}^2}{b} + \frac{\sigma^2}{abn}$$

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n E\{Y_{ijk}^2\} &= abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + abn\sigma_{\beta^*}^2 + abn\sigma_{\alpha\beta^*}^2 + abn\sigma^2 \\
n \sum_{i=1}^a \sum_{j=1}^b E\{\bar{Y}_{ij^*}^2\} &= abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + abn\sigma_{\beta^*}^2 + abn\sigma_{\alpha\beta^*}^2 + ab\sigma^2 \\
bn \sum_{i=1}^a E\{\bar{Y}_{i\bullet\bullet}^2\} &= abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + an\sigma_{\beta^*}^2 + an\sigma_{\alpha\beta^*}^2 + a\sigma^2 \\
an \sum_{j=1}^b E\{\bar{Y}_{\bullet j^*}^2\} &= abn\mu^2 + abn\sigma_{\beta^*}^2 + b\sigma^2 \\
abn E\{\bar{Y}_{\bullet\bullet\bullet}^2\} &= abn\mu^2 + an\sigma_{\beta^*}^2 + \sigma^2 \\
E\{MS_A\} &= \frac{1}{a-1} \left[\left(abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + an\sigma_{\beta^*}^2 + an\sigma_{\alpha\beta^*}^2 + a\sigma^2 \right) - \left(abn\mu^2 + an\sigma_{\beta^*}^2 + n\sigma_{\alpha\beta^*}^2 + \sigma^2 \right) \right] = \sigma^2 + n\sigma_{\alpha\beta^*}^2 + \frac{bn \sum_{i=1}^a \alpha_i^2}{a-1} \\
E\{MS_B\} &= \frac{1}{b-1} \left[\left(abn\mu^2 + abn\sigma_{\beta^*}^2 + b\sigma^2 \right) - \left(abn\mu^2 + an\sigma_{\beta^*}^2 + \sigma^2 \right) \right] = \sigma^2 + an\sigma_{\beta^*}^2 \\
E\{MS_{AB}\} &= \frac{1}{(a-1)(b-1)} \times \\
&\left\{ \left[\left(abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + abn\sigma_{\beta^*}^2 + abn\sigma_{\alpha\beta^*}^2 + ab\sigma^2 \right) - \left(abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + an\sigma_{\beta^*}^2 + an\sigma_{\alpha\beta^*}^2 + a\sigma^2 \right) \right] + \right. \\
&\left. \left[- \left(abn\mu^2 + abn\sigma_{\beta^*}^2 + b\sigma^2 \right) + \left(abn\mu^2 + an\sigma_{\beta^*}^2 + \sigma^2 \right) \right] \right\} = \sigma^2 + \frac{an\sigma_{\alpha\beta^*}^2}{a-1} = \sigma^2 + n\sigma_{\alpha\beta}^2 \\
E\{MS_{ERR}\} &= \frac{1}{ab(n-1)} \left[\left(abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + abn\sigma_{\beta^*}^2 + abn\sigma_{\alpha\beta^*}^2 + abn\sigma^2 \right) - \left(abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + abn\sigma_{\beta^*}^2 + abn\sigma_{\alpha\beta^*}^2 + ab\sigma^2 \right) \right] = \sigma^2
\end{aligned}$$

Note that for the restricted model, if we test for a main effect for the random factor B, we are testing for a different variance than in the unrestricted model, and the correct error term is MS_{ERR} , as opposed to MS_{AB} as would be done for the unrestricted model. This effects the error term and degrees of freedom:

$$H_0 : \sigma_{\beta^*}^2 = 0 \Rightarrow \sigma_{\beta^*}^2 + \frac{\sigma_{\alpha\beta^*}^2}{a} = 0 \quad TS : F_B = \frac{MS_B}{MS_{ERR}} \quad RR : F_B \geq F_{1-\alpha; b-1, ab(n-1)} \quad \text{P-value} = P(F_{b-1, ab(n-1)} \geq F_B)$$

7.5. Matrix Form for the Navigational Techniques Example

Here we consider the mixed model with 2 fixed factors: Navigational Technique ($a = 4$) and Input Method ($b = 2$), and one random factor: Subject ($c = 36$). There was one replication per subject for each combination of Navigation Technique and Input Method ($n = 1$). The model can be written as:

$$\begin{aligned}
Y_{ijk} &= \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \gamma_k + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + \varepsilon_{ijk} \quad i = 1, 2, 3, 4; j = 1, 2; k = 1, 2, \dots, 36 \\
\sum_{i=1}^4 \alpha_i &= \sum_{j=1}^2 \beta_j = \sum_{i=1}^4 (\alpha\beta)_{ij} = \sum_{j=1}^2 (\alpha\beta)_{ij} = 0 \quad \{\gamma\} \perp \{(\alpha\gamma)\} \perp \{(\beta\gamma)\} \perp \{\varepsilon\} \\
\gamma_k &\sim NID(0, \sigma_{\gamma}^2) \quad (\alpha\gamma)_{ik} \sim NID(0, \sigma_{\alpha\gamma}^2) \quad (\beta\gamma)_{jk} \sim NID(0, \sigma_{\beta\gamma}^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \\
\text{Matrix Form: } &\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\varepsilon}
\end{aligned}$$

Note that this is an unrestricted model.

7.6. Likelihood Ratio Tests for Variance Components

An alternative test for variance components can be conducted based on the log-likelihood (technically joint density of \mathbf{Y} and \mathbf{u}) evaluated at the estimated parameters. The test involves fitting the model with and without the particular random effect, and comparing the log-likelihood. $\chi_{obs}^2 = -2(\ln L_0 - \ln L_A) = -2(l_0 - l_A)$

Example: Navigational Techniques of Web Maps

We test the significance of the interaction variance components between the fixed factors and the random (subject) effects. $H_0^{AC} : \sigma_{AC}^2 = 0$ $H_0^{BC} : \sigma_{BC}^2 = 0$

R Program:

```
navmap <- read.table("http://www.stat.ufl.edu/~winner/data/navtechmap1.dat",
  header=F, col.names=c("navtech", "inpmeth", "subj", "tasktime"))
attach(navmap)
navtech <- factor(navtech); inpmeth <- factor(inpmeth); subj <- factor(subj)
library(lmerTest)
navmap.mod2 <- lmer(tasktime ~ navtech + inpmeth + navtech:inpmeth +
  (1|subj) + (1|navtech:subj) + (1|inpmeth:subj))
logLik(navmap.mod2)
navmap.mod3 <- lmer(tasktime ~ navtech + inpmeth + navtech:inpmeth +
  (1|subj) + (1|navtech:subj))
logLik(navmap.mod3)
navmap.mod4 <- lmer(tasktime ~ navtech + inpmeth + navtech:inpmeth +
  (1|subj) + (1|inpmeth:subj))
logLik(navmap.mod4)
rand(navmap.mod2)
```

R Output

```
> logLik(navmap.mod2)
'log Lik.' -1420.12 (df=12)
> logLik(navmap.mod3)
'log Lik.' -1424.224 (df=11)
> logLik(navmap.mod4)
'log Lik.' -1422.47 (df=11)
> rand(navmap.mod2)
Analysis of Random effects Table:
      Chi.sq Chi.DF p.value
subj      0.00     1  1.000
navtech:subj  4.70     1  0.030 *
inpmeth:subj  8.21     1  0.004 **
```

Note that by comparing models 2 and 3, you get the following test statistics, which are also computed directly with the **rand** option in the **lmerTest** package. The p-values computed by R are based on the chi-square distribution with 1 degree of freedom. These p-values are conservative for strictly 1-sided tests.

$$\chi_{BC}^2 = -2((-1424.224) - (-1420.12)) = 8.21$$

$$\chi_{AC}^2 = -2((-1422.47) - (-1420.12)) = 4.70$$

Data Sources:

Women's Professional Bowling Scores:
www.pba.com

J.R. Hudson (1968). "Institute of Brewing: Analysis Committee Measurement of Head-Retention in Bottled Beer," *Journal of the Institute of Brewing*, Vol. 74, Issue 3, pp. 275-285.

F.-G. Wu, H. Lin, M. You (2011). "The Enhanced Navigator for the Touch Screen: A Comparative Study on Navigational Techniques of Web Maps," *Displays*, Vol. 32, pp. 284-295.

Chapter 8 – Designs with Nested Factors

So far, all of the multi-factor designs considered have been **crossed**. That means the same levels of Factor B were used within each level of Factor A, and vice versa. For example, in the Navigation Technique Experiment, the same 2 input methods were used for each navigational technique, and vice versa. Further, each subject received all 8 treatments.

Many studies involve **nested** factors (as well as possibly crossed factors). These factors have different levels within levels of the nesting factor. For instance, a study comparing test scores among school districts may sample various schools within each district, and possibly classrooms within schools. Also, in many repeated measures designs, subjects will be assigned to receive one treatment, and observed at multiple time points. In this case, subjects are nested within treatments, and crossed with time.

8.1. Two-Factor Nested Designs

We begin with a 2-factor design, where Factor A has a levels and Factor B has b_i levels within the i^{th} level of Factor A. We will assume a balanced design such that within each level of factor B there are n replications. The model can be fixed (Factors A and B observed at all levels of interest), random (Factors A and B observed at samples of levels), or mixed (A at all levels of interest, B at a sample of levels). As before, in all cases the Analysis of Variance is computed in the same manner, but the Expected Mean Squares will depend on the type of factors included.

Fixed Effects Model:

$$\begin{aligned}
 Y_{ijk} &= \mu + \alpha_i + \beta_{j(i)} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b_i; k = 1, \dots, n \quad \sum_{i=1}^a b_i \alpha_i = \sum_{j=1}^{b_1} \beta_{j(1)} = \dots = \sum_{j=1}^{b_a} \beta_{j(a)} = 0 \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \\
 SS_A &= \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n (\bar{Y}_{i..} - \bar{Y}...)^2 = n \sum_{i=1}^a b_i \bar{Y}_{i..}^2 - N \bar{Y}...^2 \quad \text{where } N = nb... = n \sum_{i=1}^a b_i \quad df_A = a - 1 \\
 SS_{B(A)} &= \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n (\bar{Y}_{ij.} - \bar{Y}_{i..})^2 = n \sum_{i=1}^a \sum_{j=1}^{b_i} \bar{Y}_{ij.}^2 - n \sum_{i=1}^a b_i \bar{Y}_{i..}^2 \quad df_{B(A)} = \sum_{i=1}^a (b_i - 1) = b... - a \\
 SS_{\text{Err}} &= \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n (Y_{ijk} - \bar{Y}_{ij.})^2 = \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n Y_{ijk}^2 - n \sum_{i=1}^a \sum_{j=1}^{b_i} \bar{Y}_{ij.}^2 \quad df_{\text{Err}} = b...(n-1) = N - b... \\
 SS_{\text{Tot}} &= \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n (Y_{ijk} - \bar{Y}...)^2 = \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n Y_{ijk}^2 - N \bar{Y}...^2 \quad df_{\text{Tot}} = N - 1 \\
 E\{Y_{ijk}\} &= \mu + \alpha_i + \beta_{j(i)} \quad E\{\bar{Y}_{ij.}\} = \mu + \alpha_i + \beta_{j(i)} \quad E\{\bar{Y}_{i..}\} = \mu + \alpha_i \quad E\{\bar{Y}...\} = \mu \\
 V\{Y_{ijk}\} &= \sigma^2 \quad V\{\bar{Y}_{ij.}\} = \frac{\sigma^2}{n} \quad V\{\bar{Y}_{i..}\} = \frac{\sigma^2}{nb_i} \quad V\{\bar{Y}...\} = \frac{\sigma^2}{N} \\
 E\{Y_{ijk}^2\} &= (\mu + \alpha_i + \beta_{j(i)})^2 + \sigma^2 \Rightarrow E\left\{\sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n Y_{ijk}^2\right\} = \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n (\mu + \alpha_i + \beta_{j(i)})^2 + N\sigma^2 = \\
 &= N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2 + 2n\mu \sum_{i=1}^a b_i \alpha_i + 2n\mu \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)} + 2n \sum_{i=1}^a \alpha_i \sum_{j=1}^{b_i} \beta_{j(i)} + N\sigma^2 = \\
 &= N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2 + N\sigma^2
 \end{aligned}$$

$$E \left\{ \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n Y_{ijk}^2 \right\} = N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2 + N\sigma^2$$

$$E \left\{ \bar{Y}_{ij\bullet}^2 \right\} = \left(\mu + \alpha_i + \beta_{j(i)} \right)^2 + \frac{\sigma^2}{n} \Rightarrow E \left\{ n \sum_{i=1}^a \sum_{j=1}^{b_i} \bar{Y}_{ij\bullet}^2 \right\} = n \sum_{i=1}^a \sum_{j=1}^{b_i} \left(\mu + \alpha_i + \beta_{j(i)} \right)^2 + N \frac{\sigma^2}{n} =$$

$$= N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2 + b \cdot \sigma^2$$

$$E \left\{ \bar{Y}_{i\bullet\bullet}^2 \right\} = \left(\mu + \alpha_i \right)^2 + \frac{\sigma^2}{nb_i} \Rightarrow E \left\{ n \sum_{i=1}^a b_i \bar{Y}_{i\bullet\bullet}^2 \right\} = N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + 2n\mu \sum_{i=1}^a b_i \alpha_i + n \sum_{i=1}^a b_i \frac{\sigma^2}{nb_i} = N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + a\sigma^2$$

$$E \left\{ \bar{Y}_{\bullet\bullet\bullet}^2 \right\} = \mu^2 + \frac{\sigma^2}{N} \Rightarrow E \left\{ N \bar{Y}_{\bullet\bullet\bullet}^2 \right\} = N\mu^2 + \sigma^2$$

$$E \{ MS_A \} = \frac{1}{a-1} \left[\left(N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + a\sigma^2 \right) - \left(N\mu^2 + \sigma^2 \right) \right] = \frac{n \sum_{i=1}^a b_i \alpha_i^2}{a-1} + \sigma^2$$

$$E \{ MS_{B(A)} \} = \frac{1}{b \cdot - a} \left[\left(N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2 + b \cdot \sigma^2 \right) - \left(N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + a\sigma^2 \right) \right] = \frac{n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2}{b \cdot - a} + \sigma^2$$

$$E \{ MS_{Err} \} = \frac{1}{N - b \cdot} \left[\left(N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2 + N\sigma^2 \right) - \left(N\mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a \sum_{j=1}^{b_i} \beta_{j(i)}^2 + b \cdot \sigma^2 \right) \right] = \sigma^2$$

Thus all tests and parameter estimates and inferences are based on using MS_{Err} as the error term.

$$H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad TS_A : F_A = \frac{MS_A}{MS_{Err}} \quad RR_A : F_A \geq F_{1-\alpha; a-1, N-b \cdot}$$

$$P\text{-Value: } P(F_{a-1, N-b \cdot} \geq F_A)$$

$$H_0^{B(A)} : \beta_{1(i)} = \dots = \beta_{b_a(a)} = 0 \quad TS_{B(A)} : F_{B(A)} = \frac{MS_{B(A)}}{MS_{Err}} \quad RR_{B(A)} : F_{B(A)} \geq F_{1-\alpha; b \cdot - a, N-b \cdot}$$

$$P\text{-Value: } P(F_{b \cdot - a, N-b \cdot} \geq F_{B(A)})$$

$$V \{ \bar{Y}_{i\bullet\bullet} \} = \frac{\sigma^2}{nb_i} \quad \hat{SE} \{ \bar{Y}_{i\bullet\bullet} \} = \sqrt{\frac{MS_{Err}}{nb_i}} \quad \text{COV} \{ \bar{Y}_{i\bullet\bullet}, \bar{Y}_{i\bullet\bullet} \} = 0$$

$$V \{ \bar{Y}_{ij\bullet} \} = \frac{\sigma^2}{n} \quad \hat{SE} \{ \bar{Y}_{ij\bullet} \} = \sqrt{\frac{MS_{Err}}{n}} \quad \text{COV} \{ \bar{Y}_{ij\bullet}, \bar{Y}_{ij\bullet} \} = 0$$

Random Effects Model:

$$Y_{ijk} = \mu + \alpha_i + \beta_{j(i)} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b_i; k = 1, \dots, n \quad \{\alpha\} \perp \{\beta\} \perp \{\varepsilon\}$$

$$\alpha_i \sim NID(0, \sigma_\alpha^2) \quad \beta_{j(i)} \sim NID(0, \sigma_\beta^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2)$$

$$E\{Y_{ijk}\} = E\{\bar{Y}_{ij\cdot}\} = E\{\bar{Y}_{i\cdot\cdot}\} = E\{\bar{Y}_{\dots}\} = \mu$$

$$V\{Y_{ijk}\} = \sigma_\alpha^2 + \sigma_\beta^2 + \sigma^2 \quad \text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\alpha^2 + \sigma_\beta^2 + \sigma^2 & i = i', j = j', k = k' \\ \sigma_\alpha^2 + \sigma_\beta^2 & i = i', j = j', k \neq k' \\ \sigma_\alpha^2 & i = i', j \neq j', \forall k, k' \\ 0 & i \neq i', \forall j, j', \forall k, k' \end{cases}$$

$$V\{\bar{Y}_{ij\cdot}\} = \frac{1}{n^2} \left[n(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma^2) + n(n-1)(\sigma_\alpha^2 + \sigma_\beta^2) \right] = \sigma_\alpha^2 + \sigma_\beta^2 + \frac{\sigma^2}{n}$$

$$V\{\bar{Y}_{i\cdot\cdot}\} = \frac{1}{n^2 b_i^2} \left[nb_i(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma^2) + n(n-1)b_i(\sigma_\alpha^2 + \sigma_\beta^2) + b_i(b_i-1)n^2\sigma_\alpha^2 \right] = \sigma_\alpha^2 + \frac{\sigma_\beta^2}{b_i} + \frac{\sigma^2}{nb_i}$$

$$V\{\bar{Y}_{\dots}\} = \frac{1}{n^2 b_\cdot^2} \left[nb_\cdot(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma^2) + n(n-1)b_\cdot(\sigma_\alpha^2 + \sigma_\beta^2) + \left(\frac{n^2 b_\cdot^2}{a} - n^2 b_\cdot \right) \sigma_\alpha^2 + \left(n^2 b_\cdot^2 - \frac{n^2 b_\cdot^2}{a} \right) (0) \right]$$

$$= \frac{\sigma_\alpha^2}{a} + \frac{\sigma_\beta^2}{b_\cdot} + \frac{\sigma^2}{nb_\cdot}$$

$$E\left\{ \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n Y_{ijk}^2 \right\} = nb_\cdot \mu^2 + nb_\cdot (\sigma_\alpha^2 + \sigma_\beta^2 + \sigma^2) = nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + nb_\cdot \sigma_\beta^2 + nb_\cdot \sigma^2$$

$$E\left\{ n \sum_{i=1}^a \sum_{j=1}^{b_i} \bar{Y}_{ij\cdot}^2 \right\} = nb_\cdot \mu^2 + nb_\cdot \left(\sigma_\alpha^2 + \sigma_\beta^2 + \frac{\sigma^2}{n} \right) = nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + nb_\cdot \sigma_\beta^2 + b_\cdot \sigma^2$$

$$E\left\{ n \sum_{i=1}^a b_i \bar{Y}_{i\cdot\cdot}^2 \right\} = nb_\cdot \mu^2 + n \sum_{i=1}^a b_i \left(\sigma_\alpha^2 + \frac{\sigma_\beta^2}{b_i} + \frac{\sigma^2}{nb_i} \right) = nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + an \sigma_\beta^2 + a \sigma^2$$

$$E\{N\bar{Y}_{\dots}^2\} = nb_\cdot \mu^2 + nb_\cdot \left(\frac{\sigma_\alpha^2}{a} + \frac{\sigma_\beta^2}{b_\cdot} + \frac{\sigma^2}{nb_\cdot} \right) = nb_\cdot \mu^2 + n \left(\frac{b_\cdot}{a} \right) \sigma_\alpha^2 + n \sigma_\beta^2 + \sigma^2$$

$$E\{MS_A\} = \frac{1}{a-1} \left[(nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + an \sigma_\beta^2 + a \sigma^2) - \left(nb_\cdot \mu^2 + n \left(\frac{b_\cdot}{a} \right) \sigma_\alpha^2 + n \sigma_\beta^2 + \sigma^2 \right) \right] = n \left(\frac{b_\cdot}{a} \right) \sigma_\alpha^2 + n \sigma_\beta^2 + \sigma^2$$

$$E\{MS_{B(A)}\} = \frac{1}{b_\cdot - a} \left[(nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + nb_\cdot \sigma_\beta^2 + b_\cdot \sigma^2) - (nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + an \sigma_\beta^2 + a \sigma^2) \right] = n \sigma_\beta^2 + \sigma^2$$

$$E\{MS_{Err}\} = \frac{1}{N - b_\cdot} \left[(nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + nb_\cdot \sigma_\beta^2 + nb_\cdot \sigma^2) - (nb_\cdot \mu^2 + nb_\cdot \sigma_\alpha^2 + nb_\cdot \sigma_\beta^2 + b_\cdot \sigma^2) \right] = \sigma^2$$

These results lead to the following tests and point estimates regarding variance components:

$$\begin{aligned}
H_0^A : \sigma_\alpha^2 = 0 \quad H_A^A : \sigma_\alpha^2 > 0 \quad TS_A : F_A = \frac{MS_A}{MS_{B(A)}} \\
RR_A : F_A \geq F_{1-\alpha; a-1, b, -a} \quad \text{P-value: } P(F_{a-1, b, -a} \geq F_A) \\
H_0^{B(A)} : \sigma_\beta^2 = 0 \quad H_A^{B(A)} : \sigma_\beta^2 > 0 \quad TS_{B(A)} : F_{B(A)} = \frac{MS_{B(A)}}{MS_{\text{Err}}} \\
RR_{B(A)} : F_{B(A)} \geq F_{1-\alpha; b, -a, N-b} \quad \text{P-value: } P(F_{b, -a, N-b} \geq F_{B(A)}) \\
\hat{\sigma}^2 = MS_{\text{Err}} \quad \hat{\sigma}_\beta^2 = \frac{MS_{B(A)} - MS_{\text{Err}}}{n} \quad \hat{\sigma}_\alpha^2 = \frac{MS_A - MS_{B(A)}}{nb_\bullet} \quad \text{where } \bar{b}_\bullet = \frac{b_\bullet}{a}
\end{aligned}$$

Mixed Effects Model (A Fixed, B Random):

$$\begin{aligned}
Y_{ijk} &= \mu + \alpha_i + \beta_{j(i)} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b_i; k = 1, \dots, n \quad \{\beta\} \perp \{\varepsilon\} \\
\sum_{i=1}^a \alpha_i &= 0 \quad \beta_{j(i)} \sim NID(0, \sigma_\beta^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \\
E\{Y_{ijk}\} &= E\{\bar{Y}_{ij\bullet}\} = E\{\bar{Y}_{i\bullet\bullet}\} = \mu + \alpha_i \quad E\{\bar{Y}_{\dots}\} = \mu \\
V\{Y_{ijk}\} &= \sigma_\beta^2 + \sigma^2 \quad \text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\beta^2 + \sigma^2 & i = i', j = j', k = k' \\ \sigma_\beta^2 & i = i', j = j', k \neq k' \\ 0 & i = i', j \neq j', \forall k, k' \\ 0 & i \neq i', \forall j, j', \forall k, k' \end{cases}
\end{aligned}$$

$$\begin{aligned}
V\{\bar{Y}_{ij\bullet}\} &= \frac{1}{n^2} \left[n(\sigma_\beta^2 + \sigma^2) + n(n-1)(\sigma_\beta^2) \right] = \sigma_\beta^2 + \frac{\sigma^2}{n} \\
V\{\bar{Y}_{i\bullet\bullet}\} &= \frac{1}{n^2 b_i^2} \left[n b_i (\sigma_\beta^2 + \sigma^2) + n(n-1) b_i (\sigma_\beta^2) + b_i (b_i - 1) n^2 (0) \right] = \frac{\sigma_\beta^2}{b_i} + \frac{\sigma^2}{n b_i} \\
V\{\bar{Y}_{\dots}\} &= \frac{1}{n^2 b_\bullet^2} \left[n b_\bullet (\sigma_\beta^2 + \sigma^2) + n(n-1) b_\bullet (\sigma_\beta^2) + \left(\frac{n^2 b_\bullet^2}{a} - n^2 b_\bullet \right) (0) + \left(n^2 b_\bullet^2 - \frac{n^2 b_\bullet^2}{a} \right) (0) \right] = \frac{\sigma_\beta^2}{b_\bullet} + \frac{\sigma^2}{n b_\bullet}
\end{aligned}$$

This leads to the following Expected Mean Squares.

$$\begin{aligned}
E \left\{ \sum_{i=1}^a \sum_{j=1}^{b_i} \sum_{k=1}^n Y_{ijk}^2 \right\} &= nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + nb \cdot (\sigma_\beta^2 + \sigma^2) = nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + nb \cdot \sigma_\beta^2 + nb \cdot \sigma^2 \\
E \left\{ n \sum_{i=1}^a \sum_{j=1}^{b_i} \bar{Y}_{ij \cdot}^2 \right\} &= nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + nb \cdot \left(\sigma_\beta^2 + \frac{\sigma^2}{n} \right) = nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + nb \cdot \sigma_\beta^2 + b \cdot \sigma^2 \\
E \left\{ n \sum_{i=1}^a b_i \bar{Y}_{i \cdot \cdot}^2 \right\} &= nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + n \sum_{i=1}^a b_i \left(\frac{\sigma_\beta^2}{b_i} + \frac{\sigma^2}{nb_i} \right) = nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + an \sigma_\beta^2 + a \sigma^2 \\
E \left\{ N \bar{Y}^2 \dots \right\} &= nb \cdot \mu^2 + nb \cdot \left(\frac{\sigma_\beta^2}{b \cdot} + \frac{\sigma^2}{nb \cdot} \right) = nb \cdot \mu^2 + n \sigma_\beta^2 + \sigma^2 \\
E \{ MS_A \} &= \frac{1}{a-1} \left[\left(nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + an \sigma_\beta^2 + a \sigma^2 \right) - \left(nb \cdot \mu^2 + n \sigma_\beta^2 + \sigma^2 \right) \right] = \frac{n \sum_{i=1}^a b_i \alpha_i^2}{a-1} + n \sigma_\beta^2 + \sigma^2 \\
E \{ MS_{B(A)} \} &= \frac{1}{b \cdot - a} \left[\left(nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + nb \cdot \sigma_\beta^2 + b \cdot \sigma^2 \right) - \left(nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + an \sigma_\beta^2 + a \sigma^2 \right) \right] = n \sigma_\beta^2 + \sigma^2 \\
E \{ MS_{Err} \} &= \frac{1}{nb \cdot - b \cdot} \left[\left(nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + nb \cdot \sigma_\beta^2 + nb \cdot \sigma^2 \right) - \left(nb \cdot \mu^2 + n \sum_{i=1}^a b_i \alpha_i^2 + nb \cdot \sigma_\beta^2 + b \cdot \sigma^2 \right) \right] = \sigma^2
\end{aligned}$$

These results lead to the following tests and point estimators regarding variance components and parameters.

$$\begin{aligned}
H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad TS_A : F_A &= \frac{MS_A}{MS_{B(A)}} \\
RR_A : F_A \geq F_{1-\alpha; a-1, b \cdot - a} \quad \text{P-value: } P(F_{a-1, b \cdot - a} \geq F_A) \\
H_0^{B(A)} : \sigma_\beta^2 = 0 \quad H_A^{B(A)} : \sigma_\beta^2 > 0 \quad TS_{B(A)} : F_{B(A)} &= \frac{MS_{B(A)}}{MS_{Err}} \\
RR_{B(A)} : F_{B(A)} \geq F_{1-\alpha; b \cdot - a, N - b \cdot} \quad \text{P-value: } P(F_{b \cdot - a, N - b \cdot} \geq F_{B(A)}) \\
\hat{\sigma}^2 = MS_{Err} \quad \hat{\sigma}_\beta^2 &= \frac{MS_{B(A)} - MS_{Err}}{n} \\
V \{ \bar{Y}_{i \cdot \cdot} \} = \frac{\sigma_\beta^2}{b_i} + \frac{\sigma^2}{nb_i} = \frac{1}{nb_i} (n \sigma_\beta^2 + \sigma^2) \quad \hat{SE} \{ \bar{Y}_{i \cdot \cdot} \} &= \sqrt{\frac{MS_{B(A)}}{nb_i}} \quad \text{COV} \{ \bar{Y}_{i \cdot \cdot}, \bar{Y}_{i' \cdot \cdot} \} = 0 \\
\hat{SE} \{ \bar{Y}_{i \cdot \cdot} - \bar{Y}_{i' \cdot \cdot} \} &= \sqrt{MS_{B(A)} \left(\frac{1}{nb_i} + \frac{1}{nb_{i'}} \right)}
\end{aligned}$$

Note that when coding levels of factor B, it is helpful to have them go from 1 to $b \cdot$ across levels of factor A as opposed to 1 to b_i within each treatment when using computer software packages.

Example: Measurements Made on Silicon Wafers from Different Batches

A study (Jensen (2002)) sampled silicon wafers and made measurements on the wafers to study variation. The characteristic being measured was not given for proprietary reasons. A sample of $a = 20$ batches (aka lots) were selected. Within each batch, a sample of $b = 2$ wafers were selected, and $n = 9$ locations on the wafer were measured. The data are given below in tabular form.

Batch	Wafer(B)	Wafer	Y_ij1	Y_ij2	Y_ij3	Y_ij4	Y_ij5	Y_ij6	Y_ij7	Y_ij8	Y_ij9
1	1	1	181.247	181.280	185.021	180.144	192.570	178.741	184.153	184.353	183.117
1	2	2	175.267	179.844	181.146	177.338	186.057	174.399	177.372	176.336	181.514
2	1	3	167.718	169.956	169.990	171.560	173.597	170.791	174.165	177.706	173.530
2	2	4	170.758	171.292	174.332	172.261	182.649	169.322	173.764	173.029	175.668
3	1	5	169.054	180.211	175.635	173.230	189.497	169.856	176.436	183.451	182.449
3	2	6	168.988	167.017	171.493	169.388	184.821	169.489	175.134	172.061	173.397
4	1	7	163.152	168.664	168.263	167.962	180.989	162.585	168.864	169.165	173.407
4	2	8	163.486	169.566	171.937	169.265	182.960	165.758	171.937	170.835	167.428
5	1	9	171.760	167.284	168.186	170.691	182.015	170.424	172.628	164.946	165.480
5	2	10	166.048	167.150	163.710	167.718	176.036	166.449	166.616	169.422	166.148
6	1	11	180.077	178.507	174.800	175.601	186.457	181.013	176.938	175.869	176.236
6	2	12	169.121	167.919	165.580	168.052	174.399	169.155	169.722	165.914	166.649
7	1	13	181.156	182.025	178.751	185.465	184.396	183.962	187.736	183.929	181.791
7	2	14	184.764	184.864	184.396	189.139	191.678	185.966	192.947	187.870	186.434
8	1	15	182.893	180.020	179.820	181.858	190.375	186.701	187.636	179.887	178.785
8	2	16	176.213	176.446	177.682	173.941	186.233	174.643	180.020	176.747	178.618
9	1	17	176.537	175.334	172.962	175.000	175.668	172.829	178.841	173.564	168.052
9	2	18	174.833	177.105	175.902	171.259	181.948	170.825	171.526	176.102	171.493
10	1	19	175.334	175.100	176.436	175.201	187.794	176.938	176.670	178.741	178.374
10	2	20	183.384	180.445	178.374	179.042	183.017	181.781	180.445	184.487	177.539
11	1	21	166.493	174.810	168.397	177.081	171.503	171.904	181.423	182.158	169.532
11	2	22	160.380	165.257	164.355	168.931	168.697	163.820	172.204	167.294	164.522
12	1	23	177.706	177.071	176.770	177.539	188.996	179.109	183.117	177.839	178.808
12	2	24	173.864	174.466	178.474	171.626	190.700	166.048	171.359	176.503	178.641
13	1	25	161.148	162.050	165.090	160.948	170.467	157.240	162.084	166.893	166.125
13	2	26	155.002	158.510	158.075	158.343	163.253	156.305	159.011	157.574	161.382
14	1	27	172.538	176.179	177.048	175.110	180.822	171.670	169.866	173.039	171.670
14	2	28	170.033	172.271	175.945	172.505	183.962	168.397	171.603	175.645	176.680
15	1	29	184.253	184.219	187.727	177.873	195.476	177.505	175.167	179.543	187.660
15	2	30	187.526	183.217	189.430	182.783	200.520	183.451	183.184	183.952	189.965
16	1	31	166.382	170.858	169.121	172.061	179.810	168.119	172.795	170.858	170.658
16	2	32	168.486	168.954	169.722	171.626	177.572	172.395	173.998	172.428	171.660
17	1	33	181.046	181.514	182.750	177.639	193.973	181.414	175.134	178.942	185.088
17	2	34	174.733	177.071	180.545	175.167	195.243	173.096	172.328	178.775	181.447
18	1	35	163.309	170.123	167.885	171.626	173.664	168.820	171.560	162.374	166.215
18	2	36	165.347	164.612	164.612	168.019	173.430	167.585	173.297	159.701	161.906
19	1	37	173.707	174.175	170.568	179.753	180.154	175.712	183.594	177.415	169.766
19	2	38	165.357	168.998	166.726	173.975	172.705	167.962	173.507	171.670	167.896
20	1	39	171.770	169.399	166.359	161.716	176.413	172.004	170.701	168.330	165.825
20	2	40	162.084	164.154	158.142	161.783	160.013	160.981	162.384	163.720	161.716

In this example, both factors A (Batch) and B (Wafer within Batch) are random effects, so that we will fit a random effects model. Below, we fit the analysis of variance and obtain tests and parameter estimates. Note that the overall sample size is $N = 20(2)(9) = 360$. The degrees of freedom are $20-1 = 19$ for Batch, $20(2-1) = 20$ for Wafer(Batch), $20(2)(9-1) = 320$ for Error, and $20(2)(9)-1 = 359$ for Total.

			Numerator	Denominator			
Source	df	SS	MS	MS	F	F(.05)	P-value
Batch	19	14050.87	739.52	97.98	7.548	2.137	0.0000
Wafer(Batch)	20	1959.63	97.98	19.03	5.149	1.603	0.0000
Error	320	6089.58	19.03				
Total	359	22100.09					

$$H_0^A : \sigma_\alpha^2 = 0 \quad H_A^A : \sigma_\alpha^2 > 0 \quad TS_A : F_A = \frac{MS_A}{MS_{B(A)}} = \frac{739.52}{97.98} = 7.548$$

$$RR_A : F_A \geq F_{1-.05;19,20} = 2.137 \quad \text{P-value: } P(F_{19,20} \geq 7.548) = .0000$$

$$H_0^{B(A)} : \sigma_\beta^2 = 0 \quad H_A^{B(A)} : \sigma_\beta^2 > 0 \quad TS_{B(A)} : F_{B(A)} = \frac{97.98}{19.03} = 5.149$$

$$RR_{B(A)} : F_{B(A)} \geq F_{1-.05;20,320} = 1.603 \quad \text{P-value: } P(F_{20,320} \geq 5.149) = .0000$$

$$\hat{\sigma}^2 = 19.03 \quad \hat{\sigma}_\beta^2 = \frac{97.98 - 19.03}{9} = 8.77 \quad \hat{\sigma}_\alpha^2 = \frac{739.52 - 97.98}{9(2)} = 35.64$$

Below is the R Program. Note that the variable **wafer_batch** takes on values 1 and 2 within each batch, while the variable **wafer** takes on the values 1 and 2 for wafers from batch 1, 3 and 4 for wafers from batch 2, ..., values 39 and 40 for wafers from batch 20.

R Program

```

wafer1 <- read.table("http://www.stat.ufl.edu/~winner/data/semicon_qual.dat",
  header=F,col.names=c("batch","wafer_batch","wafer","replic","y.meas"))
attach(wafer1)

batch <- factor(batch)
wafer_batch <- factor(wafer_batch)
wafer <- factor(wafer)

wafer.mod1 <- aov(y.meas ~ batch + batch/wafer)
summary(wafer.mod1)

wafer.mod2 <- aov(y.meas ~ batch + Error(wafer))
summary(wafer.mod2)

library(lmerTest)

wafer.mod3 <- lmer(y.meas ~ 1 + (1|batch/wafer))
summary(wafer.mod3)

```

Note that **wafer.mod1** uses the wrong error term (MS_{Err}) when testing for Batch effects.

R Output

```
> wafer.mod1 <- aov(y.meas ~ batch + batch/wafer)
> summary(wafer.mod1)
      Df Sum Sq Mean Sq F value    Pr(>F)
batch   19  14051    739.5   38.861 < 2e-16 ***
batch:wafer 20   1960     98.0    5.149 3.71e-11 ***
Residuals 320   6090     19.0
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
>
> wafer.mod2 <- aov(y.meas ~ batch + Error(wafer))
> summary(wafer.mod2)

Error: wafer
      Df Sum Sq Mean Sq F value    Pr(>F)
batch   19  14051    739.5   7.548 1.78e-05 ***
Residuals 20   1960     98.0
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Error: Within
      Df Sum Sq Mean Sq F value    Pr(>F)
Residuals 320   6090     19.03

> wafer.mod3 <- lmer(y.meas ~ 1 + (1|batch/wafer))
> summary(wafer.mod3)
Linear mixed model fit by REML t-tests use Satterthwaite approximations to
degrees of freedom [merModLmerTest]
Formula: y.meas ~ 1 + (1 | batch/wafer)

REML criterion at convergence: 2184.6

Scaled residuals:
    Min       1Q   Median       3Q      Max
-2.2897 -0.5826 -0.1729  0.4287  3.7529

Random effects:
 Groups      Name      Variance Std.Dev.
wafer:batch (Intercept)  8.772    2.962
batch       (Intercept) 35.641    5.970
Residual    19.030     4.362
Number of obs: 360, groups: wafer:batch, 40; batch, 20

Fixed effects:
              Estimate Std. Error      df t value Pr(>|t|)
(Intercept)  174.342      1.433   19.000   121.6 <2e-16 ***
---
```

Note that for the random effects model, when we estimate the population mean, we have the following.

$$\begin{aligned} \text{Parameter: } \mu \quad \text{Estimator: } \hat{\mu} = \bar{Y}_{\dots} \quad \text{Note: } b_{\cdot} = ab = 20(2) = 40 \\ V\{\bar{Y}_{\dots}\} = \frac{\sigma_{\alpha}^2}{a} + \frac{\sigma_{\beta}^2}{ab} + \frac{\sigma^2}{abn} \quad E\{MS_A\} = \frac{nb_{\cdot}}{a} \sigma_{\alpha}^2 + n\sigma_{\beta}^2 + \sigma^2 = nb\sigma_{\alpha}^2 + n\sigma_{\beta}^2 + \sigma^2 \\ \Rightarrow V\{\bar{Y}_{\dots}\} = \frac{E\{MS_A\}}{abn} \Rightarrow SE\{\bar{Y}_{\dots}\} = \sqrt{\frac{MS_A}{abn}} = \sqrt{\frac{739.52}{20(2)(9)}} = 1.433 \end{aligned}$$

Example – Mean Water Depths in Florida Swamps

A study (Ewel and Wickenheiser (1988)) classified Florida swamps into one of $a = 3$ size categories (Small, Medium, and Large). Within each size category, $b = 3$ swamps were selected. Within each swamp, $n = 27$ depth measurements were made at random locations. For this analysis, we treat Factor A (size) as Fixed, Factor B (swamp, nested within size) as Random, and replicate measurements, as always, as Random. The following table gives the means and variances of the depths for each of the $ab = 9$ swamps. These data have been simulated from approximate means and SDs from the published paper.

	Swamp Size		
Swamp#	Small	Medium	Large
1	48.0 (15.12)	110.2 (8.16)	128.8 (15.33)
2	36.3 (20.84)	103.0 (11.43)	137.2 (10.29)
3	72.2 (20.58)	106.1 (15.38)	192.3 (14.81)

The Sums of Squares, Expected Mean Squares and Analysis of Variance are given below.

$$a = 3 \quad b = 3 \quad n = 27 \quad N = abn = 243$$

Swamp Size: $SS_A = bn \sum_{i=1}^a (\bar{y}_{i..} - \bar{y}_{...})^2 = 81 \sum_{i=1}^3 (\bar{y}_{i..} - \bar{y}_{...})^2 \quad df_A = a - 1 = 3 - 1 = 2$

$$E(MS_A) = \sigma^2 + n\sigma_\beta^2 + \frac{bn \sum_{i=1}^a \alpha_i^2}{a-1} = \sigma^2 + 27\sigma_\beta^2 + \frac{81 \sum_{i=1}^3 \alpha_i^2}{2}$$

Swamp(Size): $SS_{B(A)} = n \sum_{i=1}^a \sum_{j=1}^b (\bar{y}_{ij.} - \bar{y}_{i..})^2 = 27 \sum_{i=1}^3 \sum_{j=1}^3 (\bar{y}_{ij.} - \bar{y}_{i..})^2 \quad df_{B(A)} = a(b-1) = 3(3-1) = 6$

$$E(MS_{B(A)}) = \sigma^2 + n\sigma_\beta^2 = \sigma^2 + 27\sigma_\beta^2$$

Error: $SS_{Err} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (y_{ijk} - \bar{y}_{ij.})^2 = \sum_{i=1}^a \sum_{j=1}^b (n-1)s_{ij}^2 = 26 \sum_{i=1}^3 \sum_{j=1}^3 s_{ij}^2 \quad df_{Err} = ab(n-1) = 3(3)(27-1) = 234$

$$E(MS_{Err}) = \sigma^2$$

Total: $SS_{Tot} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (y_{ijk} - \bar{y}_{...})^2 = SSA + SSB(A) + SSE \quad df_{Tot} = abn - 1 = 3(3)(27) - 1 = 242$

i	j(i)	Ybar(ij)	Ybar(i*)	Ybar(**)	Ybar(i*)-Ybar(**)	Ybar(ij)-Ybar(i*)	S(ij)	n(Y(i*)-Y(**))^2	n(Y(ij)-Y(i*))^2	(n-1)S(ij)^2
1	1(1)	48.0	52.17	103.79	-51.62	-4.17	15.12	71951.05	468.75	5943.97
1	2(1)	36.3	52.17	103.79	-51.62	-15.87	20.84	71951.05	6797.28	11291.95
1	3(1)	72.2	52.17	103.79	-51.62	20.03	20.58	71951.05	10836.03	11011.95
2	1(2)	110.2	106.43	103.79	2.64	3.77	8.16	188.81	383.07	1731.23
2	2(2)	103.0	106.43	103.79	2.64	-3.43	11.43	188.81	318.27	3396.77
2	3(2)	106.1	106.43	103.79	2.64	-0.33	15.38	188.81	3.00	6150.15
3	1(3)	128.8	152.77	103.79	48.98	-23.97	15.33	64768.21	15508.83	6110.23
3	2(3)	137.2	152.77	103.79	48.98	-15.57	10.29	64768.21	6542.67	2752.99
3	3(3)	192.3	152.77	103.79	48.98	39.53	14.81	64768.21	42197.88	5702.74
Sum	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	410724.24	83055.78	54091.97

Source	df	SS	MS	F	P-value
Swamp Size A	2	410724.24	205362.12	14.84	0.0048
Swamp(Size) B(A)	6	83055.78	13842.63	59.88	0.0000
Error	234	54091.97	231.16		
Total	242	547871.99			

$$H_0^A : \alpha_1 = \alpha_2 = \alpha_3 = 0 \quad (\text{No Swamp Size Effect}) \quad H_A^A : \text{Not all } \alpha_i = 0$$

$$\text{T.S. : } F_{obs}^A = \frac{MS_A}{MS_{B(A)}} = \frac{205362.12}{13842.63} = 14.84$$

$$\text{P-Value: } P(F_{2,6} \geq 14.84) = .0048$$

$$H_0^B : \sigma_\beta^2 = 0 \quad (\text{No variation among swamp levels within swamp sizes}) \quad H_A^B : \sigma_\beta^2 > 0$$

$$\text{T.S. : } F_{obs}^B = \frac{MS_{B(A)}}{MS_{Err}} = \frac{13842.63}{231.16} = 59.88$$

$$\text{P-Value: } P(F_{6,234} \geq 59.88) \approx .0000$$

Next, we make pairwise comparisons among the swamp sizes in terms of mean depths and estimate the Swamp within Size and Error Variance Components.

$$\hat{SE}\{\bar{Y}_{i..}\} = \sqrt{\frac{MS_{B(A)}}{bn}} = 13.07 \quad \hat{SE}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \sqrt{MS_{B(A)} \left(\frac{2}{bn}\right)} = 18.49$$

Bonferroni's Method $\left(\binom{a}{2} = \binom{3}{2} = 3 \text{ Comparisons} \right)$ - Simultaneous 95% CI's for $\alpha_i - \alpha_{i'}$:

$$(\bar{y}_{i..} - \bar{y}_{i'..}) \pm t_{0.05/2(3),6} \sqrt{MS_{B(A)} \left(\frac{2}{bn}\right)} \equiv (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 3.287(18.49) \equiv (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 60.78$$

Swamp Sizes	Difference	SE(Diff)	LB(Bon)	UB(Bon)
Large-Medium	46.33	18.49	-14.45	107.11
Large-Small	100.60	18.49	39.82	161.38
Medium-Small	54.27	18.49	-6.51	114.85

$$E(MS_{Err}) = \sigma^2 \Rightarrow \hat{\sigma}^2 = MS_{Err} = 231.16 \Rightarrow \hat{\sigma} = \sqrt{231.16} = 15.2$$

$$E(MS_{B(A)}) = \sigma^2 + n\sigma_\beta^2 \Rightarrow \hat{\sigma}_\beta^2 = \frac{MS_{B(A)} - MS_{Err}}{n} = \frac{13842.63 - 231.16}{27} = 504.13 \Rightarrow \hat{\sigma}_\beta = 22.5$$

R Program:

```
swamp1 <-  
read.table("http://www.stat.ufl.edu/~winner/data/swamp1.dat", header=F,  
           col.names=c("swamp.sz", "swamp.id", "water.lvl"))  
attach(swamp1)  
  
swamp.sz <- factor(swamp.sz)  
swamp.id <- factor(swamp.id)  
  
round(tapply(water.lvl, swamp.id, mean), 2)  
round(tapply(water.lvl, swamp.id, sd), 2)  
  
swamp.aov1 <- aov(water.lvl ~ swamp.sz + swamp.sz/swamp.id)  
# This provides ANOVA, not appropriate F-test for swamp.sz  
summary(swamp.aov1)  
  
swamp.aov2 <- aov(water.lvl ~ swamp.sz + Error(swamp.id))  
# This provides appropriate F-test for swamp.sz  
summary(swamp.aov2)  
  
library(lmerTest)  
  
swamp.aov3 <- lmer(water.lvl ~ swamp.sz + (1|swamp.sz:swamp.id))  
summary(swamp.aov3)  
anova(swamp.aov3)  
lsmeans(swamp.aov3)  
diff1smeans(swamp.aov3)
```

R Output:

```
> round(tapply(water.lvl, swamp.id, mean), 2)  
 1      2      3      4      5      6      7      8      9  
48.0 36.3 72.2 110.2 103.0 106.1 128.8 137.2 192.3  
> round(tapply(water.lvl, swamp.id, sd), 2)  
 1      2      3      4      5      6      7      8      9  
15.12 20.84 20.58 8.16 11.43 15.38 15.33 10.29 14.81  
>  
> swamp.aov1 <- aov(water.lvl ~ swamp.sz + swamp.sz/swamp.id)  
> # This provides ANOVA, not appropriate F-test for swamp.sz  
> summary(swamp.aov1)  
              Df Sum Sq Mean Sq F value Pr(>F)  
swamp.sz      2 410724  205362  888.38 <2e-16 ***  
swamp.sz:swamp.id 6  83058   13843   59.88 <2e-16 ***  
Residuals    234  54092     231  
---  
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1  
>  
> swamp.aov2 <- aov(water.lvl ~ swamp.sz + Error(swamp.id))  
> # This provides appropriate F-test for swamp.sz  
> summary(swamp.aov2)  
  
Error: swamp.id  
              Df Sum Sq Mean Sq F value Pr(>F)  
swamp.sz      2 410724  205362  14.84 0.00476 **  
Residuals    6  83058   13843  
---  
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1  
  
Error: within  
              Df Sum Sq Mean Sq F value Pr(>F)  
Residuals    234  54092     231.2  
>
```

Continued

$$\begin{array}{l}
\boldsymbol{\varepsilon} = \begin{bmatrix} \boldsymbol{\varepsilon}_{11} \\ \boldsymbol{\varepsilon}_{12} \\ \boldsymbol{\varepsilon}_{13} \\ \boldsymbol{\varepsilon}_{21} \\ \boldsymbol{\varepsilon}_{22} \\ \boldsymbol{\varepsilon}_{23} \\ \boldsymbol{\varepsilon}_{31} \\ \boldsymbol{\varepsilon}_{32} \\ \boldsymbol{\varepsilon}_{33} \end{bmatrix}
\end{array}
\quad
E\{\mathbf{Y}\} = \mathbf{X}\boldsymbol{\beta} \quad
V\{\mathbf{Y}\} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \sigma^2\mathbf{I}_{243} \quad
\mathbf{G} = \sigma_{\beta}^2 V\{\mathbf{u}\} = \sigma_{\beta}^2 \mathbf{I}_9$$

$$\mathbf{Z}\mathbf{G}\mathbf{Z}' = \sigma_{\beta}^2 \begin{bmatrix}
\mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27} & \mathbf{0}_{27 \times 27} \\
\mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{0}_{27 \times 27} & \mathbf{1}_{27 \times 27}
\end{bmatrix}$$

Here we obtain the **estimates** of the (fixed) elements of $\boldsymbol{\beta}$ and the **predictions** of the (random) elements of \mathbf{u} , based on the ANOVA (and REML) estimates of σ^2 and σ_{β}^2 . We use the **sum** contrast restriction in R, that the elements of $\boldsymbol{\beta}$ are interpreted as follows: $\beta_0 = \mu$ $\beta_1 = \alpha_1$ $\beta_2 = \alpha_2 \Rightarrow -(\beta_1 + \beta_2) = \alpha_3$ and \mathbf{X} is of the form given below, along with the mixed model equation estimates:

$$\mathbf{X} = \begin{bmatrix} \mathbf{1}_{81 \times 1} & \mathbf{1}_{81 \times 1} & \mathbf{0}_{81 \times 1} \\ \mathbf{1}_{81 \times 1} & \mathbf{0}_{81 \times 1} & \mathbf{1}_{81 \times 1} \\ \mathbf{1}_{81 \times 1} & -\mathbf{1}_{81 \times 1} & -\mathbf{1}_{81 \times 1} \end{bmatrix} \quad \hat{\sigma}^2 = 231.2 \quad \hat{\sigma}_{\beta}^2 = 504.1$$

$$\begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{Z} \\ \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{Z} + \hat{\mathbf{G}}^{-1} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{y} \\ \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix} \quad
V \left\{ \begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} \right\} = \begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{Z} \\ \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{Z} + \hat{\mathbf{G}}^{-1} \end{bmatrix}^{-1}$$

	X'(R^-1)X			X'(R^-1)Z									
	1.0510	0.0000	0.0000	0.1168	0.1168	0.1168	0.1168	0.1168	0.1168	0.1168	0.1168	0.1168	
	0.0000	0.7007	0.3503	0.1168	0.1168	0.1168	0.0000	0.0000	0.0000	-0.1168	-0.1168	-0.1168	
	0.0000	0.3503	0.7007	0.0000	0.0000	0.0000	0.1168	0.1168	0.1168	-0.1168	-0.1168	-0.1168	
Z'(R^-1)X	0.1168	0.1168	0.0000	0.1188	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	Z'(R^-1)Z
	0.1168	0.1168	0.0000	0.0000	0.1188	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	+G^-1
	0.1168	0.1168	0.0000	0.0000	0.0000	0.1188	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
	0.1168	0.0000	0.1168	0.0000	0.0000	0.0000	0.1188	0.0000	0.0000	0.0000	0.0000	0.0000	
	0.1168	0.0000	0.1168	0.0000	0.0000	0.0000	0.0000	0.1188	0.0000	0.0000	0.0000	0.0000	
	0.1168	0.0000	0.1168	0.0000	0.0000	0.0000	0.0000	0.0000	0.1188	0.0000	0.0000	0.0000	
	0.1168	-0.1168	-0.1168	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1188	0.0000	0.0000	
	0.1168	-0.1168	-0.1168	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1188	0.0000	
	0.1168	-0.1168	-0.1168	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1188	

X'(R^-1)Y		beta,u	StdError
109.0864		103.7892	7.547354
-35.2448		-51.6226	10.67357
-16.2323		2.645226	10.67357
5.60558	Z'(R^-1)Y	-4.09671	13.1775
4.239144		-15.602	13.1775
8.431661		19.69872	13.1775
12.86959		3.704481	13.1775
12.02868		-3.37599	13.1775
12.39061		-0.32849	13.1775
15.04152		-23.5662	13.1775
16.0224		-15.3073	13.1775
22.45722		38.8735	13.1775

V(beta,u)												
56.9626	0.0000	0.0000	-56.0111	-56.0111	-56.0111	-56.0111	-56.0111	-56.0111	-56.0111	-56.0111	-56.0111	-56.0111
0.0000	113.9251	-56.9626	-112.0222	-112.0222	-112.0222	56.0111	56.0111	56.0111	56.0111	56.0111	56.0111	56.0111
0.0000	-56.9626	113.9251	56.0111	56.0111	56.0111	-112.0222	-112.0222	-112.0222	56.0111	56.0111	56.0111	56.0111
-56.0111	-112.0222	56.0111	173.6466	165.2267	165.2267	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
-56.0111	-112.0222	56.0111	165.2267	173.6466	165.2267	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
-56.0111	-112.0222	56.0111	165.2267	165.2267	173.6466	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
-56.0111	56.0111	-112.0222	0.0000	0.0000	0.0000	173.6466	165.2267	165.2267	0.0000	0.0000	0.0000	0.0000
-56.0111	56.0111	-112.0222	0.0000	0.0000	0.0000	165.2267	173.6466	165.2267	0.0000	0.0000	0.0000	0.0000
-56.0111	56.0111	-112.0222	0.0000	0.0000	0.0000	165.2267	165.2267	173.6466	0.0000	0.0000	0.0000	0.0000
-56.0111	56.0111	56.0111	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	173.6466	165.2267	165.2267
-56.0111	56.0111	56.0111	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	165.2267	173.6466	165.2267
-56.0111	56.0111	56.0111	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	165.2267	165.2267	173.6466

R Program (Continuation of Previous): Note that `se.ranef` does not provide the standard errors obtained above for random effects, which match those from **SAS Proc Mixed**.

```

library(lmerTest)
library(arm)

options(contrasts=c("contr.sum", "contr.poly"))
swamp.aov3 <- lmer(water.lv1 ~ swamp.sz + (1|swamp.sz:swamp.id))
summary(swamp.aov3)
anova(swamp.aov3)
lsmeans(swamp.aov3)
diff1smeans(swamp.aov3)
ranef(swamp.aov3)
se.coef(swamp.aov3)
se.fixef(swamp.aov3)
se.ranef(swamp.aov3)

```

R Output:

```
Random effects:
  Groups             Name      Variance Std.Dev.
swamp.sz:swamp.id (Intercept) 504.1    22.45
Residual              231.2    15.20
Number of obs: 243, groups:  swamp.sz:swamp.id, 9

Fixed effects:
              Estimate Std. Error      df t value Pr(>|t|)
(Intercept)  103.789      7.548    6.000  13.751 9.2e-06 ***
swamp.sz1    -51.623     10.674    6.000  -4.836 0.00289 **
swamp.sz2     2.645     10.674    6.000   0.248 0.81254
---

Correlation of Fixed Effects:
              (Intr) swmp.1
swamp.sz1    0.000
swamp.sz2    0.000 -0.500
> anova(swamp.aov3)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
              Sum Sq Mean Sq NumDF DenDF F.value  Pr(>F)
swamp.sz 6858.7  3429.3      2      6  14.835 0.004759 **
---

> lsmeans(swamp.aov3)
Least Squares Means table:
              swamp.sz Estimate Standard Error DF t-value Lower CI Upper CI p-value
swamp.sz 1  1      1      52.17      13.07 6      3.99      20.2      84.2      0.007
swamp.sz 2  2      2     106.43      13.07 6      8.14      74.4     138.4     2e-04
swamp.sz 3  3      3     152.77      13.07 6     11.69     120.8    184.8    <2e-16

> diff1smeans(swamp.aov3)
Differences of LSMEANS:
              Estimate Standard Error      DF t-value Lower CI Upper CI p-value
swamp.sz 1 - 2      -54.3      18.5      6.0  -2.94  -99.5  -9.03  0.026
swamp.sz 1 - 3     -100.6     18.5      6.0  -5.44 -145.8 -55.36 0.002
swamp.sz 2 - 3      -46.3     18.5      6.0  -2.51  -91.6  -1.09  0.046

> ranef(swamp.aov3)
$`swamp.sz:swamp.id`
(Intercept)
1:1 -4.0967233
1:2 -15.6020733
1:3  19.6987966
2:4   3.7044954
2:5  -3.3760001
2:6  -0.3284954
3:7 -23.5663258
3:8 -15.3073258
3:9  38.8736515

> se.coef(swamp.aov3)
$fixef
[1] 7.547635 10.673968 10.673968

$`swamp.sz:swamp.id`
(Intercept)
1:1  2.901487
1:2  2.901487
1:3  2.901487
2:4  2.901487
2:5  2.901487
2:6  2.901487
3:7  2.901487
3:8  2.901487
3:9  2.901487
```

Note that the Correlation of the fixed effects can be obtained from the upper left 3x3 submatrix of $V\left\{\hat{\beta}, \hat{u}\right\}$.

V(beta)		
56.9626	0.0000	0.0000
0.0000	113.9251	-56.9626
0.0000	-56.9626	113.9251

$$\text{COV}\left\{\hat{\beta}_0, \hat{\beta}_1\right\} = \text{COV}\left\{\hat{\beta}_0, \hat{\beta}_2\right\} = 0 \quad \text{CORR}\left\{\hat{\beta}_1, \hat{\beta}_2\right\} = \frac{-56.9626}{\sqrt{113.9251^2}} = -0.5000$$

To obtain the Sum of Squares for Treatments and F-statistic computed by R, use the following computations.

$$\mathbf{K}' = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \hat{\beta} = \begin{bmatrix} \hat{\mu} \\ \hat{\alpha}_1 \\ \hat{\alpha}_2 \end{bmatrix} \quad \hat{V}^* \left\{ \hat{\beta} \right\} = \frac{1}{\hat{\sigma}^2} \hat{V} \left\{ \hat{\beta} \right\}$$

$$SS_A = \left(\mathbf{K}' \hat{\beta} \right)' \left(\mathbf{K}' \hat{V}^* \left\{ \hat{\beta} \right\} \mathbf{K} \right)^{-1} \left(\mathbf{K}' \hat{\beta} \right) \quad F_A = \frac{SS_A}{\hat{\sigma}^2}$$

				Beta-hat
K'				103.7892
0	1	0		-51.6226
0	0	1		2.645226
K'B	(K'V*K)^-1	SS	F	
-51.6226	2.705403	1.352702	6859.094	14.83625
2.645226	1.352702	2.705403		
	V*(beta)			
	0.246420	0.000000	0.000000	
	0.000000	0.492841	-0.246420	
	0.000000	-0.246420	0.492841	

8.2. Models with Crossed and Nested Factors

More complex models can contain both crossed and nested factors. Consider a model with Factor A, Factor B nested within A, and Factor C crossed with Factors A and B. Here we will assume that Factor A has a levels, Factor B has b levels within each level of A, and Factor C has c levels. Further, we assume there are n replicates at each combination of Factors C and B (within A). The model and sums of squares are written as follows.

$$Y_{ijkl} = \mu + \alpha_i + \beta_{j(i)} + \gamma_k + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk(i)} + \varepsilon_{l(ijk)} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c; l = 1, \dots, n$$

$$SS_A = bcn \sum_{i=1}^a (\bar{Y}_{i\dots} - \bar{Y}_{\dots})^2 \quad df_A = a - 1$$

$$SS_{B(A)} = cn \sum_{i=1}^a \sum_{j=1}^b (\bar{Y}_{ij\dots} - \bar{Y}_{i\dots})^2 \quad df_{B(A)} = a(b-1)$$

$$SS_C = abn \sum_{k=1}^c (\bar{Y}_{\dots k} - \bar{Y}_{\dots})^2 \quad df_C = c - 1$$

$$SS_{AC} = bn \sum_{i=1}^a \sum_{k=1}^c (\bar{Y}_{i\dots k} - \bar{Y}_{i\dots} - \bar{Y}_{\dots k} + \bar{Y}_{\dots})^2 \quad df_{AC} = (a-1)(c-1)$$

$$SS_{BC(A)} = n \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c (\bar{Y}_{ijk\dots} - \bar{Y}_{ij\dots} - \bar{Y}_{i\dots k} + \bar{Y}_{i\dots})^2 \quad df_{BC(A)} = a(b-1)(c-1)$$

$$SS_{\text{Err}} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^n (Y_{ijkl} - \bar{Y}_{ijk\dots})^2 \quad df_{\text{Err}} = abc(n-1)$$

$$SS_{\text{Tot}} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^n (Y_{ijkl} - \bar{Y}_{\dots})^2 \quad df_{\text{Tot}} = abc n - 1$$

Clearly, this can be generalized to b_i levels of Factor B within the i^{th} level of Factor A. Also, Expected Mean Squares will depend on whether Factor levels effects are fixed parameters or random variables. Algorithms exist for obtaining Expected Mean Squares for complex models such as these.

One method, based on the Unrestricted Model is as follows (from Kuehl, 2000):

1. Write the appropriate linear model
2. Set up a 2-way table with rows for each model term (except μ), and column for each subscript
3. For each column, give the number of factor levels and **F**ixed or **R**andom identifier
4. Add column at end for components (θ^2 for fixed effects, σ^2 for random effects)
5. If column subscript does not appear in the row term, enter the number of levels of the column subscript
6. If a subscript is in brackets for a row term, place a 1 in the cell under the subscript
7. For each row, if any row subscript matches the column subscript, enter 0 if both: the column represents a Fixed factor and there is a fixed row component of variation (θ^2)
8. Enter 1 in all remaining cells
9. Determining Expected Mean Squares:
 - a. Include σ^2 with a coefficient of 1 for all terms
 - b. Of the other variance components, include only those whose model terms include subscripts of the effect of interest
 - c. Cover columns of non-bracketed subscripts for the row effect of interest

- d. The coefficient for each component in the $E\{MS\}$ is the product of the remaining columns of the row for that effect.

Example: Bowling Scores for Professional Bowlers by Oil Pattern and Bowling Center

The Professional Bowling Association (PBA) has 15 traditional tournaments per year (as well as several others with different formats). The tournaments are played at 15 different bowling centers. There are many PBA bowlers, however, not all bowlers play at all tournaments. Tournaments involve 2 preliminary rounds, each made up of 7 games (games involve 10 frames with a perfect score being 300). After these rounds, the leading bowlers move on in the tournament. There are 5 oiling patterns (Chameleon, Cheetah, Scorpion, Shark, and Viper), each is used at 3 of the tournaments. Set up this model/design, with respect to factors, and effects and variances to be estimated. Note that we consider only 37 bowlers who competed in all tournaments. Each observation is a 7 game total for a bowler at a tourney in a 7-game preliminary round.

In this example, we will denote Oil Pattern as (Fixed) Factor A with $a = 5$ levels, Bowling Center, nested within Oil Pattern as Factor B, with $b = 3$ Centers per Pattern, and Bowler as (Random) Factor C, with $c = 37$ levels. Note that Bowling Center could be Fixed if these are the only centers of interest (for instance, if these centers are the same ones used each season for the PBA), or could be Random if they are considered a sample from a population of centers. We will consider both cases. The Analysis of Variance is given below, with $n = 2$ replicates per treatment.

$$Y_{ijkl} = \mu + \alpha_i + \beta_{j(i)} + \gamma_k + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk(i)} + \varepsilon_{l(ijk)} \quad i = 1, \dots, 5; j = 1, 2, 3; k = 1, \dots, 37; l = 1, 2$$

$$SS_A = 3(37)(2) \sum_{i=1}^5 (\bar{y}_{i\dots} - \bar{y}_{\dots})^2 = 337.1 \quad df_A = 5 - 1 = 4 \quad MS_A = 84.27$$

$$SS_{B(A)} = 37(2) \sum_{i=1}^5 \sum_{j=1}^3 (\bar{y}_{ij\dots} - \bar{y}_{i\dots})^2 = 97.7 \quad df_{B(A)} = 5(3 - 1) = 10 \quad MS_{B(A)} = 5(3 - 1) = 9.77$$

$$SS_C = 5(3)(2) \sum_{k=1}^{37} (\bar{y}_{\dots k} - \bar{y}_{\dots})^2 = 84.4 \quad df_C = 37 - 1 = 36 \quad MS_C = 2.35$$

$$SS_{AC} = 3(2) \sum_{i=1}^5 \sum_{k=1}^{37} (\bar{y}_{i\dots k} - \bar{y}_{i\dots} - \bar{y}_{\dots k} + \bar{y}_{\dots})^2 = 129.3 \quad df_{AC} = (5 - 1)(37 - 1) = 144 \quad MS_{AC} = 0.90$$

$$SS_{BC(A)} = 2 \sum_{i=1}^5 \sum_{j=1}^3 \sum_{k=1}^{37} (\bar{y}_{ijk\dots} - \bar{y}_{ij\dots} - \bar{y}_{i\dots k} + \bar{y}_{i\dots})^2 = 321.1 \quad df_{BC(A)} = 5(3 - 1)(37 - 1) = 360 \quad MS_{BC(A)} = 0.89$$

$$SS_{Err} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^n (y_{ijkl} - \bar{y}_{ijk\dots})^2 = 296.3 \quad df_{Err} = 5(3)(37)(2 - 1) = 555 \quad MS_{Err} = 0.53$$

$$SS_{Tot} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^n (y_{ijkl} - \bar{y}_{\dots})^2 = 1265.9 \quad df_{Tot} = 5(3)(37)(2) - 1 = 1109$$

R Program (Does not report correct F-tests for Mixed Model)

```
pbahasse <-
read.fwf(file="http://www.stat.ufl.edu/~winner/computing/sas/pbahasse.dat",
         width=c(8,8,8,8,8,8),

col.names=c("score","tourney","rep","bowler","oil","touney_oil"))
attach(pbahasse)

tourney <- factor(tourney, levels=1:15)
bowler <- factor(bowler, levels=1:37)
oil <- factor(oil, levels=1:5)
score <- score/100

pba.aov <- aov(score ~ oil*bowler*tourney)

summary(pba.aov)
```

R Output

```
> pba.aov <- aov(score ~ oil*bowler*tourney)
>
> summary(pba.aov)
              Df Sum Sq Mean Sq F value    Pr(>F)
oil              4   337.1    84.27 157.858 < 2e-16 ***
bowler           36    84.4     2.35   4.394 9.55e-15 ***
tourney          10    97.7     9.77  18.293 < 2e-16 ***
oil:bowler       144  129.3     0.90   1.682 1.67e-05 ***
bowler:tourney  360  321.1     0.89   1.671 2.72e-08 ***
Residuals       555  296.3     0.53
---
```

Next, we compute the Expected Mean Squares; first with Bowling Center as Fixed, then with Bowling Center as Random. In each case, we treat Oil Pattern as Fixed, and Bowler as Random.

Steps 1-4:

$$Y_{ijkl} = \mu + \alpha_i + \beta_{j(i)} + \gamma_k + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk(i)} + \varepsilon_{l(ijk)} \quad i = 1, \dots, 5; j = 1, 2, 3; k = 1, \dots, 37; l = 1, 2$$

	Fixed/Random	Fixed	Fixed	Random	Random	
	Levels	a=5	b=3	c=37	n=2	
Source	Effect\Subscript	i	j	k	l	Component
A	α_i					θ_A^2
B(A)	$\beta_{j(i)}$					$\theta_{B(A)}^2$
C	γ_k					σ_C^2
AC	$(\alpha\gamma)_{ik}$					σ_{AC}^2
BC(A)	$(\beta\gamma)_{jk(i)}$					$\sigma_{BC(A)}^2$
Error	$\varepsilon_{l(ijk)}$					σ^2

Note that the Fixed Components for Oil Pattern and Bowling Center are:

$$\theta_A^2 = \frac{\sum_{i=1}^a \alpha_i^2}{a-1} = \frac{\sum_{i=1}^a \alpha_i^2}{5-1} = 0.25 \sum_{i=1}^a \alpha_i^2 \quad \theta_{B(A)}^2 = \frac{\sum_{i=1}^a \sum_{j=1}^b \beta_{j(i)}^2}{a(b-1)} = \frac{\sum_{i=1}^a \sum_{j=1}^b \beta_{j(i)}^2}{5(3-1)} = 0.10 \sum_{i=1}^a \sum_{j=1}^b \beta_{j(i)}^2$$

Step 5: If a column subscript does not appear in row effect, enter the number of levels corresponding to the subscript of the column.

	Fixed/Random	Fixed	Fixed	Random	Random	
	Levels	a=5	b=3	c=37	n=2	
Source	Effect\Subscript	i	j	k	1	Component
A	α_i		3	37	2	θ_A^2
B(A)	$\beta_{j(i)}$			37	2	$\theta_{B(A)}^2$
C	γ_k	5	3		2	σ_C^2
AC	$(\alpha\gamma)_{ik}$		3		2	σ_{AC}^2
BC(A)	$(\beta\gamma)_{jk(i)}$				2	$\sigma_{BC(A)}^2$
Error	$\epsilon_{l(ijk)}$					σ^2

Step 6: If a subscript is bracketed in a row effect, place a 1 in cells under the bracketed subscripts:

	Fixed/Random	Fixed	Fixed	Random	Random	
	Levels	a=5	b=3	c=37	n=2	
Source	Effect\Subscript	i	j	k	1	Component
A	α_i		3	37	2	θ_A^2
B(A)	$\beta_{j(i)}$	1		37	2	$\theta_{B(A)}^2$
C	γ_k	5	3		2	σ_C^2
AC	$(\alpha\gamma)_{ik}$		3		2	σ_{AC}^2
BC(A)	$(\beta\gamma)_{jk(i)}$	1			2	$\sigma_{BC(A)}^2$
Error	$\epsilon_{l(ijk)}$	1	1	1		σ^2

Steps 7-8: For each row, if any row subscript matches the column subscript, enter 0 if both: the column represents a Fixed factor and there is a fixed row component of variation (θ^2). Enter 1 in all remaining cells

	Fixed/Random	Fixed	Fixed	Random	Random	
	Levels	a=5	b=3	c=37	n=2	
Source	Effect\Subscript	i	j	k	1	Component
A	α_i	0	3	37	2	θ_A^2
B(A)	$\beta_{j(i)}$	1	0	37	2	$\theta_{B(A)}^2$
C	γ_k	5	3	1	2	σ_C^2
AC	$(\alpha\gamma)_{ik}$	1	3	1	2	σ_{AC}^2
BC(A)	$(\beta\gamma)_{jk(i)}$	1	1	1	2	$\sigma_{BC(A)}^2$
Error	$\epsilon_{l(ijk)}$	1	1	1	1	σ^2

Step 9: Determining Expected Mean Squares:

- Include σ^2 with a coefficient of 1 for all terms
- Of the other variance components, include only those whose model terms include subscripts of the effect of interest
- Cover columns of non-bracketed subscripts for the row effect of interest
- The coefficient for each component in the $E\{MS\}$ is the product of the remaining columns of the row for that effect.

$$\begin{aligned}
 E\{MS_A\} &= \sigma^2 + 1(2)\sigma_{BC(A)}^2 + 3(2)\sigma_{AC}^2 + 3(37)(2)\theta_A^2 = \sigma^2 + 2\sigma_{BC(A)}^2 + 6\sigma_{AC}^2 + 222\theta_A^2 \\
 E\{MS_{B(A)}\} &= \sigma^2 + 1(2)\sigma_{BC(A)}^2 + 1(37)(2)\theta_{B(A)}^2 = \sigma^2 + 2\sigma_{BC(A)}^2 + 74\theta_{B(A)}^2 \\
 E\{MS_C\} &= \sigma^2 + 1(2)\sigma_{BC(A)}^2 + 3(2)\sigma_{AC}^2 + 5(3)(2)\sigma_C^2 = \sigma^2 + 2\sigma_{BC(A)}^2 + 6\sigma_{AC}^2 + 30\sigma_C^2 \\
 E\{MS_{AC}\} &= \sigma^2 + 1(2)\sigma_{BC(A)}^2 + 3(2)\sigma_{AC}^2 = \sigma^2 + 2\sigma_{BC(A)}^2 + 6\sigma_{AC}^2 \\
 E\{MS_{BC(A)}\} &= \sigma^2 + 1(2)\sigma_{BC(A)}^2 = \sigma^2 + 2\sigma_{BC(A)}^2 \\
 E\{MS_{Err}\} &= \sigma^2
 \end{aligned}$$

Making use of these Expected Mean Squares, we can test for fixed effects, and estimate all variance components.

$$\begin{aligned}
 H_0^A : \theta_A^2 = 0 \quad H_A^A : \theta_A^2 = 0 \quad TS : F_A = \frac{MS_A}{MS_{AC}} = \frac{84.27}{0.90} = 93.633 \quad RR : F_A \geq F_{.95;4,144} = 2.435 \\
 H_0^{B(A)} : \theta_{B(A)}^2 = 0 \quad H_A^{B(A)} : \theta_{B(A)}^2 = 0 \quad TS : F_{B(A)} = \frac{MS_{B(A)}}{MS_{BC(A)}} = \frac{9.77}{0.89} = 10.978 \quad RR : F_{B(A)} \geq F_{.95;10,360} = 1.857 \\
 \hat{\sigma}_C^2 = \frac{MS_C - MS_{AC}}{abn} = \frac{2.35 - 0.90}{30} = 0.0483 \quad \hat{\sigma}_{AC}^2 = \frac{MS_{AC} - MS_{BC(A)}}{bn} = \frac{0.90 - 0.89}{6} = 0.0017 \\
 \hat{\sigma}_{BC(A)}^2 = \frac{MS_{BC(A)} - MS_{Err}}{n} = \frac{0.89 - 0.53}{2} = 0.18 \quad \hat{\sigma}^2 = MS_{Err} = 0.53
 \end{aligned}$$

Data Sources:

C.R. Jensen (2002). "Variance Component Calculations: Common Methods and Misapplications in the Semiconductor Industry," *Quality Engineering*, Vol. 14, #4, pp. 647-657.

K.C. Ewel and L.P. Wickenheiser (1988). "Effect of Swamp Size on Growth Rates of Cypress (Taxodium Distichum) Trees," *American Midland Naturalist*, Vol. 120, #2, pp.362-370

Men's Professional Bowling Scores:
www.pba.com

Chapter 9 – Block Designs

In this chapter, we consider various designs with blocking factors. Blocks are generally thought of as groups of experimental units that are homogeneous. For instance, in an agricultural field study, blocks may be plots of land that can be broken into subunits that are similar with respect to soil, sun exposure, moisture, etc. In an industrial experiment, blocks may be batches of raw material. In a pharmacokinetic study, blocks may be individual subjects. In other settings, blocks can be constructed among individuals based on demographic or other characteristics. In complete block designs, each treatment is assigned at random to (at least) one unit within each block. In latin square designs, there are 2 blocking factors. In graeco-latin square designs, there are 3 blocking factors. In incomplete block designs, the number of treatments exceeds the number of units per block, so that not every treatment appears in each block.

Depending on the experimental setting, blocks can be either fixed or random. In most cases, it seems reasonable to assume they are random (see e.g. Littell, Milliken, Stroup, and Wolfinger (1996), p. 1). Further, treatments are usually assumed fixed in block designs, and their effects are the primary interest in inference, although the variance (and standard deviation) of block effects may be of interest as well. Note that by placing units into blocks, then assigning treatments at random to units within blocks, this can be considered a randomization restriction, as compared to a Completely Randomized Design. Any factorial structure can also be run in a block design. However, as the number of treatments (combinations of factor levels) increases, it is more difficult to find blocks of sufficient size to contain all treatments.

9.1. Randomized Complete Block Design (RCBD)

In a Randomized Complete Block Design, we have t treatments to be compared and b blocks that are each made up of t experimental units. These units can be subjects when feasible, or groups of individual (homogeneous) units. Note that we are changing our notation for number of treatments and number of replicates per treatment from previous chapters to reflect the treatment and block structure. The model can be written as follows.

$$Y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij} \quad i = 1, \dots, t; \quad j = 1, \dots, b \quad \sum_{i=1}^t \tau_i = 0 \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad \varepsilon_{ij} \sim NID(0, \sigma^2) \quad \{\beta_j\} \perp \{\varepsilon_{ij}\}$$

Note that this is simply a mixed effects model with 1 replicate per combination of levels for factors A and B. Here we obtain the mean and variance of sample means, and the variance of the difference between 2 treatment means. Again, keep in mind we are treating block effects as random effects.

$$E\{Y_{ij}\} = \mu + \tau_i \quad V\{Y_{ij}\} = \sigma_\beta^2 + \sigma^2 \quad \text{COV}\{Y_{ij}, Y_{i', j'}\} = \begin{cases} \sigma_\beta^2 + \sigma^2 & i = i', j = j' \\ \sigma_\beta^2 & i \neq i', j = j' \\ 0 & \forall i, i', j \neq j' \end{cases}$$

$$E\{\bar{Y}_{i\cdot}\} = \frac{1}{b} b(\mu + \tau_i) = \mu + \tau_i$$

$$V\{\bar{Y}_{i\cdot}\} = \frac{1}{b^2} \left[\sum_{j=1}^b V\{Y_{ij}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ij}, Y_{i, j'}\} \right] = \frac{1}{b^2} \left[b(\sigma_\beta^2 + \sigma^2) + b(b-1)(0) \right] = \frac{\sigma_\beta^2 + \sigma^2}{b}$$

$$E\{\bar{Y}_{\cdot j}\} = \frac{1}{t} \sum_{i=1}^t (\mu + \tau_i) = \mu$$

$$V\{\bar{Y}_{\cdot j}\} = \frac{1}{t^2} \left[\sum_{i=1}^t V\{Y_{ij}\} + 2 \sum_{i=1}^{t-1} \sum_{i'=i+1}^t \text{COV}\{Y_{ij}, Y_{i',j}\} \right] = \frac{1}{t^2} \left[t(\sigma_\beta^2 + \sigma^2) + t(t-1)\sigma_\beta^2 \right] = \frac{t\sigma_\beta^2 + \sigma^2}{t}$$

$$E\{\bar{Y}_{\cdot\cdot}\} = \frac{1}{tb} \sum_{i=1}^t \sum_{j=1}^b (\mu + \tau_i) = \mu$$

$$V\{\bar{Y}_{\cdot\cdot}\} = \frac{1}{(tb)^2} \left[\sum_{i=1}^t \sum_{j=1}^b V\{Y_{ij}\} + 2 \sum_{i=1}^{t-1} \sum_{i'=i+1}^t \sum_{j=1}^b \text{COV}\{Y_{ij}, Y_{i',j}\} + 2 \sum_{i=1}^t \sum_{i'=1}^t \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ij}, Y_{i',j'}\} \right] =$$

$$= \frac{1}{(tb)^2} \left[bt(\sigma_\beta^2 + \sigma^2) + bt(t-1)\sigma_\beta^2 + b(b-1)t^2(0) \right] = \frac{t\sigma_\beta^2 + \sigma^2}{bt}$$

$$i \neq i': \text{COV}\{\bar{Y}_{i\cdot}, \bar{Y}_{i'\cdot}\} = \frac{1}{b^2} \text{COV}\{Y_{i1} + \dots + Y_{ib}, Y_{i'1} + \dots + Y_{i'b}\} = \frac{1}{b^2} \left[b\sigma_\beta^2 + b(b-1)(0) \right] = \frac{\sigma_\beta^2}{b}$$

$$\Rightarrow V\{\bar{Y}_{i\cdot} - \bar{Y}_{i'\cdot}\} = 2 \left(\frac{\sigma_\beta^2 + \sigma^2}{b} \right) - 2 \left(\frac{\sigma_\beta^2}{b} \right) = 2 \left(\frac{\sigma^2}{b} \right)$$

Note that the variance of a treatment mean is a function of the variance components for blocks and error. Had blocks been fixed, the variance would have been σ^2/b . This is a problem with some standard software packages output. The variance of the difference between two means is the same, whether blocks are fixed or random.

Next, we obtain the Analysis of Variance and the expected mean squares. Again, this is a special case of the general mixed effects model.

$$SS_{\text{Trts}} = b \sum_{i=1}^t (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 = b \sum_{i=1}^t \bar{Y}_{i\cdot}^2 - bt\bar{Y}_{\cdot\cdot}^2 \quad df_{\text{Trts}} = t-1$$

$$SS_{\text{Blks}} = t \sum_{j=1}^b (\bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot})^2 = t \sum_{j=1}^b \bar{Y}_{\cdot j}^2 - bt\bar{Y}_{\cdot\cdot}^2 \quad df_{\text{Blks}} = b-1$$

$$SS_{\text{Err}} = \sum_{i=1}^t \sum_{j=1}^b (Y_{ij} - \bar{Y}_{i\cdot} - \bar{Y}_{\cdot j} + \bar{Y}_{\cdot\cdot})^2 = \sum_{i=1}^t \sum_{j=1}^b Y_{ij}^2 - b \sum_{i=1}^t \bar{Y}_{i\cdot}^2 - t \sum_{j=1}^b \bar{Y}_{\cdot j}^2 + bt\bar{Y}_{\cdot\cdot}^2 \quad df_{\text{Err}} = (t-1)(b-1)$$

$$E \left\{ \sum_{i=1}^t \sum_{j=1}^b Y_{ij}^2 \right\} = \sum_{i=1}^t \sum_{j=1}^b \left[(\sigma_\beta^2 + \sigma^2) + (\mu + \tau_i)^2 \right] = bt(\sigma_\beta^2 + \sigma^2) + bt\mu^2 + b \sum_{i=1}^t \tau_i^2 \quad \left(\sum_{i=1}^t \tau_i = 0 \right)$$

$$E \left\{ b \sum_{i=1}^t \bar{Y}_{i\cdot}^2 \right\} = b \sum_{i=1}^t \left[\left(\frac{\sigma_\beta^2 + \sigma^2}{b} \right) + (\mu + \tau_i)^2 \right] = t(\sigma_\beta^2 + \sigma^2) + bt\mu^2 + b \sum_{i=1}^t \tau_i^2$$

$$E \left\{ t \sum_{j=1}^b \bar{Y}_{\cdot j}^2 \right\} = t \sum_{j=1}^b \left[\left(\frac{t\sigma_\beta^2 + \sigma^2}{t} \right) + \mu^2 \right] = tb\sigma_\beta^2 + b\sigma^2 + bt\mu^2$$

$$E \left\{ bt\bar{Y}_{\cdot\cdot}^2 \right\} = tb \left[\left(\frac{t\sigma_\beta^2 + \sigma^2}{tb} \right) + \mu^2 \right] = t\sigma_\beta^2 + \sigma^2 + bt\mu^2$$

$$\begin{aligned}
E\{SS_{\text{Trts}}\} &= \left[t(\sigma_\beta^2 + \sigma^2) + bt\mu^2 + b\sum_{i=1}^t \tau_i^2 \right] - [t\sigma_\beta^2 + \sigma^2 + bt\mu^2] = (t-1)\sigma^2 + b\sum_{i=1}^t \tau_i^2 \\
\Rightarrow E\{MS_{\text{Trts}}\} &= \sigma^2 + \frac{b\sum_{i=1}^t \tau_i^2}{t-1} \\
E\{SS_{\text{Blks}}\} &= [tb\sigma_\beta^2 + b\sigma^2 + tb\mu^2] - [t\sigma_\beta^2 + \sigma^2 + tb\mu^2] = t(b-1)\sigma_\beta^2 + (b-1)\sigma^2 \\
\Rightarrow E\{MS_{\text{Blks}}\} &= \sigma^2 + t\sigma_\beta^2 \\
E\{SS_{\text{Err}}\} &= \\
&= \left[tb(\sigma_\beta^2 + \sigma^2) + tb\mu^2 + b\sum_{i=1}^t \tau_i^2 \right] - \left[t(\sigma_\beta^2 + \sigma^2) + tb\mu^2 + b\sum_{i=1}^t \tau_i^2 \right] - [tb\sigma_\beta^2 + b\sigma^2 + tb\mu^2] + [t\sigma_\beta^2 + \sigma^2 + tb\mu^2] = \\
&= (tb - t - b + 1)\sigma^2 = (t-1)(b-1)\sigma^2 \Rightarrow E\{MS_{\text{Err}}\} = \sigma^2
\end{aligned}$$

Next, we can estimate the variance components, and make inferences concerning model parameters. To test for treatment effects, we can conduct the F-test, comparing Treatment and Error Mean Squares. We can also test whether the Block variance component is 0.

$$\begin{aligned}
\hat{\sigma}^2 &= MS_{\text{Err}} \quad \hat{\sigma}_\beta^2 = \frac{MS_{\text{Blks}} - MS_{\text{Err}}}{t} \\
\hat{\mu} &= \bar{Y}_{..} \Rightarrow V\{\hat{\mu}\} = V\{\bar{Y}_{..}\} = \frac{t\sigma_\beta^2 + \sigma^2}{tb} \quad \hat{V}\{\hat{\mu}\} = \frac{t\sigma_\beta^2 + \sigma^2}{tb} \\
\hat{\tau}_i &= \bar{Y}_{i.} - \bar{Y}_{..} \Rightarrow V\{\hat{\tau}_i\} = V\{\bar{Y}_{i.} - \bar{Y}_{..}\} = V\{\bar{Y}_{i.}\} + V\{\bar{Y}_{..}\} - 2\text{COV}\{\bar{Y}_{i.}, \bar{Y}_{..}\} \\
\text{COV}\{\bar{Y}_{i.}, \bar{Y}_{..}\} &= \text{COV}\left\{\bar{Y}_{i.}, \frac{1}{t}\sum_{i'=1}^t \bar{Y}_{i' \cdot}\right\} = \frac{1}{t} [V\{\bar{Y}_{i.}\} + (t-1)\text{COV}\{\bar{Y}_{i.}, \bar{Y}_{i' \cdot}\}] = \frac{1}{t} \left[\frac{\sigma_\beta^2 + \sigma^2}{b} + (t-1)\frac{\sigma_\beta^2}{b} \right] = \frac{t\sigma_\beta^2 + \sigma^2}{tb} \\
\Rightarrow V\{\hat{\tau}_i\} &= V\{\bar{Y}_{i.} - \bar{Y}_{..}\} = \frac{\sigma_\beta^2 + \sigma^2}{b} + \frac{t\sigma_\beta^2 + \sigma^2}{tb} - 2\frac{t\sigma_\beta^2 + \sigma^2}{tb} = \frac{(t\sigma_\beta^2 + t\sigma^2) - (t\sigma_\beta^2 + \sigma^2)}{tb} = \frac{(t-1)\sigma^2}{tb} \\
\Rightarrow \hat{V}\{\hat{\tau}_i\} &= \frac{(t-1)MS_{\text{Err}}}{tb} \\
\hat{\tau}_i - \hat{\tau}_{i'} &= \bar{Y}_{i.} - \bar{Y}_{i' \cdot} \Rightarrow V\{\hat{\tau}_i - \hat{\tau}_{i'}\} = V\{\bar{Y}_{i.} - \bar{Y}_{i' \cdot}\} = \frac{2\sigma^2}{b} \Rightarrow \hat{V}\{\hat{\tau}_i - \hat{\tau}_{i'}\} = \frac{2MS_{\text{Err}}}{b} \\
\hat{\mu} + \hat{\tau}_i &= \bar{Y}_{i.} \Rightarrow V\{\hat{\mu} + \hat{\tau}_i\} = V\{\bar{Y}_{i.}\} = \frac{\sigma_\beta^2 + \sigma^2}{b} \Rightarrow \hat{V}\{\hat{\mu} + \hat{\tau}_i\} = \frac{MS_{\text{Blks}} + (t-1)MS_{\text{Err}}}{tb} \\
H_0: \tau_1 = \dots = \tau_t = 0 \quad H_A: \text{Not all } \tau_i = 0 \quad TS: F_{\text{Trts}} &= \frac{MS_{\text{Trts}}}{MS_{\text{Err}}} \quad RR: F_{\text{Trts}} \geq F_{1-\alpha; t-1, (t-1)(b-1)} \\
H_0: \sigma_\beta^2 = 0 \quad H_A: \sigma_\beta^2 > 0 \quad TS: F_{\text{Blks}} &= \frac{MS_{\text{Blks}}}{MS_{\text{Err}}} \quad RR: F_{\text{Blks}} \geq F_{1-\alpha; b-1, (t-1)(b-1)}
\end{aligned}$$

9.2. Matrix Form of RCBD

Assume the data are ordered by treatment first, then by block within treatment. The matrix form is given below.

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\varepsilon}$$

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \\ \vdots \\ \mathbf{Y}_t \end{bmatrix} \quad \mathbf{Y}_i = \begin{bmatrix} Y_{i1} \\ Y_{i2} \\ \vdots \\ Y_{ib} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \vdots \\ \alpha_t \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} \mathbf{1}_b & \mathbf{1}_b & \mathbf{0}_b & \cdots & \mathbf{0}_b \\ \mathbf{1}_b & \mathbf{0}_b & \mathbf{1}_b & \cdots & \mathbf{0}_b \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{1}_b & \mathbf{0}_b & \mathbf{0}_b & \cdots & \mathbf{1}_b \end{bmatrix} \quad \mathbf{u} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_b \end{bmatrix} \quad \mathbf{Z} = \begin{bmatrix} \mathbf{I}_b \\ \mathbf{I}_b \\ \vdots \\ \mathbf{I}_b \end{bmatrix}$$

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_t \end{bmatrix} \quad \boldsymbol{\varepsilon}_i = \begin{bmatrix} \varepsilon_{i1} \\ \varepsilon_{i2} \\ \vdots \\ \varepsilon_{ib} \end{bmatrix}$$

Note that \mathbf{X} is not full rank in this form. The usual constraints from the 1-Way ANOVA can be applied.

Example: Food Pinching Efficiency for 6 Lengths of Chopsticks in 31 Subjects

A study (Hsu and Wu (1991)) was conducted to measure food pinching efficiency among $t = 6$ lengths of chopsticks (180mm, 210, 240, 270, 300, 330) in $b = 31$ subjects. Each subject used each length chopstick (hopefully in random order), and the response measured was the number of peanuts successfully picked up and dropped in a cup. Technically the response is discrete, but data have been simulated that preserve the authors' Analysis of Variance that are continuous. The data given in tabular form and ANOVA computations are given below.

$$SS_{\text{Trts}} = 31 \left[(24.94 - 25.01)^2 + \dots + (24.00 - 25.01)^2 \right] = 106.858 \quad df_{\text{Trts}} = 6 - 1 = 5 \quad MS_{\text{Trts}} = \frac{106.858}{5} = 21.3716$$

$$SS_{\text{Blks}} = 6 \left[(22.11 - 25.01)^2 + \dots + (27.23 - 25.01)^2 \right] = 2277.54 \quad df_{\text{Blks}} = 31 - 1 = 30 \quad MS_{\text{Blks}} = \frac{2277.54}{30} = 75.9182$$

$$SS_{\text{Err}} = \left[(19.55 - 24.94 - 22.11 + 25.01)^2 + \dots + (27.52 - 24.00 - 27.23 + 25.01)^2 \right] = 634.634 \quad df_{\text{Err}} = 5(30) = 150$$

$$MS_{\text{Err}} = \frac{634.634}{150} = 4.2309$$

ANOVA						
SOURCE	df	SS	MS	F	F(.05)	P-value
Treatments	5	106.86	21.37	5.0513	2.2745	0.0003
Blocks	30	2277.54	75.92	17.9438	1.5354	0.0000
Error	150	634.63	4.23			
Total	185	3019.04				

subject	Chpstk1	Chpstk2	Chpstk3	Chpstk4	Chpstk5	Chpstk6	SubjMean
1	19.55	23.53	21.34	24.40	22.50	21.32	22.11
2	27.24	26.39	29.94	25.88	23.10	26.18	26.46
3	28.76	30.90	32.95	27.97	28.26	25.93	29.13
4	31.19	26.05	29.40	24.54	25.55	28.61	27.56
5	21.91	23.27	22.32	22.66	16.71	20.54	21.24
6	27.62	29.17	28.36	28.94	27.88	26.44	28.07
7	29.46	30.93	28.49	30.72	31.07	29.36	30.01
8	26.35	17.55	22.24	16.70	23.44	19.77	21.01
9	26.69	32.55	36.15	30.27	28.82	31.69	31.03
10	30.22	28.87	30.62	26.29	27.77	24.64	28.07
11	27.81	26.53	26.53	22.33	24.54	22.09	24.97
12	23.46	25.26	27.95	24.85	24.55	23.42	24.92
13	23.64	25.65	31.49	24.33	27.78	28.63	26.92
14	27.85	29.39	30.24	24.50	26.14	26.30	27.40
15	20.62	23.26	24.80	22.67	23.44	22.89	22.95
16	25.35	24.77	26.43	22.28	26.44	22.68	24.66
17	28.00	25.42	29.35	23.80	27.47	30.92	27.49
18	23.49	23.65	21.15	25.36	24.94	20.74	23.22
19	27.77	32.22	29.18	29.50	29.68	27.24	29.27
20	18.48	18.86	21.60	20.19	24.33	17.12	20.10
21	23.01	21.75	25.39	20.14	25.42	23.63	23.22
22	22.66	23.07	22.26	21.09	24.64	20.91	22.44
23	23.24	22.30	24.85	24.78	22.78	23.49	23.57
24	22.82	27.04	24.56	24.74	26.50	24.86	25.09
25	17.94	22.24	16.35	22.73	18.71	16.28	19.04
26	26.67	24.87	22.96	21.08	22.86	21.52	23.33
27	28.98	30.85	25.82	25.70	25.09	27.22	27.28
28	21.48	21.15	19.46	19.79	19.72	17.41	19.84
29	14.47	16.47	23.60	16.82	17.05	16.42	17.47
30	28.29	29.05	33.10	31.15	30.91	28.22	30.12
31	27.97	26.99	27.13	27.84	25.92	27.52	27.23
ChstkMn	24.94	25.48	26.32	24.32	24.97	24.00	25.01

$$\hat{\sigma}^2 = 4.2309 \quad \hat{\sigma}_\beta^2 = \frac{75.9182 - 4.2309}{6} = 11.95$$

$$\hat{\tau}_1 = 24.94 - 25.01 = -0.07 \quad \hat{\tau}_2 = 0.47 \quad \hat{\tau}_3 = 1.31 \quad \hat{\tau}_4 = -0.69 \quad \hat{\tau}_5 = -0.04 \quad \hat{\tau}_6 = -1.01$$

$$\hat{V}\left\{\hat{\tau}_i\right\} = \frac{(6-1)4.2309}{6(31)} = 0.1137 \quad SE\left\{\hat{\tau}_i\right\} = \sqrt{0.1137} = 0.3372$$

$$\hat{V}\left\{\hat{\tau}_i - \hat{\tau}_{i'}\right\} = \frac{2(4.2309)}{31} = 0.2730 \quad SE\left\{\hat{\tau}_i - \hat{\tau}_{i'}\right\} = \sqrt{0.2730} = 0.5225$$

Tukey's HSD: $q_{.95;6,150} = 4.088$ $HSD = 4.088\sqrt{\frac{4.2309}{31}} = 1.5102$

Bonferroni MSD: $t_{1-.05/(2(15)),150} = 2.983$ $MSD = 2.983\sqrt{\frac{2(4.2309)}{31}} = 1.5586$

$$\hat{V}\left\{\hat{\mu} + \hat{\tau}_i\right\} = \frac{75.9182 + (6-1)4.2309}{6(31)} = \frac{97.0727}{186} = 0.5219 \quad \hat{V}\left\{\hat{\mu} + \hat{\tau}_i\right\} = \sqrt{0.5219} = 0.7224$$

Based on both Tukey's HSD and Bonferroni MSD, length 3 is significantly better than lengths 4 and 6. The difference between lengths 2 and 6 is just short of significance.

R Program

```
cs.rbd <- read.table("http://www.stat.ufl.edu/~winner/data/chopstick2_rcb.dat",
  header=F,col.names=c("y.cs","trt.cs","blk.cs"))
attach(cs.rbd)

trt.cs <- factor(trt.cs); blk.cs <- factor(blk.cs)

options(contrasts=c("contr.sum","contr.poly"))
cs.mod1 <- aov(y.cs ~ trt.cs + blk.cs)
summary.lm(cs.mod1)
anova(cs.mod1)
TukeyHSD(cs.mod1,"trt.cs")
```

R Output

```
> cs.mod1 <- aov(y.cs ~ trt.cs + blk.cs)
> summary.lm(cs.mod1)

Coefficients:
(Intercept)  Estimate Std. Error t value Pr(>|t|)
trt.cs1      -0.07043   0.33724  -0.209 0.834856
trt.cs2       0.47828   0.33724   1.418 0.158207
trt.cs3       1.31731   0.33724   3.906 0.000141 ***
trt.cs4      -0.68172   0.33724  -2.021 0.045012 *
trt.cs5      -0.03753   0.33724  -0.111 0.911547
blk.cs1      -2.89892   0.82608  -3.509 0.000593 ***
...
blk.cs30      5.11441   0.82608   6.191 5.45e-09 ***
---
Residual standard error: 2.057 on 150 degrees of freedom
Multiple R-squared:  0.7898,    Adjusted R-squared:  0.7407
F-statistic: 16.1 on 35 and 150 DF,  p-value: < 2.2e-16

> anova(cs.mod1)
Analysis of Variance Table
Response: y.cs
      Df Sum Sq Mean Sq F value    Pr(>F)
trt.cs   5  106.86   21.372   5.0513 0.0002623 ***
blk.cs  30 2277.54   75.918  17.9438 < 2.2e-16 ***
Residuals 150  634.63    4.231

> TukeyHSD(cs.mod1,"trt.cs")
Tukey multiple comparisons of means
95% family-wise confidence level

      diff      lwr      upr      p adj
2-1  0.54870968 -0.9595748  2.05699418 0.8999148
3-1  1.38774194 -0.1205426  2.89602644 0.0904885
4-1 -0.61129032 -2.1195748  0.89699418 0.8503866
5-1  0.03290323 -1.4753813  1.54118773 0.9999999
6-1 -0.93548387 -2.4437684  0.57280063 0.4749602
3-2  0.83903226 -0.6692522  2.34731676 0.5959492
4-2 -1.16000000 -2.6682845  0.34828450 0.2346843
5-2 -0.51580645 -2.0240910  0.99247805 0.9213891
6-2 -1.48419355 -2.9924781  0.02409096 0.0565555
4-3 -1.99903226 -3.5073168 -0.49074775 0.0025803
5-3 -1.35483871 -2.8631232  0.15344579 0.1053005
6-3 -2.32322581 -3.8315103 -0.81494130 0.0002412
5-4  0.64419355 -0.8640910  2.15247805 0.8199855
6-4 -0.32419355 -1.8324781  1.18409096 0.9893780
6-5 -0.96838710 -2.4766716  0.53989741 0.4349561
```

The following program portion, making use of the **multcomp** package, gives the Tukey comparisons and graphical output of the differences.

R Program

```
install.packages("multcomp")
require(multcomp)

cs.glht <- glht(cs.mod1, linfct = mcp(trt.cs="Tukey"))
summary(cs.glht) # the summary of the tests
confint(cs.glht)

windows(width=5,height=3,pointsize=10)
plot(cs.glht)
title(sub="Chopstick Efficiency Data",adj=0)
mtext("Tukey Honest Significant Differences",side=3,line=0.5)
```

R Output

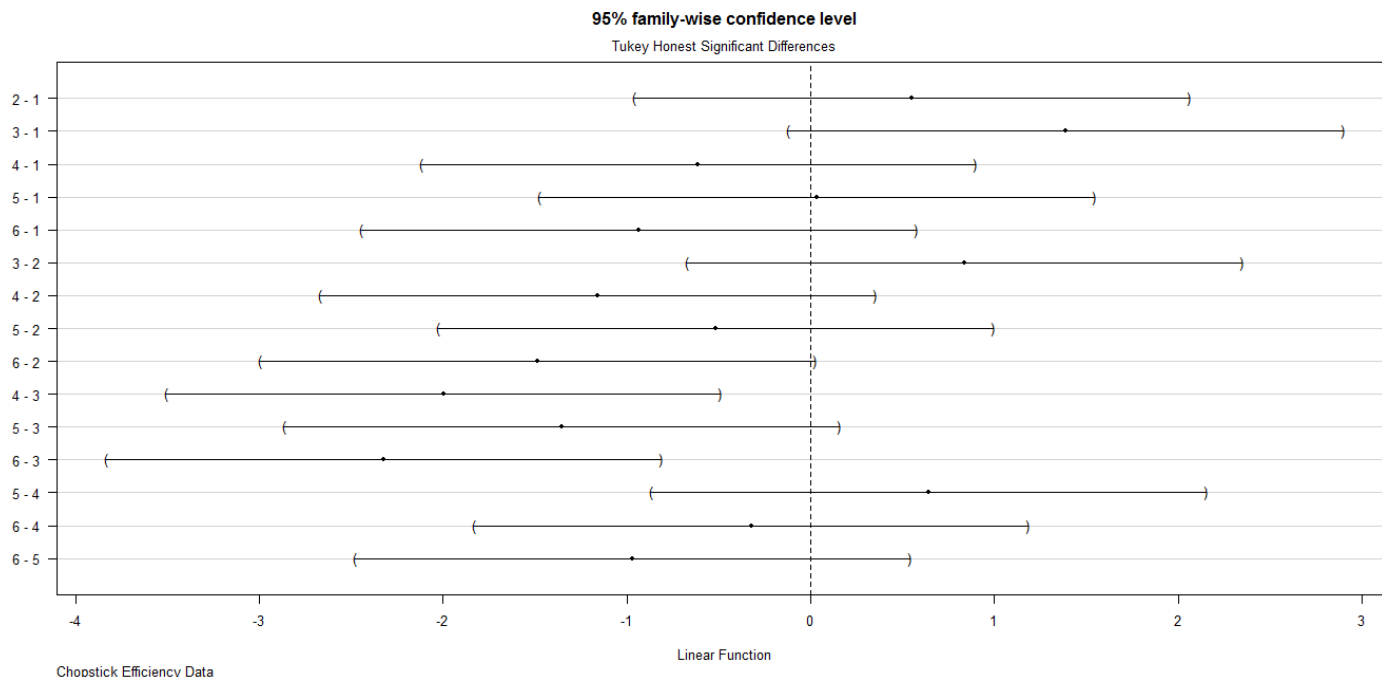
```
Linear Hypotheses:
      Estimate Std. Error t value Pr(>|t|)
2 - 1 == 0    0.5487    0.5225   1.050  0.8999
3 - 1 == 0    1.3877    0.5225   2.656  0.0904 .
4 - 1 == 0   -0.6113    0.5225  -1.170  0.8504
5 - 1 == 0    0.0329    0.5225   0.063  1.0000
6 - 1 == 0   -0.9355    0.5225  -1.791  0.4750
3 - 2 == 0    0.8390    0.5225   1.606  0.5959
4 - 2 == 0   -1.1600    0.5225  -2.220  0.2347
5 - 2 == 0   -0.5158    0.5225  -0.987  0.9214
6 - 2 == 0   -1.4842    0.5225  -2.841  0.0564 .
4 - 3 == 0   -1.9990    0.5225  -3.826  0.0026 **
5 - 3 == 0   -1.3548    0.5225  -2.593  0.1054
6 - 3 == 0   -2.3232    0.5225  -4.447 <0.001 ***
5 - 4 == 0    0.6442    0.5225   1.233  0.8200
6 - 4 == 0   -0.3242    0.5225  -0.621  0.9894
6 - 5 == 0   -0.9684    0.5225  -1.854  0.4350
```

Quantile = 2.8866

95% family-wise confidence level

Linear Hypotheses:

```
      Estimate lwr      upr
2 - 1 == 0  0.54871 -0.95943  2.05685
3 - 1 == 0  1.38774 -0.12040  2.89589
4 - 1 == 0 -0.61129 -2.11943  0.89685
5 - 1 == 0  0.03290 -1.47524  1.54105
6 - 1 == 0 -0.93548 -2.44363  0.57266
3 - 2 == 0  0.83903 -0.66911  2.34718
4 - 2 == 0 -1.16000 -2.66814  0.34814
5 - 2 == 0 -0.51581 -2.02395  0.99234
6 - 2 == 0 -1.48419 -2.99234  0.02395
4 - 3 == 0 -1.99903 -3.50718 -0.49089
5 - 3 == 0 -1.35484 -2.86298  0.15331
6 - 3 == 0 -2.32323 -3.83137 -0.81508
5 - 4 == 0  0.64419 -0.86395  2.15234
6 - 4 == 0 -0.32419 -1.83234  1.18395
6 - 5 == 0 -0.96839 -2.47653  0.53976
```



Results of the analysis using the **lmerTest** package is given below.

R Program

```
library(lmerTest)
options(contrasts=c("contr.sum","contr.poly"))

cs.mod2 <- lmer(y.cs ~ trt.cs + (1|blk.cs))
summary(cs.mod2)
anova(cs.mod2)
if(require(pbkrtest))
anova(cs.mod2,ddf="Kenward-Roger")
lsmeans(cs.mod2)
diff1smeans(cs.mod2)
```

R Output

```
> summary(cs.mod2)
Formula: y.cs ~ trt.cs + (1 | blk.cs)

REML criterion at convergence: 881.3

Random effects:
 Groups   Name      Variance Std.Dev.
 blk.cs  (Intercept)  11.948   3.457
 Residual                    4.231   2.057
Number of obs: 186, groups: blk.cs, 31

Fixed effects:
      Estimate Std. Error    df t value Pr(>|t|)
(Intercept)  25.00559    0.63888 30.00000  39.140 < 2e-16 ***
trt.cs1      -0.07043    0.33724 150.00000  -0.209  0.834856
trt.cs2       0.47828    0.33724 150.00000   1.418  0.158207
trt.cs3       1.31731    0.33724 150.00000   3.906  0.000141 ***
trt.cs4      -0.68172    0.33724 150.00000  -2.021  0.045012 *
trt.cs5      -0.03753    0.33724 150.00000  -0.111  0.911547
```

```

> anova(cs.mod2)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value    Pr(>F)
trt.cs 106.86  21.372     5   150  5.0513 0.0002623 ***

> if(require(pbkrtest))
+ anova(cs.mod2,ddf="Kenward-Roger")
Loading required package: pbkrtest
Analysis of Variance Table of type 3 with Kenward-Roger
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value    Pr(>F)
trt.cs 106.86  21.372     5   150  5.0513 0.0002623 ***

> lsmeans(cs.mod2)
Least Squares Means table:
      trt.cs Estimate Standard Error   DF t-value Lower CI Upper CI p-value
trt.cs 1     1.0   24.935      0.722 48.3  34.520    23.5    26.4 <2e-16
trt.cs 2     2.0   25.484      0.722 48.3  35.280    24.0    26.9 <2e-16
trt.cs 3     3.0   26.323      0.722 48.3  36.440    24.9    27.8 <2e-16
trt.cs 4     4.0   24.324      0.722 48.3  33.670    22.9    25.8 <2e-16
trt.cs 5     5.0   24.968      0.722 48.3  34.560    23.5    26.4 <2e-16
trt.cs 6     6.0   24.000      0.722 48.3  33.220    22.5    25.5 <2e-16

> diff1smeans(cs.mod2)
Differences of LSMEANS:
      Estimate Standard Error   DF t-value Lower CI Upper CI p-value
trt.cs 1 - 2    -0.5     0.5225 150.0   -1.05  -1.5810  0.484  0.295
trt.cs 1 - 3    -1.4     0.5225 150.0   -2.66  -2.4201 -0.355  0.009
trt.cs 1 - 4     0.6     0.5225 150.0    1.17  -0.4210  1.644  0.244
trt.cs 1 - 5     0.0     0.5225 150.0   -0.06  -1.0652  0.999  0.950
trt.cs 1 - 6     0.9     0.5225 150.0    1.79  -0.0968  1.968  0.075
trt.cs 2 - 3    -0.8     0.5225 150.0   -1.61  -1.8714  0.193  0.110
trt.cs 2 - 4     1.2     0.5225 150.0    2.22   0.1277  2.192  0.028
trt.cs 2 - 5     0.5     0.5225 150.0    0.99  -0.5165  1.548  0.325
trt.cs 2 - 6     1.5     0.5225 150.0    2.84   0.4519  2.517  0.005
trt.cs 3 - 4     2.0     0.5225 150.0    3.83   0.9667  3.031  2e-04
trt.cs 3 - 5     1.4     0.5225 150.0    2.59   0.3225  2.387  0.010
trt.cs 3 - 6     2.3     0.5225 150.0    4.45   1.2909  3.356 <2e-16
trt.cs 4 - 5    -0.6     0.5225 150.0   -1.23  -1.6765  0.388  0.220
trt.cs 4 - 6     0.3     0.5225 150.0    0.62  -0.7081  1.357  0.536
trt.cs 5 - 6     1.0     0.5225 150.0    1.85  -0.0639  2.001  0.066

```

9.3. Relative Efficiency of RCBD

The purpose of running a Randomized Complete Block Design is to remove the block variation from the error variation in the responses. When blocks are highly variable, we can remove a large amount of error variation relative to a Completely Randomized Design. A measure of the efficiency gain of the RCBD to a CRD is obtained as follows.

- 1) Compute estimate of σ^2 from the RCBD: $s_{RCBD}^2 = MS_{Err}$ $df_{RCBD} = (t-1)(b-1)$
- 2) Obtain estimate of σ^2 had it been a CRD: $s_{CRD}^2 = \frac{(b-1)MS_{Blks} + b(t-1)MS_{Err}}{bt-1}$ $df_{CRD} = t(b-1)$
- 3) Relative Efficiency (not corrected for df): $RE = \frac{s_{CRD}^2}{s_{RCBD}^2}$
- 4) Correction Factor: $CF = \frac{(df_{RCBD} + 1)(df_{CRD} + 3)}{(df_{RCBD} + 3)(df_{CRD} + 1)}$
- 5) Multiply results from parts 3) and 4): $RE^* = RE \times CF$

The interpretation of the relative efficiency is to determine how many subjects per treatment would be needed for a CRD to have the same standard error of the difference between means (or any contrast) as the RCBD had.

Example: Food Pinching Efficiency for 6 Lengths of Chopsticks in 31 Subjects

$$MS_{\text{Err}} = 4.2309 = s_{\text{RCBD}}^2 \quad MS_{\text{Blks}} = 75.9182 \quad t = 6 \quad b = 31 \quad df_{\text{RCBD}} = (6-1)(31-1) = 150$$

$$s_{\text{CRD}}^2 = \frac{(31-1)75.9182 + 31(6-1)4.2309}{6(31)-1} = \frac{2277.5460 + 655.7895}{185} = \frac{2933.3355}{185} = 15.5587 \quad df_{\text{CRD}} = 6(31-1) = 180$$

$$RE = \frac{15.5587}{4.2309} = 3.7476 \quad CF = \frac{(150+1)(180+3)}{(150+3)(180+1)} = \frac{27633}{27693} = 0.9978 \quad RE^* = 3.7476(0.9978) = 3.7395$$

Thus, had this experiment been conducted as a Completely Randomized Design, there would need to have been $31(3.7395) = 116$ subjects per treatment (696 total across treatments) to have the same precision in comparing treatment means. The blocking appears to have been very efficient.

9.4. Friedman's Rank-Based Nonparametric Test

When data are not normally distributed, and/or contain excessive outliers, a nonparametric, rank-based test can be used. This test was developed by renowned economist Milton Friedman. The test is similar to the Kruskal-Wallis test for the 1-Way ANOVA. Friedman's test is conducted as follows.

- 1) Rank the measurements for the t treatments from 1 (smallest) to t (largest) within blocks. Tied observations receive the average of the ranks they would have received if not tied.
- 2) Sum the ranks for each treatment across blocks: T_1, T_2, \dots, T_t s.t. $\sum_{i=1}^t T_i = b(1 + \dots + t) = \frac{bt(t+1)}{2}$
- 3) Test $H_0 : M_1 = \dots = M_t$ vs $H_A : \text{Not all } M_i \text{ are equal}$, where M_i is population median for Trt i
- 4) Test Statistic: $F_r = \frac{12}{bt(t+1)} \sum_{i=1}^t T_i^2 - 3b(t+1)$
- 5) Rejection Region: $F_r \geq \chi_{1-\alpha; t-1}^2$
- 6) If Reject H_0 , conclude $M_i \neq M_j$, if $|\bar{T}_i - \bar{T}_j| \geq z_{1-(\alpha/2C)} \sqrt{\frac{t(t+1)}{6b}}$ where: $\bar{T}_i = \frac{T_i}{b}$ and $C = \frac{t(t-1)}{2}$

Example: Food Pinching Efficiency for 6 Lengths of Chopsticks in 31 Subjects

For the chopstick experiment, we get the ranks of the food pinching efficiencies within each subject. For Subject 1, we have the following responses:

subject	Chpstk1	Chpstk2	Chpstk3	Chpstk4	Chpstk5	Chpstk6
1	19.55	23.53	21.34	24.40	22.50	21.32

The ranks for Chopsticks 1-6 for this individual are: 1, 5, 3, 6, 4, 2.
The complete table of ranks is given below.

Rank_C1	Rank_C2	Rank_C3	Rank_C4	Rank_C5	Rank_C6
1	5	3	6	4	2
5	4	6	2	1	3
4	5	6	2	3	1
6	3	5	1	2	4
3	6	4	5	1	2
2	6	4	5	3	1
3	5	1	4	6	2
6	2	4	1	5	3
1	5	6	3	2	4
5	4	6	2	3	1
6	4.5	4.5	2	3	1
2	5	6	4	3	1
1	3	6	2	4	5
4	5	6	1	2	3
1	4	6	2	5	3
4	3	5	1	6	2
4	2	5	1	3	6
3	4	2	6	5	1
2	6	3	4	5	1
2	3	5	4	6	1
3	2	5	1	6	4
4	5	3	2	6	1
3	1	6	5	2	4
1	6	2	3	5	4
3	5	2	6	4	1
6	5	4	1	3	2
5	6	3	2	1	4
6	5	2	4	3	1
1	3	6	4	5	2
2	3	6	5	4	1
6	2	3	5	1	4
105	127.5	135.5	96	112	75
T1	T2	T3	T4	T5	T6

For testing whether the population medians differ among the 6 lengths, we compute the test statistic, rejection region, and Bonferroni minimum significant difference for comparing mean ranks among the $C = 6(5)/2 = 15$ pairs of chopstick lengths.

$$\begin{aligned}
 TS: F_r &= \frac{12}{31(6)(7)} \left[(105)^2 + (127.5)^2 + (135.5)^2 + (96)^2 + (112)^2 + (75)^2 \right] - 3(31)(7) \\
 &= \frac{876318}{1302} - 651 = 673.0553 - 651 = 22.0553 \\
 RR: F_r &\geq \chi_{.95;5}^2 = 11.0705 \quad \text{P-value} = P(\chi_5^2 \geq 22.0553) = .0005 \\
 z_{1-(.05/(2(15)))} &= 2.9352 \Rightarrow \text{Conclude } M_i \neq M_{i'} \text{ if } |\bar{T}_i - \bar{T}_{i'}| \geq 2.9352 \sqrt{\frac{6(7)}{6(31)}} = 2.9352(0.4752) = 1.3948
 \end{aligned}$$

The ordered rank means are given below, along with lines adjoining not significantly different means.

CS6	CS4	CS1	CS5	CS2	CS3
2.4194	3.0968	3.3871	3.6129	4.1129	4.3710

Chopticks 2 and 3 are significantly better than chopstick 6. No other pairs are significantly different. The R Program and output for Friedman's Test (not including the post-hoc comparisons) are given below.

R Program

```
cs.rbd <- read.table("http://www.stat.ufl.edu/~winner/data/chopstick2_rcb.dat",
                    header=F,col.names=c("y.cs","trt.cs","blk.cs"))
attach(cs.rbd)

trt.cs <- factor(trt.cs); blk.cs <- factor(blk.cs)

friedman.test(y.cs ~ trt.cs | blk.cs)
```

R Output

```
> friedman.test(y.cs ~ trt.cs | blk.cs)

Friedman rank sum test

data: y.cs and trt.cs and blk.cs
Friedman chi-squared = 22.0756, df = 5, p-value = 0.0005065
```

9.5. Latin Square Design

A Latin Square design has 2 blocking factors. In its purest form, each blocking factor will have the same number of levels as the treatment factor. When the number of treatments is small, squares can be replicated to obtain more observations. The blocking factors can be fixed or random, the variance of individual treatment means will depend on whether or not one or both blocking factors is (are) random. The variance of the difference between 2 treatment means will not (as in the RCBD).

The key to the Latin Square Design is that each treatment appears once in each level of the row and column blocking factors. Suppose we have an experiment with $t = 5$ levels (say A,B,C,D,E), and the row and column blocking factors each has 5 levels. Then the design could look like this.

Row\Column	Col1	Col2	Col3	Col4	Col5
Row1	A	B	C	D	E
Row2	B	C	D	E	A
Row3	C	D	E	A	B
Row4	D	E	A	B	C
Row5	E	A	B	C	D

Each treatment appears once in each row and once in each column. While there are 3 factors, each with t levels, there are only t^2 observations (one in each row/column combination). We give the model here.

$$Y_{ij}^k = \mu + \tau_k + \rho_i + \gamma_j + \varepsilon_{ij}^k \quad i=1, \dots, t; j=1, \dots, t; k=1, \dots, t \quad \varepsilon_{ij}^k \sim NID(0, \sigma^2)$$

$\mu \equiv$ Overall Mean Response

$\tau_k \equiv$ Effect of Treatment k which appears in Row i and Column j $\sum_{k=1}^t \tau_k = 0$

$\rho_i \equiv$ Effect of Row Blocking Factor Level i Fixed $\Rightarrow \sum_{i=1}^t \rho_i = 0$ Random $\Rightarrow \rho_i \sim NID(0, \sigma_\rho^2)$

$\gamma_j \equiv$ Effect of Column Blocking Factor Level j Fixed $\Rightarrow \sum_{j=1}^t \gamma_j = 0$ Random $\Rightarrow \gamma_j \sim NID(0, \sigma_\gamma^2)$

When Row and/or Column factors are Random: $\{\rho_i\} \perp \{\gamma_j\} \perp \{\varepsilon_{ij}^k\}$

The mean and covariance structure for the data for 3 scenarios corresponding to whether rows and columns are fixed or random effects are given here.

$$Y_{ij}^k = \mu + \tau_k + \rho_i + \gamma_j + \varepsilon_{ij}^k \quad i=1, \dots, t; j=1, \dots, t; k=1, \dots, t$$

Rows and Columns Fixed:

$$E\{Y_{ij}^k\} = \mu + \tau_k + \rho_i + \gamma_j \quad \text{COV}\{Y_{ij}^k, Y_{i'j'}^{k'}\} = \begin{cases} \sigma^2 & i=i'; j=j'; k=k' \\ 0 & \text{otherwise} \end{cases}$$

Rows Fixed and Columns Random:

$$E\{Y_{ij}^k\} = \mu + \tau_k + \rho_i \quad \text{COV}\{Y_{ij}^k, Y_{i'j'}^{k'}\} = \begin{cases} \sigma_\rho^2 + \sigma^2 & i=i'; j=j'; k=k' \\ \sigma_\rho^2 & i \neq i'; j=j'; k=k' \\ 0 & \text{otherwise} \end{cases}$$

Rows and Columns Random:

$$E\{Y_{ij}^k\} = \mu + \tau_k \quad \text{COV}\{Y_{ij}^k, Y_{i'j'}^{k'}\} = \begin{cases} \sigma_\rho^2 + \sigma_\gamma^2 + \sigma^2 & i=i'; j=j'; k=k' \\ \sigma_\rho^2 & i=i'; j \neq j'; k \neq k' \\ \sigma_\gamma^2 & i \neq i'; j=j'; k \neq k' \\ 0 & \text{otherwise} \end{cases}$$

To obtain the Analysis of Variance, consider the Fixed Effects model, although the sums of squares are the same for all cases.

$$\begin{aligned}
 \hat{Y}_{ij}^k &= \hat{\mu} + \hat{\tau}_k + \hat{\rho}_i + \hat{\gamma}_j \quad \text{define: } n_{ij}^k = \begin{cases} 1 & \text{if Trt } k \text{ occurs in row } i, \text{ column } j \\ 0 & \text{otherwise} \end{cases} \\
 \bar{Y}_k &= \frac{1}{t} \sum_{i=1}^t \sum_{j=1}^t n_{ij}^k Y_{ij}^k & \bar{Y}_{i\cdot} &= \frac{1}{t} \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k Y_{ij}^k & \bar{Y}_{\cdot j} &= \frac{1}{t} \sum_{i=1}^t \sum_{k=1}^t n_{ij}^k Y_{ij}^k & \bar{Y}_{\cdot\cdot} &= \frac{1}{t^2} \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k Y_{ij}^k \\
 \hat{\mu} &= \bar{Y}_{\cdot\cdot} & \hat{\tau}_k &= \bar{Y}_k - \bar{Y}_{\cdot\cdot} & \hat{\rho}_i &= \bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot} & \hat{\gamma}_j &= \bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot} \\
 SS_{\text{Tot}} &= \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k (Y_{ij}^k - \bar{Y}_{\cdot\cdot})^2 = \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k (Y_{ij}^k)^2 - t^2 \bar{Y}_{\cdot\cdot}^2 & df_{\text{Tot}} &= t^2 - 1 \\
 SS_{\text{Trts}} &= t \sum_{k=1}^t (\bar{Y}_k - \bar{Y}_{\cdot\cdot})^2 = t \sum_{k=1}^t \bar{Y}_k^2 - t^2 \bar{Y}_{\cdot\cdot}^2 & df_{\text{Trts}} &= t - 1 \\
 SS_{\text{Rows}} &= t \sum_{i=1}^t (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 = t \sum_{i=1}^t \bar{Y}_{i\cdot}^2 - t^2 \bar{Y}_{\cdot\cdot}^2 & df_{\text{Rows}} &= t - 1 \\
 SS_{\text{Cols}} &= t \sum_{j=1}^t (\bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot})^2 = t \sum_{j=1}^t \bar{Y}_{\cdot j}^2 - t^2 \bar{Y}_{\cdot\cdot}^2 & df_{\text{Cols}} &= t - 1 \\
 SS_{\text{Err}} &= \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left(Y_{ij}^k - \hat{Y}_{ij}^k \right)^2 = \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left(Y_{ij}^k - [\bar{Y}_{\cdot\cdot} + \bar{Y}_k - \bar{Y}_{\cdot\cdot} + \bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot} + \bar{Y}_{\cdot j} - \bar{Y}_{\cdot\cdot}] \right)^2 = \\
 &= \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left(Y_{ij}^k - \bar{Y}_k - \bar{Y}_{i\cdot} - \bar{Y}_{\cdot j} + 2\bar{Y}_{\cdot\cdot} \right)^2 = \\
 &= \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k (Y_{ij}^k)^2 - t \sum_{k=1}^t \bar{Y}_k^2 - t \sum_{i=1}^t \bar{Y}_{i\cdot}^2 - t \sum_{j=1}^t \bar{Y}_{\cdot j}^2 + 2t^2 \bar{Y}_{\cdot\cdot}^2 = SS_{\text{Tot}} - SS_{\text{Trts}} - SS_{\text{Rows}} - SS_{\text{Cols}} \\
 \Rightarrow df_{\text{Err}} &= (t^2 - 1) - 3(t - 1) = (t + 1)(t - 1) - 3(t - 1) = (t - 1)(t + 1 - 3) = (t - 1)(t - 2)
 \end{aligned}$$

Note that for any given treatment, we have the following (since it appears in each row and column once).

$$\begin{aligned}
 \bar{Y}_k &= \frac{1}{t} \sum_{i=1}^t \sum_{j=1}^t n_{ij}^k Y_{ij}^k \quad \text{where } n_{ij}^k = \begin{cases} 1 & \text{if Treatment } k \text{ appears in Row } i, \text{ Column } j \\ 0 & \text{Otherwise} \end{cases} \\
 \Rightarrow \bar{Y}_k &= \frac{1}{t} \left[t\mu + t\tau_k + \sum_{i=1}^t \rho_i + \sum_{j=1}^t \gamma_j + \sum_{i=1}^t \sum_{j=1}^t n_{ij}^k \varepsilon_{ij}^k \right] \\
 \text{Rows and Columns Fixed: } E\{\bar{Y}_k\} &= \mu + \tau_k & V\{\bar{Y}_k\} &= \frac{t\sigma^2}{t^2} = \frac{\sigma^2}{t} \\
 \text{Rows Fixed and Columns Random: } E\{\bar{Y}_k\} &= \mu + \tau_k & V\{\bar{Y}_k\} &= \frac{t\sigma_\gamma^2 + t\sigma^2}{t^2} = \frac{\sigma_\gamma^2 + \sigma^2}{t} \\
 \text{Rows and Columns Random: } E\{\bar{Y}_k\} &= \mu + \tau_k & V\{\bar{Y}_k\} &= \frac{t\sigma_\rho^2 + t\sigma_\gamma^2 + t\sigma^2}{t^2} = \frac{\sigma_\rho^2 + \sigma_\gamma^2 + \sigma^2}{t}
 \end{aligned}$$

Thus, the variance of a treatment mean depends on whether row and column blocking factors are fixed or random. Note that the variance of the difference in treatment means will be the same, regardless of whether row

and column blocking factors are fixed or random. This is due to the covariance structure and the fact that each pair of treatments occurs together once in rows and columns.

Rows and Columns Fixed:

$$V\{\bar{Y}_k\} = \frac{\sigma^2}{t} \quad \text{COV}\{\bar{Y}_k, \bar{Y}_{k'}\} = 0 \quad (k \neq k')$$

$$\Rightarrow V\{\bar{Y}_k - \bar{Y}_{k'}\} = \frac{2\sigma^2}{t} \Rightarrow \hat{SE}\{\bar{Y}_k - \bar{Y}_{k'}\} = \sqrt{\frac{2MS_{\text{Err}}}{t}}$$

Rows Fixed and Columns Random:

$$V\{\bar{Y}_k\} = \frac{\sigma^2 + \sigma_\gamma^2}{t} \quad \text{COV}\{Y_{ij}^k, Y_{i'j}^{k'}\} = \sigma_\gamma^2 \quad (1 \text{ per column, over } t \text{ columns})$$

$$\Rightarrow \text{COV}\{\bar{Y}_k, \bar{Y}_{k'}\} = \frac{1}{t^2} t \sigma_\gamma^2 = \frac{\sigma_\gamma^2}{t}$$

$$\Rightarrow V\{\bar{Y}_k - \bar{Y}_{k'}\} = 2 \frac{\sigma^2 + \sigma_\gamma^2}{t} - 2 \frac{\sigma_\gamma^2}{t} = \frac{2\sigma^2}{t} \Rightarrow \hat{SE}\{\bar{Y}_k - \bar{Y}_{k'}\} = \sqrt{\frac{2MS_{\text{Err}}}{t}}$$

Rows and Columns Random:

$$V\{\bar{Y}_k\} = \frac{\sigma^2 + \sigma_\gamma^2 + \sigma_\rho^2}{t} \quad \text{COV}\{Y_{ij}^k, Y_{i'j}^{k'}\} = \sigma_\gamma^2 \quad \text{COV}\{Y_{ij}^k, Y_{ij'}^{k'}\} = \sigma_\rho^2$$

$$\Rightarrow \text{COV}\{Y_{i\cdot}^k, Y_{i\cdot}^{k'}\} = t \sigma_\gamma^2 \quad \text{COV}\{Y_{\cdot j}^k, Y_{\cdot j}^{k'}\} = t \sigma_\rho^2 \Rightarrow \text{COV}\{\bar{Y}_k, \bar{Y}_{k'}\} = t \sigma_\gamma^2 + t \sigma_\rho^2$$

$$\Rightarrow \text{COV}\{\bar{Y}_k, \bar{Y}_{k'}\} = \frac{1}{t^2} t (\sigma_\gamma^2 + \sigma_\rho^2) = \frac{\sigma_\gamma^2 + \sigma_\rho^2}{t}$$

$$\Rightarrow V\{\bar{Y}_k - \bar{Y}_{k'}\} = 2 \frac{\sigma^2 + \sigma_\gamma^2 + \sigma_\rho^2}{t} - 2 \frac{\sigma_\gamma^2 + \sigma_\rho^2}{t} = \frac{2\sigma^2}{t} \Rightarrow \hat{SE}\{\bar{Y}_k - \bar{Y}_{k'}\} = \sqrt{\frac{2MS_{\text{Err}}}{t}}$$

The expected mean squares for the 3 cases are given below. Their derivations are similar to the Randomized Complete Block Design.

$$SS_{\text{Err}} = \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left(Y_{ij}^k - \bar{Y}_k - \bar{Y}_{i\cdot} - \bar{Y}_{\cdot j} + 2\bar{Y}_{\cdot\cdot} \right)^2$$

Note: $\sum_{i=1}^t n_{ij}^k = \sum_{j=1}^t n_{ij}^k = 1$ $\sum_{i=1}^t \sum_{j=1}^t n_{ij}^k = \sum_{i=1}^t \sum_{k=1}^t n_{ij}^k = \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k = t$ $\sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k = t^2$

$$SS_{\text{Err}} = \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left(Y_{ij}^k \right)^2 - t \sum_{k=1}^t \bar{Y}_k^2 - t \sum_{i=1}^t \bar{Y}_{i\cdot}^2 - t \sum_{j=1}^t \bar{Y}_{\cdot j}^2 + 2t^2 \bar{Y}_{\cdot\cdot}^2$$

$$SS_{\text{Trts}} = t \sum_{k=1}^t \left(\bar{Y}_k - \bar{Y}_{\cdot\cdot} \right)^2 = t \sum_{k=1}^t \bar{Y}_k^2 - t^2 \bar{Y}_{\cdot\cdot}^2$$

Rows and Columns Fixed:

$$n_{ij}^k = 1: \quad E\{n_{ij}^k Y_{ij}^k\} = \mu + \tau_k + \rho_i + \gamma_j \quad V\{n_{ij}^k Y_{ij}^k\} = \sigma^2 \quad E\{n_{ij}^k (Y_{ij}^k)^2\} = (\mu + \tau_k + \rho_i + \gamma_j)^2 + \sigma^2$$

$$E\{\bar{Y}_k\} = \mu + \tau_k \quad V\{\bar{Y}_k\} = \frac{\sigma^2}{t} \quad E\{\bar{Y}_k^2\} = (\mu + \tau_k)^2 + \frac{\sigma^2}{t}$$

$$E\{\bar{Y}_{i\cdot}\} = \mu + \rho_i \quad V\{\bar{Y}_{i\cdot}\} = \frac{\sigma^2}{t} \quad E\{\bar{Y}_{i\cdot}^2\} = (\mu + \rho_i)^2 + \frac{\sigma^2}{t}$$

$$E\{\bar{Y}_{\cdot j}\} = \mu + \gamma_j \quad V\{\bar{Y}_{\cdot j}\} = \frac{\sigma^2}{t} \quad E\{\bar{Y}_{\cdot j}^2\} = (\mu + \gamma_j)^2 + \frac{\sigma^2}{t}$$

$$E\{\bar{Y}_{\cdot\cdot}\} = \mu \quad V\{\bar{Y}_{\cdot\cdot}\} = \frac{\sigma^2}{t^2} \quad E\{\bar{Y}_{\cdot\cdot}^2\} = \mu^2 + \frac{\sigma^2}{t^2}$$

$$E\{SS_{\text{Err}}\} = \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left[\mu^2 + \tau_k^2 + \rho_i^2 + \gamma_j^2 + 2\mu\tau_k + 2\mu\rho_i + 2\mu\gamma_j + 2\tau_k\rho_i + 2\tau_k\gamma_j + 2\rho_i\gamma_j + \sigma^2 \right]$$

$$- \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left[\mu^2 + \tau_k^2 + 2\mu\tau_k + \frac{\sigma^2}{t} \right] - t \sum_{i=1}^t \sum_{k=1}^t n_{ij}^k \left[\mu^2 + \rho_i^2 + 2\mu\rho_i + \frac{\sigma^2}{t} \right] - t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left[\mu^2 + \gamma_j^2 + 2\mu\gamma_j + \frac{\sigma^2}{t} \right] + 2t^2 \left[\mu^2 + \frac{\sigma^2}{t^2} \right] =$$

$$\mu^2 [t^2 - t^2 - t^2 - t^2 + 2t^2] + \sum_{k=1}^t \tau_k^2 [t-t] + \sum_{i=1}^t \rho_i^2 [t-t] + \sum_{j=1}^t \gamma_j^2 [t-t] + \sigma^2 [t^2 - t - t - t + 2] = \sigma^2 [t^2 - 3t + 2]$$

$$= \sigma^2 (t-1)(t-2) \Rightarrow E\{MS_{\text{Err}}\} = E\left\{ \frac{SS_{\text{Err}}}{(t-1)(t-2)} \right\} = \sigma^2$$

$$E\{SS_{\text{Trts}}\} = \sum_{i=1}^t \sum_{j=1}^t \sum_{k=1}^t n_{ij}^k \left[\mu^2 + \tau_k^2 + 2\mu\tau_k + \frac{\sigma^2}{t} \right] - t^2 \left[\mu^2 + \frac{\sigma^2}{t^2} \right] = \mu^2 [t^2 - t^2] + t \sum_{k=1}^t \tau_k^2 + \sigma^2 [t-1]$$

$$\Rightarrow E\{MS_{\text{Trts}}\} = E\left\{ \frac{SS_{\text{Trts}}}{t-1} \right\} = \sigma^2 + \frac{t \sum_{k=1}^t \tau_k^2}{t-1}$$

For this model (as well as the other two cases), we can test for treatment effects and make pairwise comparisons among means as follow.

$$H_0: \tau_1 = \dots = \tau_t = 0 \quad H_A: \text{Not all } \tau_i = 0$$

$$\text{Test Statistic: } F_{\text{Trts}} = \frac{MS_{\text{Trts}}}{MS_{\text{Err}}} \quad \text{Rejection Region: } F_{\text{Trts}} \geq F_{1-\alpha; t-1, (t-1)(t-2)} \quad \text{P-value: } P\left(F_{t-1, (t-1)(t-2)} \geq F_{\text{Trts}}\right)$$

$$\hat{SE}\{\bar{Y}_k - \bar{Y}_{k'}\} = \sqrt{\frac{2MS_{\text{Err}}}{t}}$$

Rows and Columns Fixed: $\hat{SE}\{\bar{Y}_k\} = \sqrt{\frac{MS_{Err}}{t}}$

Rows Fixed and Columns Random: $\hat{SE}\{\bar{Y}_k\} = \sqrt{\frac{\hat{\sigma}^2 + \hat{\sigma}_\gamma^2}{t}} \quad \hat{\sigma}^2 = MS_{Err} \quad \hat{\sigma}_\gamma^2 = \frac{MS_{Cols} - MS_{Err}}{t}$

Rows and Columns Random: $\hat{SE}\{\bar{Y}_k\} = \sqrt{\frac{\hat{\sigma}^2 + \hat{\sigma}_\gamma^2 + \hat{\sigma}_\rho^2}{t}} \quad \hat{\sigma}_\rho^2 = \frac{MS_{Rows} - MS_{Err}}{t}$

Example: Hominy Sales by Shelf Space, Store, Week

A marketing experiment was conducted (Cox (1964)) to compare the effects of shelf space (4 to 14 by 2 units). The experiment was conducted as a Latin Square Design with $t = 6$. The Row factor was Store and the Column factor was Week. Each shelf space (4,6,8,10,12,14) was assigned to each store once, and to each week once. The data and design are given below. It seems reasonable to treat Store and Week as random effects.

Hominy	Week1	Week2	Week3	Week4	Week5	Week6	Mean	Trt	Mean
Store1	140	150	71	111	121	127	120.00	4	78.17
Store2	131	126	130	188	133	154	143.67	6	88.00
Store3	67	94	49	93	112	161	96.00	8	83.50
Store4	109	134	96	123	127	84	112.17	10	101.83
Store5	58	71	59	62	49	27	54.33	12	120.67
Store6	37	36	52	58	38	51	45.33	14	99.33
Mean	90.33	101.83	76.17	105.83	96.67	100.67	95.25	Mean	95.25

The sums of squares and Analysis of Variance are given below.

$$\sum_{i=1}^6 \sum_{j=1}^6 \sum_{k=1}^6 n_{ij}^k (y_{ij}^k)^2 = 140^2 + \dots + 51^2 = 388763 \quad 6 \sum_{k=1}^6 \bar{y}_k^{-2} = 333743.17 \quad 6 \sum_{i=1}^6 \bar{y}_i^{-2} = 371068.17$$

$$6 \sum_{j=1}^6 \bar{y}_{\cdot j}^{-2} = 330062.50 \quad 6^2 \bar{Y}_{\cdot\cdot}^{-2} = 326612.25$$

$$SS_{Trts} = 333743.17 - 326612.25 = 7130.92 \quad df_{Trts} = 6 - 1 = 5$$

$$SS_{Rows} = 371068.17 - 326612.25 = 44455.92 \quad df_{Rows} = 6 - 1 = 5$$

$$SS_{Cols} = 330062.50 - 326612.25 = 3450.25 \quad df_{Cols} = 6 - 1 = 5$$

$$SS_{Err} = 388763.00 - 333743.17 - 371068.17 - 330062.50 + 2(326612.25) = 7113.67 \quad df_{Err} = (6-1)(6-2) = 20$$

Source	df	SS	MS	F	F(.95)	P-value
Shelf Space (Trts)	5	7130.92	1426.18	4.010	2.711	0.0111
Store (Rows)	5	44455.92	8891.18			
Week (Columns)	5	3450.25	690.05			
Error	20	7113.67	355.68			
Total	35	62150.75				

The variance components for the store, week, and error terms are computed below, as well as the variance for the shelf space means and their pairwise differences.

$$\begin{aligned} \text{Error: } \hat{\sigma}^2 &= MS_{\text{Err}} = 355.68 \\ \text{Store (Row): } \hat{\sigma}_\rho^2 &= \frac{MS_{\text{Rows}} - MS_{\text{Err}}}{t} = \frac{8891.18 - 355.68}{6} = 1422.58 \\ \text{Week (Column): } \hat{\sigma}_\gamma^2 &= \frac{MS_{\text{Cols}} - MS_{\text{Err}}}{t} = \frac{690.05 - 355.68}{6} = 55.73 \\ \hat{V}\{\bar{Y}_k\} &= \frac{\hat{\sigma}_\rho^2 + \hat{\sigma}_\gamma^2 + \hat{\sigma}^2}{t} = \frac{1422.58 + 55.73 + 355.68}{6} = 305.67 \Rightarrow SE\{\bar{Y}_k\} = \sqrt{305.67} = 17.48 \\ \hat{V}\{\bar{Y}_k - \bar{Y}_{k'}\} &= \frac{2\hat{\sigma}^2}{t} = \frac{2(355.68)}{6} = 118.56 \Rightarrow SE\{\bar{Y}_k - \bar{Y}_{k'}\} = \sqrt{118.56} = 10.89 \\ \text{Tukey's HSD for comparing all pairs of shelf space: } q_{.95;6,20} &= 4.445 \Rightarrow HSD = \frac{4.445}{\sqrt{2}}(10.89) = 34.22 \end{aligned}$$

12 units is significantly higher than 4, 6, and 8. No other lengths are significantly different.

R Program:

```
shsp <- read.table("http://www.stat.ufl.edu/~winner/data/shelfspace.dat",
  header=F, col.names=c("product", "store", "week", "shelf", "sales"))
attach(shsp)

h.product <- product[product==1]; h.product <- factor(h.product)
h.store <- store[product==1]; h.store <- factor(h.store)
h.week <- week[product==1]; h.week <- factor(h.week)
h.shelf <- shelf[product==1]; h.shelf <- factor(h.shelf)
h.sales <- sales[product==1]

print(cbind(h.product, h.store, h.week, h.shelf, h.sales))

hom.mod1 <- aov(h.sales ~ h.shelf + h.store + h.week)
anova(hom.mod1)
summary.lm(hom.mod1)
TukeyHSD(hom.mod1, "h.shelf")

library(lmerTest)

hom.mod2 <- lmer(h.sales ~ h.shelf + (1|h.store) + (1|h.week))
anova(hom.mod2)
summary(hom.mod2)
lsmeans(hom.mod2)
diff1smeans(hom.mod2)
```

R Output:

Output based on **aov** function:

```
> hom.mod1 <- aov(h.sales ~ h.shelf + h.store + h.week)
> anova(hom.mod1)
Analysis of Variance Table

Response: h.sales
      Df Sum Sq Mean Sq F value    Pr(>F)
h.shelf  5   7131  1426.2   4.0097  0.01107 *
h.store  5  44456  8891.2  24.9975 5.788e-08 ***
h.week   5   3450   690.1   1.9401  0.13235
Residuals 20   7114   355.7

> summary.lm(hom.mod1)

Call:
aov(formula = h.sales ~ h.shelf + h.store + h.week)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  98.000     12.573   7.794 1.74e-07 ***
h.shelf6     9.833      10.889   0.903 0.377229
h.shelf8     5.333      10.889   0.490 0.629598
h.shelf10    23.667     10.889   2.174 0.041925 *
h.shelf12    42.500     10.889   3.903 0.000882 ***
h.shelf14    21.167     10.889   1.944 0.066107 .
h.store2     23.667     10.889   2.174 0.041925 *
h.store3    -24.000     10.889  -2.204 0.039394 *
h.store4    -7.833      10.889  -0.719 0.480212
h.store5    -65.667     10.889  -6.031 6.77e-06 ***
h.store6    -74.667     10.889  -6.857 1.16e-06 ***
h.week2     11.500     10.889   1.056 0.303490
h.week3    -14.167     10.889  -1.301 0.208029
h.week4     15.500     10.889   1.424 0.170002
h.week5      6.333      10.889   0.582 0.567302
h.week6     10.333      10.889   0.949 0.353945

Residual standard error: 18.86 on 20 degrees of freedom
Multiple R-squared:  0.8855,    Adjusted R-squared:  0.7997
F-statistic: 10.32 on 15 and 20 DF,  p-value: 2.388e-06

> TukeyHSD(hom.mod1,"h.shelf")
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = h.sales ~ h.shelf + h.store + h.week)

$h.shelf
      diff          lwr          upr      p adj
6-4     9.833333 -24.392262  44.05893 0.9412015
8-4     5.333333 -28.892262  39.55893 0.9960032
10-4    23.666667 -10.558929  57.89226 0.2923835
12-4    42.500000   8.274404  76.72560 0.0098394
14-4    21.166667 -13.058929  55.39226 0.4062688
8-6    -4.500000 -38.725596  29.72560 0.9982094
10-6    13.833333 -20.392262  48.05893 0.7970127
12-6    32.666667  -1.558929  66.89226 0.0667654
14-6    11.333333 -22.892262  45.55893 0.8983484
10-8    18.333333 -15.892262  52.55893 0.5570249
12-8    37.166667   2.941071  71.39226 0.0284716
14-8    15.833333 -18.392262  50.05893 0.6953024
12-10   18.833333 -15.392262  53.05893 0.5293742
14-10   -2.500000 -36.725596  31.72560 0.9998973
14-12  -21.333333 -55.558929  12.89226 0.3980112
```

Output from **lmer** function in **lmerTest** package:

```

> hom.mod2 <- lmer(h.sales ~ h.shelf + (1|h.store) + (1|h.week))
> anova(hom.mod2)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value Pr(>F)
h.shelf 7130.9 1426.2     5     20  4.0097 0.01107 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary(hom.mod2)
Linear mixed model fit by REML t-tests use Satterthwaite approximations to degrees of
freedom [
merModLmerTest]
Formula: h.sales ~ h.shelf + (1 | h.store) + (1 | h.week)

REML criterion at convergence: 291.5

Random effects:
  Groups   Name      Variance Std.Dev.
h.store (Intercept) 1422.58  37.717
h.week  (Intercept)   55.73   7.465
Residual                    355.68  18.860
Number of obs: 36, groups: h.store, 6; h.week, 6

Fixed effects:
      Estimate Std. Error   df t value Pr(>|t|)
(Intercept)  78.167    17.483  7.565  4.471 0.002391 **
h.shelf6     9.833    10.889 20.000  0.903 0.377229
h.shelf8     5.333    10.889 20.000  0.490 0.629598
h.shelf10    23.667    10.889 20.000  2.174 0.041925 *
h.shelf12    42.500    10.889 20.000  3.903 0.000882 ***
h.shelf14    21.167    10.889 20.000  1.944 0.066107 .

> lsmeans(hom.mod2)
Least Squares Means table:
      h.shelf Estimate Standard Error DF t-value Lower CI Upper CI p-value
h.shelf 4      4.0      78.17      17.48 7.6 4.47 37.4 119 0.002 **
h.shelf 6      5.0      88.00      17.48 7.6 5.03 47.3 129 0.001 **
h.shelf 8      6.0      83.50      17.48 7.6 4.78 42.8 124 0.002 **
h.shelf 10     1.0     101.83     17.48 7.6 5.82 61.1 143 5e-04 ***
h.shelf 12     2.0     120.67     17.48 7.6 6.90 79.9 161 2e-04 ***
h.shelf 14     3.0      99.33     17.48 7.6 5.68 58.6 140 6e-04 ***

> diff1smeans(hom.mod2)
Differences of LSMEANS:
      Estimate Standard Error DF t-value Lower CI Upper CI p-value
h.shelf 4 - 6      -9.8      10.89  20.0 -0.90 -32.55 12.880 0.377
h.shelf 4 - 8      -5.3      10.89  20.0 -0.49 -28.05 17.380 0.630
h.shelf 4 - 10     -23.7     10.89  20.0 -2.17 -46.38 -0.954 0.042 *
h.shelf 4 - 12     -42.5     10.89  20.0 -3.90 -65.21 -19.787 9e-04 ***
h.shelf 4 - 14     -21.2     10.89  20.0 -1.94 -43.88  1.546 0.066 .
h.shelf 6 - 8       4.5      10.89  20.0  0.41 -18.21 27.213 0.684
h.shelf 6 - 10     -13.8     10.89  20.0 -1.27 -36.55  8.880 0.218
h.shelf 6 - 12     -32.7     10.89  20.0 -3.00 -55.38 -9.954 0.007 **
h.shelf 6 - 14     -11.3     10.89  20.0 -1.04 -34.05 11.380 0.310
h.shelf 8 - 10     -18.3     10.89  20.0 -1.68 -41.05  4.380 0.108
h.shelf 8 - 12     -37.2     10.89  20.0 -3.41 -59.88 -14.454 0.003 **
h.shelf 8 - 14     -15.8     10.89  20.0 -1.45 -38.55  6.880 0.161
h.shelf 10 - 12    -18.8     10.89  20.0 -1.73 -41.55  3.880 0.099 .
h.shelf 10 - 14     2.5      10.89  20.0  0.23 -20.21 25.213 0.821
h.shelf 12 - 14    21.3      10.89  20.0  1.96 -1.38 44.047 0.064 .

```

9.6. Relative Efficiency of Latin Square Design

The efficiency of the Latin Square Design can be computed relative to a Completely Randomized Design, or Randomized Complete Block Designs with only the Row Blocking factor or Column Blocking factor. Here we give formulas for the estimated error variances, degrees of freedom, and Relative Efficiencies for the 3 cases.

$$\text{Latin Square: } s_{LS}^2 = MS_{ERR} \quad df_{LS} = (t-1)(t-2)$$

RCBD with Rows as Blocks:

$$s_{RCBD,ROW}^2 = \frac{(t-1)MS_{COLS} + (t-1)^2 MS_{ERR}}{t(t-1)} = \frac{MS_{COLS} + (t-1)MS_{ERR}}{t} \quad df_{RCBD,ROW} = (t-1)^2$$

$$RE_{RCBD,ROW} = \frac{s_{RCBD,ROW}^2}{s_{LS}^2} \quad CF_{RCBD,ROW} = \frac{((t-1)(t-2)+1)((t-1)^2+3)}{((t-1)(t-2)+3)((t-1)^2+1)} \quad RE_{RCBD,ROW}^* = RE_{RCBD,ROW} CF_{RCBD,ROW}$$

RCBD with Columns as Blocks:

$$s_{RCBD,COL}^2 = \frac{(t-1)MS_{ROWS} + (t-1)^2 MS_{ERR}}{t(t-1)} = \frac{MS_{ROWS} + (t-1)MS_{ERR}}{t} \quad df_{RCBD,COL} = (t-1)^2$$

$$RE_{RCBD,COL} = \frac{s_{RCBD,COL}^2}{s_{LS}^2} \quad CF_{RCBD,COL} = \frac{((t-1)(t-2)+1)((t-1)^2+3)}{((t-1)(t-2)+3)((t-1)^2+1)} \quad RE_{RCBD,COL}^* = RE_{RCBD,COL} CF_{RCBD,COL}$$

CRD:

$$s_{CRD}^2 = \frac{(t-1)(MS_{COLS} + MS_{ROWS}) + (t-1)(t-2)MS_{ERR}}{t(t-1)} = \frac{MS_{COLS} + MS_{ROWS} + (t-2)MS_{ERR}}{t} \quad df_{CRD} = t(t-1)$$

$$RE_{CRD} = \frac{s_{CRD}^2}{s_{LS}^2} \quad CF_{CRD} = \frac{((t-1)(t-2)+1)(t(t-1)+3)}{((t-1)(t-2)+3)(t(t-1)+1)} \quad RE_{CRD}^* = RE_{CRD} CF_{CRD}$$

Example: Hominy Sales by Shelf Space, Store, Week

We compute the 3 Relative Efficiency measures for the shelf space latin square experiment. The latin square design is highly efficient. This is particularly with respect to Store as a Blocking factor, not so much with respect to Week as a Blocking factor.

$$MS_{ERR} = 355.68 \quad MS_{COLS} = 690.05 \quad MS_{ROWS} = 8891.18 \quad t = 6$$

$$\text{Latin Square: } s_{LS}^2 = 355.68 \quad df_{LS} = (6-1)(6-2) = 20$$

RCBD with Rows as Blocks:

$$s_{RCBD,ROW}^2 = \frac{690.05 + (6-1)355.68}{6} = 411.41 \quad df_{RCBD,ROW} = (6-1)^2 = 25$$

$$RE_{RCBD,ROW} = \frac{411.41}{355.68} = 1.16 \quad CF_{RCBD,ROW} = \frac{((6-1)(6-2)+1)((6-1)^2+3)}{((6-1)(6-2)+3)((6-1)^2+1)} = \frac{21(28)}{23(26)} = 0.983 \quad RE_{RCBD,ROW}^* = 1.14$$

RCBD with Columns as Blocks:

$$s_{RCBD,COL}^2 = \frac{8891.18 + (6-1)355.68}{6} = 1778.26 \quad df_{RCBD,COL} = (6-1)^2 = 25$$

$$RE_{RCBD,COL} = \frac{1778.26}{355.68} = 5.00 \quad CF_{RCBD,COL} = 0.983 \quad RE_{RCBD,COL}^* = 4.92$$

CRD:

$$s_{CRD}^2 = \frac{690.05 + 8891.18 + (6-2)355.68}{6} = 1833.99 \quad df_{CRD} = 6(6-1) = 30$$

$$RE_{CRD} = \frac{1833.99}{355.68} = 5.16 \quad CF_{CRD} = \frac{((6-1)(6-2)+1)(6(6-1)+3)}{((6-1)(6-2)+3)(6(6-1)+1)} = \frac{21(33)}{23(31)} = 0.972 \quad RE_{CRD}^* = 5.02$$

9.7. Incomplete Block Designs

When the number of treatments increases, it is often difficult to find blocks that have as many homogeneous sub-units as treatments. Also, in some cases it is logistically impossible or inconvenient to assign all treatments within blocks. Sporting events also often can involve only 2 teams from a larger group of teams, and matches can be treated as incomplete blocks. First we consider the **Balanced Incomplete Block Design (BIB)** then we briefly describe the **Partially Balanced Incomplete Block Design (PBIB)**. Note that even when the design is unbalanced with random blocks, these models can be fit as a general mixed model.

Balanced Incomplete Block Design

In this design, there are t treatments and b blocks of $k < t$ subunits. Each treatment is observed in $r < b$ replicates. This requires that the total number of observations will be $N = tr = bk$. Clearly, Balanced Incomplete Block Designs are limited to certain specific combinations of levels of t , r , b , and k . A further restriction is that each treatment occurs in r blocks with $k-1$ remaining positions in each block. These must be evenly distributed among the $t-1$ remaining treatments. Let λ represent the number of blocks that each pair of treatments occur in together. From this, we obtain the following restrictions for a BIB.

$$\text{Number of Treatments Appearing in Blocks with a Given Treatment: } \lambda(t-1) = r(k-1) \Rightarrow \lambda = \frac{r(k-1)}{(t-1)}$$

Plans for various numbers of treatments and blocks (and block sizes) are available, in particular, see Cochran and Cox (1957) for a wide variety of designs.

The statistical model for a BIB design and a general linear test for treatment effects (adjusted for blocks) is given below.

Full Model: $Y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij} \quad i = 1, \dots, t \quad j = 1, \dots, b$ (Note: Not all pairs (i, j))	
$H_0 : \tau_1 = \dots = \tau_t = 0 \quad H_A : \text{Not all } \tau_i = 0$	
$SS_{\text{Err(F)}} = \sum_{i=1}^t \sum_{j=1}^b \left(Y_{ij} - \left(\hat{\mu} + \hat{\tau}_i + \hat{\beta}_j \right) \right)^2$	$df_F = N - (1 + (t-1) + (b-1)) = rt - t - b + 1$
Reduced Model: $Y_{ij} = \mu + \beta_j + \varepsilon_{ij} \quad i = 1, \dots, t \quad j = 1, \dots, b$	
$SS_{\text{Err(R)}} = \sum_{i=1}^t \sum_{j=1}^b \left(Y_{ij} - \left(\hat{\mu} + \hat{\beta}_j \right) \right)^2$	$df_R = N - (1 + (b-1)) = rt - b$
Test Statistic: $F_{\text{obs}} = \frac{\left[\frac{SS_{\text{Err(R)}} - SS_{\text{Err(F)}}}{df_R - df_F} \right]}{\left[\frac{SS_{\text{Err(F)}}}{df_F} \right]} = \frac{\left[\frac{SS_{\text{Err(R)}} - SS_{\text{Err(F)}}}{t-1} \right]}{\left[\frac{SS_{\text{Err(F)}}}{t(r-1) - (b-1)} \right]} \stackrel{H_0}{\sim} F_{t-1, t(r-1) - (b-1)}$	

Next, we obtain least squares estimates of the model parameters under the assumption of fixed block effects. The corresponding Analysis of Variance is suitable for either fixed or random blocks. This analysis is referred to as the **intra-block analysis**.

Fixed Blocks: $n_{ij} Y_{ij} = n_{ij} (\mu + \tau_i + \beta_j + \varepsilon_{ij}) \quad i = 1, \dots, t; j = 1, \dots, b$	$n_{ij} = \begin{cases} 1 & \text{if Trt } i \text{ in Blk } j \\ 0 & \text{otherwise} \end{cases}$	$\sum_{i=1}^t \tau_i = \sum_{j=1}^b \beta_j = 0$
Random Blocks: $n_{ij} Y_{ij} = n_{ij} (\mu + \tau_i + \beta_j^* + \varepsilon_{ij}^*)$	$\beta_j^* = \beta_j - \bar{\beta}$	$\varepsilon_{ij}^* = \varepsilon_{ij} + \bar{\beta}$
	$\sum_{i=1}^t \tau_i = 0$	$\beta_j \sim NID(0, \sigma_\beta^2)$
$Q = \sum_{i=1}^t \sum_{j=1}^b n_{ij} \varepsilon_{ij}^2 = \sum_{i=1}^t \sum_{j=1}^b n_{ij} (Y_{ij} - \mu - \tau_i - \beta_j)^2$		
$\frac{\partial Q}{\partial \mu} = -2 \sum_{i=1}^t \sum_{j=1}^b n_{ij} (Y_{ij} - \mu - \tau_i - \beta_j) \stackrel{\text{set}}{=} 0 \Rightarrow \sum_{i=1}^t \sum_{j=1}^b n_{ij} Y_{ij} = N \hat{\mu} + r \sum_{i=1}^t \hat{\tau}_i + k \sum_{j=1}^b \hat{\beta}_j$		
$\Rightarrow Y_{..} = N \hat{\mu} \Rightarrow \hat{\mu} = \bar{Y}_{..}$		
$\frac{\partial Q}{\partial \tau_i} = -2 \sum_{j=1}^b n_{ij} (Y_{ij} - \mu - \tau_i - \beta_j) \stackrel{\text{set}}{=} 0 \Rightarrow \sum_{j=1}^b n_{ij} Y_{ij} = Y_{i.} = r \hat{\mu} + r \hat{\tau}_i + \sum_{j=1}^b n_{ij} \hat{\beta}_j \quad i = 1, \dots, t$		
$\frac{\partial Q}{\partial \beta_j} = -2 \sum_{i=1}^t n_{ij} (Y_{ij} - \mu - \tau_i - \beta_j) \stackrel{\text{set}}{=} 0 \Rightarrow \sum_{i=1}^t n_{ij} Y_{ij} = Y_{.j} = k \hat{\mu} + \sum_{i=1}^t n_{ij} \hat{\tau}_i + k \hat{\beta}_j \quad j = 1, \dots, b$		
$\Rightarrow \hat{\beta}_j = \frac{1}{k} Y_{.j} - \hat{\mu} - \frac{1}{k} \sum_{i=1}^t n_{ij} \hat{\tau}_i$		
$\Rightarrow k Y_{i.} = kr \hat{\mu} + kr \hat{\tau}_i + k \sum_{j=1}^b n_{ij} \left[\frac{1}{k} Y_{.j} - \hat{\mu} - \frac{1}{k} \sum_{i=1}^t n_{ij} \hat{\tau}_i \right]$		

$$kY_{i\bullet} = kr\hat{\mu} + kr\hat{\tau}_i + k \sum_{j=1}^b n_{ij} \left[\frac{1}{k} Y_{\bullet j} - \hat{\mu} - \frac{1}{k} \sum_{i'=1}^t n_{i'j} \hat{\tau}_{i'} \right]$$

Consider the Last Term: $\sum_{j=1}^b n_{ij} \left[Y_{\bullet j} - k\hat{\mu} - \sum_{i'=1}^t n_{i'j} \hat{\tau}_{i'} \right]$

1) $\sum_{j=1}^b n_{ij} Y_{\bullet j} = B_i \equiv$ Sum of Block Totals that Trt i appears in

2) $\sum_{j=1}^b n_{ij} k\hat{\mu} = k\hat{\mu} n_{i\bullet} = k\hat{\mu} r = kr\hat{\mu}$

3) $\sum_{j=1}^b \sum_{i'=1}^t n_{ij} n_{i'j} \hat{\tau}_{i'} = \sum_{j=1}^b n_{ij}^2 \hat{\tau}_i + \sum_{j=1}^b \sum_{\substack{i'=1 \\ i' \neq i}}^t n_{ij} n_{i'j} \hat{\tau}_{i'}$ $n_{ij} n_{i'j} = \begin{cases} 1 & \text{if Trts } i, i' \text{ in Blk } j \\ 0 & \text{otherwise} \end{cases}$

Notes: (a) $\sum_{i=1}^t \hat{\tau}_i = 0 \Rightarrow -\hat{\tau}_i = \sum_{\substack{i'=1 \\ i' \neq i}}^t \hat{\tau}_{i'}$ (b): $\sum_{j=1}^b n_{ij} n_{i'j} = \lambda \quad \forall i \neq i'$

$$\Rightarrow \sum_{j=1}^b \sum_{i'=1}^t n_{ij} n_{i'j} \hat{\tau}_{i'} = \sum_{j=1}^b n_{ij} \hat{\tau}_i + \sum_{\substack{i'=1 \\ i' \neq i}}^t \hat{\tau}_{i'} \sum_{j=1}^b n_{ij} n_{i'j} = r\hat{\tau}_i + \lambda \sum_{\substack{i'=1 \\ i' \neq i}}^t \hat{\tau}_{i'} = (r - \lambda) \hat{\tau}_i$$

$$kY_{i\bullet} = kr\hat{\mu} + kr\hat{\tau}_i + B_i - kr\hat{\mu} - (r - \lambda) \hat{\tau}_i$$

$$\Rightarrow kY_{i\bullet} - B_i = \hat{\tau}_i [kr - (r - \lambda)] = \hat{\tau}_i [r(k - 1) + \lambda] = \hat{\tau}_i [\lambda(t - 1) + \lambda] = \hat{\tau}_i \lambda t$$

$$\Rightarrow \hat{\tau}_i = \frac{kY_{i\bullet} - B_i}{\lambda t} = \frac{kQ_i}{\lambda t} \quad Q_i = Y_{i\bullet} - \frac{1}{k} B_i$$

The estimated treatment effect depends only on the comparisons within blocks that the treatment occurred in. It does not make use of any observations from blocks it did not occur in. This is why it is called an **intra-block analysis**.

The Analysis of Variance for either fixed or random blocks is given below. Note that the variance of an estimated treatment effect will depend on whether blocks are fixed or random.

Full Model: $SS_{\text{Err(F)}} = \sum_{i=1}^t \sum_{j=1}^b n_{ij} \left(Y_{ij} - \hat{\mu} - \hat{\tau}_i - \hat{\beta}_j^{\text{Full}} \right)^2$ $\hat{\beta}_j^{\text{Full}} = \bar{Y}_{\bullet j} - \bar{Y}_{\bullet\bullet} - \frac{1}{k} \sum_{i=1}^t n_{ij} \hat{\tau}_i$

Reduced Model: $SS_{\text{Err(R)}} = \sum_{i=1}^t \sum_{j=1}^b n_{ij} \left(Y_{ij} - \hat{\mu} - \hat{\beta}_j^{\text{Reduced}} \right)^2$ $\hat{\beta}_j^{\text{Reduced}} = \bar{Y}_{\bullet j} - \bar{Y}_{\bullet\bullet}$

Difference: $SS_{\text{Err(R)}} - SS_{\text{Err(F)}} = SS_{\text{Trts(Adj)}} =$

$$= SS_{\text{Trts(Adj)}} = \frac{k \sum_{i=1}^t Q_i^2}{\lambda t} \quad Q_i = Y_{i\bullet} - \frac{1}{k} B_i \quad \frac{1}{k} B_i \equiv \text{Sum of Block Means containing Trt } i$$

Next, we consider the estimated treatment means for the fixed and random block cases, as well as the estimated differences among means, as well as contrasts among means. First, we consider the fixed blocks case.

$$\text{COV}\{Y_{ij}, Y_{i',j'}\} = \begin{cases} \sigma^2 & i=i', j=j' \\ 0 & \text{otherwise} \end{cases}$$

$$\hat{\mu}_i = \hat{\mu} + \hat{\tau}_i = \frac{1}{rt} Y_{..} + \frac{k}{\lambda t} Y_{i.} - \frac{1}{\lambda t} B_i \quad B_i = \sum_{j=1}^b n_{ij} Y_{.j}$$

Note that: $Y_{..}$ has rt observations, $Y_{i.}$ has r observations, B_i has rk observations

$$\Rightarrow V\{Y_{..}\} = rt\sigma^2 \quad V\{Y_{i.}\} = r\sigma^2 \quad V\{B_i\} = rk\sigma^2$$

$$\Rightarrow \text{COV}\{Y_{..}, Y_{i.}\} = r\sigma^2 \quad \text{COV}\{Y_{..}, B_i\} = rk\sigma^2 \quad \text{COV}\{Y_{i.}, B_i\} = r\sigma^2$$

$$\begin{aligned} \Rightarrow V\{\hat{\mu}_i\} &= \left(\frac{1}{rt}\right)^2 rt\sigma^2 + \left(\frac{k}{\lambda t}\right)^2 r\sigma^2 + \left(\frac{1}{\lambda t}\right)^2 rk\sigma^2 + 2\left(\frac{k}{rt\lambda t}\right) r\sigma^2 - 2\left(\frac{1}{rt\lambda t}\right) rk\sigma^2 - 2k\left(\frac{1}{\lambda t}\right)^2 r\sigma^2 = \\ &= \sigma^2 \left[\frac{1}{rt} + \frac{k^2 r + rk - 2rk}{(\lambda t)^2} + \frac{2rk - 2rk}{rt\lambda t} \right] = \sigma^2 \left[\frac{1}{rt} + \frac{k^2 r - rk}{(\lambda t)^2} \right] = \sigma^2 \left[\frac{1}{rt} + \left(\frac{kr}{\lambda t}\right) \frac{k-1}{\lambda t} \right] \end{aligned}$$

$$\text{Recall: } \lambda(t-1) = r(k-1) \Rightarrow \lambda = \frac{r(k-1)}{(t-1)} \Rightarrow \frac{1}{\lambda} = \frac{(t-1)}{r(k-1)}$$

$$\Rightarrow V\{\hat{\mu}_i\} = \sigma^2 \left[\frac{1}{rt} + \left(\frac{kr}{\lambda t}\right) \left(\frac{k-1}{t}\right) \left(\frac{(t-1)}{r(k-1)}\right) \right] = \sigma^2 \left[\frac{1}{rt} + \left(\frac{kr}{\lambda t}\right) \left(\frac{1}{t}\right) \left(\frac{(t-1)}{r}\right) \right] = \sigma^2 \left(\frac{1}{rt}\right) \left[1 + \frac{kr(t-1)}{\lambda t} \right]$$

$$V\{\hat{\mu}_i - \hat{\mu}_{i'}\} = V\left\{ \left(\frac{k}{\lambda t} Y_{i.} - \frac{1}{\lambda t} B_i \right) - \left(\frac{k}{\lambda t} Y_{i'.} - \frac{1}{\lambda t} B_{i'} \right) \right\} = V\left\{ \frac{k}{\lambda t} Y_{i.} - \frac{1}{\lambda t} B_i - \frac{k}{\lambda t} Y_{i'.} + \frac{1}{\lambda t} B_{i'} \right\}$$

Note that: $Y_{i.}$ and B_i share r observations, $Y_{i.}$ and $Y_{i'.}$ share 0, $Y_{i.}$ and $B_{i'}$ share λ , B_i and $B_{i'}$ share λk

$$\Rightarrow V\{\hat{\mu}_i - \hat{\mu}_{i'}\} = \frac{\sigma^2}{(\lambda t)^2} [k^2 r + kr + k^2 r + kr - 2kr - 2k^2(0) + 2k\lambda + 2k\lambda - 2k\lambda - 2kr] =$$

$$\Rightarrow V\{\hat{\mu}_i - \hat{\mu}_{i'}\} = \frac{2\sigma^2 k}{(\lambda t)^2} [kr + \lambda - r] = \frac{2\sigma^2 k}{(\lambda t)^2} [r(k-1) + \lambda] = \frac{2\sigma^2 k}{(\lambda t)^2} [\lambda(t-1) + \lambda] = \frac{2\sigma^2 k}{(\lambda t)^2} \lambda t = \frac{2\sigma^2 k}{\lambda t}$$

$$SE\{\hat{\mu}_i\} = \sqrt{\frac{MS_{\text{Err}}}{rt} \left[1 + \frac{kr(t-1)}{\lambda t} \right]} \quad SE\{\hat{\mu}_i - \hat{\mu}_{i'}\} = \sqrt{\frac{2MS_{\text{Err}}k}{\lambda t}}$$

The method of deriving the variances and standard errors for the random blocks case involves the fact that measurements from the same block are now correlated. This effects the variances and covariances of the overall total, treatment totals, and block totals for individual treatments.

$$\text{COV}\{Y_{ij}, Y_{i',j'}\} = \begin{cases} \sigma_\beta^2 + \sigma^2 & i=i', j=j' \\ \sigma_\beta^2 & i \neq i', j=j' \\ 0 & \text{otherwise} \end{cases}$$

$$\hat{\mu}_i = \hat{\mu} + \hat{\tau}_i = \frac{1}{rt} Y_{..} + \frac{k}{\lambda t} Y_{i.} - \frac{1}{\lambda t} B_i \quad B_i = \sum_{j=1}^b n_{ij} Y_{.j}$$

Note that: $Y_{..}$ has rt observations, $Y_{i.}$ has r observations, B_i has rk observations

$Y_{..}$ and $Y_{i.}$ share r observations directly, and $r(k-1)$ common block terms

$Y_{..}$ and B_i share rk observations directly, and $rk(k-1)$ common block terms

$Y_{i.}$ and B_i share r observations directly, and $r(k-1)$ common block terms

$$\Rightarrow V\{Y_{..}\} = rt(\sigma_\beta^2 + \sigma^2) + rt(k-1)\sigma_\beta^2 = rtk\sigma_\beta^2 + rt\sigma^2$$

$$\Rightarrow V\{Y_{i.}\} = r(\sigma_\beta^2 + \sigma^2) = r\sigma_\beta^2 + r\sigma^2$$

$$\Rightarrow V\{B_i\} = rk(\sigma_\beta^2 + \sigma^2) + rk(k-1)\sigma_\beta^2 = rk^2\sigma_\beta^2 + rk\sigma^2$$

$$\Rightarrow \text{COV}\{Y_{..}, Y_{i.}\} = r(\sigma_\beta^2 + \sigma^2) + r(k-1)\sigma_\beta^2 = rk\sigma_\beta^2 + r\sigma^2$$

$$\Rightarrow \text{COV}\{Y_{..}, B_i\} = rk(\sigma_\beta^2 + \sigma^2) + rk(k-1)\sigma_\beta^2 = rk^2\sigma_\beta^2 + rk\sigma^2$$

$$\Rightarrow \text{COV}\{Y_{i.}, B_i\} = r(\sigma_\beta^2 + \sigma^2) + r(k-1)\sigma_\beta^2 = rk\sigma_\beta^2 + r\sigma^2$$

$$V\{\hat{\mu}_i\} = \left(\frac{1}{tr}\right)^2 [rtk\sigma_\beta^2 + rt\sigma^2] + \left(\frac{k}{\lambda t}\right)^2 [r\sigma_\beta^2 + r\sigma^2] + \left(\frac{1}{\lambda t}\right)^2 [rk^2\sigma_\beta^2 + rk\sigma^2] +$$

$$+ 2\left(\frac{k}{tr\lambda t}\right)[rk\sigma_\beta^2 + r\sigma^2] - 2\left(\frac{1}{tr\lambda t}\right)[rk^2\sigma_\beta^2 + rk\sigma^2] - 2\frac{k}{(\lambda t)^2}[rk\sigma_\beta^2 + r\sigma^2] =$$

$$= \left(\frac{1}{tr}\right)[k\sigma_\beta^2 + \sigma^2] + \left(\frac{1}{\lambda t}\right)^2 [\sigma_\beta^2(rk^2 + rk^2 - 2rk^2) + \sigma^2(rk^2 + rk - 2rk)] +$$

$$+ \left(\frac{1}{tr\lambda t}\right)[\sigma_\beta^2(2rk^2 - 2rk^2) + \sigma^2(2rk - 2rk)]$$

$$= \left(\frac{1}{tr}\right)[k\sigma_\beta^2 + \sigma^2] + \left(\frac{1}{\lambda t}\right)^2 [\sigma^2(rk^2 - rk)] = \left(\frac{1}{tr}\right)[k\sigma_\beta^2 + \sigma^2] + \left(\frac{1}{\lambda t}\right)^2 [\sigma^2 rk(k-1)] =$$

$$= \left(\frac{1}{tr}\right)[k\sigma_\beta^2 + \sigma^2] + \sigma^2 \left[\left(\frac{rk}{\lambda t}\right) \frac{k-1}{\lambda t} \right] = \left(\frac{1}{tr}\right)[k\sigma_\beta^2 + \sigma^2] + \sigma^2 \left[\left(\frac{rk}{\lambda t}\right) \left(\frac{k-1}{t}\right) \left(\frac{t-1}{r(k-1)}\right) \right] =$$

$$= \sigma_\beta^2 \left(\frac{k}{tr}\right) + \sigma^2 \left(\frac{1}{tr}\right) \left[1 + \frac{rk(t-1)}{\lambda t} \right] = \left(\frac{1}{tr}\right) \left[k\sigma_\beta^2 + \sigma^2 \left(1 + \frac{rk(t-1)}{\lambda t} \right) \right]$$

$$V\{\hat{\mu}_i - \hat{\mu}_{i'}\} = V\left\{ \left(\frac{k}{\lambda t} Y_{i.} - \frac{1}{\lambda t} B_i \right) - \left(\frac{k}{\lambda t} Y_{i'.} - \frac{1}{\lambda t} B_{i'} \right) \right\} = V\left\{ \frac{k}{\lambda t} Y_{i.} - \frac{1}{\lambda t} B_i - \frac{k}{\lambda t} Y_{i'.} + \frac{1}{\lambda t} B_{i'} \right\}$$

$Y_{i.}$ and B_i share r observations directly, and $r(k-1)$ common block terms

$Y_{i.}$ and $Y_{i'.}$ share 0 observations directly, and λ common block terms

$Y_{i.}$ and $B_{i'}$ share λ observations directly, and $\lambda(k-1)$ common block terms

B_i and $B_{i'}$ share λk observations directly, and $\lambda k(k-1)$ common block terms

$$\begin{aligned}
\Rightarrow V\left\{\hat{\mu}_i - \hat{\mu}_i\right\} &= 2\left(\frac{k}{\lambda t}\right)^2 [r\sigma_\beta^2 + r\sigma^2] + 2\left(\frac{1}{\lambda t}\right)^2 [rk^2\sigma_\beta^2 + rk\sigma^2] - 2\left(\frac{k}{(\lambda t)^2}\right) [rk\sigma_\beta^2 + r\sigma^2] \\
&- 2\left(\frac{k}{\lambda t}\right)^2 [\lambda\sigma_\beta^2] + 2\left(\frac{k}{(\lambda t)^2}\right) [\lambda k\sigma_\beta^2 + \lambda\sigma^2] + 2\left(\frac{k}{(\lambda t)^2}\right) [\lambda k\sigma_\beta^2 + \lambda\sigma^2] - 2\left(\frac{1}{\lambda t}\right)^2 [\lambda k^2\sigma_\beta^2 + \lambda k\sigma^2] \\
&- 2\left(\frac{k}{(\lambda t)^2}\right) [rk\sigma_\beta^2 + r\sigma^2] \\
&= \frac{2}{(\lambda t)^2} \left[\sigma_\beta^2 (k^2 r + k^2 r - k^2 r - k^2 \lambda + k^2 \lambda + k^2 \lambda - k^2 \lambda - k^2 r) + \sigma^2 (k^2 r + kr - kr + k\lambda + k\lambda - k\lambda - kr) \right] \\
&= \frac{2}{(\lambda t)^2} \left[\sigma_\beta^2 (0) + \sigma^2 (k^2 r + k\lambda - kr) \right] = \frac{2k\sigma^2}{(\lambda t)^2} [kr + \lambda - r] = \frac{2k\sigma^2}{(\lambda t)^2} [r(k-1) + \lambda] = \frac{2k\sigma^2}{(\lambda t)^2} [\lambda(t-1) + \lambda] = \\
&= \frac{2k\sigma^2}{(\lambda t)^2} [\lambda t] = \frac{2k\sigma^2}{\lambda t}
\end{aligned}$$

For any Contrast: $\sum_{i=1}^t w_i = 0 \quad \hat{\zeta} = \sum_{i=1}^t w_i \hat{\mu}_i \Rightarrow V\left\{\hat{\zeta}\right\} = \frac{k\sigma^2}{\lambda t} \sum_{i=1}^t w_i^2$

$$SE\left\{\hat{\mu}_i\right\} = \sqrt{\left[\frac{1}{tr} \left[k \sigma_\beta^2 + \sigma^2 \left(1 + \frac{rk(t-1)}{\lambda t} \right) \right] \right]} \quad \hat{\sigma}^2 = MS_{Err} \quad \hat{\sigma}_\beta^2 = \frac{(b-1)(MS_{Blks(Adj)} - MS_{Err})}{tr - t}$$

$$SE\left\{\hat{\mu}_i - \hat{\mu}_i\right\} = \sqrt{\frac{2kMS_{Err}}{\lambda t}}$$

Example: Tomato Yields with 21 Varieties in 21 Blocks

A tomato trial was conducted among $t = 21$ varieties of tomatoes in $b = 21$ blocks of size $k = 5$ plots per block (Yates (1940)). Each variety was replicated $r = 5$ times, and each pair of varieties occurred together in $\lambda = 1$ block. The data in spreadsheet form, as well as intermediate computations are given below. The overall mean is 50.28 and the total corrected sum of squares is 23691.5. For this analysis we will treat blocks as random.

Trt/BLK	r/k	Y _{..j}	Y _{.i.}	B _i	Q _i	tau _{i-hat}	mu _{i-hat}
1	5	173.06	205.00	1123.55	-19.71	-4.6929	45.5903
2	5	211.50	306.50	1316.18	43.26	10.3010	60.5841
3	5	266.75	200.00	1142.75	-28.55	-6.7976	43.4855
4	5	164.50	242.75	1244.75	-6.20	-1.4762	48.8070
5	5	246.80	213.50	1296.50	-45.80	-10.9048	39.3784
6	5	305.50	279.75	1325.67	14.62	3.4800	53.7631
7	5	242.00	252.00	1179.86	16.03	3.8162	54.0993
8	5	211.00	305.75	1271.30	51.49	12.2595	62.5427
9	5	226.75	317.80	1366.55	44.49	10.5929	60.8760
10	5	232.50	335.62	1452.37	45.15	10.7490	61.0322
11	5	227.50	125.25	1048.31	-84.41	-20.0981	30.1850
12	5	211.00	241.50	1211.50	-0.80	-0.1905	50.0927
13	5	204.50	185.25	1290.00	-72.75	-17.3214	32.9617
14	5	222.25	353.50	1484.37	56.63	13.4824	63.7655
15	5	277.75	217.31	1188.31	-20.35	-4.8457	45.4374
16	5	258.00	287.75	1297.75	28.20	6.7143	56.9974
17	5	291.00	198.25	1095.75	-20.90	-4.9762	45.3070
18	5	419.62	315.75	1379.62	39.83	9.4824	59.7655
19	5	270.50	185.75	1239.31	-62.11	-14.7886	35.4946
20	5	312.50	224.50	1151.00	-5.70	-1.3571	48.9260
21	5	304.75	286.25	1293.25	27.60	6.5714	56.8546

$$y_{\bullet j} = \sum_{i=1}^{21} n_{ij} y_{ij} \quad Y_{i\bullet} = \sum_{j=1}^{21} n_{ij} y_{ij} \quad B_i = \sum_{j=1}^{21} n_{ij} y_{\bullet j}$$

$$Q_i = Y_{i\bullet} - \left(\frac{1}{k}\right) B_i = y_{i\bullet} - \left(\frac{1}{5}\right) B_i$$

$$\hat{\tau}_i = \frac{kQ_i}{\lambda t} = \frac{5Q_i}{1(21)}$$

$$SS_{Blks} = k \sum_{j=1}^b (\bar{y}_{\bullet j} - \bar{y}_{\bullet\bullet})^2 = 12790.13$$

$$SS_{Trts(Adj)} = \frac{k \sum_{i=1}^t Q_i^2}{\lambda t} = \frac{5 \sum_{i=1}^{21} Q_i^2}{1(21)} = 8538.17$$

$$SS_{Err} = 2363.20$$

Block	Trt	Yield	Block	Trt	Yield	Block	Trt	Yield
1	2	51.50	8	1	40.50	15	4	47.50
1	7	36.75	8	2	58.50	15	9	65.00
1	11	21.00	8	3	35.25	15	12	51.00
1	15	41.56	8	4	45.50	15	15	49.75
1	19	22.25	8	5	31.25	15	18	64.50
2	1	50.75	9	1	40.50	16	3	38.75
2	10	52.50	9	18	49.00	16	7	55.00
2	11	32.25	9	19	38.50	16	12	51.25
2	12	44.00	9	20	47.75	16	14	57.50
2	13	32.00	9	21	51.00	16	21	55.50
3	5	51.75	10	4	51.25	17	5	43.00
3	9	58.50	10	6	47.25	17	7	67.00
3	11	29.75	10	11	24.75	17	13	46.00
3	14	70.75	10	16	58.75	17	16	64.50
3	20	56.00	10	21	50.50	17	18	70.50
4	3	37.25	11	1	39.50	18	2	68.25
4	8	37.25	11	14	55.25	18	6	74.00
4	11	17.50	11	15	37.75	18	10	98.12
4	17	26.75	11	16	48.25	18	14	93.25
4	18	45.75	11	17	46.75	18	18	86.00
5	1	33.75	12	4	36.50	19	2	67.00
5	6	45.75	12	7	44.00	19	9	66.00
5	7	49.25	12	10	51.75	19	13	31.75
5	8	55.25	12	17	35.25	19	17	49.00
5	9	62.80	12	20	43.50	19	21	56.75
6	5	46.50	13	3	42.50	20	4	62.00
6	8	78.00	13	6	50.25	20	8	82.25
6	10	59.00	13	13	30.75	20	13	44.75
6	15	49.50	13	15	38.75	20	14	76.75
6	21	72.50	13	20	42.25	20	19	46.75
7	2	61.25	14	5	41.00	21	3	46.25
7	8	53.00	14	6	62.50	21	9	65.50
7	12	45.00	14	12	50.25	21	10	74.25
7	16	47.75	14	17	40.50	21	16	68.50
7	20	35.00	14	19	28.00	21	19	50.25

To test for treatment (variety) effects, controlling for blocks, we use the F-test, based on the treatment (adjusted for blocks) sum of squares, and the error sum of squares. Below we give the Analysis of Variance and the F-test for treatment effects. The Error degrees of freedom for the full model are given below.

$$df_{Full} = rt - t - b + 1 = 5(21) - 21 - 21 + 1 = 64$$

Source	df	SS	MS	F	F(0.95)	P-value
Blocks	20	12790.13	639.51			
Trts Blocks	20	8538.17	426.91	11.562	1.737	0.0000
Trts	20	14222.31	711.12			
Blocks Trts	20	7105.99	355.30			
Error	64	2363.20	36.92			
Total	104	23691.50				

The estimated variance components, as well as the estimated standard errors for treatment means and their differences, are computed below.

$$\hat{\sigma}^2 = MS_{\text{Err}} = 36.92 \quad \hat{\sigma}_\beta^2 = \frac{(b-1)(MS_{\text{Blks(Adj)}} - MS_{\text{Err}})}{tr - t} = \frac{(21-1)(355.30 - 36.92)}{21(5) - 21} = \frac{6367.6}{84} = 75.80$$

$$SE\left\{\hat{\mu}_i\right\} = \sqrt{\left[\frac{1}{21(5)}\left[5(75.80) + 36.92\left(1 + \frac{5(5)(21-1)}{1(21)}\right)\right]\right]} = \sqrt{\frac{1294.97}{105}} = \sqrt{12.33} = 3.51$$

$$SE\left\{\hat{\mu}_i - \hat{\mu}_j\right\} = \sqrt{\frac{2(5)36.92}{1(21)}} = \sqrt{17.58} = 4.19$$

The R Program and output are given below. Note that the F-test for variety effects gives a slightly higher value (based on EGLS) and the ANOVA based F-test. We will see an adjustment that can be made in terms of the estimated treatment effects below that makes use of the fact that blocks are random.

R Program

```
tomato <- read.csv("http://www.stat.ufl.edu/~winner/data/yates_tomato_bibd.csv",
                  header=T)
attach(tomato); names(tomato)

Block <- factor(Block)
Trt <- factor(Trt)

tomato.mod1 <- aov(Yield ~ Block + Trt)
anova(tomato.mod1)

tomato.mod2 <- aov(Yield ~ Trt + Block)
anova(tomato.mod2)

library(lmerTest)
tomato.mod3 <- lmer(Yield ~ Trt + (1|Block))
summary(tomato.mod3)
anova(tomato.mod3)
lsmeans(tomato.mod3)
diff.lsmeans(tomato.mod3)
rand(tomato.mod3)
```

R Output

```
> tomato.mod1 <- aov(Yield ~ Block + Trt)
> anova(tomato.mod1)
Analysis of Variance Table

Response: Yield
      Df Sum Sq Mean Sq F value    Pr(>F)
Block  20 12790.1   639.51  17.319 < 2.2e-16 ***
Trt    20   8538.2   426.91  11.562 2.376e-14 ***
Residuals 64  2363.2    36.92
---
> tomato.mod2 <- aov(Yield ~ Trt + Block)
> anova(tomato.mod2)
Analysis of Variance Table

Response: Yield
      Df Sum Sq Mean Sq F value    Pr(>F)
Trt    20 14222.3   711.12  19.2584 < 2.2e-16 ***
Block  20   7106.0   355.30   9.6222 1.489e-12 ***
Residuals 64  2363.2    36.92
```

Continued (Partial) Output:

```

> tomato.mod3 <- lmer(Yield ~ Trt + (1|Block))
> summary(tomato.mod3)
Linear mixed model fit by REML t-tests use Satterthwaite approximations to
degrees of freedom [merModLmerTest]
Formula: Yield ~ Trt + (1 | Block)

REML criterion at convergence: 620.6

Scaled residuals:
    Min       1Q   Median       3Q      Max
-2.31074 -0.57607 -0.02352  0.51519  2.43916

Random effects:
 Groups Name          Variance Std.Dev.
Block  (Intercept)  75.80    8.707
Residual                    36.92    6.077
Number of obs: 105, groups: Block, 21

Fixed effects:
            Estimate Std. Error    df t value Pr(>|t|)
(Intercept)  45.1132     3.4922  79.3000  12.918 < 2e-16 ***
Trt2         15.5453     4.1582  66.1600   3.738 0.000389 ***
Trt3         -1.9899     4.1582  66.1600  -0.479 0.633833
.
Trt20         3.3944     4.1582  66.1600   0.816 0.417260
Trt21        11.7824     4.1582  66.1600   2.834 0.006097 **

> anova(tomato.mod3)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value    Pr(>F)
Trt  8935.1  446.76    20 66.158  12.099 4.441e-15 ***

> lsmeans(tomato.mod3)
Least Squares Means table:
      Trt Estimate Standard Error    DF t-value Lower CI Upper CI p-value
Trt 1  1.0    45.11      3.49 79.3   12.92   38.2   52.1 <2e-16 ***
Trt 2 12.0    60.66      3.49 79.3   17.37   53.7   67.6 <2e-16 ***
.
Trt 20 13.0   48.51      3.49 79.3   13.89   41.6   55.5 <2e-16 ***
Trt 21 14.0   56.90      3.49 79.3   16.29   49.9   63.8 <2e-16 ***

> diff1smeans(tomato.mod3)
Differences of LSMEANS:
      Estimate Standard Error    DF t-value Lower CI Upper CI p-value
Trt 1 - 2    -15.5      4.158  66.2   -3.74  -23.847  -7.2434  4e-04 ***
Trt 1 - 3     2.0      4.158  66.2    0.48  -6.312  10.2918  0.634
.
Trt 19 - 21  -21.2      4.158  66.2   -5.11  -29.531 -12.9272 <2e-16 ***
Trt 20 - 21   -8.4      4.158  66.2   -2.02  -16.690  -0.0863  0.048 *

> rand(tomato.mod3)
Analysis of Random effects Table:
      Chi.sq Chi.DF p.value
Block  48.5     1 3e-12 ***

```

When blocks are random, a second analysis that can be conducted is an **inter-block analysis**. This provides a second set of estimates of the $\{\tau_i\}$ that can be combined with the intra-block estimates. We can then take a weighted average of the two estimates, with weights being proportional to the reciprocal of their variances. We describe the method below. The sketch of the derivation of the Expected Mean Squares makes use of some of the results from the intra-block analysis given above.

$$Y_{\cdot j} = \sum_{i=1}^t n_{ij} Y_{ij} = k\mu + \sum_{i=1}^t n_{ij} \tau_i + \left\{ k\beta_j + \sum_{i=1}^t n_{ij} \varepsilon_{ij} \right\} \quad n_{ij} = \begin{cases} 1 & \text{if Trt } i \text{ occurs in Blk } j \\ 0 & \text{otherwise} \end{cases}$$

$$= k\mu + \sum_{i=1}^t n_{ij} \tau_i + \eta_j \quad \eta_j \sim N(0, k^2 \sigma_\beta^2 + k\sigma^2) \quad \sum_{i=1}^t \tau_i = 0$$

This leads to OLS estimators:

$$Q = \sum_{j=1}^b \eta_j^2 = \sum_{j=1}^b \left(Y_{\cdot j} - k\mu - \sum_{i=1}^t n_{ij} \tau_i \right)^2 = \sum_{j=1}^b Q_j$$

$$Q_j = \left(Y_{\cdot j} - k\mu - \sum_{i=1}^t n_{ij} \tau_i \right)^2 = Y_{\cdot j}^2 + k^2 \mu^2 + \sum_{i=1}^t n_{ij}^2 \tau_i^2 + 2 \sum_{i=1}^{t-1} \sum_{i'=i+1}^t n_{ij} n_{i'j} \tau_i \tau_{i'} - 2Y_{\cdot j} k\mu - 2Y_{\cdot j} \sum_{i=1}^t n_{ij} \tau_i + 2k\mu \sum_{i=1}^t n_{ij} \tau_i$$

$$\frac{\partial Q_j}{\partial \mu} = 2k^2 \mu - 2Y_{\cdot j} k + 2k \sum_{i=1}^t n_{ij} \tau_i \Rightarrow \sum_{j=1}^b \frac{\partial Q_j}{\partial \mu} = 2k^2 \mu b - 2k \sum_{j=1}^b Y_{\cdot j} + 2k \sum_{j=1}^b \sum_{i=1}^t n_{ij} \tau_i \stackrel{\text{set}}{=} 0$$

$$\Rightarrow kb \tilde{\mu} - Y_{\cdot\cdot} + 0 = 0 \Rightarrow \tilde{\mu} = \frac{Y_{\cdot\cdot}}{kb} = \bar{Y}_{\cdot\cdot}$$

If Treatment l appears in Block $j \Rightarrow n_{lj} = 1$:

$$\frac{\partial Q_j}{\partial \tau_l} = 2\tau_l + 2 \sum_{i \neq l} n_{ij} \tau_i - 2Y_{\cdot j} + 2k\mu \Rightarrow \sum_{j=1}^b \frac{\partial Q_j}{\partial \tau_l} = 2r\tau_l + 2 \sum_{j=1}^b \sum_{i \neq l} n_{ij} n_{lj} \tau_i - 2 \sum_{j=1}^b n_{lj} Y_{\cdot j} + 2k\mu r \stackrel{\text{set}}{=} 0$$

$$\Rightarrow r\tau_l + \lambda \sum_{i \neq l} \tau_i - \sum_{j=1}^b n_{lj} Y_{\cdot j} + k\tilde{\mu} r = 0 \Rightarrow (r - \lambda)\tau_l + \lambda \sum_{i=1}^t \tau_i + B_l r + k\tilde{\mu} r = (r - \lambda)\tau_l + B_l r + k\tilde{\mu} r$$

$$\Rightarrow \tilde{\tau}_l = \frac{B_l - rk\tilde{\mu}}{r - \lambda} \quad B_l = \sum_{j=1}^b n_{lj} Y_{\cdot j}$$

$$V\{\tilde{\tau}_l\} = \left(\frac{1}{r - \lambda} \right)^2 \left[V\{B_l\} + r^2 k^2 V\{\tilde{\mu}\} - 2rk \text{COV}\{B_l, \tilde{\mu}\} \right] =$$

$$= \left(\frac{1}{r - \lambda} \right)^2 \left[rk^2 \sigma_\beta^2 + rk\sigma^2 + r^2 k^2 \left(\frac{k}{tr} \sigma_\beta^2 + \frac{1}{tr} \sigma^2 \right) - 2kr \left(\frac{1}{tr} \right) (rk^2 \sigma_\beta^2 + rk\sigma^2) \right] =$$

$$= \left(\frac{1}{r - \lambda} \right)^2 \left[\sigma_\beta^2 \left(rk^2 \left(1 - \frac{k}{t} \right) \right) + \sigma^2 \left(rk \left(1 - \frac{k}{t} \right) \right) \right]$$

$$\lambda(t-1) = r(k-1) \Rightarrow \lambda = r \left(\frac{k-1}{t-1} \right) \Rightarrow r - \lambda = r \left[1 - \frac{k-1}{t-1} \right] = r \left[\frac{(t-1) - (k-1)}{t-1} \right] = r \left(\frac{t-k}{t-1} \right)$$

$$\Rightarrow V\{\tilde{\tau}_l\} = \left(\frac{1}{r^2} \right) \left(\frac{t-1}{t-k} \right)^2 \left[\sigma_\beta^2 \left(rk^2 \left(\frac{t-k}{t} \right) \right) + \sigma^2 \left(rk \left(\frac{t-k}{t} \right) \right) \right] = \left(\frac{1}{r} \right) \left(\frac{t-1}{t-k} \right) \left[\sigma_\beta^2 \left(k^2 \left(\frac{t-1}{t} \right) \right) + \sigma^2 \left(k \left(\frac{t-1}{t} \right) \right) \right] =$$

$$= \frac{\sigma_\beta^2 \left(k^2 \left(\frac{t-1}{t} \right) \right) + \sigma^2 \left(k \left(\frac{t-1}{t} \right) \right)}{r - \lambda}$$

$$V\{\tilde{\tau}_l - \tilde{\tau}_{l'}\} = V\left\{ \frac{B_l - B_{l'}}{r - \lambda} \right\} = \left(\frac{1}{r - \lambda} \right)^2 \left[V\{B_l\} + V\{B_{l'}\} - 2\text{COV}\{B_l, B_{l'}\} \right] =$$

$$= \left(\frac{1}{r - \lambda} \right)^2 \left[2r(k^2 \sigma_\beta^2 + k\sigma^2) - 2\lambda(k^2 \sigma_\beta^2 + k\sigma^2) \right] = \left(\frac{1}{r - \lambda} \right)^2 2(r - \lambda)(k^2 \sigma_\beta^2 + k\sigma^2) = \frac{2(k^2 \sigma_\beta^2 + k\sigma^2)}{r - \lambda}$$

$$SS_{\text{Blks(Adj)}} = \frac{k \sum_{i=1}^t Q_i^2}{\lambda t} + \frac{\sum_{j=1}^b Y_{.j}^2}{k} - \frac{\sum_{i=1}^t Y_{i.}^2}{r}$$

$$Q_i = Y_{i.} - \frac{1}{k} \sum_{j=1}^b n_{ij} Y_{.j} = Y_{i.} - \frac{1}{k} B_i \Rightarrow Q_i^2 = Y_{i.}^2 + \frac{1}{k^2} B_i^2 - \frac{2}{k} Y_{i.} B_i$$

$$E\{Y_{i.}\} = r(\mu + \tau_i) \quad V\{Y_{i.}\} = r(\sigma_\beta^2 + \sigma^2) \Rightarrow E\{Y_{i.}^2\} = r^2 \mu^2 + r^2 \tau_i^2 + 2r^2 \mu \tau_i + r\sigma_\beta^2 + r\sigma^2$$

$$E\{B_i\} = r(\mu + \tau_i) + \lambda \sum_{i \neq i} (\mu + \tau_{i'}) = \mu(r + \lambda(t-1)) + r\tau_i + \lambda \sum_{i \neq i} \tau_{i'} = \mu(r + r(k-1)) + (r-\lambda)\tau_i = \mu kr + (r-\lambda)\tau_i$$

$$V\{B_i\} = rk^2 \sigma_\beta^2 + rk\sigma^2 \Rightarrow E\{B_i^2\} = \mu^2 k^2 r^2 + (r-\lambda)^2 \tau_i^2 + 2\mu kr(r-\lambda)\tau_i + rk^2 \sigma_\beta^2 + rk\sigma^2$$

$$\text{COV}\{Y_{i.}, B_i\} = rk\sigma_\beta^2 + r\sigma^2 \Rightarrow E\{Y_{i.}, B_i\} = \text{COV}\{Y_{i.}, B_i\} + E\{Y_{i.}\}E\{B_i\} =$$

$$= rk\sigma_\beta^2 + r\sigma^2 + [r(\mu + \tau_i)][\mu kr + (r-\lambda)\tau_i] = \mu^2 kr^2 + r(r-\lambda)\tau_i^2 + \mu r(kr + (r-\lambda))\tau_i + rk\sigma_\beta^2 + r\sigma^2$$

$$E\{Q_i^2\} = \mu^2 \left[r^2 + \frac{k^2 r^2}{k^2} - \frac{2kr^2}{k} \right] + \tau_i^2 \left[r^2 + \frac{(r-\lambda)^2}{k^2} - \frac{2r(r-\lambda)}{k} \right] + \tau_i \left[2r^2 \mu + \frac{2\mu kr(r-\lambda)}{k^2} - \frac{2\mu r(kr + (r-\lambda))}{k} \right] +$$

$$+ \sigma_\beta^2 \left[r + \frac{rk^2}{k^2} - \frac{2rk}{k} \right] + \sigma^2 \left[r + \frac{rk}{k^2} - \frac{2r}{k} \right] = \tau_i^2 \left(\frac{rk - (r-\lambda)}{k} \right)^2 + C\tau_i + \sigma^2 r \left(\frac{k-1}{k} \right) =$$

$$= \tau_i^2 \left(\frac{r(k-1) + \lambda}{k} \right)^2 + C\tau_i + \sigma^2 r \left(\frac{k-1}{k} \right) = \tau_i^2 \left(\frac{\lambda(t-1) + \lambda}{k} \right)^2 + C\tau_i + \sigma^2 \left(\frac{\lambda(t-1)}{k} \right) = \tau_i^2 \left(\frac{\lambda t}{k} \right)^2 + C\tau_i + \sigma^2 \left(\frac{\lambda(t-1)}{k} \right)$$

$$E\left\{ \frac{k \sum_{i=1}^t Q_i^2}{\lambda t} \right\} = \left(\frac{k}{\lambda t} \right) \sum_{i=1}^t \tau_i^2 \left(\frac{\lambda t}{k} \right)^2 + C \sum_{i=1}^t \tau_i + \left(\frac{k}{\lambda t} \right) t \sigma^2 \left(\frac{\lambda(t-1)}{k} \right) = \left(\frac{\lambda t}{k} \right) \sum_{i=1}^t \tau_i^2 + \sigma^2 (t-1)$$

$$E\{Y_{.j}\} = k\mu + \sum_{i=1}^t n_{ij} \tau_i \quad V\{Y_{.j}\} = \sigma_\beta^2 k^2 + \sigma^2 k \quad [E\{Y_{.j}\}]^2 = \mu^2 k^2 + \left[\sum_{i=1}^t n_{ij}^2 \tau_i^2 + \sum_{i=1}^t \sum_{i \neq i'} n_{ij} n_{i'j} \tau_i \tau_{i'} \right] + 2k\mu \sum_{i=1}^t n_{ij} \tau_i$$

$$E\{Y_{.j}^2\} = \mu^2 k^2 + \sum_{i=1}^t n_{ij}^2 \tau_i^2 + \sum_{i=1}^t \sum_{i \neq i'} n_{ij} n_{i'j} \tau_i \tau_{i'} + 2k\mu \sum_{i=1}^t n_{ij} \tau_i + \sigma_\beta^2 k^2 + \sigma^2 k$$

$$E\left\{ \sum_{j=1}^b Y_{.j}^2 \right\} = \mu^2 k^2 b + \sum_{i=1}^t \tau_i^2 \sum_{j=1}^b n_{ij}^2 + \sum_{i=1}^t \sum_{i \neq i'} \tau_i \tau_{i'} \sum_{j=1}^b n_{ij} n_{i'j} + 2k\mu \sum_{i=1}^t \tau_i \sum_{j=1}^b n_{ij} + \sigma_\beta^2 k^2 b + \sigma^2 kb =$$

$$= \mu^2 k^2 b + r \sum_{i=1}^t \tau_i^2 + \lambda \sum_{i=1}^t \tau_i \sum_{i \neq i'} \tau_{i'} + 2k\mu r \sum_{i=1}^t \tau_i + \sigma_\beta^2 k^2 b + \sigma^2 kb = \mu^2 k^2 b + r \sum_{i=1}^t \tau_i^2 + \lambda \sum_{i=1}^t \tau_i (-\tau_i) + 0 + \sigma_\beta^2 k^2 b + \sigma^2 kb$$

$$E\left\{ \frac{\sum_{j=1}^b Y_{.j}^2}{k} \right\} = \mu^2 kb + \left(\frac{r-\lambda}{k} \right) \sum_{i=1}^t \tau_i^2 + \sigma_\beta^2 kb + \sigma^2 b$$

$$E\left\{ \frac{\sum_{i=1}^t Y_{i.}^2}{r} \right\} = \mu^2 rt + r \sum_{i=1}^t \tau_i^2 + \sigma_\beta^2 t + \sigma^2 t$$

$$E\{SS_{\text{Blks(Adj)}}\} = \mu^2 [0 + N - N] + \sum_{i=1}^t \tau_i^2 \left[\left(\frac{\lambda t}{k} \right) + \left(\frac{r-\lambda}{k} \right) - \frac{rk}{k} \right] + \sigma_\beta^2 [0 + N - t] + \sigma^2 [t - 1 + b - t] =$$

$$= \sum_{i=1}^t \tau_i^2 \left[\frac{\lambda(t-1) - r(k-1)}{k} \right] + \sigma_\beta^2 (N - t) + \sigma^2 (n - 1) = 0 + \sigma_\beta^2 (N - t) + \sigma^2 (b - 1) \Rightarrow E\{MS_{\text{Blks(Adj)}}\} = \sigma_\beta^2 \left(\frac{N-t}{b-1} \right) + \sigma^2$$

$$\text{For any Contrast: } \sum_{i=1}^t w_i = 0: \quad \tilde{\zeta} = \sum_{i=1}^t w_i \tilde{\tau}_i \quad V\left\{\tilde{\zeta}\right\} = \frac{k^2 \sigma_\beta^2 + k \sigma^2}{r - \lambda} \sum_{i=1}^t w_i^2$$

$$E\{MS_{\text{Err}}\} = \sigma^2 \quad E\{MS_{\text{Blks(Adj)}}\} = \sigma^2 + \left(\frac{N-t}{b-1}\right) \sigma_\beta^2$$

$$\Rightarrow \hat{\sigma}^2 = MS_{\text{Err}} \quad \hat{\sigma}_\beta^2 = (MS_{\text{Blks(Adj)}} - MS_{\text{Err}}) \left(\frac{b-1}{N-t}\right) \quad SE\left\{\tilde{\zeta}\right\} = \sqrt{\frac{k^2 \hat{\sigma}_\beta^2 + k \hat{\sigma}^2}{r - \lambda} \sum_{i=1}^t w_i^2}$$

The intra-block and inter-block estimators of any contrast can be combined, with weights that sum to 1, and that are inversely proportional to their respective variances.

$$\bar{\zeta} = \frac{\left[\frac{1}{V\left\{\hat{\zeta}\right\}} \hat{\zeta} + \frac{1}{V\left\{\tilde{\zeta}\right\}} \tilde{\zeta} \right]}{\left[\frac{1}{V\left\{\hat{\zeta}\right\}} + \frac{1}{V\left\{\tilde{\zeta}\right\}} \right]} \quad V\left\{\bar{\zeta}\right\} = \frac{1}{\left[\frac{1}{V\left\{\hat{\zeta}\right\}} + \frac{1}{V\left\{\tilde{\zeta}\right\}} \right]} = \frac{V\left\{\hat{\zeta}\right\} V\left\{\tilde{\zeta}\right\}}{V\left\{\hat{\zeta}\right\} + V\left\{\tilde{\zeta}\right\}}$$

where:

$$\hat{\zeta} = \sum_{i=1}^t w_i \hat{\tau}_i \quad V\left\{\hat{\zeta}\right\} = \frac{\sigma^2 k}{\lambda t} \sum_{i=1}^t w_i^2 \quad \hat{\tau}_i = \frac{k}{\lambda t} Y_{i\cdot} - \frac{1}{\lambda t} B_i$$

$$\tilde{\zeta} = \sum_{i=1}^t w_i \tilde{\tau}_i \quad V\left\{\tilde{\zeta}\right\} = \frac{k^2 \sigma_\beta^2 + k \sigma^2}{r - \lambda} \sum_{i=1}^t w_i^2 \quad \tilde{\tau}_i = \frac{B_i - r k \bar{y}_{..}}{r - \lambda}$$

$$\hat{\sigma}_\beta^2 = (MS_{\text{BLKS(Adj)}} - MS_{\text{Err}}) \left(\frac{b-1}{N-t}\right) \quad \hat{\sigma}^2 = MS_{\text{Err}}$$

Example: Tomato Yields with 21 Varieties in 21 Blocks

A tomato trial was conducted among $t = 21$ varieties of tomatoes in $b = 21$ blocks of size $k = 5$ plots per block. Each variety was replicated $r = 5$ times, and each pair of varieties occurred together in $\lambda = 1$ block. The data in spreadsheet form, as well as intermediate computations are given below. The overall mean is 50.28 and the total corrected sum of squares is 23691.5. For this analysis we will treat blocks as random. Here we obtain the inter-block estimates for each variety effect.

i/j	Y_j	T_j	W_j	B_i	tau_i-tilde
1	173.06	1086.81	-44.30	1123.55	-33.3821
2	211.50	1092.62	-7.02	1316.18	14.7754
3	266.75	1234.55	19.84	1142.75	-28.5821
4	164.50	1145.00	-64.50	1244.75	-3.0821
5	246.80	1360.30	-25.26	1296.50	9.8554
6	305.50	1358.43	33.81	1325.67	17.1479
7	242.00	1366.00	-31.20	1179.86	-19.3046
8	211.00	1167.75	-22.55	1271.30	3.5554
9	226.75	1217.25	-16.70	1366.55	27.3679
10	232.50	1221.75	-11.85	1452.37	48.8229
11	227.50	1261.81	-24.86	1048.31	-52.1921
12	211.00	1253.12	-39.62	1211.50	-11.3946
13	204.50	1106.81	-16.86	1290.00	8.2304
14	222.25	1118.75	-1.50	1484.37	56.8229
15	277.75	1335.11	10.73	1188.31	-17.1921
16	258.00	1333.25	-8.65	1297.75	10.1679
17	291.00	1254.25	40.15	1095.75	-40.3321
18	419.62	1591.12	101.40	1379.62	30.6354
19	270.50	1294.05	11.69	1239.31	-4.4421
20	312.50	1273.00	57.90	1151.00	-26.5196
21	304.75	1326.92	39.37	1293.25	9.0429

$$\hat{\sigma}^2 = MS_{\text{Err}} = 36.92 \quad \hat{\sigma}_\beta^2 = \frac{(b-1)(MS_{\text{Blks(Adj)}} - MS_{\text{Err}})}{tr-t} = \frac{(21-1)(355.30 - 36.92)}{21(5) - 21} = \frac{6367.6}{84} = 75.80$$

$$\hat{SE}\{\tilde{\tau}_i\} = \sqrt{\frac{1}{5-1} \left[(5^2)(75.80) \left(\frac{21-1}{21} \right) + 5(36.92) \left(\frac{21-1}{21} \right) \right]} = \sqrt{\frac{1804.76 + 175.81}{4}} = \sqrt{495.14} = 22.25$$

$$\hat{SE}\{\tilde{\tau}_i - \tilde{\tau}_{i'}\} = \sqrt{\frac{2 \left[(5^2)(75.80) + 5(36.92) \right]}{5-1}} = \sqrt{\frac{4159.20}{4}} = \sqrt{1039.80} = 32.25$$

Weights for combining intra- and inter-block Contrasts:

$$\hat{V}\left\{\hat{\zeta}\right\} = \frac{5(36.92)}{1(21)} \sum_{i=1}^t w_i^2 = 8.79 \sum_{i=1}^t w_i^2 \quad \hat{V}\left\{\tilde{\zeta}\right\} = \frac{(5^2)(75.80) + 5(36.92)}{5-1} \sum_{i=1}^t w_i^2 = 519.90 \sum_{i=1}^t w_i^2$$

$$\Rightarrow \bar{\zeta} = \frac{\left[\frac{1}{8.79} \hat{\zeta} + \frac{1}{519.90} \tilde{\zeta} \right]}{\left[\frac{1}{8.79} + \frac{1}{519.90} \right]} = 0.9834 \hat{\zeta} + 0.0166 \tilde{\zeta} \quad \hat{V}(\bar{\zeta}) = \frac{\left(8.79 \sum_{i=1}^g w_i^2 \right) \left(519.90 \sum_{i=1}^g w_i^2 \right)}{\left(8.79 \sum_{i=1}^g w_i^2 \right) + \left(519.90 \sum_{i=1}^g w_i^2 \right)} = 8.64 \sum_{i=1}^t w_i^2$$

$$\text{For pairwise variety comparisons: } \bar{\tau}_i - \bar{\tau}_{i'} : \sum_{i=1}^t w_i^2 = 2 \quad \hat{SE}\{\bar{\tau}_i - \bar{\tau}_{i'}\} = \sqrt{2(8.64)} = 4.157$$

Often the inter-block analysis is more work than gain. For this example, there is virtually no difference between intra-block and combined estimates. Note that the standard error of the difference between variety means for Estimated Generalized Least Squares (from the **diffsmeans** statement in the **lmerTest** package) is very close to the combined estimate.

Additional Incomplete Block Designs

When there are 2 blocking factors, as in a latin square design, it may be that we can have one blocking factor that has the same number (or a multiple) of levels as the treatment factor, but the other blocking factor has fewer levels than the treatment factor. For instance, we may wish to compare 7 brands of tires, based on 7 cars, but only 4 tire positions on each car.

As a second example, in sensory studies, it is well known that raters cannot provide reliable ratings when comparing too many products. In a Sensory Informed Design (SID), researchers wished to compare 12 varieties of white bread (on many criteria), with each rater being exposed to 4 of the varieties for assessments (Franczak, *et al* (2015)). It was found that if each bread was going to be exposed the same time in each of the order positions (1,2,3,4), there would need to be 396 subjects, and each variety would occur 33 times in each position, for a total of 132 times among the subjects.

A sports example is the schedules among most premier football (soccer) leagues around the world. One blocking factor is the game, the other is whether the game is home or away for a given team. Each game can have only 2 of the teams in the league, one team is the home team, the other is the visiting (away) team. For a league with 20 teams, each team plays the remaining 19 teams twice: once at home, once away. There are a total of $2 \binom{20}{2} = 2(190) = 380$ games played in the season. Each pair of teams occur together twice in a block, once each as the Home/Away team.

The **partially balanced incomplete block design (PBIB)** breaks treatments into groups. Treatments within groups appear a certain number of times together in blocks, treatments in different groups appear fewer times together in blocks. Clearly the standard error of the difference between 2 treatment means will depend on whether they are in the same group. Cochran and Cox (1957, p. 456) describe an experiment comparing Yields (pound per plot) of 15 varieties of cotton in 15 blocks of size 4. In this design, each treatment is observed 4 times, and appears along with $4(4-1) = 12$ other treatments in blocks. Thus, each treatment is not observed with $14-12 = 2$ other treatments.

A sports example involves Major League Baseball in the U.S. circa 1970s. There were 2 leagues: the American and National. Within each league, there were 2 divisions: the East and West, with 6 teams in each division. Each game involved 2 teams. There were no “inter-league games,” each team played only within their league. Teams played the 5 remaining teams within their division 18 times (9 at home, 9 away), and the 6 teams in the other division within their league 12 times (6 at home, 6 away). Thus, each team played $5(18) + 6(12) = 162$ games per season, 81 at home, 81 away. Expansion and inter-league play have wreaked havoc on the simplistic balance of Major League Baseball since those days.

Example: Cotton Varieties in a PBIB

The data for the cotton trial described above were analyzed with the following “association scheme”: (1,6,11), (2,7,12), (3,8,13), (4,9,14) (5,10,15). Treatments within the same “grouping” do not appear together in a block, treatments from different groupings appear once together in a block. Below is the R program and (partial) output for the analysis. Note that the standard error for the difference between 2 means is higher for pairs of treatments in the same “grouping” than for pairs from different “groupings.”

R Program

```
cotton <-
read.table("http://www.stat.ufl.edu/~winner/data/cc_cotton_pbib.dat",
  header=F, col.names=c("c.blk", "c.trt", "c.yld"))
attach(cotton)

c.blk <- factor(c.blk); c.trt <- factor(c.trt)

cotton.mod1 <- aov(c.yld ~ c.blk + c.trt)
anova(cotton.mod1)

library(lmerTest)

cotton.mod2 <- lmer(c.yld ~ c.trt + (1|c.blk))
summary(cotton.mod2)
anova(cotton.mod2)
lsmeans(cotton.mod2)
difflsmeans(cotton.mod2)
rand(cotton.mod2)
```

Partial R Output

```
> anova(cotton.mod1)
Analysis of Variance Table

Response: c.yld
      Df Sum Sq Mean Sq F value    Pr(>F)
c.blk  14  4.8393  0.34567   4.0122 0.0006194 ***
c.trt  14  1.4892  0.10637   1.2347 0.3012021
Residuals 31  2.6708  0.08615

> summary(cotton.mod2)
Linear mixed model fit by REML t-tests use Satterthwaite approximations to
degrees of freedom [merModLmerTest]
Formula: c.yld ~ c.trt + (1 | c.blk)

Random effects:
 Groups      Name          Variance Std.Dev.
c.blk      (Intercept)  0.04652  0.2157
Residual                    0.08556  0.2925
Number of obs: 60, groups: c.blk, 15

Fixed effects:
              Estimate Std. Error      df t value Pr(>|t|)
(Intercept)  2.81752     0.16641  44.14000  16.931 <2e-16 ***
c.trt2      -0.41221     0.22206  36.25000  -1.856  0.0716 .
c.trt3      -0.36258     0.22206  36.25000  -1.633  0.1112
c.trt4      -0.03369     0.22206  36.25000  -0.152  0.8802
c.trt5      -0.01262     0.22206  36.25000  -0.057  0.9550
c.trt6       0.09317     0.22720  37.70000   0.410  0.6841
c.trt7      -0.02854     0.22206  36.25000  -0.129  0.8985
c.trt8      -0.03592     0.22206  36.25000  -0.162  0.8724
c.trt9       0.07379     0.22206  36.25000   0.332  0.7416
c.trt10     -0.32646     0.22206  36.25000  -1.470  0.1501
c.trt11      0.08118     0.22720  37.70000   0.357  0.7229
c.trt12      0.23530     0.22206  36.25000   1.060  0.2963
c.trt13     -0.19975     0.22206  36.25000  -0.900  0.3743
c.trt14     -0.32621     0.22206  36.25000  -1.469  0.1505
c.trt15      0.04171     0.22206  36.25000   0.188  0.8521

> difflsmeans(cotton.mod2)
Differences of LSMEANS:
      Estimate Standard Error      DF t-value Lower CI Upper CI p-value
c.trt 1 - 2      0.4          0.2221  36.3    1.86   -0.0380  0.8625  0.072
c.trt 1 - 3      0.4          0.2221  36.3    1.63   -0.0877  0.8128  0.111
c.trt 1 - 4      0.0          0.2221  36.3    0.15   -0.4166  0.4839  0.880
c.trt 1 - 5      0.0          0.2221  36.3    0.06   -0.4376  0.4629  0.955
c.trt 1 - 6     -0.1          0.2272  37.7   -0.41   -0.5532  0.3669  0.684
c.trt 1 - 7      0.0          0.2221  36.3    0.13   -0.4217  0.4788  0.898
c.trt 1 - 8      0.0          0.2221  36.3    0.16   -0.4143  0.4862  0.872
c.trt 1 - 9     -0.1          0.2221  36.3   -0.33   -0.5240  0.3765  0.742
c.trt 1 - 10     0.3          0.2221  36.3    1.47   -0.1238  0.7767  0.150
c.trt 1 - 11    -0.1          0.2272  37.7   -0.36   -0.5412  0.3789  0.723
c.trt 1 - 12    -0.2          0.2221  36.3   -1.06   -0.6856  0.2150  0.296
c.trt 1 - 13     0.2          0.2221  36.3    0.90   -0.2505  0.6500  0.374
c.trt 1 - 14     0.3          0.2221  36.3    1.47   -0.1240  0.7765  0.150
c.trt 1 - 15     0.0          0.2221  36.3   -0.19   -0.4920  0.4085  0.852
```



```
> rand(cotton.mod2)
Analysis of Random effects Table:
  Chi.sq Chi.DF p.value
c.blk    5.88     1    0.02 *
```

Data/Design Sources:

S-H. Hsu and S-P.Wu (1991). "An Investigation for Determining the Optimum Length of Chopsticks," *Applied Ergonomics*, Vol. 22, #6, pp. 395-400.

K. Cox (1964). "The Responsiveness to Shelf Space Changes in Supermarkets," *Journal of Marketing Research*, Vol.1 #2, pp. 63-67.

F. Yates (1940). "The Recovery of Inter-Block Information in Balanced Incomplete Block Designs," *Annals of Eugenics*, Vol. 10, #1, pp. 317-325.

B.C. Franczak, R.P. Browne, P.D. McNicholas, C.J. Findlay (2015). "Product Selection for Liking Studies: The Sensory Informed Design," *Food Quality and Preference*, Vol. 44, pp. 36-43.

W.G. Cochran and G.M. Cox (1957). *Experimental Designs*, 2nd Ed., Wiley, NY. p. 456.

Chapter 10 – Multi-Factor Designs

Many research studies use multiple factors at 2 or a few levels to determine which have the largest impact and which factors interact on the response variable. In this chapter, we describe full factorial, fractional factorial, response surface, and mixture designs. To begin, we will assume we have k factors, each at 2 levels (low/high or present/absent). These can be generalized to more than 2 levels, which we consider in response surface and mixture designs.

10.1. 2^k Full Factorial Designs

In these designs, all combinations of the k factors are observed, with the overall sample size $n = 2^k$. Each factor (A,B,C,...) will have 2 levels, and the observations (experimental runs) can be labeled to reflect whether the given factors are at their low or high levels. Suppose we have 4 factors: A, B, C, and D, then the experiment will have $2^4 = 16$ runs. When all 4 factors are at their low (absent) level, it is common to label the run as (1). When factor A is at its high (present) level, and the remaining factors are at their low levels, the run is often labelled as a . When all factors are at their high levels, the run would be labelled as $abcd$. A common way of reporting the experimental result is as follows, where “-1” implies the factor is at its low level, “1” implies it is at its high level. The experimental runs would be conducted in random order.

Run	Label	A	B	C	D
1	(1)	-1	-1	-1	-1
2	a	1	-1	-1	-1
3	b	-1	1	-1	-1
4	ab	1	1	-1	-1
5	c	-1	-1	1	-1
6	ac	1	-1	1	-1
7	bc	-1	1	1	-1
8	abc	1	1	1	-1
9	d	-1	-1	-1	1
10	ad	1	-1	-1	1
11	bd	-1	1	-1	1
12	abd	1	1	-1	1
13	cd	-1	-1	1	1
14	acd	1	-1	1	1
15	bcd	-1	1	1	1
16	abcd	1	1	1	1

To model the “A effect” we compute a multiple of the difference between the runs when A is at its high level and when it is at its low level.

$$(a + ab + ac + abc + ad + abd + acd + abcd) - ((1) + b + c + bc + d + bd + cd + bcd)$$

Two-way interactions are modelled by determining whether the two factors are both at the same (low/high) level versus when one is at its high level and the other is at its low level. For instance the “A effect” when B is at its low level is $(a + ac + ad + acd) - ((1) + c + d + cd)$. The “A effect” when B is at its high level is $(ab + abc + abd + abcd) - (b + bc + bd + bcd)$. When we take the difference between the “A effect” when B is at its high level minus the “A effect” when B is at its low level, we get a multiple of the “AB interaction effect”.

$$\begin{aligned} & \left[(ab + abc + abd + abcd) - (b + bc + bd + bcd) \right] - \left[(a + ac + ad + acd) - ((1) + c + d + cd) \right] \\ & = (ab + abc + abd + abcd + (1) + c + d + cd) - (b + bc + bd + bcd + a + ac + ad + acd) \end{aligned}$$

This takes the difference between the runs when A and B appear at the same (low/high) level and the runs when A and B are at opposite (low/high) levels. The columns corresponding to A and B in the above spreadsheet can be multiplied to give the AB contrast.

For a 3-way interaction, consider the AB interaction when C is absent and when C is present.

$$\begin{aligned} \text{C Absent: } & ((1) + ab + d + abd) - (a + b + ad + bd) \\ \text{C Present: } & ((c + abc + cd + abcd) - (ac + bc + acd + bcd)) \\ \text{C Present - C Absent: } & (a + b + c + abc + ad + bd + cd + abcd) - ((1) + ab + bc + d + abd + acd + bcd) \end{aligned}$$

This takes the difference between the cases when an odd number of the factors A, B, and C are at their high levels and the cases when an even number are at their high levels. The columns corresponding to A, B, and C can be multiplied to give the ABC contrast. This generalizes to interactions among any number of factors.

Run	Label	A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD
1	(1)	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1	-1	-1	1
2	a	1	-1	-1	-1	1	1	1	1	1	1	1	1	1	-1	-1
3	b	-1	1	-1	-1	-1	1	1	1	1	1	1	1	-1	1	-1
4	ab	1	1	-1	-1	-1	1	1	1	1	1	-1	-1	1	1	1
5	c	-1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	-1
6	ac	1	-1	1	-1	1	-1	1	-1	1	-1	-1	1	-1	1	1
7	bc	-1	1	1	-1	-1	-1	1	-1	1	-1	-1	1	1	-1	1
8	abc	1	1	1	-1	-1	-1	1	-1	1	-1	1	-1	-1	-1	-1
9	d	-1	-1	-1	1	1	1	-1	1	-1	-1	-1	1	1	1	-1
10	ad	1	-1	-1	1	1	1	-1	1	-1	-1	1	-1	-1	1	1
11	bd	-1	1	-1	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
12	abd	1	1	-1	1	-1	1	-1	1	-1	-1	-1	1	-1	-1	-1
13	cd	-1	-1	1	1	1	-1	-1	-1	-1	1	1	1	-1	-1	1
14	acd	1	-1	1	1	1	-1	-1	-1	-1	1	-1	-1	1	-1	-1
15	bcd	-1	1	1	1	-1	-1	-1	-1	-1	1	-1	-1	-1	1	-1
16	abcd	1	1	1	1	-1	-1	-1	-1	-1	1	1	1	1	1	1

Note that each contrast has half of the measurements with a +1 coefficient and half of the measurements with a -1 coefficient. We obtain the following estimated effects and sums of squares as follow.

$$\begin{aligned} \hat{A} &= \frac{1}{2^{4-1}} \left[(a + ab + ac + abc + ad + abd + acd + abcd) - ((1) + b + c + bc + d + bd + cd + abcd) \right] \\ V\{\hat{A}\} &= \left(\frac{1}{2^{4-1}} \right)^2 2^4 \sigma^2 = \frac{1}{2^{4-2}} \sigma^2 \Rightarrow SE\{\hat{A}\} = \sqrt{\frac{1}{2^{4-2}} MS_{\text{Err}}} \\ SS_A &= 2^{4-1} \left[(\bar{Y}_{A=+1} - \bar{Y})^2 + (\bar{Y}_{A=-1} - \bar{Y})^2 \right] = 2^{4-1} \left[\left(\bar{Y}_{A=+1} - \frac{1}{2}(\bar{Y}_{A=+1} + \bar{Y}_{A=-1}) \right)^2 + \left(\bar{Y}_{A=-1} - \frac{1}{2}(\bar{Y}_{A=+1} + \bar{Y}_{A=-1}) \right)^2 \right] = \\ & 2^{4-1} \left[\left(\frac{1}{2}(\bar{Y}_{A=+1} - \bar{Y}_{A=-1}) \right)^2 + \left(\frac{1}{2}(\bar{Y}_{A=-1} - \bar{Y}_{A=+1}) \right)^2 \right] = \frac{2^{4-1}}{4} 2 \left(\hat{A} \right)^2 = 2^{4-2} \left(\hat{A} \right)^2 \\ \text{In general, if there are } k \text{ Factors: } & SE\{\hat{A}\} = \sqrt{\frac{1}{2^{k-2}} MS_{\text{Err}}} \quad SS_A = 2^{k-2} \left(\hat{A} \right)^2 \\ \text{If the "data" are means of } r \text{ replicates at each "run": } & SE\{\hat{A}\} = \sqrt{\frac{1}{r 2^{k-2}} MS_{\text{Err}}} \quad SS_A = r 2^{k-2} \left(\hat{A} \right)^2 \end{aligned}$$

Similar computations are made for other main effects and interactions.

Example: Factors Relating to Pb(II) Adsorption onto Walnut Shells

A study was conducted (Saadat and Karimi-Jashni (2011)), with 4 factors, each at 2 levels: pH (2, 10), walnut shell adsorption dose (1 g/l, 20 g/l), initial metal concentration (10 mg/l, 90 mg/l), and temperature (15°C, 45°C). The response measured was percent Pb(II) removal. The experiment was done in $r = 2$ replicates. Data below include the mean and standard deviation for the 2 observations at each combination of factor levels.

Trt	A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD	Mean	SD
1	-1	-1	-1	-1	-1	1	1	1	1	1	-1	-1	-1	-1	1	5.31	1.94
2	1	-1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	-1	-1	53.25	1.09
3	-1	1	-1	-1	-1	1	1	-1	-1	1	1	1	-1	1	-1	83.68	4.79
4	1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	1	1	1	88.97	1.02
5	-1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	-1	1.25	0.08
6	1	-1	1	-1	-1	1	-1	-1	1	-1	-1	1	-1	1	1	76.62	1.78
7	-1	1	1	-1	-1	-1	-1	1	1	-1	-1	1	1	-1	1	64.22	5.37
8	1	1	1	-1	1	1	-1	1	-1	-1	1	-1	-1	-1	-1	80.27	0.38
9	-1	-1	-1	1	1	1	-1	1	-1	-1	-1	1	1	1	-1	7.23	2.01
10	1	-1	-1	-1	1	-1	-1	1	1	-1	-1	1	-1	1	1	54.00	6.55
11	-1	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	-1	1	85.54	2.19
12	1	1	-1	1	1	-1	1	-1	1	-1	-1	1	-1	-1	-1	91.01	0.65
13	-1	-1	1	1	1	1	-1	-1	-1	1	1	1	-1	-1	1	1.81	0.24
14	1	-1	1	1	-1	1	1	-1	-1	1	-1	-1	1	-1	-1	78.23	1.74
15	-1	1	1	1	1	-1	-1	1	1	1	-1	-1	-1	1	-1	65.91	4.86
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	81.16	1.98
Effect	36.07	45.3825	-2.44	1.415	-25.555	9.7025	-0.0925	-11.97	0.205	-0.2275	-4.5675	-0.0625	0.155	-0.1025	-0.4	MSErr	9.00
SE{Eff}	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06		
t	34.01	42.79	-2.30	1.33	-24.10	9.15	-0.09	-11.29	0.19	-0.21	-4.31	-0.06	0.15	-0.10	-0.38		
SS{Effect}	10408.36	16476.57	47.6288	16.0178	5224.464	753.1081	0.06845	1146.247	0.3362	0.41405	166.8965	0.03125	0.1922	0.08405	1.28		
F	1156.69	1831.06	5.29	1.78	580.60	83.69	0.01	127.38	0.04	0.05	18.55	0.00	0.02	0.01	0.14		

Here is a summary of the calculations for MS_{Err} and for factor A (pH).

$$k = 4 \Rightarrow t = 2^4 = 16 \quad r = 2 \Rightarrow n = 16(2) = 32 \quad df_{Err} = n - t = 32 - 16 = 16$$

$$SS_{Err} = \sum_{i=1}^t (n_i - 1) s_i^2 = (2 - 1) [1.94^2 + \dots + 1.98^2] = 143.9744 \quad MS_{Err} = \frac{143.9744}{16} = 8.9984 \approx 9.00$$

$$\hat{A} = \frac{1}{2^{4-1}} \left[(53.25 + 88.97 + 76.62 + 80.27 + 54.00 + 91.01 + 78.23 + 81.16) - (5.31 + 83.68 + 1.25 + 64.22 + 7.23 + 85.54 + 1.81 + 65.91) \right]$$

$$= \frac{1}{8} (603.51 - 314.95) = \frac{288.56}{8} = 36.07$$

$$SE\{\hat{A}\} = \sqrt{\frac{1}{2(2^{4-2})} 9.00} = \sqrt{\frac{9}{8}} = 1.0606 \Rightarrow t_A = \frac{\hat{A}}{SE\{\hat{A}\}} = \frac{36.07}{1.061} = 34.01 \quad t_{.975;16} = 2.120$$

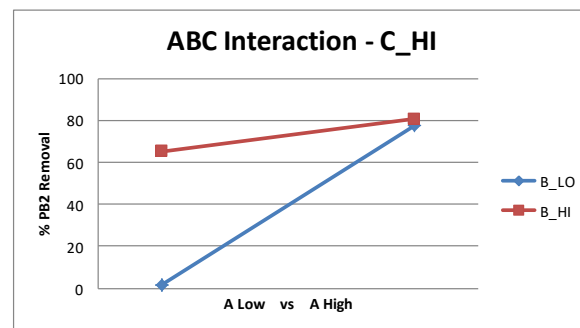
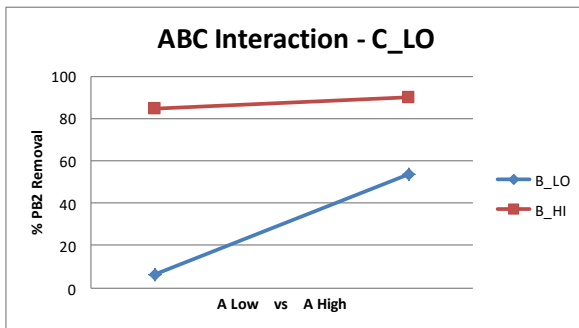
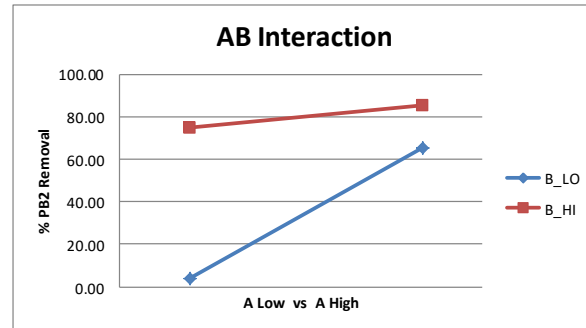
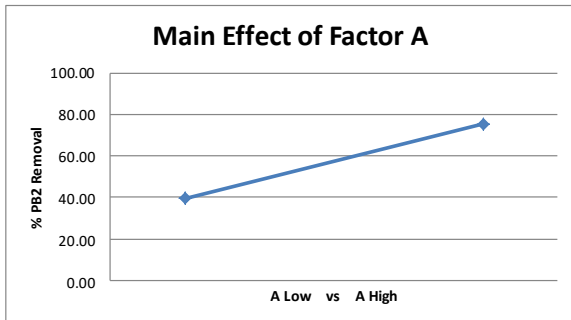
$$SS_A = 2(2^{4-2})(36.07^2) = 10408.36 \Rightarrow F_A = \frac{10408.36/1}{9.00} = 1156.48 \quad F_{.95;1,16} = 4.49$$

Note that if we have only 1 replicate per treatment, there are 0 degrees of freedom for error, and we cannot conduct the t- or F-tests for treatment effects, unless we assume higher order interactions are negligible, and use their sums of squares to estimate Error.

Factors A (pH), B (walnut shell adsorption dose), and C (Initial metal concentration) are all important, as well as all of their 2-Way and 3-Way interactions. Factor D (Temperature) and all of its interactions with A, B, and

C are not significant. We could fit a simpler model removing those terms and increase our error degrees of freedom.

Here we include plots to demonstrate main effects and interactions involving Factor A (pH).



The upper left plot demonstrates the Factor A (pH) main effect, namely that there is a higher level of Pb2 removal at high pH than at low pH. The upper right plot demonstrates the 2-way interaction between factors A (pH) and B (walnut shell adsorption dose), namely that the pH effect is larger (steeper) when the adsorption dose is at its low level. The plot also demonstrates that the high level of adsorption dose has a higher level of Pb2 removal than the low level of adsorption dose. The bottom 2 plots show that the 2-way interaction between Factors A and B differ for the 2 levels of Factor C (initial metal concentration).

Below, we run the analysis in R, and use a Complete versus Reduced model to test whether we can simultaneously drop all factor D terms. Note that the program reads in the raw data, not the mean and standard deviations for the 16 treatments.

R Program

```
walnut <- read.csv("http://www.stat.ufl.edu/~winner/data/pb2_walnut.csv",
  header=T)
attach(walnut); names(walnut)

pH <- factor(pH)
adsorb_dose <- factor(adsorb_dose)
metal_conc <- factor(metal_conc)
temp_c <- factor(temp)

options(contrasts=c("contr.sum", "contr.poly"))

walnut.mod1 <- aov(pb2_remove ~ pH*adsorb_dose*metal_conc*temp_c)
anova(walnut.mod1)
summary.lm(walnut.mod1)

walnut.mod2 <- aov(pb2_remove ~ pH*adsorb_dose*metal_conc)
anova(walnut.mod2)
summary.lm(walnut.mod2)

anova(walnut.mod2, walnut.mod1)
```

R Output

```
> anova(walnut.mod1)
Analysis of Variance Table

Response: pb2_remove

Df Sum Sq Mean Sq F value Pr(>F)
pH 1 10408.4 10408.4 1156.6900 2.373e-16 ***
adsorb_dose 1 16476.6 16476.6 1831.0556 < 2.2e-16 ***
metal_conc 1 47.6 47.6 5.2930 0.0351999 *
temp_c 1 16.0 16.0 1.7801 0.2008202
pH:adsorb_dose 1 5224.5 5224.5 580.5992 5.319e-14 ***
pH:metal_conc 1 753.1 753.1 83.6936 9.337e-08 ***
adsorb_dose:metal_conc 1 1146.2 1146.2 127.3834 4.975e-09 ***
pH:temp_c 1 0.1 0.1 0.0076 0.9315808
adsorb_dose:temp_c 1 0.3 0.3 0.0374 0.8491619
metal_conc:temp_c 1 0.4 0.4 0.0460 0.8328609
pH:adsorb_dose:metal_conc 1 166.9 166.9 18.5473 0.0005431 ***
pH:adsorb_dose:temp_c 1 0.0 0.0 0.0035 0.9537370
pH:metal_conc:temp_c 1 0.2 0.2 0.0214 0.8856297
adsorb_dose:metal_conc:temp_c 1 0.1 0.1 0.0093 0.9242074
pH:adsorb_dose:metal_conc:temp_c 1 1.3 1.3 0.1422 0.7110124
Residuals 16 144.0 9.0

> summary.lm(walnut.mod1)
Coefficients:

(Intercept) 57.40375 0.53028 108.251 < 2e-16 ***
pH1 -18.03500 0.53028 -34.010 2.37e-16 ***
adsorb_dose1 -22.69125 0.53028 -42.791 < 2e-16 ***
metal_conc1 1.22000 0.53028 2.301 0.035200 *
temp_c1 -0.70750 0.53028 -1.334 0.200820
pH1:adsorb_dose1 -12.77750 0.53028 -24.096 5.32e-14 ***
pH1:metal_conc1 4.85125 0.53028 9.148 9.34e-08 ***
adsorb_dose1:metal_conc1 -5.98500 0.53028 -11.286 4.97e-09 ***
pH1:temp_c1 -0.04625 0.53028 -0.087 0.931581
adsorb_dose1:temp_c1 0.10250 0.53028 0.193 0.849162
metal_conc1:temp_c1 -0.11375 0.53028 -0.215 0.832861
pH1:adsorb_dose1:metal_conc1 2.28375 0.53028 4.307 0.000543 ***
pH1:adsorb_dose1:temp_c1 0.03125 0.53028 0.059 0.953737
pH1:metal_conc1:temp_c1 -0.07750 0.53028 -0.146 0.885630
adsorb_dose1:metal_conc1:temp_c1 0.05125 0.53028 0.097 0.924207
pH1:adsorb_dose1:metal_conc1:temp_c1 -0.20000 0.53028 -0.377 0.711012
```

```
> anova(walnut.mod2)
Analysis of Variance Table

Response: pb2_remove

Df Sum Sq Mean Sq F value Pr(>F)
pH 1 10408.4 10408.4 1538.1963 < 2.2e-16 ***
adsorb_dose 1 16476.6 16476.6 2434.9851 < 2.2e-16 ***
metal_conc 1 47.6 47.6 7.0388 0.01392 *
pH:adsorb_dose 1 5224.5 5224.5 772.0959 < 2.2e-16 ***
pH:metal_conc 1 753.1 753.1 111.2979 1.711e-10 ***
adsorb_dose:metal_conc 1 1146.2 1146.2 169.3978 2.285e-12 ***
pH:adsorb_dose:metal_conc 1 166.9 166.9 24.6647 4.527e-05 ***
Residuals 24 162.4 6.8

> summary.lm(walnut.mod2)

Coefficients:

(Intercept) 57.4037 0.4598 124.833 < 2e-16 ***
pH1 -18.0350 0.4598 -39.220 < 2e-16 ***
adsorb_dose1 -22.6912 0.4598 -49.346 < 2e-16 ***
metal_conc1 1.2200 0.4598 2.653 0.0139 *
pH1:adsorb_dose1 -12.7775 0.4598 -27.787 < 2e-16 ***
pH1:metal_conc1 4.8512 0.4598 10.550 1.71e-10 ***
adsorb_dose1:metal_conc1 -5.9850 0.4598 -13.015 2.28e-12 ***
pH1:adsorb_dose1:metal_conc1 2.2837 0.4598 4.966 4.53e-05 ***

Residual standard error: 2.601 on 24 degrees of freedom
Multiple R-squared: 0.9953, Adjusted R-squared: 0.9939
F-statistic: 722.5 on 7 and 24 DF, p-value: < 2.2e-16

>
> anova(walnut.mod2, walnut.mod1)
Analysis of Variance Table

Model 1: pb2_remove ~ pH * adsorb_dose * metal_conc
Model 2: pb2_remove ~ pH * adsorb_dose * metal_conc * temp_c
Res.Df RSS Df Sum of Sq F Pr(>F)
1 24 162.40
2 16 143.97 8 18.424 0.2559 0.9717
```

Note that by using the **contr.sum** contrast, the effects computed on the spreadsheet are twice as large as the estimated effects in the R output. The standard errors differ by a factor of 2, and the corresponding t-statistics are identical. The effects computed by taking the difference between high and low means of the factor are comparable to $\hat{\alpha}_{\text{High}} - \hat{\alpha}_{\text{Low}}$. R is reporting $\hat{\alpha}_{\text{Low}}$ subject to $\hat{\alpha}_{\text{High}} = -\hat{\alpha}_{\text{Low}}$ and $\hat{A} = \hat{\alpha}_{\text{High}} - \hat{\alpha}_{\text{Low}} = -2\hat{\alpha}_{\text{Low}}$.

To obtain the interaction plots in R, include the following commands at the bottom of the previous program. These are crude plots, with some time consuming effort they can be made extremely elegant.

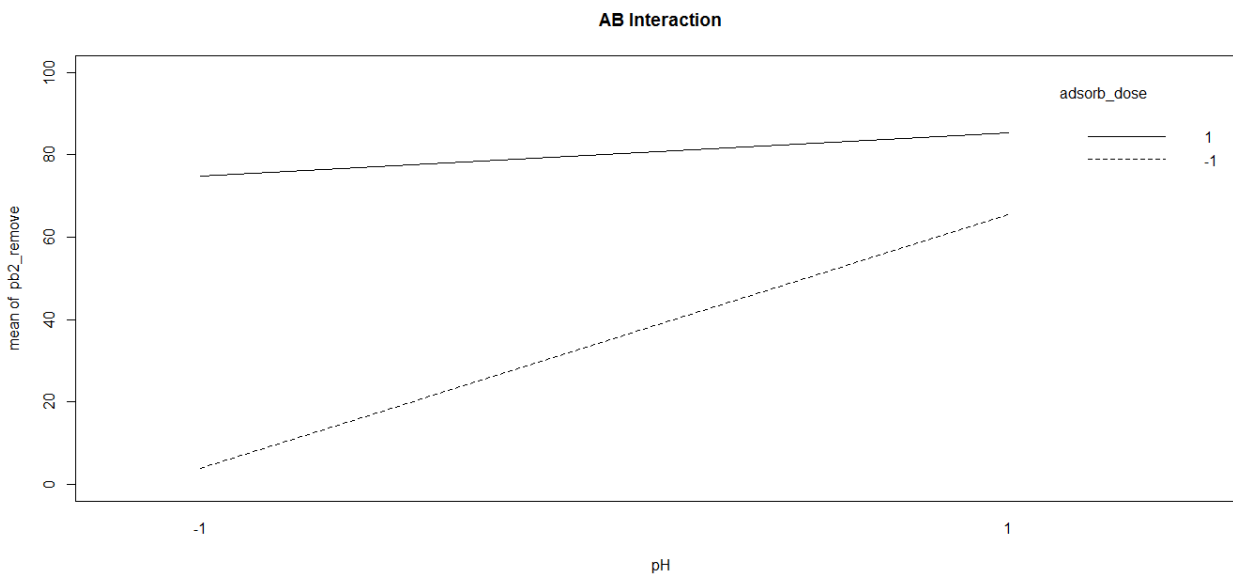
R Commands

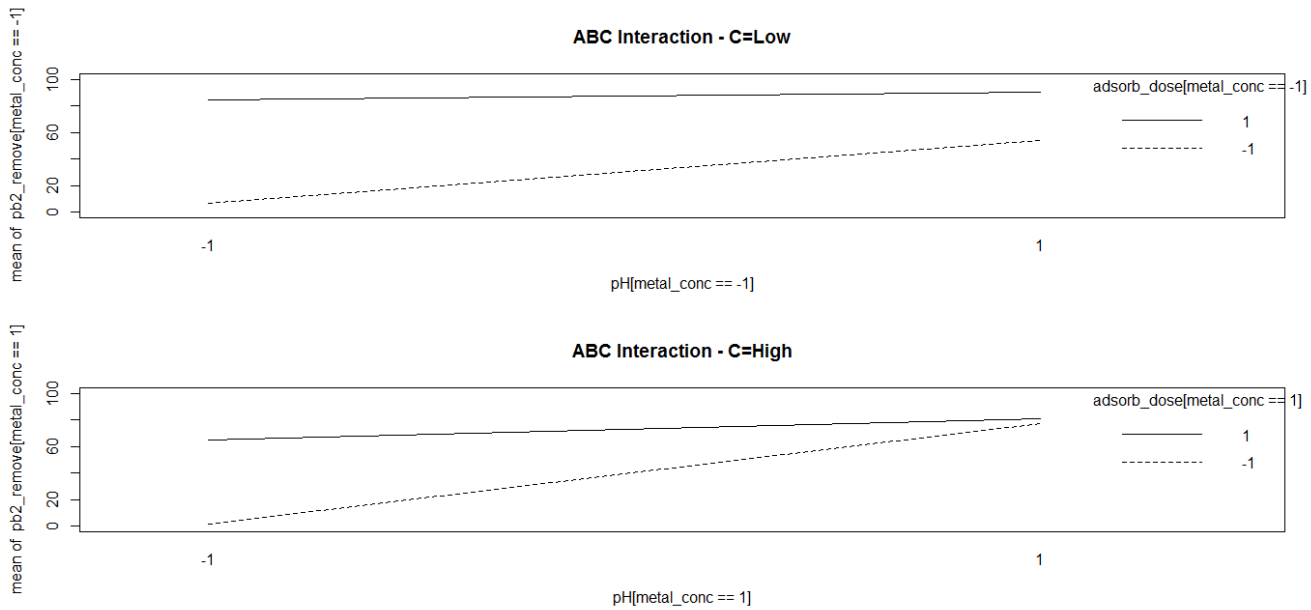
```
interaction.plot(pH,adsorb_dose,pb2_remove,ylim=c(0,100),
main="AB Interaction")

par(mfrow=c(2,1))

interaction.plot(pH[metal_conc==1],adsorb_dose[metal_conc==1],
pb2_remove[metal_conc==1],ylim=c(0,100),main="ABC Interaction - C=Low")

interaction.plot(pH[metal_conc==1],adsorb_dose[metal_conc==1],
pb2_remove[metal_conc==1],ylim=c(0,100),main="ABC Interaction - C=High")
```





Factorials in Incomplete Blocks

In many practical cases, as k increases, it is not possible to conduct a factorial as a complete block design when it is wished to increase precision of estimates. This can be a result of the fact that as block size increases, homogeneity of block “sub-units” will decrease, or because people cannot make assessments of many treatments, or because batches of raw material are not large enough to be split into 2^k individual components. Often, we can repeat the resulting incomplete factorial design various times.

Going back to the previous scenario, where we have $k = 4$ factors, each at 2 levels. First, suppose that we can construct blocks of 8 treatments, due to the nature of the experiment. Below we consider 4 of the

$\binom{16}{8} = \frac{16!}{8!8!} = 12870$ ways we could choose 8 treatments from the 16 for block 1. All of these choices are not arbitrary, as they will keep most (but not all) effects unaffected by the blocking structure.

Case 1			Case 2			Case 3			Case 4	
Block 1	Block 2		Block 1	Block 2		Block 1	Block 2		Block 1	Block 2
a	(1)		(1)	a		a	(1)		(1)	a
ab	b		ab	b		b	ab		ab	b
ac	c		c	ac		c	ac		ac	c
abc	bc		abc	bc		abc	bc		bc	abc
ad	d		d	ad		ad	d		ad	d
abd	bd		abd	bd		bd	abd		bd	abd
acd	cd		cd	acd		cd	acd		cd	acd
abcd	bcd		abcd	bcd		abcd	bcd		abcd	bcd

The problem arises that for each of these designs, the difference between Block 1 and Block 2 means will be the same as (confounded with) one of our main or interaction effects. However, for each of these “well-behaved” cases, all other effects will be unaffected by the blocking structure. Recall the goal of blocking is to reduce experimental error, thus increasing power to determine effects. For each of these cases, we will determine which effect is confounded with the block effect, by taking the differences in Block 1 and Block 2 means, and comparing with the +/- structure of the original spreadsheet. Note that as there are 2 blocks, the block sum of squares would have 1 degree of freedom, so there will be 1 confounded effect.

Case 1: $\left[(a + ab + ac + abc + ad + abd + acd + abcd) - ((1) + b + c + bc + d + bd + cd + bcd) \right] = \hat{A}$
Case 2: $\left[((1) + ab + c + abc + d + abd + cd + abcd) - (a + b + ac + bc + ad + bd + acd + bcd) \right] = \hat{AB}$
Case 3: $\left[(a + b + c + abc + ad + bd + cd + abcd) - ((1) + ab + ac + bc + d + abd + acd + bcd) \right] = \hat{ABC}$
Case 4: $\left[((1) + ab + ac + bc + ad + bd + cd + abcd) - (a + b + c + abc + d + abd + acd + bcd) \right] = \hat{ABCD}$

Thus, Case 1 is problematic, as the Block effect is confounded with the main effect for Factor A. Note that Case 4 is “best” in the sense that only the highest order interaction (the least important in the hierarchy) is confounded with the blocks.

Further note that Factor B is not confounded in any of the cases. That is, Factor B occurs at its high and low levels 4 times in each of the 2 blocks for each case. Thus, any block effects will balance out when obtaining its estimated effect. This also holds for any other main effect or interaction that is not confounded with blocks.

Sums of squares are computed as before and whether or not there is an error sum of squares, depends on whether there is more than 1 replicate of the experiment. We will work through a computations for an example from Cochran and Cox (1957). More details on the construction of these designs, as well as other issues such as partial confounding, where different effects are confounded in different replicates can be found in Montgomery (200?), Cochran and Cox (1957), Kuehl (2000), and Oehlert (????). Further, these sources also include factorials with factors at 2 or 3 levels: $2^{k_2}3^{k_3}$ designs. We will consider response surface designs with numeric factors at various numbers of levels below.

Example – Bean Yields in a 2⁴ Factorial Confounded in Blocks

Cochran and Cox (1957, pp. 188-192) report bean yields from Rothamsted Experimental Station from 1936. The experiment had 4 factors, each at 2 levels. Dung (D: 0, 10 tons/acre), Nitrochalk (N: 0, 0.4 cwt N/acre), Superphosphate (P: 0, 0.6 cwt P₂O₅/acre), and Muriate of potash (K: 0, 1.0 cwt K₂O/acre).

The experiment thus had $2^4 = 16$ treatments, and was conducted in blocks of size 8. There were 2 replicates, thus a total of $N = 2(16) = 32$ observations. Within each block, the 4-way interaction was confounded with blocks. Note that the blocks are nested within replicates, such that the 2 blocks from replicate 1 differ from the blocks from replicate 2. The error sum of squares will be obtained by the sum of the interaction effects between replicates and each of the non-confounded effects (main and interaction). Thus, there will be $(2-1)*(15-1) = 14$ error degrees of freedom. First, we run the analysis through a spreadsheet, then will run it in R.

	Replicate1	Replicate1	Replicate2	Replicate2	
Treatment	Block	Yield	Block	Yield	TrtSum
d	1	53	3	42	95
n	1	42	3	47	89
p	1	45	3	39	84
k	1	55	3	50	105
dnp	1	48	3	52	100
dnk	1	41	3	34	75
dpk	1	55	3	44	99
npk	1	36	3	43	79
	BlkMean	46.875	BlkMean	43.875	
(1)	2	58	4	57	115
dn	2	41	4	42	83
dp	2	50	4	52	102
dk	2	43	4	52	95
np	2	50	4	39	89
nk	2	44	4	43	87
pk	2	51	4	56	107
dnpk	2	44	4	54	98
	BlkMean	47.625	BlkMean	49.375	
	RepMean	47.25	RepMean	46.625	
			OverallMean	46.9375	

Trt	A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD	TotYld	MeanYld	Trt
1	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1	-1	-1	1	115	57.5	(1)
2	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1	1	1	-1	-1	95	47.5	d
3	-1	1	-1	-1	-1	-1	1	1	-1	-1	1	1	-1	1	-1	89	44.5	n
4	1	1	-1	-1	1	-1	-1	-1	-1	-1	-1	-1	1	1	1	83	41.5	dn
5	-1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	-1	84	42.0	p
6	1	-1	1	-1	-1	1	-1	-1	-1	-1	-1	-1	-1	1	1	102	51.0	dp
7	-1	1	1	-1	-1	-1	-1	1	1	-1	-1	-1	1	1	-1	89	44.5	np
8	1	1	1	-1	1	1	-1	1	-1	-1	1	-1	-1	-1	-1	100	50.0	dnp
9	-1	-1	-1	1	1	1	-1	1	-1	-1	-1	1	1	1	-1	105	52.5	k
10	1	-1	-1	1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	95	47.5	dk
11	-1	1	-1	1	-1	1	-1	-1	-1	1	-1	-1	1	-1	1	87	43.5	nk
12	1	1	-1	1	1	-1	1	-1	1	-1	-1	1	-1	-1	-1	75	37.5	dnk
13	-1	-1	1	1	1	-1	-1	-1	-1	1	1	1	-1	-1	1	107	53.5	pk
14	1	-1	1	1	-1	1	1	-1	-1	1	-1	-1	1	-1	-1	99	49.5	dpk
15	-1	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1	1	-1	79	39.5	npk
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	98	49.0	dnpk
Effect	-0.500	-6.375	0.875	-0.750	2.000	5.500	-0.875	3.125	-2.000	1.750	0.500	1.125	-1.375	-2.000	3.125			
SS(Eff)	2.000	325.125	6.125	4.500	32.000	242.000	6.125	78.125	32.000	24.500	2.000	10.125	15.125	32.000	78.125			

The estimated effects were computed as before, taking the sum of the products of the ± 1 's for each effect column with the mean yield for that row's treatment. The sum of squares for each effect is computed as before as well, keeping in mind each yield is based on 2 replicates. The Effect and sum of squares for ABCD is not relevant, being confounded with blocks within each replicate. Here we compute the Total, Replicate, Block(Rep), and Error (by subtraction) sums of squares.

$$SS_{Tot} = \left[(53 - 46.9375)^2 + \dots + (54 - 46.9375)^2 \right] = 1277.875 \quad df_{Tot} = 32 - 1 = 31$$

$$SS_{Reps} = 16 \left[(47.25 - 46.9375)^2 + (46.625 - 46.9375)^2 \right] = 3.125 \quad df_{Reps} = 2 - 1 = 1$$

$$SS_{Blks(Reps)} = 8 \left[(46.875 - 47.25)^2 + (47.625 - 47.25)^2 + (43.875 - 46.625)^2 + (49.375 - 46.625)^2 \right] = 123.25$$

$$df_{Blks(Reps)} = 2(2 - 1) = 2$$

$$SS_{Trts} = SS_A + \dots + SS_{BCD} = 2.00 + \dots + 32.00 = 811.750 \quad df_{Trts} = (2^4 - 1) - 1 = 15 - 1 = 14$$

$$SS_{Err} = 1277.875 - 3.125 - 123.25 - 811.75 = 339.75 \quad df_{Err} = (2 - 1)(14) = 14 \Rightarrow MS_{Err} = \frac{339.75}{14} = 24.27$$

The critical F-value for 1 and 14 degrees of freedom is $F_{.95;1,14} = 4.160$. This implies that Factor B (Nitrochalk) and the AC (Dung/Superphosphate) interaction are the important effects.

R Program

```
bean <- read.csv("http://www.stat.ufl.edu/~winner/data/bean_factorial_cc.csv",
                header=T)
attach(bean); names(bean)

Dung <- factor(Dung); Nchalk <- factor(Nchalk)
Phos <- factor(Phos); Kmur <- factor(Kmur)
Block <- factor(Block); Replicate <- factor(Replicate)

options(contrasts=c("contr.sum","contr.poly"))

bean.mod1 <- aov(Yield ~ Replicate + Block:Replicate +
                Dung*Nchalk*Phos*Kmur - Dung:Nchalk:Phos:Kmur)
anova(bean.mod1)
```

R Output

```
> anova(bean.mod1)
Analysis of Variance Table

Response: Yield
      Df Sum Sq Mean Sq F value    Pr(>F)
Replicate  1  3.13    3.13  0.1288 0.725064
Dung       1  2.00    2.00  0.0824 0.778258
Nchalk    1 325.13  325.13 13.3974 0.002572 **
Phos      1  6.12    6.12  0.2524 0.623205
Kmur      1  4.50    4.50  0.1854 0.673303
Replicate:Block 2 123.25  61.63  2.5394 0.114564
Dung:Nchalk  1  32.00   32.00  1.3186 0.270083
Dung:Phos   1 242.00  242.00  9.9720 0.006982 **
Nchalk:Phos  1  78.13   78.13  3.2193 0.094393 .
Dung:Kmur   1  6.13    6.13  0.2524 0.623205
Nchalk:Kmur  1  32.00   32.00  1.3186 0.270083
Phos:Kmur   1  24.50   24.50  1.0096 0.332058
Dung:Nchalk:Phos  1  2.00    2.00  0.0824 0.778258
Dung:Nchalk:Kmur  1 10.13   10.13  0.4172 0.528774
Dung:Phos:Kmur   1 15.12   15.12  0.6233 0.443007
Nchalk:Phos:Kmur  1  32.00   32.00  1.3186 0.270083
Residuals    14 339.75   24.27
```

To analyze a design where different effects are confounded in the different replicates, so these effects are only “partially confounded” can be messy. Kuehl (2000, Section 11.3) provides a worked out example.

As a second example, suppose that instead of being able to construct 2 incomplete blocks of size 8 for a 2^4 factorial, the block sizes can only be of size 4. This again could be due to logistics such as batch sizes or time to complete runs, or simply homogeneity of sub-units within blocks. Now, instead of one effect being confounded with blocks, 3 will be. Here, we provide merely an example, see Montgomery (2001), Kuehl (2000), or any number of experimental design textbooks and/or software packages for rules and/or computer based designs.

Consider the following table, where we assign 1 to the treatments where the main effect factor is present and 0 (as opposed to -1) when it is absent. Our goal is to confound the 2 interactions AD and BC with blocks, and we will find that a third factor is “naturally” confounded. We will go through the steps to construct the blocks, following Kuehl (2000, Section 11.4) that gives a detailed description.

1. Define the effects that will “manually” be used to confound with blocks. We use AD and BC here.
2. Set up a column for treatment labels, and k columns (4 in this case) for “coefficients” of the treatment labels for the contrast to be confounded: x_A, x_B, \dots

- Set up columns for the effects to be “manually confounded” (2 in this case), and for each, sum the “coefficients” from step 2 for that treatment (row) and that effect. $L_{AD} = x_A + x_D$ and $L_{BC} = x_B + x_C$
- Set up two columns that takes $(L_{AD} \text{ mod } 2)$ and $(L_{BC} \text{ mod } 2)$.
Note that $(0 \text{ mod } 2) = 0$, $(1 \text{ mod } 2) = 1$, and $(2 \text{ mod } 2) = 0$. It is “the remainder after division.”
- Group treatments that have common $(L_{AD} \text{ mod } 2)$ and $(L_{BC} \text{ mod } 2)$ into the same block.

Treatment	x_A	x_B	x_C	x_D	L_AD	L_BC	L_AD mod 2	L_BC mod 2	Block
(1)	0	0	0	0	0	0	0	0	1
a	1	0	0	0	1	0	1	0	2
b	0	1	0	0	0	1	0	1	3
ab	1	1	0	0	1	1	1	1	4
c	0	0	1	0	0	1	0	1	3
ac	1	0	1	0	1	1	1	1	4
bc	0	1	1	0	0	2	0	0	1
abc	1	1	1	0	1	2	1	0	2
d	0	0	0	1	1	0	1	0	2
ad	1	0	0	1	2	0	0	0	1
bd	0	1	0	1	1	1	1	1	4
abd	1	1	0	1	2	1	0	1	3
cd	0	0	1	1	1	1	1	1	4
acd	1	0	1	1	2	1	0	1	3
bcd	0	1	1	1	1	2	1	0	2
abcd	1	1	1	1	2	2	0	0	1

Thus, the 4 blocks would be as follows.

Block1	Block2	Block3	Block4
(1)	a	b	ab
bc	abc	c	ac
ad	d	abd	bd
abcd	bcd	acd	cd

Further, note that within each block, the treatments all have either an even or odd number of factors at their high levels (Blocks 1 and 4 are even, Blocks 2 and 3 are odd). Thus the 4-factor interaction, which is the “product” of the 2 interactions that were used to create the blocks. Many software packages can quickly construct designs such as these, making the actual process described here obsolete, yet interesting from a historical perspective.

10.2. Fractional Factorial Designs

In many “screening experiments,” there can be quite a few factors to be simultaneously varied. As the number of factors increases, the number of treatments or experimental runs needed to complete a full factorial gets very large very quickly (doubling with each additional two level factor). This can become cost prohibitive or simply impossible to be conducted. Fortunately, researchers are typically only interested in main effects and lower order interactions, and not particularly interested in the many higher order interactions. Thus, often, they can actually conduct only a fraction of the full factorial design. In general, we will label this a 2^{k-p} factorial design.

When running a fractional factorial, factors are confounded, or “aliased.” That is, their effects are indistinguishable. The goal is typically to be able to run a “small” experiment and still obtain estimates of main effects and lower order interactions, under the assumption that higher order interactions are negligible. Then, once a smaller set of important factors are identified, a follow up larger study will be conducted with those factors.

The mechanics of choosing factorial designs have been automated by design software, here we simply describe the process briefly, then discuss the nature of the aliasing. Then, we will go through a numeric example based on a larger, published study. The process begins by setting up incomplete blocks as described above. Next, one block is selected, and those treatments within the block are run in an experiment. If in the 2^4 case, we construct 2 blocks of 8 treatments, select one of them, we have a 2^{4-1} fractional factorial design. Consider the blocks described above that confounded the 4-way interactions.

Block1	(1)	ab	ac	bc	ad	bd	cd	abcd
Block2	a	b	c	abc	d	abd	acd	bcd

Suppose we flipped a coin, and chose to run Block 2 as a one-half fraction of the full factorial. Below we give the effect estimates for each effect.

$\hat{A} = \frac{1}{4}[(a + abc + abd + acd) - (b + c + d + bcd)]$	$\hat{B} = \frac{1}{4}[(b + abc + abd + bcd) - (a + c + d + acd)]$
$\hat{C} = \frac{1}{4}[(c + abc + acd + bcd) - (a + b + d + abd)]$	$\hat{D} = \frac{1}{4}[(d + abd + acd + bcd) - (a + b + c + abc)]$
$\hat{AB} = \frac{1}{4}[(c + abc + d + abd) - (a + b + acd + bcd)]$	$\hat{AC} = \frac{1}{4}[(b + abc + d + acd) - (a + c + abd + bcd)]$
$\hat{AD} = \frac{1}{4}[(b + c + abd + acd) - (a + abc + d + bcd)]$	$\hat{BC} = \frac{1}{4}[(a + abc + d + bcd) - (b + c + abd + acd)]$
$\hat{BD} = \frac{1}{4}[(a + c + abd + bcd) - (b + abc + d + acd)]$	$\hat{CD} = \frac{1}{4}[(a + b + acd + bcd) - (c + abc + d + abd)]$
$\hat{ABC} = \frac{1}{4}[(a + b + c + abc) - (d + abd + acd + bcd)]$	$\hat{ABD} = \frac{1}{4}[(a + b + d + abd) - (c + abc + acd + bcd)]$
$\hat{ACD} = \frac{1}{4}[(a + c + d + acd) - (b + abc + abd + bcd)]$	$\hat{BCD} = \frac{1}{4}[(b + c + d + bcd) - (a + abc + abd + acd)]$

Note the following equalities:

$\hat{A} = -\hat{BCD}$	$\hat{B} = -\hat{AC}$	$\hat{C} = -\hat{ABD}$	$\hat{D} = -\hat{ABC}$	$\hat{AB} = -\hat{CD}$	$\hat{AC} = -\hat{BD}$	$\hat{AD} = -\hat{BC}$
------------------------	-----------------------	------------------------	------------------------	------------------------	------------------------	------------------------

Note that the “negatives” occur because we selected the second of the 2 blocks; had we selected the first block, the pairs of effects would be the same, just the equalities would have been “positive.” The pattern goes as follows, where “I” acts as 1 in multiplication of labels. The “exponents” of the factor labels in the multiplications are based on mod 2 arithmetic. That is: $A^{(0 \bmod 2)} = A^0 = I$, $A^{(1 \bmod 2)} = A^1 = A$, $A^{(2 \bmod 2)} = A^0 = I$.

1. Set “I” equal to the effects used to create the incomplete blocks
2. If there were 2 blocks used, multiply them together using the mod 2 arithmetic described above, and the new created one is the “generalized interaction.” These $2 + 1 = 3 = 2^2 - 1$ effects are unestimable.
3. If there were 3 used, create generalized interactions based on all 3 pairs of effects used, as well as the product of all 3. These $3 + 3 + 1 = 7 = 2^3 - 1$ effects are unestimable
4. If there were p used, create generalized interactions based on all $\binom{p}{2}$ pairs, $\binom{p}{3}$ triples, ... 1 p -tuple.

These $2^p - 1$ effects are unestimable.

5. For each effect, multiply it by I, and the $2^p - 1$ effects generated above by the mod 2 arithmetic. Each effect is aliased with the $2^p - 1$ effects generated from the multiplication(s).

For this example, the 4-way interaction was confounded with blocks. By choosing Block 2, we chose the treatments where the coefficients of the terms for ABCD were negative as all treatments had an odd number of factors at their high levels. Thus, we have $I = -ABCD$. We obtain the alias structure directly as follows.

$$AI = A = -A^2BCD = -A^0BCD = -BCD \quad \text{similarly: } B = -ACD, C = -ABD, D = -ABC \quad AB = -CD, \text{ and so on.}$$

Next consider a quarter fraction, 2^{4-2} based on selecting block 3 from the above confounding structure, where AD and BC were confounded with blocks. Block 3 contained the following 4 treatments: b, c, abd, acd . Within these treatments, the AD coefficients are +1 and the BC coefficients are -1. The generalized interaction is the product of AD and -BC, or -ABCD. Thus, the defining relation is $I = AD = -BC = -ABCD$. We obtain the following aliases for estimable main effects and 2 way interactions.

$$A = D = -ABC = -BCD, \quad B = ABD = -C = ACD, \quad AB = BD = -AC = -CD$$

Clearly, this would be problematic in a practical setting as main effects are aliased with one another. There are many classes of fractional factorial designs that have been constructed. They are classified by their “resolution.” The most common are the following 3 types.

- **Resolution III:** No pairs of main effects are confounded, but main effects are confounded with 2-factor interactions, and pairs of 2-factor interactions are confounded.
- **Resolution IV:** No main effects are confounded with other main effects or 2-factor interactions, pairs of 2-factor interactions are confounded.
- **Resolution V:** No pairs of main effects or 2-factor interactions are confounded with one another, 2-factor interactions are confounded with 3-factor interactions.

The half-fraction 2^{4-1} with $I = -ABCD$ described above is Resolution IV, the quarter fraction 2^{4-2} meets none of these criteria.

Two major classes of fractional factorial designs that are widely applied are **Plackett-Burman Designs** and **Taguchi Orthogonal Arrays**. These layouts are available in many textbooks, software programs, and internet websites. We will include examples of both types below.

Plackett-Burman designs for 2-level factorial designs are used to estimate main effects when interactions can be ignored. They have a total of $N = 4m$ observations, where m is an integer, and there are up to $k = N-1$ factors. These designs can be extended to cases when all factors either 3,4,5, or 7 levels.

Taguchi Orthogonal arrays can be used when factors have either all the same or varying numbers of levels. They are designs that allow for having less than the full factorial possible treatments.

Example – 8 Factor Study of Beer Malting in 12 Runs – Plackett-Burman Design

A Plackett-Burman design in 12 runs can facilitate up to 11 2-level factors. The design, in terms of +/- 1^s is given below. A beer malting study (Meng, *et al* (2007)) had 8 factors, each at 2 levels: A = Steeping Temp (14,18C), B = Steeping Time (24,48hrs), C = Germination Temp (12,20C), D = Peroxide Hydrogen Conc (0,0.2g/l), E = Germination Time (4,8days), F = Withering Temp (35,50C), G = Drying Temp (55,65C), H = Kilning Temp (70,90C). The response measured was Superoxide Dismutase (SOD) Activity (U/g). The experiment consisted of taking 8 columns from the 11 factor Plackett-Burman Design.

Run	Factor1	Factor2	Factor3	Factor4	Factor5	Factor6	Factor7	Factor8	Factor9	Factor10	Factor11
1	1	1	-1	1	1	1	-1	-1	-1	1	-1
2	-1	1	1	-1	1	1	1	-1	-1	-1	1
3	1	-1	1	1	-1	1	1	1	-1	-1	-1
4	-1	1	-1	1	1	-1	1	1	1	-1	-1
5	-1	-1	1	-1	1	1	-1	1	1	1	-1
6	-1	-1	-1	1	-1	1	1	-1	1	1	1
7	1	-1	-1	-1	1	-1	1	1	-1	1	1
8	1	1	-1	-1	-1	1	-1	1	1	-1	1
9	1	1	1	-1	-1	-1	1	-1	1	1	-1
10	-1	1	1	1	-1	-1	-1	1	-1	1	1
11	1	-1	1	1	1	-1	-1	-1	1	-1	1
12	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1

The data for the malting experiment are given below, where $Y' = \frac{Y}{100}$ for ease of computational interpretations.

Run	A	B	C	D	E	F	G	H	Y	Y'=Y/100
1	1	-1	1	-1	-1	-1	1	1	1058	10.58
2	1	1	-1	1	-1	-1	-1	1	1107	11.07
3	-1	1	1	-1	1	-1	-1	-1	1254	12.54
4	1	-1	1	1	-1	1	-1	-1	911	9.11
5	1	1	-1	1	1	-1	1	-1	1122	11.22
6	1	1	1	-1	1	1	-1	1	1338	13.38
7	-1	1	1	1	-1	1	1	-1	1303	13.03
8	-1	-1	1	1	1	-1	1	1	980	9.80
9	-1	-1	-1	1	1	1	-1	1	706	7.06
10	1	-1	-1	-1	1	1	1	-1	642	6.42
11	-1	1	-1	-1	-1	1	1	1	1102	11.02
12	-1	-1	-1	-1	-1	-1	-1	-1	588	5.88
Effect	0.408	3.902	2.628	0.245	-0.045	-0.178	0.505	0.785	SS_Err	SS_Tot
SS{Effect}	0.500	45.669	20.724	0.180	0.006	0.095	0.765	1.849	0.442	70.231
SE{Effect}	0.222	0.222	0.222	0.222	0.222	0.222	0.222	0.222	MS_Err	
t{Effect}	1.843	17.608	11.862	1.106	-0.203	-0.805	2.279	3.543	0.147	
F{Effect}	3.396	310.047	140.698	1.223	0.041	0.648	5.194	12.551		

The effect, standard error, and sum of squares are computed as follows for Factor A.

$$\hat{A} = \left[\left(\frac{10.58 + 11.07 + 9.11 + 11.22 + 13.38 + 6.42}{6} \right) - \left(\frac{12.54 + 13.03 + 9.80 + 7.06 + 11.02 + 5.88}{6} \right) \right] =$$

$$= \frac{61.78 - 59.33}{6} = \frac{2.45}{6} = 0.4083 \quad MS_{Err} = \frac{SS_{Err}}{N - k - 1} = \frac{0.442}{12 - 8 - 1} = \frac{0.442}{3} = 0.1473$$

$$V\{\hat{A}\} = \left(\frac{1}{6} \right)^2 12\sigma^2 = \frac{\sigma^2}{3} \quad \text{In general: } V\{\hat{A}\} = \left(\frac{2}{N} \right)^2 N\sigma^2 = \frac{4\sigma^2}{N}$$

$$SE\{\hat{A}\} = \sqrt{\frac{4MS_{Err}}{N}} = \sqrt{\frac{4(0.1473)}{12}} = \sqrt{0.0491} = 0.2216$$

$$SS_A = 6 \left[\left(\bar{Y}_{Lo} - \frac{\bar{Y}_{Lo} + \bar{Y}_{Hi}}{2} \right)^2 + \left(\bar{Y}_{Hi} - \frac{\bar{Y}_{Lo} + \bar{Y}_{Hi}}{2} \right)^2 \right] = 6(2) \left(\frac{\bar{Y}_{Hi} - \bar{Y}_{Lo}}{2} \right)^2 = \frac{12}{4} (\hat{A})^2 = 3(0.4083)^2 = 0.5001$$

$$\text{In General: } SS_A = \frac{N}{2} (2) \left(\frac{1}{4} \right) (\hat{A})^2 = \frac{N}{4} (\hat{A})^2$$

The R program and corresponding output are given below.

R Program

```
malt_sod <- read.table("http://www.stat.ufl.edu/~winner/data/malt_sod_pb.dat",
  header=F,col.names=c("runnum","A","B","C","D","E","F","G","H","SOD"))
attach(malt_sod)

A <- factor(A); B <- factor(B); C <- factor(C); D <- factor(D)
E <- factor(E); F <- factor(F); G <- factor(G); H <- factor(H)
SODc <- SOD/100

options(contrasts=c("contr.sum","contr.poly"))
sod.mod1 <- aov(SODc ~ A+B+C+D+E+F+G+H)
anova(sod.mod1)
summary.lm(sod.mod1)
```

R Output

```
> anova(sod.mod1)
Analysis of Variance Table

Response: SODc
  Df Sum Sq Mean Sq  F value    Pr(>F)
A   1  0.500   0.500    3.3959 0.1625843
B   1 45.669  45.669   310.0466 0.0003993 ***
C   1 20.724  20.724   140.6979 0.0012884 **
D   1  0.180   0.180    1.2225 0.3495693
E   1  0.006   0.006    0.0412 0.8520634
F   1  0.095   0.095    0.6477 0.4797999
G   1  0.765   0.765    5.1941 0.1070284
H   1  1.849   1.849   12.5506 0.0382901 *
Residuals  3  0.442   0.147
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary.lm(sod.mod1)

Call:
aov(formula = SODc ~ A + B + C + D + E + F + G + H)

Residuals:
    1     2     3     4     5     6     7     8
0.28583 -0.23750  0.08750  0.03917  0.23750 -0.08750 -0.03917 -0.28583
    9    10    11    12
0.28583 -0.23750  0.03917 -0.08750

Coefficients:
(Intercept) 10.09250  0.11079  91.094 2.92e-06 ***
A1          -0.20417  0.11079  -1.843 0.162584
B1          -1.95083  0.11079 -17.608 0.000399 ***
C1          -1.31417  0.11079 -11.862 0.001288 **
D1          -0.12250  0.11079  -1.106 0.349569
E1           0.02250  0.11079   0.203 0.852063
F1           0.08917  0.11079   0.805 0.479800
G1          -0.25250  0.11079  -2.279 0.107028
H1          -0.39250  0.11079  -3.543 0.038290 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.3838 on 3 degrees of freedom
Multiple R-squared:  0.9937,    Adjusted R-squared:  0.9769
F-statistic: 59.22 on 8 and 3 DF,  p-value: 0.003238
```


Example – 3-Factors at 3 Levels: Grass Trimming Machine – Taguchi Orthogonal Array

An example of a 3^3 factorial design, conducted in $3^{3-1} = 9$ runs is an experiment with 3 factors, each at 3 levels in grass trimmers (Mallick (2010)). The factors are A: length of thread (1=100, 2=150, 3=200mm), B: engine speed (1=3000, 2=4000, 3=5000rpm), and C: material of handle (1=wood, 2=aluminum, 3=acrylonitrile butadiene styrene (ABS) pipe). The response was a hand-arm vibration score. A full factorial design would need $3^3 = 27$ runs. This is an example of a Taguchi L9 orthogonal array for a fractional factorial design. The design and data are given below.

Run	A	B	C	Y	Trt	Mean
1	1	1	1	2.348	A1	2.9687
2	1	2	2	4.350	A2	3.5567
3	1	3	3	2.208	A3	3.9270
4	2	1	3	2.729	B1	3.0923
5	2	2	1	4.410	B2	3.9987
6	2	3	2	3.531	B3	3.3613
7	3	1	2	4.200	C1	3.7010
8	3	2	3	3.236	C2	4.0270
9	3	3	1	4.345	C3	2.7243
					All	3.4841

Here, we will analyze the main effects analysis with the following model.

$$Y = \mu + \alpha_i + \beta_j + \gamma_k + \varepsilon \quad \sum_{i=1}^3 \alpha_i = \sum_{j=1}^3 \beta_j = \sum_{k=1}^3 \gamma_k = 0$$

We compute the Analysis of Variance, and test for main effects among factors A, B, and C.

$$\begin{aligned}
 SS_A &= 3 \left[(2.9687 - 3.4841)^2 + (3.5567 - 3.4841)^2 + (3.9270 - 3.4841)^2 \right] = \\
 &= 3 [0.2656 + 0.0053 + 0.1962] = 3(0.4671) = 1.4013 \quad df_A = 3 - 1 = 2 \quad MS_A = \frac{1.4013}{2} = 0.7007 \\
 SS_B &= 3 \left[(3.0923 - 3.4841)^2 + (3.9987 - 3.4841)^2 + (3.3613 - 3.4841)^2 \right] = \\
 &= 3 [0.1535 + 0.2648 + 0.0151] = 3(0.4334) = 1.3002 \quad df_B = 3 - 1 = 2 \quad MS_B = \frac{1.3002}{2} = 0.6501 \\
 SS_C &= 3 \left[(3.7010 - 3.4841)^2 + (4.0270 - 3.4841)^2 + (2.7243 - 3.4841)^2 \right] = \\
 &= 3 [0.0470 + 0.2947 + 0.5773] = 3(0.9190) = 2.7570 \quad df_C = 3 - 1 = 2 \quad MS_C = \frac{2.7570}{2} = 1.3785 \\
 SS_{Tot} &= \left[(2.348 - 3.4841)^2 + \dots + (4.345 - 3.4841)^2 \right] = 6.4138 \quad df_{Tot} = 9 - 1 = 8 \\
 SS_{Err} &= 6.4138 - 1.4013 - 1.3002 - 2.7570 = 0.9953 \quad df_{Err} = 8 - 3(2) = 2 \quad MS_{Err} = \frac{0.9953}{2} = 0.4777 \\
 F_A &= \frac{0.7007}{0.4777} = 1.4668 \quad F_B = \frac{0.6501}{0.4777} = 1.3609 \quad F_C = \frac{1.3785}{0.4777} = 2.8857 \quad F_{0.95;2,2} = 19.00
 \end{aligned}$$

Clearly, none of the effects are significant based on this very small experiment. We compute the effect estimates and standard errors, based on the matrix form of the model. First, we give the X matrix and β vector, then the estimates, standard errors and t-statistics, along with intermediate computations.

X0	A1	A2	B1	B2	C1	C2		Beta
1	1	0	1	0	1	0		μ
1	1	0	0	1	0	1		α_1
1	1	0	-1	-1	-1	-1		α_2
1	0	1	1	0	-1	-1		β_1
1	0	1	0	1	1	0		β_2
1	0	1	-1	-1	0	1		γ_1
1	-1	-1	1	0	0	1		γ_2
1	-1	-1	0	1	-1	-1		
1	-1	-1	-1	-1	1	0		

X'X								X'Y		
9	0	0	0	0	0	0	0	31.357		
0	6	3	0	0	0	0	0	-2.875		
0	3	6	0	0	0	0	0	-1.111		
0	0	0	6	3	0	0	0	-0.807		
0	0	0	3	6	0	0	0	1.912		
0	0	0	0	0	6	3	0	2.930		
0	0	0	0	0	3	6	0	3.908		
INV(X'X)								Beta-hat	StdErr	t
0.111111	0	0	0	0	0	0	0	3.4841	0.2304	15.1226
0	0.222222	-0.111111	0	0	0	0	0	-0.5154	0.3258	-1.5820
0	-0.111111	0.222222	0	0	0	0	0	0.0726	0.3258	0.2227
0	0	0	0.222222	-0.111111	0	0	0	-0.3918	0.3258	-1.2024
0	0	0	-0.111111	0.222222	0	0	0	0.5146	0.3258	1.5793
0	0	0	0	0	0.222222	-0.111111	0	0.2169	0.3258	0.6657
0	0	0	0	0	-0.111111	0.222222	0	0.5429	0.3258	1.6662
Y'IY	Ybar	Y'(1/n)JY	Y'PY	SS_Tot	SS_Reg	SS_Err	MS_Err			
115.6651	3.4841	109.2513	114.7097	6.4138	5.4584	0.9554	0.4777			

Below we give the R program and output for this analysis.

R Program

```

grasstrim <- read.table("http://www.stat.ufl.edu/~winner/data/grasstrim.dat",
  header=F,col.names=c("runnum","A","B","C","Y"))
attach(grasstrim)

A <- factor(A); B <- factor(B); C <- factor(C)
options(contrasts=c("contr.sum","contr.poly"))

grasstrim.mod1 <- aov(Y ~ A+B+C)
anova(grasstrim.mod1)
summary.lm(grasstrim.mod1)

```

R Output

```
> anova(grasstrim.mod1)
Analysis of Variance Table

Response: Y
      Df Sum Sq Mean Sq F value Pr(>F)
A       2  1.40129  0.70065  1.4667 0.4054
B       2  1.29999  0.65000  1.3606 0.4236
C       2  2.75709  1.37855  2.8857 0.2574
Residuals 2  0.95544  0.47772
> summary.lm(grasstrim.mod1)

Call:
aov(formula = Y ~ A + B + C)

Residuals:
     1     2     3     4     5     6     7     8     9
-0.4458  0.3239  0.1219  0.3239  0.1219 -0.4458  0.1219 -0.4458  0.3239

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.48411    0.23039  15.123  0.00434 **
A1          -0.51544    0.32582  -1.582  0.25447
A2           0.07256    0.32582   0.223  0.84445
B1          -0.39178    0.32582  -1.202  0.35224
B2           0.51456    0.32582   1.579  0.25504
C1           0.21689    0.32582   0.666  0.57412
C2           0.54289    0.32582   1.666  0.23759
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.6912 on 2 degrees of freedom
Multiple R-squared:  0.851,    Adjusted R-squared:  0.4041
F-statistic: 1.904 on 6 and 2 DF,  p-value: 0.3836
```

10.3. Analyzing Effects from Full and Fractional Factorial Designs

We have shown t-tests and F-tests for effects when there is an error term in the model. Note that these often have very few degrees of freedom in most cases. An alternative approach is based on the fact that if no effects exist in the population, the estimated effects will be normally distributed around a mean of 0. The normality of the effects is based on the assumption that the original measurements are normal. When the main effects and 2-factor interactions can be “independently” estimated, as in a full factorial, or Resolution V fractional factorial, we can make a normal probability plot of the main and 2-factor interaction effects to determine which, if any, are larger (positive or negative) than would be expected under the hypothesis of no effects. This method does not need an estimate of the error variance to be conducted.

Example – 2⁵⁻¹ Experiment on Crush Radius on Motorcycle Front Wheels

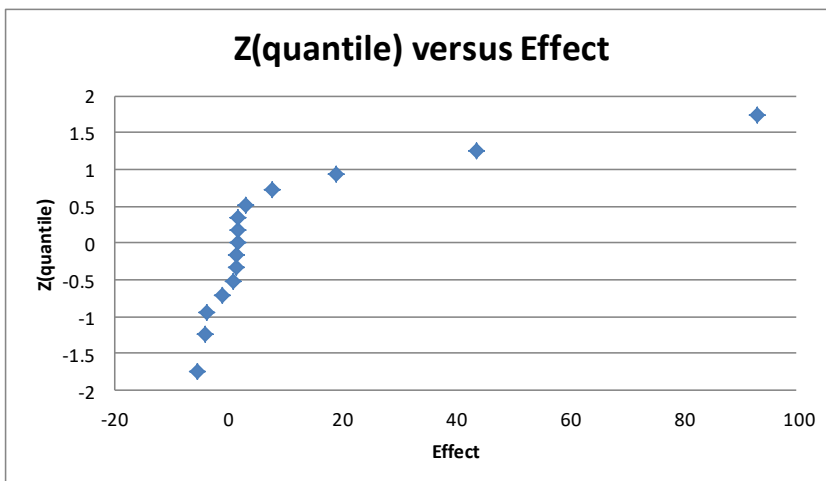
An experiment (Tan, *et al* (2009)) was conducted as a 2⁵⁻¹ fractional factorial with $r = 4$ replicates measuring crush radius on the front wheel of motorcycles. There were 5 factors in the study, S: impact speed (3, 6 meters/sec), M: impact mass (51.18, 108.33kg), P: tire pressure (148, 252kPa), G: striker contact geometry (0.03, 0.10 radius), and D: impact offset distance (0.0, 0.108 meters height). The 5-factor interaction was confounded with blocks (I=SMPGD), so that 2-factor interactions are confounded with 3-factor interactions and main effects are confounded with 4-factor interactions (Resolution V). We will work with the treatment means and standard deviations here. Note that due to replication, we can conduct the t- and F-tests along with the normal probability plots. The data, effect estimates, and t- and F-tests are given below.

Trt	S	M	P	G	D	SM	SP	SG	SD	MP	MG	MD	PG	PD	GD	Y_Mean	Y_SD
1	-1	-1	-1	-1	-1	1	1	1	1	-1	1	1	-1	1	-1	4.25	0.500
2	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	83.00	2.160
3	-1	1	-1	-1	-1	-1	-1	1	1	1	-1	-1	-1	1	1	38.00	2.449
4	1	1	-1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	-1	128.50	7.000
5	-1	-1	1	-1	-1	-1	1	-1	1	1	-1	1	1	-1	-1	3.50	0.577
6	1	-1	1	-1	-1	1	-1	1	-1	1	-1	1	-1	-1	1	73.00	6.683
7	-1	1	1	-1	-1	1	-1	-1	1	-1	1	-1	1	-1	1	19.00	2.449
8	1	1	1	-1	-1	1	1	1	-1	-1	1	-1	-1	-1	1	146.25	3.500
9	-1	-1	-1	-1	1	-1	1	1	-1	1	1	-1	1	-1	1	4.50	0.577
10	1	-1	-1	-1	1	1	-1	-1	1	1	1	-1	-1	-1	1	86.50	5.447
11	-1	1	-1	-1	1	1	-1	1	-1	-1	1	1	-1	-1	1	28.75	1.500
12	1	1	1	-1	1	-1	1	-1	1	-1	-1	1	-1	-1	1	144.50	3.873
13	-1	-1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	3.25	0.500
14	1	-1	1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	69.25	7.932
15	-1	1	1	1	1	-1	-1	-1	-1	1	1	1	-1	1	-1	28.00	3.367
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	143.25	2.754
Effect	93.125	43.625	-4.063	1.563	-3.813	19.063	1.375	1.625	0.875	3.250	1.625	-5.500	-1.063	1.688	7.688	SS_Err	757.5
SE{Effect}	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993	df_Err	48
t{Effect}	93.768	43.926	-4.091	1.573	-3.839	19.194	1.384	1.636	0.881	3.272	1.636	-5.538	-1.070	1.699	7.741	MS_Err	15.781
SS{Effect}	138756.3	30450.3	264.1	39.1	232.6	5814.1	30.3	42.3	12.3	169.0	42.3	484.0	18.1	45.6	945.6		
F{Effect}	8792.475	1929.521	16.733	2.475	14.737	368.416	1.917	2.677	0.776	10.709	2.677	30.669	1.145	2.887	59.917		

We order and rank the effects from smallest (large/negative) to largest (large/positive). Next, obtain the

“quantile” for each effect: $q = \frac{\text{rank} - 0.375}{\text{\#effects} + 0.25}$ and the “z-score” corresponding to each quantile. Finally, plot the effects on the X-axis versus the z-scores on the y-axis.

Label	Effect	Rank	quantile	Z(qntl)	Effect	Z(qntl)
MD	-5.5	1	0.040984	-1.73938	-5.5	-1.73938
P	-4.0625	2	0.106557	-1.24505	-4.0625	-1.24505
D	-3.8125	3	0.172131	-0.94578	-3.8125	-0.94578
PG	-1.0625	4	0.237705	-0.7137	-1.0625	-0.7137
SD	0.875	5	0.303279	-0.51499	0.875	-0.51499
SP	1.375	6	0.368852	-0.33489	1.375	-0.33489
G	1.5625	7	0.434426	-0.16512	1.5625	-0.16512
SG	1.625	8	0.5	0	1.625	0
MG	1.625	9	0.565574	0.165116	1.625	0.165116
PD	1.6875	10	0.631148	0.334894	1.6875	0.334894
MP	3.25	11	0.696721	0.514994	3.25	0.514994
GD	7.6875	12	0.762295	0.713705	7.6875	0.713705
SM	19.0625	13	0.827869	0.945777	19.0625	0.945777
M	43.625	14	0.893443	1.245046	43.625	1.245046
S	93.125	15	0.959016	1.739384	93.125	1.739384



The largest three effects (S, M, and SM) are clearly well away from the “line” formed by the remaining effects. The R Program for the analysis is given below.

R Program

```

mw <- read.table("http://www.stat.ufl.edu/~winner/data/mtrcyclewheel.dat",
  header=F,col.names=c("Mw.trt","S","M","P","G","D","Y","runorder"))
attach(mw)

S <- factor(S); M <- factor(M); P <- factor(P); G <- factor(G); D <- factor(D)

options(contrasts=c("contr.sum","contr.poly"))

mw.mod1 <- aov(Y ~ S+M+P+G+D+S:M+S:P+S:G+S:D+M:P+M:G+M:D+P:G+P:D+G:D)
anova(mw.mod1)
summary.lm(mw.mod1)

effects.mod1 <- coefficients(mw.mod1)[-1]      ### Removes mean estimate
effects.mod1 <- 2*effects.mod1                ### Effects are 2*beta
effects.mod1[1:5] <- -1*effects.mod1[1:5]     ### Main effects are -2*beta
effects.mod1

qqnorm(effects.mod1); qqline(effects.mod1)

```

R Output

```

> anova(mw.mod1)
Analysis of Variance Table

Response: Y

```

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
S	1	138756	138756	8792.4752	< 2.2e-16	***
M	1	30450	30450	1929.5208	< 2.2e-16	***
P	1	264	264	16.7327	0.0001635	***
G	1	39	39	2.4752	0.1222203	
D	1	233	233	14.7366	0.0003615	***
S:M	1	5814	5814	368.4158	< 2.2e-16	***
S:P	1	30	30	1.9168	0.1726091	
S:G	1	42	42	2.6772	0.1083340	
S:D	1	12	12	0.7762	0.3826847	
M:P	1	169	169	10.7089	0.0019797	**
M:G	1	42	42	2.6772	0.1083340	
M:D	1	484	484	30.6693	1.263e-06	***
P:G	1	18	18	1.1446	0.2900425	
P:D	1	46	46	2.8871	0.0957632	.
G:D	1	946	946	59.9168	5.442e-10	***
Residuals	48	757	16			

```

---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary.lm(mw.mod1)

Coefficients:

```

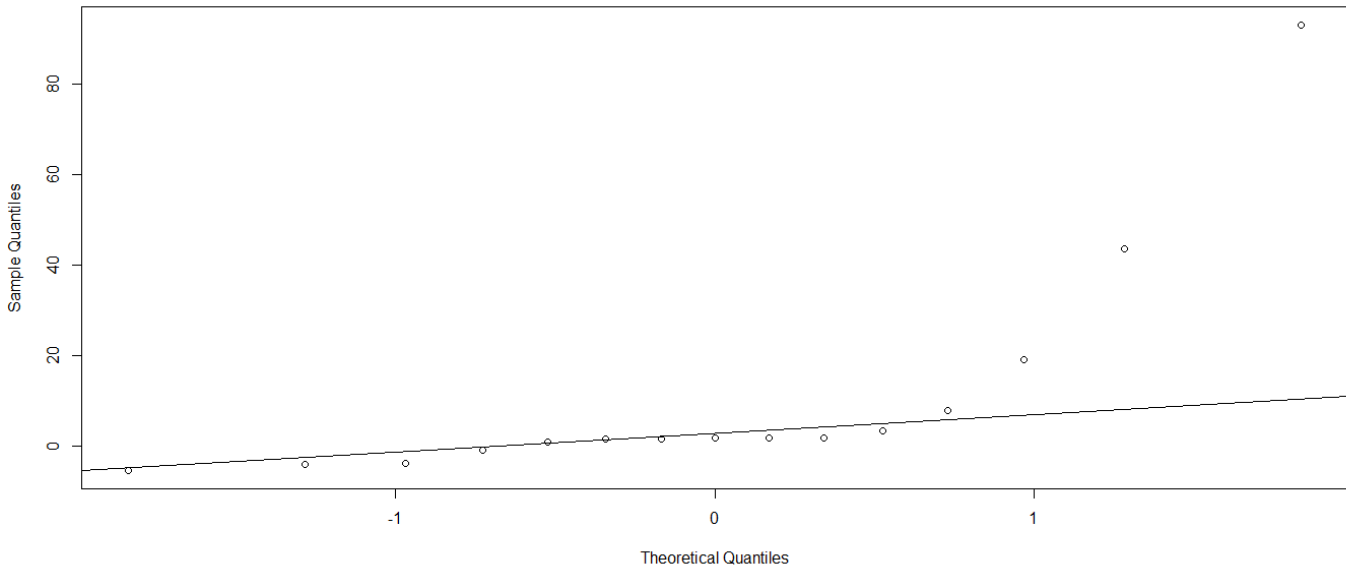
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	62.7188	0.4966	126.304	< 2e-16 ***
S1	-46.5625	0.4966	-93.768	< 2e-16 ***
M1	-21.8125	0.4966	-43.926	< 2e-16 ***
P1	2.0313	0.4966	4.091	0.000163 ***
G1	-0.7812	0.4966	-1.573	0.122220
D1	1.9062	0.4966	3.839	0.000361 ***
S1:M1	9.5312	0.4966	19.194	< 2e-16 ***
S1:P1	0.6875	0.4966	1.384	0.172609
S1:G1	0.8125	0.4966	1.636	0.108334
S1:D1	0.4375	0.4966	0.881	0.382685
M1:P1	1.6250	0.4966	3.272	0.001980 **
M1:G1	0.8125	0.4966	1.636	0.108334
M1:D1	-2.7500	0.4966	-5.538	1.26e-06 ***
P1:G1	-0.5312	0.4966	-1.070	0.290042
P1:D1	0.8438	0.4966	1.699	0.095763 .
G1:D1	3.8437	0.4966	7.741	5.44e-10 ***

```

Residual standard error: 3.973 on 48 degrees of freedom
Multiple R-squared:  0.9957,    Adjusted R-squared:  0.9944
F-statistic: 749.2 on 15 and 48 DF,  p-value: < 2.2e-16

```

Normal Q-Q Plot



Note that the **qqnorm** and **qqline** options put the effects on the vertical axis and the theoretical quantiles on the horizontal axis. The three largest effects show up very clearly on the plot.

10.4. Response Surface Designs

When all factors are numeric and have more than 2 levels, experimentation is often conducted to optimize (maximize or minimize) the mean response. The model is fit as a polynomial regression. Two widely used classes of response surface designs are **Central Composite Designs (CCD)** and **Box-Behnken Designs (BBD)**. As with fractional factorial designs, there are many textbooks, software packages, and internet websites that have these designs for various numbers of factors. In virtually all cases, regardless of the units and levels that the original factors take on, the designs are typically “coded” with each factor centered at 0. The models are usually second order polynomials including main effects, 2-factor interactions, and quadratic terms. Occasionally third order polynomial models are fit. The second order model is as follows.

$$E\{Y\} = \beta_0 + \sum_{i=1}^k \beta_i X_i + \sum_{i=1}^{k-1} \sum_{i'=i+1}^k \beta_{ii'} X_i X_{i'} + \sum_{i=1}^k \beta_{ii} X_i^2 = \beta_0 + \mathbf{x}'\boldsymbol{\beta}_1 + \mathbf{x}'\boldsymbol{\beta}_2 \mathbf{x}$$

where: $\mathbf{x} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_k \end{bmatrix}$ $\boldsymbol{\beta}_1 = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}$ $\boldsymbol{\beta}_2 = \begin{bmatrix} \beta_{11} & \beta_{12}/2 & \cdots & \beta_{1k}/2 \\ \beta_{12}/2 & \beta_{22} & \cdots & \beta_{2k}/2 \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{1k}/2 & \beta_{2k}/2 & \cdots & \beta_{kk} \end{bmatrix}$

$$\text{Fitted (OLS) Values: } \hat{Y} = \hat{\beta}_0 + \sum_{i=1}^k \hat{\beta}_i X_i + \sum_{i=1}^{k-1} \sum_{i'=i+1}^k \hat{\beta}_{ii'} X_i X_{i'} + \sum_{i=1}^k \hat{\beta}_{ii} X_i^2 = \hat{\beta}_0 + \mathbf{x}'\hat{\boldsymbol{\beta}}_1 + \mathbf{x}'\hat{\boldsymbol{\beta}}_2 \mathbf{x}$$

$$\frac{\partial \hat{Y}}{\partial \mathbf{x}} = \hat{\boldsymbol{\beta}}_1 + 2\hat{\boldsymbol{\beta}}_2 \mathbf{x} \stackrel{\text{set}}{=} \mathbf{0} \Rightarrow \mathbf{x}^* = -\frac{1}{2} \hat{\boldsymbol{\beta}}_2^{-1} \hat{\boldsymbol{\beta}}_1$$

is the "optimal" point for maximizing or minimizing the surface.

Central Composite Designs

In a central composite design, typically we begin with k factors, each at 3 equally spaced levels, coded as -1/0/+1. A 2^k factorial is set up at each combination of +/-1 for the k factors, then there are $2k$ points with all but 1 factor at its 0 level and the remaining factor at +/- α where α is commonly $\sqrt{2}$ or $\sqrt{3}$, finally there are c center points where all factors are at their 0 levels. The center points allow for a goodness-of-fit F-test to be conducted.

Example – 3 Factor CCD to Optimize Moisture Content in Fried Potato Chips

An experiment (Song, *et al* (2007)) had three factors, A: Vacuum microwave pre-drying time (minutes), B: Vacuum Temperature (°C), and C: Frying Time (minutes). The $k = 3$ “axial” points were set at $\alpha = 1.682$. The data, design and coded levels are given below. There were 3 response variables: Moisture Content, Fat Content, and Breaking Strength. We will analyze Moisture Content. Note that there are $c = 6$ center points.

Run	A	B	C	Moisture	Fat	Break	Level	A	B	C
1	-1	-1	-1	27.52	23.12	1337.2	-1.682	0.95	83.18	11.59
2	-1	-1	1	9.08	28.69	974.6	-1	3	90	15
3	-1	1	-1	14.55	27.82	886.7	0	6	100	20
4	-1	1	1	8.13	32.56	748.9	1	9	110	25
5	1	-1	-1	13.95	17.04	1040.3	1.682	11.05	116.82	28.41
6	1	-1	1	8.57	20.97	813.1				
7	1	1	-1	3.28	20.42	719.3				
8	1	1	1	2.97	24.98	656.8				
9	-1.682	0	0	13.02	27.58	1007.8				
10	1.682	0	0	6.87	19.01	903.3				
11	0	-1.682	0	16.08	20.85	1153.4				
12	0	1.682	0	6.03	24.92	488.5				
13	0	0	-1.682	17.69	20.39	1308				
14	0	0	1.682	5.52	24.32	517.3				
15	0	0	0	7.9	22.83	759.9				
16	0	0	0	8.01	23.94	682				
17	0	0	0	7.73	21.27	715				
18	0	0	0	7.86	21.88	735.2				
19	0	0	0	8.13	22.56	636				
20	0	0	0	8.05	22.98	652.7				

The matrix form of this analysis is given below. The X matrix has a column for the intercept, 3 columns for linear effects, 3 columns for 2-factor interactions, and 3 columns for quadratic terms.

X										Y
1	-1	-1	-1	1	1	1	1	1	1	27.52
1	-1	-1	1	1	1	-1	-1	1	1	9.08
1	-1	1	-1	-1	1	-1	1	1	1	14.55
1	-1	1	1	-1	-1	1	1	1	1	8.13
1	1	-1	-1	-1	-1	1	1	1	1	13.95
1	1	-1	1	1	-1	1	-1	1	1	8.57
1	1	1	-1	1	-1	-1	1	1	1	3.28
1	1	1	1	1	1	1	1	1	1	2.97
1	-1.682	0	0	0	0	0	2.829124	0	0	13.02
1	1.682	0	0	0	0	0	2.829124	0	0	6.87
1	0	-1.682	0	0	0	0	0	2.829124	0	16.08
1	0	1.682	0	0	0	0	0	2.829124	0	6.03
1	0	0	-1.682	0	0	0	0	0	2.829124	17.69
1	0	0	1.682	0	0	0	0	0	2.829124	5.52
1	0	0	0	0	0	0	0	0	0	7.9
1	0	0	0	0	0	0	0	0	0	8.01
1	0	0	0	0	0	0	0	0	0	7.73
1	0	0	0	0	0	0	0	0	0	7.86
1	0	0	0	0	0	0	0	0	0	8.13
1	0	0	0	0	0	0	0	0	0	8.05

The ordinary least squares estimates, and intermediate calculations are given below. Further, we give the Analysis of Variance, with sequential blocks: linear, 2-factor interactions, and quadratic terms.

X\X										X\Y			
20	0	0	0	0	0	0	13.65825	13.65825	13.65825		200.94		
0	13.65825	0	0	0	0	0	0	0	0		-40.8543		
0	0	13.65825	0	0	0	0	0	0	0		-47.0941		
0	0	0	13.65825	0	0	0	0	0	0		-51.0199		
0	0	0	0	8	0	0	0	0	0		-2.35		
0	0	0	0	0	8	0	0	0	0		19.17		
0	0	0	0	0	0	8	0	0	0		17.09		
13.65825	0	0	0	0	0	0	24.00789	8	8		144.3213		
13.65825	0	0	0	0	0	0	8	24.00789	8		150.6019		
13.65825	0	0	0	0	0	0	8	8	24.00789		153.714		
INV(X\X)											Beta-hat	Std Error	t
0.166343	0	0	0	0	0	0	-0.05679	-0.05679	-0.05679		7.947906	0.596584	13.32237
0	0.073216	0	0	0	0	0	0	0	0		-2.99118	0.395796	-7.55738
0	0	0.073216	0	0	0	0	0	0	0		-3.44803	0.395796	-8.71164
0	0	0	0.073216	0	0	0	0	0	0		-3.73547	0.395796	-9.43785
0	0	0	0	0.125	0	0	0	0	0		-0.29375	0.517159	-0.56801
0	0	0	0	0	0.125	0	0	0	0		2.39625	0.517159	4.633487
0	0	0	0	0	0	0.125	0	0	0		2.13625	0.517159	4.13074
-0.05679	0	0	0	0	0	0	0.069365	0.006895	0.006895		0.698212	0.385246	1.812381
-0.05679	0	0	0	0	0	0	0.006895	0.069365	0.006895		1.09056	0.385246	2.830816
-0.05679	0	0	0	0	0	0	0.006895	0.006895	0.069365		1.284966	0.385246	3.335446
Y\Y	Ybar	Y'(1/n)Y	Y'PY	SS_Tot	SS_Err	SS_Reg	df_Err	MS_Err					
2639.276	10.047	2018.844	2617.88	620.4318	21.39628	599.0355	10	2.139628					
B1		B2				INV(B2)				X*	Original*		
-2.99118		0.698212	-0.14688	1.198125		-0.14572	-0.82162	0.818835		-0.10505	5.684862		
-3.44803		-0.14688	1.09056	1.068125		-0.82162	0.301194	0.515722		0.253694	102.5369		
-3.73547		1.198125	1.068125	1.284966		0.818835	0.515722	-0.41396		1.340592	26.70296		

Model	SS_Tot	SS_Err	SS_Reg	#Parms	df_Err
Linear	620.4318	145.2638	475.1680	4	16
Linear, 2-FI	620.4318	62.1289	558.3029	7	13
Linear, 2-FI, Quadratic	620.4318	21.3963	599.0355	10	10

First, we test whether the linear terms are significant as a group (we know they are from the t-tests). Second, we test whether the 2-factor interactions are significant, given a model containing linear terms. Third, we test whether the quadratic terms are significant, given the linear and 2-factor interaction terms.

$$\text{Model 1: } E\{Y\} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$$

$$\text{Model 2: } E\{Y\} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3$$

$$\text{Model 3: } E\{Y\} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \beta_{33} X_3^2$$

$$\text{Model 1: } H_0^1 : \beta_1 = \beta_2 = \beta_3 = 0 \quad \text{Test Stat: } F_{obs}^1 = \frac{\left[\frac{475.1680}{3} \right]}{\left[\frac{145.2638}{16} \right]} = \frac{158.3893}{9.0790} = 17.45 \quad F_{0.95;3,16} = 3.24$$

$$\text{Model 2: } H_0^2 : \beta_{12} = \beta_{13} = \beta_{23} = 0 \quad \text{Test Stat: } F_{obs}^2 = \frac{\left[\frac{145.2638 - 62.1289}{16 - 13} \right]}{\left[\frac{62.1289}{13} \right]} = \frac{27.7116}{4.7791} = 5.80 \quad F_{0.95;3,13} = 3.41$$

$$\text{Model 3: } H_0^3 : \beta_{11} = \beta_{22} = \beta_{33} = 0 \quad \text{Test Stat: } F_{obs}^3 = \frac{\left[\frac{62.1289 - 21.3963}{13 - 10} \right]}{\left[\frac{21.3963}{10} \right]} = \frac{13.5775}{2.1396} = 6.35 \quad F_{0.95;3,10} = 3.71$$

All 3 “groups” of parameters are significant.

We next conduct the F-test for lack-of-fit for the second order model. This is an extension of the test conducted for simple linear regression models. The test involves decomposing the error sum of squares into “pure error” which represents variation of individual measurements at the same X-levels and “lack of fit” which represents differences between fitted values and group means. For this example, the overall sample size is $n = 20$, there are $c = 15$ distinct X-levels (14 distinct combinations, 6 replicates at the center). The regression model for the second order response surface has $p' = 10$ parameters. The EXCEL spreadsheet is given below, along with the formula for the test.

Y	Yhat	GrpMean	Residual	PureError	LackFit
27.52	25.4351	27.5200	2.0849	0.0000	2.0849
9.08	8.8991	9.0800	0.1809	0.0000	0.1809
14.55	14.8540	14.5500	-0.3040	0.0000	-0.3040
8.13	6.8631	8.1300	1.2669	0.0000	1.2669
13.95	15.2477	13.9500	-1.2977	0.0000	-1.2977
8.57	8.2968	8.5700	0.2732	0.0000	0.2732
3.28	3.4916	3.2800	-0.2116	0.0000	-0.2116
2.97	5.0857	2.9700	-2.1157	0.0000	-2.1157
13.02	14.9544	13.0200	-1.9344	0.0000	-1.9344
6.87	4.8921	6.8700	1.9779	0.0000	1.9779
16.08	16.8328	16.0800	-0.7528	0.0000	-0.7528
6.03	5.2336	6.0300	0.7964	0.0000	0.7964
17.69	17.8663	17.6900	-0.1763	0.0000	-0.1763
5.52	5.3002	5.5200	0.2198	0.0000	0.2198
7.9	7.9479	7.9467	-0.0479	-0.0467	-0.0012
8.01	7.9479	7.9467	0.0621	0.0633	-0.0012
7.73	7.9479	7.9467	-0.2179	-0.2167	-0.0012
7.86	7.9479	7.9467	-0.0879	-0.0867	-0.0012
8.13	7.9479	7.9467	0.1821	0.1833	-0.0012
8.05	7.9479	7.9467	0.1021	0.1033	-0.0012
		Sum	0.0000	0.0000	0.0000
		SumSq	21.3963	0.1049	21.2913
		df	10.0000	5.0000	5.0000
		MeanSq	2.1396	0.0210	4.2583
		F(LOF)	202.9036		
		F(0.95)	5.0503		

There is strong evidence that the second order polynomial model does not give an adequate fit. A higher order model may fit better.

The second order model fits better for the responses: fat content and breaking strength.

of Distinct X-Levels: c @ j^{th} level: Sample Size = n_j Fitted Value = \hat{Y}_j Mean Value = \bar{Y}_j

of Parameters in Regression Model = p' Overall Sample Size: $n = \sum_{j=1}^c n_j$

$$Y_{ij} - \hat{Y}_j = (Y_{ij} - \bar{Y}_j) + (\bar{Y}_j - \hat{Y}_j) \Rightarrow (Y_{ij} - \hat{Y}_j)^2 = (Y_{ij} - \bar{Y}_j)^2 + (\bar{Y}_j - \hat{Y}_j)^2 + 2(Y_{ij} - \bar{Y}_j)(\bar{Y}_j - \hat{Y}_j)$$

$$\begin{aligned} \Rightarrow \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \hat{Y}_j)^2 &= \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \bar{Y}_j)^2 + \sum_{j=1}^c \sum_{i=1}^{n_j} (\bar{Y}_j - \hat{Y}_j)^2 + 2 \sum_{j=1}^c (\bar{Y}_j - \hat{Y}_j) \sum_{i=1}^{n_j} (Y_{ij} - \bar{Y}_j) = \\ &= \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \bar{Y}_j)^2 + \sum_{j=1}^c n_j (\bar{Y}_j - \hat{Y}_j)^2 + 0 \end{aligned}$$

$$\text{Error Sum of Squares: } SS_{\text{Err}} = \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \hat{Y}_j)^2 \quad df_{\text{Err}} = n - p'$$

$$\text{Pure Error Sum of Squares: } SS_{\text{PE}} = \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \bar{Y}_j)^2 \quad df_{\text{PE}} = n - c$$

$$\text{Lack of Fit Sum of Squares: } SS_{\text{LF}} = \sum_{j=1}^c \sum_{i=1}^{n_j} (\bar{Y}_j - \hat{Y}_j)^2 = \sum_{j=1}^c n_j (\bar{Y}_j - \hat{Y}_j)^2 \quad df_{\text{LF}} = c - p'$$

$$H_0: E\{Y\} = \beta_0 + \sum_{i=1}^k \beta_i X_i + \sum_{i=1}^{k-1} \sum_{i'=i+1}^k \beta_{ii'} X_i X_{i'} + \sum_{i=1}^k \beta_{ii} X_i^2 \quad \text{Test Stat: } F_{\text{LF}} = \frac{\left[\frac{SS_{\text{LF}}}{c - p'} \right]}{\left[\frac{SS_{\text{PE}}}{n - c} \right]} = \frac{MS_{\text{LF}}}{MS_{\text{PE}}} \stackrel{H_0}{\sim} F_{c-p', n-c}$$

Below we give the R Program and Output for this analysis. It makes use of the **rsm** package which provides a very simple way to analyze a response design. Note that the program uses the data in its original units. We will transform the coded values to the original values in the program.

R Program

```
potato <- read.table("http://www.stat.ufl.edu/~winner/data/potatochip_dry_rsm.dat",
  header=F,col.names=c("runnum","c.drytime","c.frytemp","c.frytime","moist","fat","break"))
attach(potato)

drytime <- 6 + 3*c.drytime          ### Center = 6  -1 = 3, +1 = 9
frytemp <- 100 + 10*c.frytemp      ### Center = 100  -1 = 90, +1 = 110
frytime <- 20 + 5*c.frytime        ### Center = 20  -1 = 15, +1 = 25

library(rsm)

potato.rsm1 <- rsm(moist ~ so(drytime,frytemp,frytime))    ### so => 2nd Order
summary(potato.rsm1)

par(mfrow=c(1,3))
contour(potato.rsm1, ~ drytime + frytemp + frytime, at=xs(potato.rsm1))
```

R Output

```
> summary(potato.rsm1)
```

```
Call:
rsm(formula = moist ~ so(drytime, frytemp, frytime))
```

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	294.5057444	46.1240767	6.3851	7.984e-05	***
drytime	-4.1438432	1.9309149	-2.1461	0.0574458	.
frytemp	-3.3216726	0.8054280	-4.1241	0.0020635	**
frytime	-8.0340392	1.2242603	-6.5624	6.373e-05	***
drytime:frytemp	-0.0097917	0.0172386	-0.5680	0.5825583	
drytime:frytime	0.1597500	0.0344773	4.6335	0.0009312	***
frytemp:frytime	0.0427250	0.0103432	4.1307	0.0020418	**
drytime^2	0.0775791	0.0428051	1.8124	0.1000131	
frytemp^2	0.0109056	0.0038525	2.8308	0.0178269	*
frytime^2	0.0513986	0.0154098	3.3354	0.0075482	**

```
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Multiple R-squared:  0.9655,    Adjusted R-squared:  0.9345
F-statistic: 31.11 on 9 and 10 DF,  p-value: 3.765e-06
```

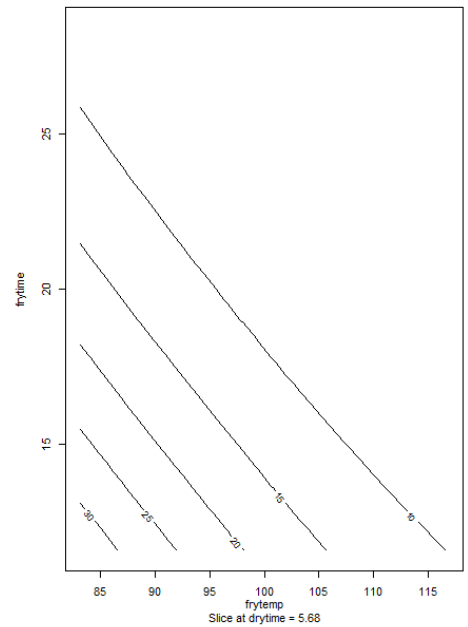
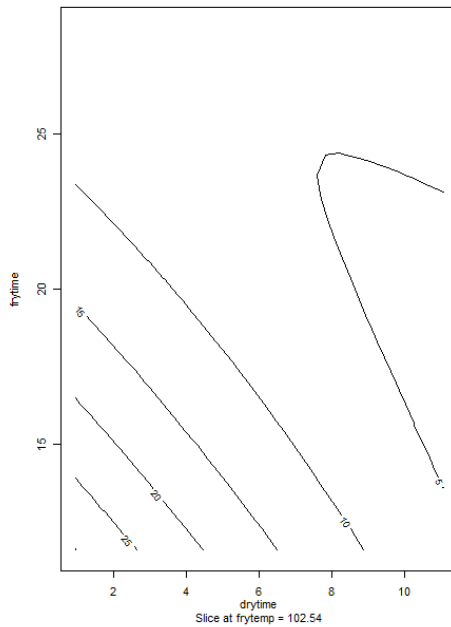
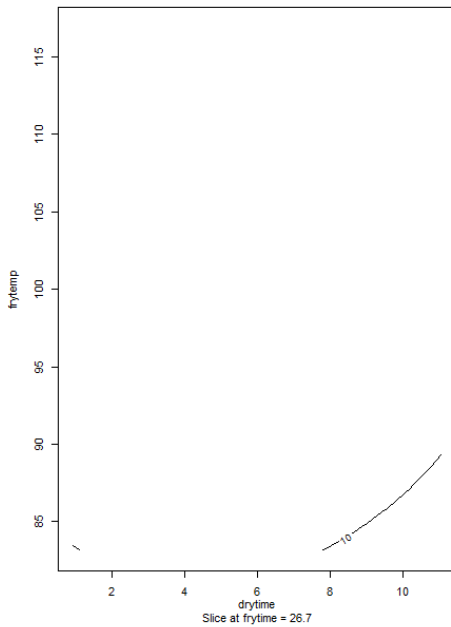
Analysis of Variance Table

Response: moist

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
FO(drytime, frytemp, frytime)	3	475.17	158.389	74.0266	3.948e-07
TWI(drytime, frytemp, frytime)	3	83.13	27.712	12.9516	0.0008857
PQ(drytime, frytemp, frytime)	3	40.73	13.578	6.3457	0.0110668
Residuals	10	21.40	2.140		
Lack of fit	5	21.29	4.258	202.9036	9.102e-06
Pure error	5	0.10	0.021		

Stationary point of response surface:

drytime	frytemp	frytime
5.684862	102.536941	26.702959



Example – CCD for Orange Juice Emulsions with 3 Factors Run in 3 Blocks

A study (Mirrhosseini and Tan (2010)) for Orange Juice emulsions was run as a CCD with 3 factors, 5 measured responses, and was run in 3 blocks. The factors were A: Gum Arabic (10.78, 13, 16.6, 20, 22.22 g/kg), B: Xanthan Gum (0.24, 0.30, 0.40, 0.50, 0.56 g/kg), and C: Orange Oil (8.73, 10, 12, 14, 15.27 g/kg). The five responses were: Y_1 = Turbidity (NTU), Y_2 = Droplet Size (nanometers), Y_3 = Polydispersity Index, Y_4 = Viscosity (mPa s), Y_5 = Density (g/cm³). The experiment was run in 3 blocks, and the data, R Program, and R Output are given below for Y_4 .

Block	A	B	C	Block1	Block2	Block3	Y1	Y2	Y3	Y4	Y5
1	20	0.5	10	1	0	0	186	1329	0.406	250.1	1.048
1	13	0.5	14	1	0	0	420	1336	0.287	230.0	1.020
1	13	0.3	10	1	0	0	168	1036	0.251	91.8	1.025
1	16.5	0.4	12	1	0	0	281	1238	0.304	178.8	1.032
1	20	0.3	14	1	0	0	385	1260	0.248	272.9	1.029
1	16.5	0.4	12	1	0	0	290	1233	0.302	181.5	1.040
2	13	0.5	10	0	1	0	185	1175	0.315	223.8	1.030
2	20	0.5	14	0	1	0	362	1572	0.295	436.4	1.036
2	20	0.3	10	0	1	0	184	1325	0.301	240.8	1.049
2	13	0.3	14	0	1	0	311	1264	0.295	176.7	1.020
2	16.5	0.4	12	0	1	0	267	1340	0.310	221.1	1.034
2	16.5	0.4	12	0	1	0	277	1350	0.321	219.0	1.035
3	16.5	0.4	12	0	0	1	253	1339	0.304	205.0	1.036
3	16.5	0.4	12	0	0	1	259	1337	0.324	223.8	1.032
3	16.5	0.24	12	0	0	1	252	1218	0.270	163.2	1.038
3	10.78	0.4	12	0	0	1	215	1203	0.289	205.5	1.019
3	16.5	0.4	15.27	0	0	1	417	1411	0.285	270.0	1.027
3	16.5	0.4	8.73	0	0	1	117	1176	0.319	168.9	1.041
3	22.22	0.4	12	0	0	1	262	1465	0.266	366.2	1.052
3	16.5	0.56	12	0	0	1	312	1466	0.335	325.1	1.033

R Program

```
oj <- read.table("http://www.stat.ufl.edu/~winner/data/orange_emul.dat",
header=F,col.names=c("blk","A","B","C","blk1","blk2","blk3","Y1","Y2","Y3","Y4","Y5"))
attach(oj)

blk <- factor(blk)

library(rsm)

oj.rsm <- rsm(Y4 ~ blk + SO(A,B,C))
summary(oj.rsm)
```

R Output

```

              Estimate Std. Error t value Pr(>|t|)
(Intercept) 1005.53717  226.86959  4.4322 0.0021905 **
blk2         52.11667    6.65863  7.8269 5.110e-05 ***
blk3         40.39077    6.22918  6.4841 0.0001913 ***
A           -81.66915   12.00906 -6.8006 0.0001377 ***
B           -950.94969  407.96903 -2.3309 0.0480914 *
C           -49.86300   22.85059 -2.1821 0.0606605 .
A:B         -4.46429   11.65017 -0.3832 0.7115570
A:C          2.27321    0.58251  3.9025 0.0045289 **
B:C          47.18750   20.38780  2.3145 0.0493415 *
AA2          2.18287    0.25860  8.4411 2.961e-05 ***
BA2         1160.92688  327.43806  3.5455 0.0075591 **
CA2          0.46948    0.79142  0.5932 0.5694284

Multiple R-squared:  0.9904,    Adjusted R-squared:  0.9772
F-statistic: 74.89 on 11 and 8 DF,  p-value: 7.847e-07

Analysis of Variance Table
Response: Y4
          Df Sum Sq Mean Sq  F value    Pr(>F)
blk       2   9097  4548.3   34.1944 0.0001203
FO(A, B, C) 3  87023 29007.6  218.0827 5.215e-08
TWI(A, B, C) 3   2758   919.2    6.9110 0.0130330
PQ(A, B, C) 3  10699  3566.3   26.8119 0.0001587
Residuals  8   1064   133.0
Lack of fit 4    190    47.5    0.2173 0.9158017
Pure error  4     874   218.5

Stationary point of response surface:
          A          B          C
13.0138170 0.2042318 11.3345823
```

Box-Behnken Designs

Box-Behnken Designs (BBD) are widely used for response surfaces and were first generated by Box and Behnken (1960). The designs involve k factors, each at 3 equally spaced numeric levels, coded as -1/0/+1. The design involves 2^k factorials at the extreme -1/+1 in incomplete blocks of size 2, augmented with multiple center points with each factor at its 0 level. In the “incomplete blocks” the $k-2$ “excluded” factors are at their 0 level. The analysis is just as that for the CCD, so we only present two examples of the design, and only include the statistical analysis based on the **rsm** package in R.

Example – Gels of Diclofenac and Curcumin for Transdermal Drug Delivery

A study (Chaudhary, *et al* (2011)) had 3 factors, each at 3 levels. The factors were A: Polymer Concentration (0.5, 1.0, 1.5 % w/w), B: Ethanol Concentration (10, 15, 20 % w/w), and C: PG Concentration (5, 10, 15 % w/w). There were three response variables: Y_1 = Flux of DDEA (mg/(cm² h)), Y_2 = Flux of CRM (μg/(cm² h)), and Y_3 = Viscosity of Gel (cP). The experiment had $n = 17$ runs. The design and data are given below.

runnum	polyconc	ethnconc	pgconc	fluxddea	fluxcrm	viscgel
1	-1	-1	0	0.67	1.48	185
2	0	0	0	0.24	1.90	1924
3	0	1	-1	0.25	3.31	2018
4	0	-1	1	0.22	2.88	2310
5	1	0	-1	0.11	3.30	3227
6	-1	1	0	0.67	1.72	145
7	-1	0	-1	0.69	1.37	143
8	0	0	0	0.23	1.87	1923
9	-1	0	1	0.67	1.52	176
10	0	0	0	0.24	1.91	1800
11	0	0	0	0.24	1.92	1921
12	1	0	1	0.17	2.98	3071
13	0	1	1	0.23	2.01	1783
14	0	0	0	0.24	1.87	1922
15	1	-1	0	0.11	3.07	3320
16	1	1	0	0.16	3.45	2801
17	0	-1	-1	0.20	1.71	2245

Note that runs 1,6,15, and 16 form the 2^2 factorial for the extreme levels of Polymer Concentration and Ethanol Concentration, and in each run PG Concentration is at its center level. The following analysis is for the response variable fluxcrm

R Program

```
transderm <- read.csv("E:\\data_articles\\transdermal_bb.csv",header=T)
attach(transderm); names(transderm)

o.polyconc <- 1 + 0.5*polyconc      # Center = 1, -1 = 0.5, +1 = 1.5
o.ethnconc <- 15 + 5*ethnconc      # Center = 15, -1 = 10, +1 = 20
o.pgconc <- 10 + 5*pgconc          # Center = 10, -1 = 5, +1 = 15

library(rsm)

transderm.rsm <- rsm(fluxcrm ~ SO(o.polyconc,o.ethnconc,o.pgconc))
summary(transderm.rsm)

par(mfrow=c(1,3))
contour(transderm.rsm, ~ o.polyconc + o.ethnconc + o.pgconc, at=xs(transderm.rsm))
```

R Output

```
> transderm.rsm <- rsm(fluxcrm ~ SO(o.polyconc,o.ethnconc,o.pgconc))
> summary(transderm.rsm)
```

```
Call:
rsm(formula = fluxcrm ~ SO(o.polyconc, o.ethnconc, o.pgconc))
```

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	0.65875000	0.17009464	3.8728	0.006109	**
o.polyconc	0.53350000	0.13499815	3.9519	0.005519	**
o.ethnconc	-0.16585000	0.01646648	-10.0720	2.041e-05	***
o.pgconc	0.23160000	0.01349981	17.1558	5.612e-07	***
o.polyconc:o.ethnconc	0.01400000	0.00503984	2.7779	0.027382	*
o.polyconc:o.pgconc	-0.04700000	0.00503984	-9.3257	3.383e-05	***
o.ethnconc:o.pgconc	-0.02470000	0.00050398	-49.0095	3.854e-10	***
o.polyconc^2	0.70200000	0.04912230	14.2909	1.954e-06	***
o.ethnconc^2	0.01442000	0.00049122	29.3553	1.371e-08	***
o.pgconc^2	0.00892000	0.00049122	18.1588	3.800e-07	***

```
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Multiple R-squared:  0.9995,    Adjusted R-squared:  0.9988
F-statistic: 1475 on 9 and 7 DF,  p-value: 1.25e-10
```

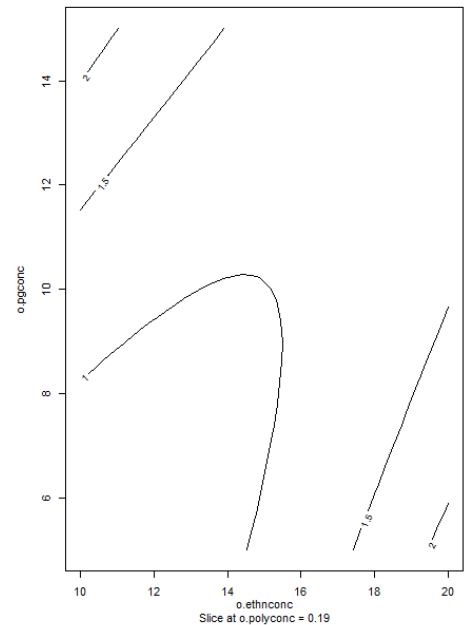
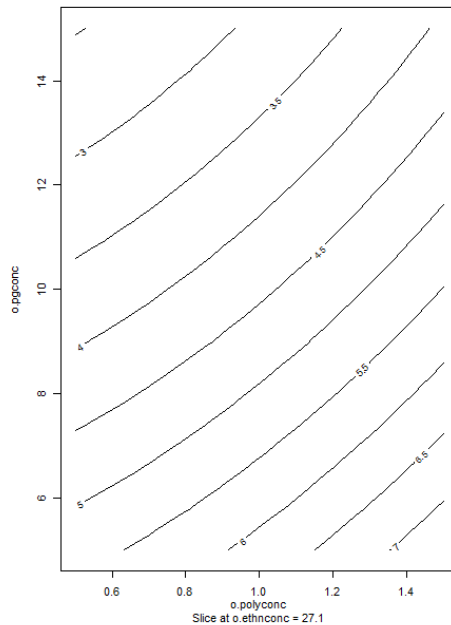
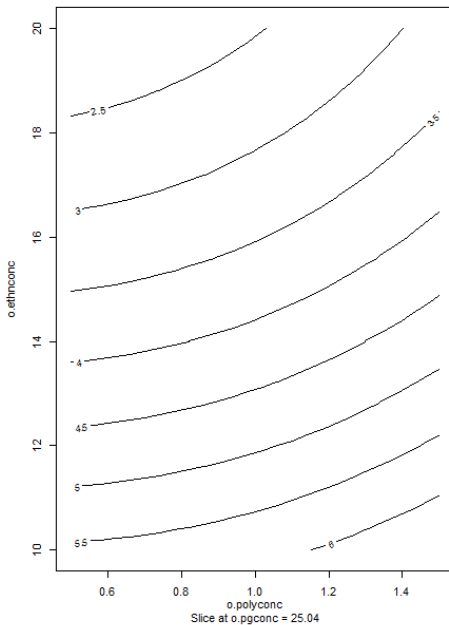
Analysis of Variance Table

Response: fluxcrm

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
FO(o.polyconc, o.ethnconc, o.pgconc)	3	5.8671	1.95569	3079.8294	2.779e-11
TWI(o.polyconc, o.ethnconc, o.pgconc)	3	1.5854	0.52845	832.2047	2.688e-09
PQ(o.polyconc, o.ethnconc, o.pgconc)	3	0.9775	0.32584	513.1268	1.450e-08
Residuals	7	0.0044	0.00064		
Lack of fit	3	0.0023	0.00078	1.4623	0.3511
Pure error	4	0.0021	0.00053		

Stationary point of response surface:

```
o.polyconc o.ethnconc o.pgconc
 0.187893 27.102321 25.036901
```



Example – Pulp and Paper Bleaching Effluent

An experiment (Sridhar, *et al* (2012)) had $k = 4$ factors, each at 3 levels, and 3 response variables. The factors are A: Current Density (5, 10, 15 mA/cm²), B: Initial pH (5,7, 9), C: Electrolyte Concentration (0, 1, 1 g/l), and D: Electrolysis Time (10, 20, 30 minutes). The responses measured are: $Y_1 =$ % Colour Removal, $Y_2 =$ % Chemical Oxygen Demand (COD) Removal, and $Y_3 =$ % Biochemical Oxygen Demand (BOD) Removal. The design is given below, with a total of $n = 29$ experimental runs. The analysis is based on the response variable % Colour Removal.

runnum	X1	X2	X3	X4	colour	cod	bod	XC1	XC2	XC3	XC4
1	15	5	1	30	81.1	71.5	67.8	0	-1	0	1
2	15	7	1	20	93.6	90.2	86.8	0	0	0	0
3	25	7	0	20	84.0	81.0	77.1	1	0	-1	0
4	15	7	1	20	93.6	90.2	86.8	0	0	0	0
5	15	7	2	10	74.0	68.6	60.6	0	0	1	-1
6	5	7	0	20	64.1	58.5	56.0	-1	0	-1	0
7	5	5	1	20	66.1	56.8	53.3	-1	-1	0	0
8	15	5	1	10	48.7	42.1	32.5	0	-1	0	-1
9	25	9	1	20	80.1	76.0	72.5	1	1	0	0
10	15	7	1	20	93.6	90.2	86.8	0	0	0	0
11	15	7	2	30	99.6	93.1	90.2	0	0	1	1
12	5	7	2	20	78.0	74.8	69.0	-1	0	1	0
13	5	7	1	10	52.6	42.0	38.0	-1	0	0	-1
14	15	5	0	20	61.2	57.0	52.3	0	-1	-1	0
15	25	7	1	30	98.5	93.6	90.9	1	0	0	1
16	15	7	1	20	93.6	90.2	86.8	0	0	0	0
17	25	7	1	10	78.2	72.0	68.0	1	0	0	-1
18	15	7	0	30	83.4	79.4	74.0	0	0	-1	1
19	15	7	1	20	93.6	90.2	86.8	0	0	0	0
20	5	7	1	30	82.0	77.2	75.4	-1	0	0	1
21	25	5	1	20	72.2	65.1	62.0	1	-1	0	0
22	15	9	1	10	49.1	45.2	41.3	0	1	0	-1
23	15	7	0	10	52.5	47.5	41.8	0	0	-1	-1
24	15	9	2	20	68.0	65.2	61.6	0	1	1	0
25	25	7	2	20	97.0	92.5	90.2	1	0	1	0
26	5	9	1	20	42.0	38.0	36.1	-1	1	0	0
27	15	9	1	30	81.2	75.6	68.7	0	1	0	1
28	15	9	0	20	60.2	56.6	53.1	0	1	-1	0
29	15	5	2	20	81.3	74.7	69.8	0	-1	1	0

R Program

```
ppb <- read.csv("http://www.stat.ufl.edu/~winner/data/pulpaperbleach.csv",header=T)
attach(ppb); names(ppb)

library(rsm)

ppb.rsm <- rsm(colour ~ SO(X1,X2,X3,X4))
summary(ppb.rsm)

par(mfrow=c(2,3))
contour(ppb.rsm, ~ X1+X2+X3+X4,at=xs(ppb.rsm))

par(mfrow=c(2,3))
persp (ppb.rsm, ~X1+X2+X3+X4, at = xs(ppb.rsm))

par(mfrow=c(2,3))
persp (ppb.rsm, ~X1+X2+X3+X4, at = xs(ppb.rsm),
contours = "col", col = rainbow(40), zlab = "% Colour Removal",
xlabs = c("Curr Dens", "pH", "Electro Conc", "Electro Time"))
```

R Output

```

> ppb.rsm <- rsm(colour ~ SO(X1,X2,X3,X4))
> summary(ppb.rsm)

Call:
rsm(formula = colour ~ SO(X1, X2, X3, X4))

      Estimate Std. Error t value Pr(>|t|)
(Intercept) -234.377083  20.508642 -11.4282 1.746e-08 ***
X1            0.894583   0.655876  1.3640  0.19411
X2           65.047917   4.191973  15.5173 3.247e-10 ***
X3           33.825000   6.293502  5.3746 9.800e-05 ***
X4            5.515833   0.691304  7.9789 1.412e-06 ***
X1:X2         0.400000   0.068182  5.8666 4.099e-05 ***
X1:X3        -0.022500   0.136365 -0.1650  0.87130
X1:X4        -0.022750   0.013636 -1.6683  0.11745
X2:X3        -1.537500   0.681825 -2.2550  0.04067 *
X2:X4        -0.003750   0.068182 -0.0550  0.95692
X3:X4        -0.132500   0.136365 -0.9717  0.34771
X1^2         -0.072458   0.010708 -6.7664 9.075e-06 ***
X2^2         -5.048958   0.267712 -18.8597 2.380e-11 ***
X3^2         -6.183333   1.070848 -5.7742 4.815e-05 ***
X4^2         -0.089833   0.010708 -8.3890 7.846e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

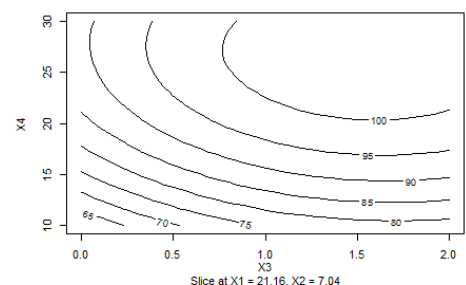
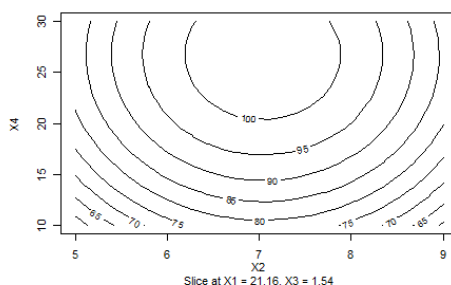
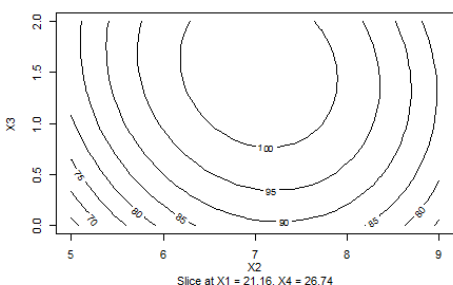
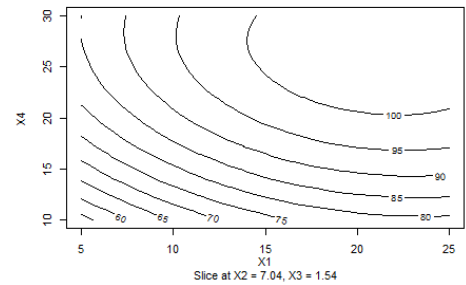
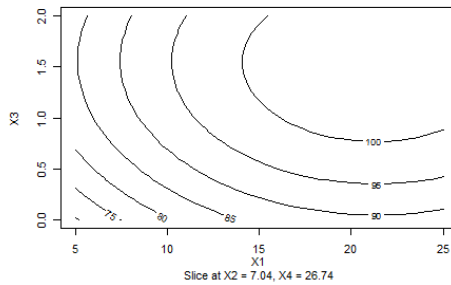
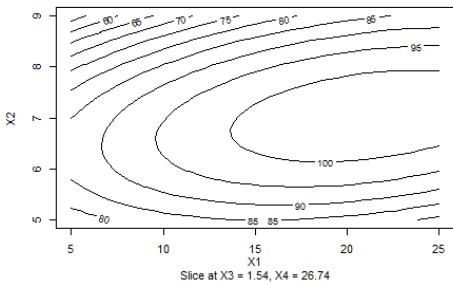
Multiple R-squared:  0.9867,    Adjusted R-squared:  0.9734
F-statistic: 74.19 on 14 and 14 DF,  p-value: 1.177e-10

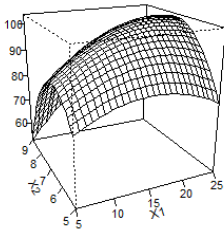
Analysis of Variance Table

Response: colour
          Df Sum Sq Mean Sq  F value    Pr(>F)
FO(X1, X2, X3, X4)  4 4522.5  1130.62 1.5200e+02 2.295e-11
TWI(X1, X2, X3, X4)  6  321.8    53.63 7.2100e+00 0.001163
PQ(X1, X2, X3, X4)  4 2881.6   720.40 9.6852e+01 4.869e-10
Residuals          14  104.1     7.44
Lack of fit        10  104.1    10.41 2.8293e+29 < 2.2e-16
Pure error          4    0.0     0.00

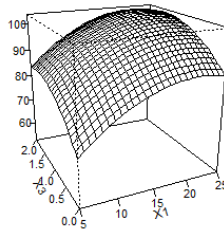
Stationary point of response surface:
      X1      X2      X3      X4
21.157655  7.036109  1.535386  26.742149

```

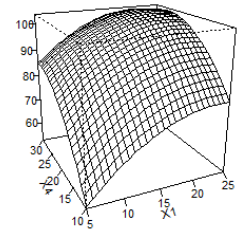




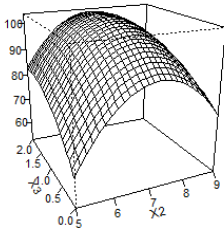
Slice at X3 = 1.54, X4 = 26.74



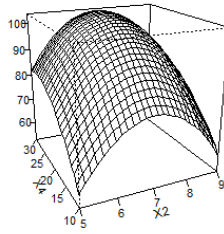
Slice at X2 = 7.04, X4 = 26.74



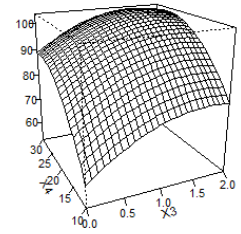
Slice at X2 = 7.04, X3 = 1.54



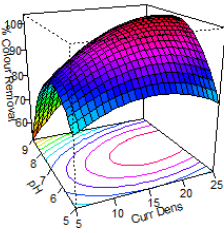
Slice at X1 = 21.16, X4 = 26.74



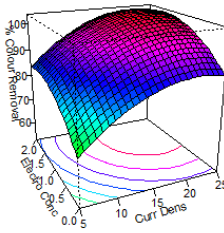
Slice at X1 = 21.16, X3 = 1.54



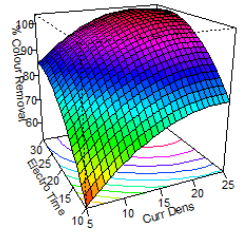
Slice at X1 = 21.16, X2 = 7.04



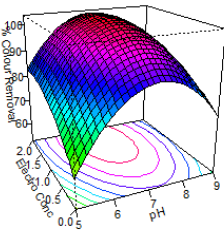
Slice at X3 = 1.54, X4 = 26.74



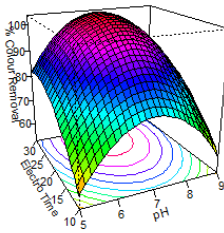
Slice at X2 = 7.04, X4 = 26.74



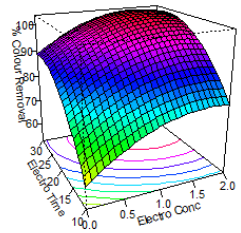
Slice at X2 = 7.04, X3 = 1.54



Slice at X1 = 21.16, X4 = 26.74



Slice at X1 = 21.16, X3 = 1.54



Slice at X1 = 21.16, X2 = 7.04

Note that the F-test for lack-of-fit strongly rejects the null hypothesis of a second-order model. The Pure Error sum of squares is virtually 0.

10.5. Mixture Designs

In many experiments, the goal is to optimize the response over various possible combinations or mixtures of “ingredients” of k factors. The levels of the input factors have a restriction that they must sum to 1. That is, they represent proportions of the ingredients in the experimental run: $X_1 + \dots + X_k = 1$. Some commonly used models that are fit include the following three (see e.g. Montgomery (2001) and Cornell (1990)). Note that these models have intercepts set equal to 0. This needs to be kept in mind when using conventional statistical regression packages.

Linear: $E\{Y\} = \sum_{i=1}^k \beta_i X_i$

Quadratic: $E\{Y\} = \sum_{i=1}^k \beta_i X_i + \sum_{i=1}^{k-1} \sum_{i'=i+1}^k \beta_{ii'} X_i X_{i'}$

Special Cubic: $E\{Y\} = \sum_{i=1}^k \beta_i X_i + \sum_{i=1}^{k-1} \sum_{i'=i+1}^k \beta_{ii'} X_i X_{i'} + \sum_{i=1}^{k-2} \sum_{i'=i+1}^{k-1} \sum_{i''=i'+1}^k \beta_{ii'i''} X_i X_{i'} X_{i''}$

Consider the linear version described above with $k = 3$ (this generalizes to the other models).

$$E\{Y\} = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 = \beta_1 (1 - X_2 - X_3) + \beta_2 X_2 + \beta_3 X_3 = \beta_1 + (\beta_2 - \beta_1) X_2 + (\beta_3 - \beta_1) X_3$$

The 3-variable regression through the origin can be written as a 2-variable regression with an intercept term. So that once we remove the correction for the mean and its 1 degree of freedom, we have $k - 1$ degrees of freedom for the linear portion of the models. We will demonstrate this below.

These designs typically are modelled as a **Simplex Lattice Mixture Design (SLMD)**, where a triangle is formed when there are $k = 3$ factors, showing the proportions of each factor at the design points. Software packages can print out “response surfaces” as contours on the triangle. See the example below making use of the **mixexp** package in R.

Example – Physiochemical and Sensory Properties of Wheat Chips

A study (Kayacier, *et al* (2014)), was conducted as a mixture experiment, relating various physiochemical (Dry Matter, Ash, Oil, Protein, Hardness) and sensory (Taste, Color, Crispness, Overall Preference) properties of wheat chips. The mixtures use in the study involved $k = 3$ ingredients: $X_1 =$ Proportion of Chickpea flour, $X_2 =$ Proportion of Pea Flour, and $X_3 =$ Proportion of Soy Flour. The physiochemical measurements for each run was the average of 4 determinations, sensory measurements were the average of 10 respondents. The mean is used as the data for the $n = 15$ mixtures under study. Here we consider the Oil response, with mean 26.7473. The design and data are given below.

Mixture	X1	X2	X3	X1X2	X1X3	X2X3	Oil
1	1	0	0	0	0	0	34.22
2	0	1	0	0	0	0	34.06
3	0	0	1	0	0	0	23.32
4	0.5	0.5	0	0.25	0	0	25.97
5	0	0.5	0.5	0	0	0.25	24.14
6	0.5	0	0.5	0	0.25	0	24.87
7	0.25	0.75	0	0.1875	0	0	30.78
8	0	0.25	0.75	0	0	0.1875	21.54
9	0.75	0	0.25	0	0.1875	0	35.44
10	0.75	0.25	0	0.1875	0	0	30.82
11	0	0.75	0.25	0	0	0.1875	25.10
12	0.25	0	0.75	0	0.1875	0	24.94
13	0.5	0.25	0.25	0.125	0.125	0.0625	27.00
14	0.25	0.5	0.25	0.125	0.0625	0.125	18.69
15	0.25	0.25	0.5	0.0625	0.125	0.125	20.32

We first consider the linear model. We will fit 2 models to obtain the correct sums of squares and F-tests. Keep in mind that when fitting a Regression through the origin, the “Total Sum of Squares” is the Uncorrected Total Sum of Squares, and the “Regression Sum of Squares” is the Model Sum of Squares. Both of these include the Correction for the mean, and R^2 is not interpreted as in a conventional regression. Here we fit the following 2 models.

$$\text{Model 1: } E\{Y\} = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$$

$$\text{Model 2: } E\{Y\} = \beta_0^* + \beta_2^* X_2 + \beta_3^* X_3 = \beta_1 + (\beta_2 - \beta_1) X_2 + (\beta_3 - \beta_1) X_3$$

$$\Rightarrow \beta_1 = \beta_0^* \quad \beta_2 = \beta_2^* + \beta_0^* \quad \beta_3 = \beta_3^* + \beta_0^*$$

$$SS_{\text{Tot2}} = SS_{\text{Tot1}} - n\bar{Y}^2 \quad SS_{\text{Reg2}} = SS_{\text{Reg1}} - n\bar{Y}^2$$

SUMMARY OUTPUT						SUMMARY OUTPUT					
Model 1						Model 2					
Regression Statistics						Regression Statistics					
Multiple R	0.9905					Multiple R	0.6685				
R Square	0.9811					R Square	0.4468				
Adjusted R Square	0.8946					Adjusted R Square	0.3546				
Standard Error	4.1842					Standard Error	4.1842				
Observations	15					Observations	15				
ANOVA						ANOVA					
	df	SS	MS	F	Significance F		df	SS	MS	F	Significance F
Regression	3	10901.00	3633.6677	207.5524	0.0000	Regression	2	169.71	84.8528	4.8467	0.0286
Residual	12	210.09	17.5072			Residual	12	210.09	17.5072		
Total	15	11111.09				Total	14	379.79			
Coefficients						Coefficients					
	Standard Err	t Stat	P-value				Standard Err	t Stat	P-value		
Intercept	0	#N/A	#N/A	#N/A		Intercept	32.5900	2.5500	12.7802	0.0000	
X1	32.5900	2.5500	12.7802	0.0000		X2	-5.1326	4.0008	-1.2829	0.2238	
X2	27.4574	2.5500	10.7675	0.0000		X3	-12.3954	4.0008	-3.0982	0.0092	
X3	20.1946	2.5500	7.9193	0.0000							

Note that the F-Statistic and R^2 for Model 1 are way higher than for Model 2. The F-test for Model 1 is testing that the mean response is 0 (not some arbitrary level μ as Model 2 is testing). Here we show the equivalence of the relations described above.

$$\text{Correction for the Mean: } CM = n\bar{y}^2 = 15(26.747333^2) = 10731.30$$

$$SS_{\text{Tot1}} = \sum_{i=1}^n y_i^2 = 11111.09 \Rightarrow SS_{\text{Tot1}} - CM = 11111.09 - 10731.30 = 379.79 = SS_{\text{Tot2}}$$

$$SS_{\text{Reg1}} = \sum_{i=1}^n \hat{y}_i^2 = 10901.00 \Rightarrow SS_{\text{Reg1}} - CM = 10901.00 - 10731.30 = 169.70 = SS_{\text{Reg2}}$$

$$\hat{\beta}_1 = 32.5900 = \hat{\beta}_0^* \quad \hat{\beta}_1 = 27.4574 = 32.5900 - 5.1326 = \hat{\beta}_0^* + \hat{\beta}_2^* \quad \hat{\beta}_1 = 20.1946 = 32.5900 - 12.3954 = \hat{\beta}_0^* + \hat{\beta}_3^*$$

Next we fit the Quadratic model: $E\{Y\} = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3$.

SUMMARY OUTPUT						
Regression Statistics						
Multiple R	0.9966					
R Square	0.9932					
Adjusted R Square	0.8783					
Standard Error	2.8951					
Observations	15					
ANOVA						
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>	
Regression	6	11035.66	1839.28	219.4439	0.0000	
Residual	9	75.43	8.38			
Total	15	11111.09				
Coefficients						
	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	
Intercept	0	#N/A	#N/A	#N/A	#N/A	
X1	36.7433	2.5191	14.5857	0.0000	31.0446	42.4420
X2	34.3433	2.5191	13.6330	0.0000	28.6446	40.0420
X3	23.6840	2.5191	9.4017	0.0000	17.9853	29.3827
X1X2	-34.8514	10.7213	-3.2507	0.0100	-59.1047	-10.5981
X1X3	-12.2086	10.7213	-1.1387	0.2842	-36.4619	12.0447
X2X3	-30.4257	10.7213	-2.8379	0.0195	-54.6790	-6.1724

The “Correct” R^2 and F-statistic are computed below.

$$CM = 10731.30 \quad SS_{\text{Tot(Corr)}} = 379.79 \quad SS_{\text{Reg}} = 11035.66 - 10731.30 = 304.36$$

$$MS_{\text{Reg}} = \frac{304.36}{6-1} = 60.87 \quad MS_{\text{Err}} = 8.38$$

$$H_0 : \text{No Linear or quadratic effects} \Rightarrow E\{Y\} = \mu$$

$$\text{Test Stat: } F_{\text{obs}} = \frac{60.87}{8.38} = 7.26 \quad F_{0.95;5,9} = 3.48 \quad P(F_{5,9} \geq 7.26) = 0.0055$$

$$R^2 = \frac{304.36}{379.79} = 0.8014$$

Here we use the **mixexp** package in R for the analysis.

R Program

```
wheat <- read.csv("http://www.stat.ufl.edu/~winner/data/sensorywheatchips.csv",
  header=T)
attach(wheat); names(wheat)

install.packages("igraph")
install.packages("mixexp")
library(mixexp)
library(daewr)

mixvars <- c("X1","X2","X3")          ### Creates group of mixvars
wheat.mod1 <- MixModel(wheat,"MY3",mixvars,2)

### Fits model, must specify: dataframe,"Y",mixvars,
### model (1=linear, 2=quadratic, 4=special cubic)
anova(wheat.mod1)
summary(wheat.mod1)

MixturePlot(X3,X2,X1,MY3,x3lab="Fraction Soy", x2lab="Fraction Pea",
  x1lab="Fraction Chickpea", corner.labs=c("Soy","Pea","Chickpea"),
  constrts=FALSE,contrs=TRUE,cols=TRUE, mod=2,n.breaks=9)
```

R Output

```
> wheat.mod1 <- MixModel(wheat,"MY3",mixvars,2)

      coefficients Std.err  t.value      Prob
X1      36.74329   2.51913  14.585702 1.438430e-07
X2      34.34329   2.51913  13.632993 2.579333e-07
X3      23.68400   2.51913   9.401657 5.965431e-06
X2:X1   -34.85143  10.72132  -3.250665 9.986732e-03
X3:X1   -12.20857  10.72132  -1.138719 2.842224e-01
X2:X3   -30.42571  10.72132  -2.837870 1.947072e-02

Residual standard error: 2.895088 on 9 degrees of freedom
Multiple R-squared: 0.8013814

> anova(wheat.mod1)
Analysis of Variance Table

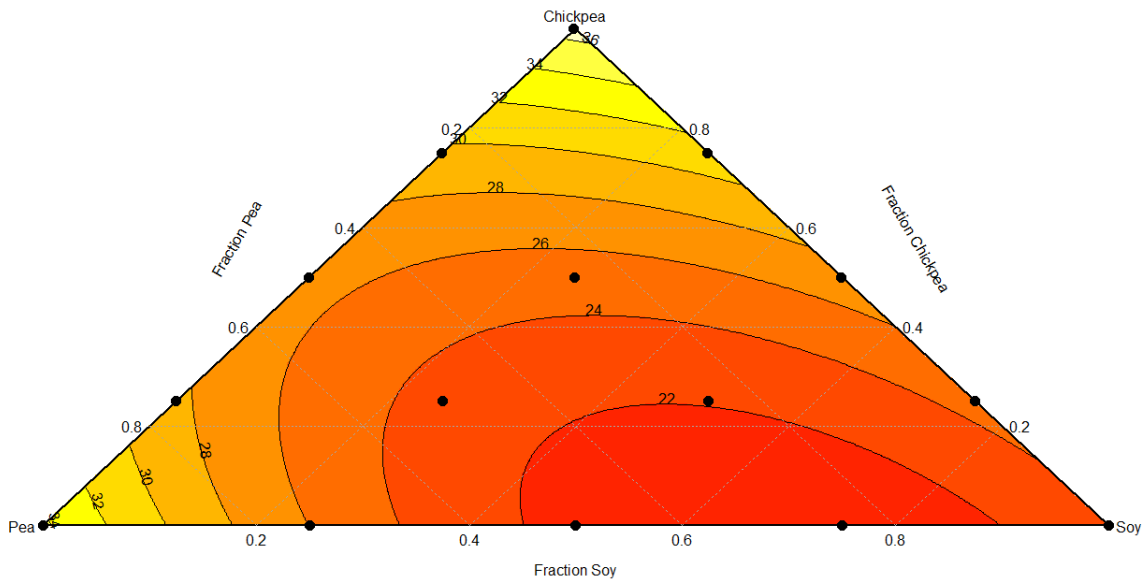
Response: MY3
      Df Sum Sq Mean Sq F value    Pr(>F)
X1      1  6869.6   6869.6  819.6067 3.769e-10 ***
X2      1  2933.5   2933.5  349.9913 1.635e-08 ***
X3      1  1098.0   1098.0  130.9998 1.151e-06 ***
X1:X2    1    63.3     63.3   7.5561 0.02252 *
X1:X3    1     3.8      3.8   0.4559 0.51653
X2:X3    1    67.5     67.5   8.0535 0.01947 *
Residuals 9    75.4      8.4
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> summary(wheat.mod1)

Call:
lm(formula = mixmodnI, data = frame)

Residuals:
    Min       1Q   Median       3Q      Max
-4.6658 -1.3299 -0.2833  1.5585  4.2506

Coefficients:
      Estimate Std. Error t value Pr(>|t|)
X1      36.743     2.519  14.586 1.44e-07 ***
X2      34.343     2.519  13.633 2.58e-07 ***
X3      23.684     2.519   9.402 5.97e-06 ***
X1:X2   -34.851    10.721  -3.251 0.00999 **
X1:X3   -12.209    10.721  -1.139 0.28422
X2:X3   -30.426    10.721  -2.838 0.01947 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.895 on 9 degrees of freedom
Multiple R-squared: 0.9932, Adjusted R-squared: 0.9887
F-statistic: 219.4 on 6 and 9 DF, p-value: 3.094e-09
```



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Chapter 11 - Split Plot Designs

In many experimental situations with 2 or more factors, it is difficult or infeasible to conduct the experiment as a Completely Randomized Design. Suppose we have 2 factors, A with a levels, B with b levels, and $N = abn$ experimental units. The logistics of the experiment may make it impossible to randomly assign the N units at random to the ab treatments, then run them in random order.

In an agricultural trial, one factor may need larger sections of land for its levels to be applied to, while the other factor may be applied to smaller sections of land. In an engineering study, one factor may be “hard to change,” while the other factor may be “easy to change.” For both of these cases, the factors will have different experimental units. The factor that needs the larger units or is harder to change is called the **Whole Plot** factor. The factor that can be applied to smaller units or is easier to change is called the **Sub Plot** factor. As the two types of factors have different units (the sub plot factor units being within the whole plot factor units), the two factors will have different error terms.

Split plot experiments can be conducted as a Completely Randomized Design, a Randomized Block Design, a Latin Square Design, or in various types of incomplete block or fractional factorial designs.

11.1. Split-Plot in a Completely Randomized Design

Suppose that Factor A is the Whole Plot Factor, with a levels. We have $N_W = an$ experimental units that we will assign at random to the levels of A in a CRD. After applying the Factor A levels to these units, we will apply the b levels of Factor B to the sub-units within the “whole” units. There will be $N = bN_W = abn$ total observations. Here we consider the case where factors A and B are fixed and the units are random. We give the model, the derivation of the Expected Mean Squares, and the Mean/Variance structure below.

$Y_{ijk} = \mu + \alpha_i + \gamma_{k(i)} + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, n$	
Factor A Effects:	$\alpha_1, \dots, \alpha_a \quad \sum_{i=1}^a \alpha_i = 0$
Factor B Effects:	$\beta_1, \dots, \beta_b \quad \sum_{j=1}^b \beta_j = 0$
AB Interaction Effects:	$(\alpha\beta)_{11}, \dots, (\alpha\beta)_{ab} \quad \sum_{i=1}^a (\alpha\beta)_{ij} = \sum_{j=1}^b (\alpha\beta)_{ij} = 0$
Whole Plot (Random) Effects:	$\gamma_{k(i)} \sim NID(0, \sigma_\gamma^2)$
Sub Plot (Random) Effects:	$\varepsilon_{ijk} \sim NID(0, \sigma^2) \quad \{\gamma_{k(i)}\} \perp \{\varepsilon_{ijk}\}$
$E\{Y_{ijk}\} = \mu + \alpha_i + \gamma_{k(i)} + \beta_j + (\alpha\beta)_{ij}$	$\text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\gamma^2 + \sigma^2 & i = i', j = j', k = k' \\ \sigma_\gamma^2 & i = i', j \neq j', k = k' \\ 0 & \text{otherwise} \end{cases}$

$$E\{Y_{ijk}\} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} \quad V\{Y_{ijk}\} = \sigma_\gamma^2 + \sigma^2 \Rightarrow E\{Y_{ijk}^2\} = \sigma_\gamma^2 + \sigma^2 + (\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij})^2$$

$$\Rightarrow E\left\{\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2\right\} = abn\sigma_\gamma^2 + abn\sigma^2 + abn\mu^2 + bn\sum_{i=1}^a \alpha_i^2 + an\sum_{j=1}^b \beta_j^2 + n\sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2$$

$$E\{\bar{Y}_{ij\bullet}\} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij}$$

$$V\{\bar{Y}_{ij\bullet}\} = V\left\{\frac{1}{n} \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{n^2} \left[\sum_{k=1}^n V\{Y_{ijk}\} + 2 \sum_{k=1}^{n-1} \sum_{k'=k+1}^n \text{COV}\{Y_{ijk}, Y_{ij'k'}\} \right] = \frac{1}{n^2} \left[n(\sigma_\gamma^2 + \sigma^2) + n(n-1)(0) \right] = \frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{n}$$

$$\Rightarrow E\{\bar{Y}_{ij\bullet}^2\} = \frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{n} + (\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij})^2$$

$$\Rightarrow n \sum_{i=1}^a \sum_{j=1}^b E\{\bar{Y}_{ij\bullet}^2\} = abn\sigma_\gamma^2 + abn\sigma^2 + abn\mu^2 + bn\sum_{i=1}^a \alpha_i^2 + an\sum_{j=1}^b \beta_j^2 + n\sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2$$

$$E\{\bar{Y}_{i\bullet k}\} = \mu + \alpha_i$$

$$V\{\bar{Y}_{i\bullet k}\} = V\left\{\frac{1}{b} \sum_{j=1}^b Y_{ijk}\right\} = \frac{1}{b^2} \left[\sum_{j=1}^b V\{Y_{ijk}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{ij'k}\} \right] = \frac{1}{b^2} \left[b(\sigma_\gamma^2 + \sigma^2) + b(b-1)(\sigma^2) \right] = \sigma_\gamma^2 + \frac{\sigma^2}{b}$$

$$\Rightarrow E\{\bar{Y}_{i\bullet k}^2\} = \sigma_\gamma^2 + \frac{\sigma^2}{b} + (\mu + \alpha_i)^2 \Rightarrow b \sum_{i=1}^a \sum_{k=1}^n E\{\bar{Y}_{i\bullet k}^2\} = abn\sigma_\gamma^2 + an\sigma^2 + abn\mu^2 + bn\sum_{i=1}^a \alpha_i^2$$

$$E\{\bar{Y}_{i\bullet\bullet}\} = \mu + \alpha_i$$

$$V\{\bar{Y}_{i\bullet\bullet}\} = V\left\{\frac{1}{bn} \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{b^2 n^2} \left[\sum_{j=1}^b \sum_{k=1}^n V\{Y_{ijk}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^n \text{COV}\{Y_{ijk}, Y_{ij'k}\} + 2 \sum_{j=1}^b \sum_{k=1}^{n-1} \sum_{k'=k+1}^n \text{COV}\{Y_{ijk}, Y_{ijk'}\} \right] =$$

$$\frac{1}{b^2 n^2} \left[bn(\sigma_\gamma^2 + \sigma^2) + b(b-1)n(\sigma^2) + bn(n-1)(0) \right] = \frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{bn}$$

$$\Rightarrow E\{\bar{Y}_{i\bullet\bullet}^2\} = \frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{bn} + (\mu + \alpha_i)^2 \Rightarrow bn \sum_{i=1}^a E\{\bar{Y}_{i\bullet\bullet}^2\} = abn\sigma_\gamma^2 + a\sigma^2 + abn\mu^2 + bn\sum_{i=1}^a \alpha_i^2$$

$$E\{\bar{Y}_{\bullet j\bullet}\} = \mu + \beta_j$$

$$V\{\bar{Y}_{\bullet j\bullet}\} = V\left\{\frac{1}{an} \sum_{i=1}^a \sum_{k=1}^n Y_{ijk}\right\} = \frac{1}{a^2 n^2} \left[\sum_{i=1}^a \sum_{k=1}^n V\{Y_{ijk}\} + 2 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{k=1}^n \text{COV}\{Y_{ijk}, Y_{i'jk}\} + 2 \sum_{i=1}^a \sum_{k=1}^{n-1} \sum_{k'=k+1}^n \text{COV}\{Y_{ijk}, Y_{ijk'}\} \right] =$$

$$\frac{1}{a^2 n^2} \left[an(\sigma_\gamma^2 + \sigma^2) + a(a-1)n(0) + bn(n-1)(0) \right] = \frac{\sigma_\gamma^2}{an} + \frac{\sigma^2}{an}$$

$$\Rightarrow E\{\bar{Y}_{\bullet j\bullet}^2\} = \frac{\sigma_\gamma^2}{an} + \frac{\sigma^2}{an} + (\mu + \beta_j)^2 \Rightarrow an \sum_{j=1}^b E\{\bar{Y}_{\bullet j\bullet}^2\} = b\sigma_\gamma^2 + b\sigma^2 + abn\mu^2 + an\sum_{j=1}^b \beta_j^2$$

$$E\{\bar{Y}_{\bullet\bullet\bullet}\} = \mu$$

$$V\{\bar{Y}_{\bullet\bullet\bullet}\} = V\left\{\frac{1}{abn} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}\right\} =$$

$$= \frac{1}{a^2 b^2 n^2} \left[\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n V\{Y_{ijk}\} + 2 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^b \sum_{k=1}^n \text{COV}\{Y_{ijk}, Y_{i'jk}\} + 2 \sum_{i=1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^n \text{COV}\{Y_{ijk}, Y_{ij'k}\} + 2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n-1} \sum_{k'=k+1}^n \text{COV}\{Y_{ijk}, Y_{ijk'}\} \right]$$

$$= \frac{1}{a^2 b^2 n^2} \left[abn(\sigma_\gamma^2 + \sigma^2) + a(a-1)bn(0) + ab(b-1)n(\sigma_\gamma^2) + abn(n-1)(0) \right] = \frac{\sigma_\gamma^2}{an} + \frac{\sigma^2}{abn}$$

$$\Rightarrow E\{\bar{Y}_{\bullet\bullet\bullet}^2\} = \frac{\sigma_\gamma^2}{an} + \frac{\sigma^2}{abn} + \mu^2 \Rightarrow abnE\{\bar{Y}_{\bullet\bullet\bullet}^2\} = b\sigma_\gamma^2 + \sigma^2 + abn\mu^2$$

$$\begin{aligned}
SS_A &= bn \sum_{i=1}^a (\bar{Y}_{i..} - \bar{Y}...)^2 = bn \sum_{i=1}^a \bar{Y}_{i..}^2 - abn \bar{Y}...^2 \\
\Rightarrow E\{SS_A\} &= \left[ab\sigma_\gamma^2 + a\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 \right] - \left[b\sigma_\gamma^2 + \sigma^2 + abn\mu^2 \right] = b(a-1)\sigma_\gamma^2 + (a-1)\sigma^2 + bn \sum_{i=1}^a \alpha_i^2 \\
\Rightarrow E\{MS_A\} &= E\left\{ \frac{SS_A}{a-1} \right\} = b\sigma_\gamma^2 + \sigma^2 + \frac{bn \sum_{i=1}^a \alpha_i^2}{a-1} \\
SS_{WPErr} &= b \sum_{i=1}^a \sum_{k=1}^n (\bar{Y}_{i.k} - \bar{Y}_{i..})^2 = b \sum_{i=1}^a \sum_{k=1}^n \bar{Y}_{i.k}^2 - bn \sum_{i=1}^a \bar{Y}_{i..}^2 \\
\Rightarrow E\{SS_{WPErr}\} &= \left[abn\sigma_\gamma^2 + an\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 \right] - \left[ab\sigma_\gamma^2 + a\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 \right] = ab(n-1)\sigma_\gamma^2 + a(n-1)\sigma^2 \\
\Rightarrow E\{MS_{WPErr}\} &= E\left\{ \frac{SS_{WPErr}}{a(n-1)} \right\} = b\sigma_\gamma^2 + \sigma^2 \\
SS_B &= an \sum_{j=1}^b (\bar{Y}_{.j.} - \bar{Y}...)^2 = an \sum_{j=1}^b \bar{Y}_{.j.}^2 - abn \bar{Y}...^2 \\
\Rightarrow E\{SS_B\} &= \left[b\sigma_\gamma^2 + b\sigma^2 + abn\mu^2 + an \sum_{j=1}^b \beta_j^2 \right] - \left[b\sigma_\gamma^2 + \sigma^2 + abn\mu^2 \right] = (b-1)\sigma^2 + an \sum_{j=1}^b \beta_j^2 \\
\Rightarrow E\{MS_B\} &= E\left\{ \frac{SS_B}{b-1} \right\} = \sigma^2 + \frac{an \sum_{j=1}^b \beta_j^2}{b-1} \\
SS_{AB} &= n \sum_{i=1}^a \sum_{j=1}^b (\bar{Y}_{ij.} - \bar{Y}_{i..} - \bar{Y}_{.j.} + \bar{Y}...)^2 = n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2 - bn \sum_{i=1}^a \bar{Y}_{i..}^2 - an \sum_{j=1}^b \bar{Y}_{.j.}^2 + abn \bar{Y}...^2 \\
\Rightarrow E\{SS_{AB}\} &= \left[ab\sigma_\gamma^2 + ab\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + an \sum_{j=1}^b \beta_j^2 + n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2 \right] - \left[ab\sigma_\gamma^2 + a\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 \right] \\
&\quad - \left[b\sigma_\gamma^2 + b\sigma^2 + abn\mu^2 + an \sum_{j=1}^b \beta_j^2 \right] + \left[b\sigma_\gamma^2 + \sigma^2 + abn\mu^2 \right] = (a-1)(b-1)\sigma^2 + n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2 \\
\Rightarrow E\{MS_{AB}\} &= E\left\{ \frac{SS_{AB}}{(a-1)(b-1)} \right\} = \sigma^2 + \frac{n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2}{(a-1)(b-1)} \\
SS_{SPErr} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (Y_{ijk} - \bar{Y}_{ij.} - \bar{Y}_{i.k} + \bar{Y}_{i..})^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n Y_{ijk}^2 - n \sum_{i=1}^a \sum_{j=1}^b \bar{Y}_{ij.}^2 - b \sum_{i=1}^a \sum_{k=1}^n \bar{Y}_{i.k}^2 + bn \sum_{i=1}^a \bar{Y}_{i..}^2 \\
\Rightarrow E\{SS_{SPErr}\} &= \left[abn\sigma_\gamma^2 + abn\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + an \sum_{j=1}^b \beta_j^2 + n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2 \right] - \\
&\quad \left[ab\sigma_\gamma^2 + ab\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 + an \sum_{j=1}^b \beta_j^2 + n \sum_{i=1}^a \sum_{j=1}^b (\alpha\beta)_{ij}^2 \right] - \\
&\quad \left[abn\sigma_\gamma^2 + an\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 \right] + \left[ab\sigma_\gamma^2 + a\sigma^2 + abn\mu^2 + bn \sum_{i=1}^a \alpha_i^2 \right] = a(b-1)(n-1)\sigma^2
\end{aligned}$$

Thus, the error term when testing for the Whole Plot Factor Effects is the Whole Plot Error term, with $a(n-1)$ degrees of freedom. The error term for testing for the Sub Plot Factor Effects and Whole Plot x Sub Plot interaction effects is the Sub Plot Error term, with $a(b-1)(n-1)$ degrees of freedom. The Sub Plot Error is also the Sub Plot x Whole Plot Unit(Whole Plot Factor) interaction.

The formal tests and variance component estimates are given below.

$$\begin{aligned}
 H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad \text{Test Stat: } F_A &= \frac{MS_A}{MS_{WPErr}} \stackrel{H_0}{\sim} F_{a-1, a(n-1)} \quad \text{P-value: } P(F_{a-1, a(n-1)} \geq F_A) \\
 H_0^B : \beta_1 = \dots = \beta_b = 0 \quad \text{Test Stat: } F_B &= \frac{MS_B}{MS_{SPErr}} \stackrel{H_0}{\sim} F_{b-1, a(b-1)(n-1)} \quad \text{P-value: } P(F_{b-1, a(b-1)(n-1)} \geq F_B) \\
 H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{ab} = 0 \quad \text{Test Stat: } F_{AB} &= \frac{MS_{AB}}{MS_{SPErr}} \stackrel{H_0}{\sim} F_{(a-1)(b-1), a(b-1)(n-1)} \quad \text{P-value: } P(F_{(a-1)(b-1), a(b-1)(n-1)} \geq F_{AB}) \\
 E\{MS_{WPErr}\} &= b\sigma_\gamma^2 + \sigma^2 \quad E\{MS_{SPErr}\} = \sigma^2 \\
 \hat{\sigma}^2 &= MS_{SPErr} \quad \hat{\sigma}_\gamma^2 = \frac{MS_{WPErr} - MS_{SPErr}}{b}
 \end{aligned}$$

The estimated variances for various types of means and their differences are derived below.

Whole Plot Factor:

$$\begin{aligned}
 V\{\bar{Y}_{i..}\} &= \frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{bn} \Rightarrow \hat{V}\{\bar{Y}_{i..}\} = \frac{\hat{\sigma}_\gamma^2}{n} + \frac{\hat{\sigma}^2}{bn} = \frac{MS_{WPErr} - MS_{SPErr}}{bn} + \frac{MS_{SPErr}}{bn} = \frac{MS_{WPErr}}{bn} \\
 i \neq i': \text{ COV}\{\bar{Y}_{i..}, \bar{Y}_{i'..}\} &= 0 \Rightarrow \hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{2MS_{WPErr}}{bn} \\
 (1-\alpha)100\% \text{ CI for } \alpha_i - \alpha_{i'} : (\bar{y}_{i..} - \bar{y}_{i'..}) &\pm t_{1-\alpha/2; a(n-1)} \sqrt{\frac{2MS_{WPErr}}{bn}}
 \end{aligned}$$

Sub Plot Factor:

$$\begin{aligned}
 V\{\bar{Y}_{\cdot j.}\} &= \frac{\sigma_\gamma^2}{an} + \frac{\sigma^2}{an} \Rightarrow \hat{V}\{\bar{Y}_{\cdot j.}\} = \frac{\hat{\sigma}_\gamma^2}{an} + \frac{\hat{\sigma}^2}{an} = \frac{MS_{WPErr} - MS_{SPErr}}{abn} + \frac{MS_{SPErr}}{an} = \frac{MS_{WPErr} + (b-1)MS_{SPErr}}{abn} \\
 j \neq j': \text{ COV}\{\bar{Y}_{\cdot j.}, \bar{Y}_{\cdot j'.}\} &= \text{COV}\left\{\frac{1}{an} \sum_{i=1}^a \sum_{k=1}^n Y_{ijk}, \frac{1}{an} \sum_{i=1}^a \sum_{k=1}^n Y_{ij'k}\right\} = \frac{1}{a^2 n^2} [an\sigma_\gamma^2 + an(n-1)(0)] = \frac{\sigma_\gamma^2}{an} \\
 \Rightarrow V\{\bar{Y}_{\cdot j.} - \bar{Y}_{\cdot j'.}\} &= 2\left(\frac{\sigma_\gamma^2}{an} + \frac{\sigma^2}{an}\right) - 2\frac{\sigma_\gamma^2}{an} = \frac{2\sigma^2}{an} \Rightarrow \hat{V}\{\bar{Y}_{\cdot j.} - \bar{Y}_{\cdot j'.}\} = \frac{2MS_{SPErr}}{an} \\
 (1-\alpha)100\% \text{ CI for } \beta_j - \beta_{j'} : (\bar{y}_{\cdot j.} - \bar{y}_{\cdot j'.}) &\pm t_{1-\alpha/2; a(b-1)(n-1)} \sqrt{\frac{2MS_{SPErr}}{an}}
 \end{aligned}$$

Simple Effects:

$$V\{\bar{Y}_{ij\bullet}\} = \frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{n} \Rightarrow \hat{V}\{\bar{Y}_{ij\bullet}\} = \frac{\hat{\sigma}_\gamma^2}{n} + \frac{\hat{\sigma}^2}{n} = \frac{MS_{WPErr} - MS_{SPErr}}{bn} + \frac{MS_{SPErr}}{n} = \frac{MS_{WPErr} + (b-1)MS_{SPErr}}{bn}$$

1) Two simple effects @ same level of Whole Plot:

$$COV\{\bar{Y}_{ij\bullet}, \bar{Y}_{i'j\bullet}\} = COV\left\{\frac{1}{n}\sum_{k=1}^n Y_{ijk}, \frac{1}{n}\sum_{k=1}^n Y_{i'jk}\right\} = \frac{1}{n^2} [n\sigma_\gamma^2 + n(n-1)(0)] = \frac{\sigma_\gamma^2}{n}$$

$$V\{\bar{Y}_{ij\bullet} - \bar{Y}_{i'j\bullet}\} = 2\left[\frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{n}\right] - 2\frac{\sigma_\gamma^2}{n} = \frac{2\sigma^2}{n} \Rightarrow \hat{V}\{\bar{Y}_{ij\bullet} - \bar{Y}_{i'j\bullet}\} = \frac{2MS_{SPErr}}{n}$$

$$(1-\alpha)100\% \text{ CI for } (\alpha\beta)_{ij} - (\alpha\beta)_{i'j}: (\bar{y}_{ij\bullet} - \bar{y}_{i'j\bullet}) \pm t_{1-\alpha/2; a(b-1)(n-1)} \sqrt{\frac{2MS_{SPErr}}{n}}$$

2) Two simple effects @ different levels of Whole Plot ($i \neq i', \forall j, j'$): $COV\{\bar{Y}_{ij\bullet}, \bar{Y}_{i'j'\bullet}\} = 0$

$$V\{\bar{Y}_{ij\bullet} - \bar{Y}_{i'j'\bullet}\} = 2\left[\frac{\sigma_\gamma^2}{n} + \frac{\sigma^2}{n}\right] \Rightarrow \hat{V}\{\bar{Y}_{ij\bullet} - \bar{Y}_{i'j'\bullet}\} = \frac{2[MS_{WPErr} + (b-1)MS_{SPErr}]}{bn}$$

$$(1-\alpha)100\% \text{ CI for } (\alpha\beta)_{ij} - (\alpha\beta)_{i'j'}: (\bar{y}_{ij\bullet} - \bar{y}_{i'j'\bullet}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2[MS_{WPErr} + (b-1)MS_{SPErr}]}{bn}}$$

$$\text{Satterthwaite's Approximate df: } v^* = \frac{(MS_{WPErr} + (b-1)MS_{SPErr})^2}{\left(\frac{(MS_{WPErr})^2}{a(n-1)} + \frac{((b-1)MS_{SPErr})^2}{a(b-1)(n-1)}\right)}$$

We analyze two examples below. The first example involves a controlled experiment with the two factors being randomly assigned to the two levels of units. The second example involves making observations on individuals from existing populations of groups.

Example – Applying Pretreatment and Wood Stains to Panels

In this example, researchers are interested in the effects of $a = 2$ Pretreatments and $b = 4$ Wood Stains on water resistance of wood panels (Potcner and Kowalski (2004)). In a balanced Completely Randomized Design, we would take $N = 8r$ panels and assign them at random to the 8 treatment combinations of Pretreatment and Stain, with r replicates per treatment. Due to the nature of conducting the experiment, it is necessary to apply Pretreatments to larger sections of panels, and it is easy to apply Stains to smaller subsections.

In this experiment, there are $n = 6$ “large” panels which serve as the Whole Plot Units, and are randomized such that 3 receive Pretreatment 1, and the other 3 receive Pretreatment 2. After applying Pretreatments to the panels, each panel is split into 4 subpanels. The 4 Wood Stains are randomly assigned to the 4 subpanels created from each panel. The water resistance of each of the $N = 24$ subpanels is measured as the response. The data and various means are given in spreadsheet form below, leading to the Analysis of Variance, tests, and estimates.

Resistance	WP_unit	Pretreat	Stain	PretrxStain	WP_mean	PreTr_Mean	Stain_Mean	PxS_Mean	All_Mean
53.5	4	2	2	22	42.000	40.650	51.350	45.400	46.358
32.5	4	2	4	24	42.000	40.650	43.883	35.733	46.358
46.6	4	2	1	21	42.000	40.650	47.350	43.633	46.358
35.4	4	2	3	23	42.000	40.650	42.850	37.833	46.358
44.6	5	2	4	24	47.750	40.650	43.883	35.733	46.358
52.2	5	2	1	21	47.750	40.650	47.350	43.633	46.358
45.9	5	2	3	23	47.750	40.650	42.850	37.833	46.358
48.3	5	2	2	22	47.750	40.650	51.350	45.400	46.358
40.8	1	1	3	13	45.275	52.067	42.850	47.867	46.358
43.0	1	1	1	11	45.275	52.067	47.350	51.067	46.358
51.8	1	1	2	12	45.275	52.067	51.350	57.300	46.358
45.5	1	1	4	14	45.275	52.067	43.883	52.033	46.358
60.9	2	1	2	12	56.175	52.067	51.350	57.300	46.358
55.3	2	1	4	14	56.175	52.067	43.883	52.033	46.358
51.1	2	1	3	13	56.175	52.067	42.850	47.867	46.358
57.4	2	1	1	11	56.175	52.067	47.350	51.067	46.358
32.1	6	2	1	21	32.200	40.650	47.350	43.633	46.358
30.1	6	2	4	24	32.200	40.650	43.883	35.733	46.358
34.4	6	2	2	22	32.200	40.650	51.350	45.400	46.358
32.2	6	2	3	23	32.200	40.650	42.850	37.833	46.358
52.8	3	1	1	11	54.750	52.067	47.350	51.067	46.358
51.7	3	1	3	13	54.750	52.067	42.850	47.867	46.358
55.3	3	1	4	14	54.750	52.067	43.883	52.033	46.358
59.2	3	1	2	12	54.750	52.067	51.350	57.300	46.358

Making use of these means (in the order they appear on the spreadsheet), we compute the Sums of Squares, Analysis of Variance, and F-tests.

$$\begin{aligned}
 a = 2 \quad b = 4 \quad n = 3 \\
 SS_A = 4(3) \left[(40.650 - 46.358)^2 + (52.067 - 46.358)^2 \right] = 782.042 \quad df_A = 2 - 1 = 1 \quad MS_A = 782.042 \\
 SS_{WPErr} = \\
 = 4 \left[(42.000 - 40.650)^2 + (47.750 - 40.650)^2 + (45.275 - 52.067)^2 + (56.175 - 52.067)^2 + (32.200 - 40.650)^2 + (54.750 - 52.067)^2 \right] = \\
 = 775.362 \quad df_{WPErr} = 2(3 - 1) = 4 \quad MS_{WPErr} = 193.841 \\
 SS_B = 2(3) \left[(51.350 - 46.358)^2 + (43.883 - 46.358)^2 + (47.350 - 46.358)^2 + (42.850 - 46.358)^2 \right] = 266.005 \\
 df_B = 4 - 1 = 3 \quad MS_B = 88.668 \\
 SS_{AB} = 3 \left[(45.400 - 40.650 - 51.350 + 46.358)^2 + \dots + (57.300 - 52.067 - 51.350 + 46.358)^2 \right] = 62.792 \\
 df_{AB} = (2 - 1)(4 - 1) = 3 \quad MS_{AB} = 20.931 \\
 SS_{SPErr} = \left[(53.5 - 45.400 - 42.000 + 40.650)^2 + \dots + (59.2 - 57.300 - 54.750 + 52.067)^2 \right] = 152.518 \\
 df_{SPErr} = 2(4 - 1)(3 - 1) = 12 \quad MS_{SPErr} = 12.710 \\
 H_0^A : \alpha_1 = \alpha_2 = 0 \quad F_A = \frac{782.042}{193.841} = 4.034 \quad F_{.95;1,4} = 7.71 \quad P(F_{1,4} \geq 4.034) = .1150 \\
 H_0^B : \beta_1 = \dots = \beta_4 = 0 \quad F_B = \frac{88.668}{12.710} = 6.976 \quad F_{.95;3,12} = 3.49 \quad P(F_{3,12} \geq 6.976) = .0057 \\
 H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{24} = 0 \quad F_{AB} = \frac{20.931}{12.710} = 1.647 \quad F_{.95;3,12} = 3.49 \quad P(F_{3,12} \geq 1.647) = .2309
 \end{aligned}$$

The Analysis of Variance table is given below, summarizing the tests computed above.

Source	df	SS	MS	F	F(.95)	P-value
Pretreatment	1	782.042	782.042	4.034	7.709	0.1150
WP Error	4	775.362	193.840			
Stain	3	266.005	88.668	6.976	3.490	0.0057
PretrtxStain	3	62.792	20.931	1.647	3.490	0.2309
SP Error	12	152.518	12.710			
Total (Corr)	23	2038.718				

The estimated variance components, means, standard errors and formulas for confidence intervals for mean differences are computed below.

$$\hat{\sigma}^2 = 12.710 \quad \hat{\sigma}_\gamma^2 = \frac{193.840 - 12.710}{4} = 45.283$$

Whole Plot Factor:

$$\hat{V}\{\bar{Y}_{i..}\} = \frac{193.840}{4(3)} = 16.153 \quad \hat{SE}\{\bar{Y}_{i..}\} = \sqrt{16.153} = 4.019$$

$$\hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{2(193.840)}{4(3)} = 32.306 \quad \hat{SE}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \sqrt{32.306} = 5.684$$

$$95\% \text{ CI for } \alpha_i - \alpha_{i'} : (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 2.776(5.684) \equiv (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 15.778$$

Sub Plot Factor:

$$\hat{V}\{\bar{Y}_{.j.}\} = \frac{193.840 + (4-1)(12.710)}{2(4)(3)} = 9.665 \quad \hat{SE}\{\bar{Y}_{.j.}\} = \sqrt{9.665} = 3.109$$

$$\hat{V}\{\bar{Y}_{.j.} - \bar{Y}_{.j'.}\} = \frac{2(12.710)}{2(3)} = 4.237 \quad \hat{SE}\{\bar{Y}_{.j.} - \bar{Y}_{.j'.}\} = \sqrt{4.237} = 2.058$$

$$95\% \text{ CI for } \beta_j - \beta_{j'} : (\bar{y}_{.j.} - \bar{y}_{.j'.}) \pm 2.179(2.058) \equiv (\bar{y}_{.j.} - \bar{y}_{.j'.}) \pm 4.485$$

Simple Effects:

$$\hat{V}\{\bar{Y}_{ij.}\} = \frac{193.840 + (4-1)(12.710)}{4(3)} = 19.331 \quad \hat{SE}\{\bar{Y}_{ij.}\} = \sqrt{19.331} = 4.397$$

1) Two simple effects @ same level of Whole Plot:

$$\hat{V}\{\bar{Y}_{ij.} - \bar{Y}_{ij'.}\} = \frac{2(12.710)}{3} = 8.473 \quad \hat{SE}\{\bar{Y}_{ij.} - \bar{Y}_{ij'.}\} = \sqrt{8.473} = 2.911$$

$$95\% \text{ CI for } (\alpha\beta)_{ij} - (\alpha\beta)_{ij'} : (\bar{y}_{ij.} - \bar{y}_{ij'.}) \pm 2.179(2.911) \equiv (\bar{y}_{ij.} - \bar{y}_{ij'.}) \pm 6.343$$

2) Two simple effects @ different levels of Whole Plot ($i \neq i', \forall j, j'$):

$$\hat{V}\{\bar{Y}_{ij.} - \bar{Y}_{i'j'.}\} = \frac{2[193.840 + (4-1)(12.710)]}{4(3)} = 38.662 \quad \hat{SE}\{\bar{Y}_{ij.} - \bar{Y}_{i'j'.}\} = \sqrt{38.662} = 6.218$$

$$(1-\alpha)100\% \text{ CI for } (\alpha\beta)_{ij} - (\alpha\beta)_{i'j'.} : (\bar{y}_{ij.} - \bar{y}_{i'j'.}) \pm 2.571(6.218) \equiv (\bar{y}_{ij.} - \bar{y}_{i'j'.}) \pm 15.986$$

$$\text{Satterthwaite's Approximate df: } \nu^* = \frac{(193.840 + (4-1)(12.710))^2}{\left(\frac{(193.840)^2}{2(3-1)} + \frac{((4-1)12.710)^2}{2(4-1)(3-1)}\right)} = \frac{53810.081}{9514.644} = 5.656$$

The R Program and Output are given here.

R Program

```
ws <- read.csv("http://www.stat.ufl.edu/~winner/data/wood_stain.csv",header=T)
attach(ws); names(ws)

WP_unit <- factor(WP_unit)
Pretreat <- factor(Pretreat)
Stain <- factor(Stain)

ws.mod1 <- aov(Resistance ~ Pretreat + Pretreat:WP_unit + Stain + Pretreat:Stain)
anova(ws.mod1)

library(lmerTest)

ws.mod3 <- lmer(Resistance ~ Pretreat*Stain + (1|Pretreat:WP_unit))
summary(ws.mod3)
anova(ws.mod3)
lsmmeans(ws.mod3)
diff.lsmmeans(ws.mod3)
rand(ws.mod3)
```

R Output

```
> anova(ws.mod1)
Analysis of Variance Table

Response: Resistance
Df Sum Sq Mean Sq F value Pr(>F)
Pretreat 1 782.04 782.04 61.5303 4.596e-06 ***
Stain 3 266.01 88.67 6.9763 0.0056928 **
Pretreat:WP_unit 4 775.36 193.84 15.2512 0.0001186 ***
Pretreat:Stain 3 62.79 20.93 1.6468 0.2309105
Residuals 12 152.52 12.71

> summary(ws.mod3)

Random effects:
Groups Name Variance Std.Dev.
Pretreat:WP_unit (Intercept) 45.28 6.729
Residual 12.71 3.565
Number of obs: 24, groups: Pretreat:WP_unit, 6

Fixed effects:
Estimate Std. Error df t value Pr(>|t|)
(Intercept) 51.0667 4.3967 5.6550 11.615 3.69e-05 ***
Pretreat2 -7.4333 6.2179 5.6550 -1.195 0.2796
Stain2 6.2333 2.9109 12.0000 2.141 0.0535 .
Stain3 -3.2000 2.9109 12.0000 -1.099 0.2932
Stain4 0.9667 2.9109 12.0000 0.332 0.7456
Pretreat2:Stain2 -4.4667 4.1166 12.0000 -1.085 0.2992
Pretreat2:Stain3 -2.6000 4.1166 12.0000 -0.632 0.5395
Pretreat2:Stain4 -8.8667 4.1166 12.0000 -2.154 0.0523 .

> anova(ws.mod3)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
Sum Sq Mean Sq NumDF DenDF F.value Pr(>F)
Pretreat 51.277 51.277 1 4 4.0345 0.114983
Stain 266.005 88.668 3 12 6.9763 0.005693 **
Pretreat:Stain 62.792 20.931 3 12 1.6468 0.230910
```

Note that the F-test for Pretreatment uses the incorrect error term and error degrees of freedom, leading to false rejection of the null hypothesis of no differences among Pretreatment effects. The Output continues below.

```

> lsmeans(ws.mod3)
Least Squares Means table:

```

	Pretreat	Stain	Estimate	Standard Error	DF	t-value	Lower CI	Upper CI	p-value
Pretreat 1	1.0	NA	52.07	4.02	4.0	12.95	40.9	63.2	2e-04 ***
Pretreat 2	2.0	NA	40.65	4.02	4.0	10.11	29.5	51.8	5e-04 ***
Stain 1	NA	1.0	47.35	3.11	5.7	15.23	39.6	55.1	<2e-16 ***
Stain 2	NA	2.0	51.35	3.11	5.7	16.52	43.6	59.1	<2e-16 ***
Stain 3	NA	3.0	42.85	3.11	5.7	13.78	35.1	50.6	<2e-16 ***
Stain 4	NA	4.0	43.88	3.11	5.7	14.12	36.2	51.6	<2e-16 ***
Pretreat:Stain 1 1	1.0	1.0	51.07	4.40	5.7	11.61	40.1	62.0	<2e-16 ***
Pretreat:Stain 2 1	2.0	1.0	43.63	4.40	5.7	9.92	32.7	54.6	1e-04 ***
Pretreat:Stain 1 2	1.0	2.0	57.30	4.40	5.7	13.03	46.4	68.2	<2e-16 ***
Pretreat:Stain 2 2	2.0	2.0	45.40	4.40	5.7	10.33	34.5	56.3	1e-04 ***
Pretreat:Stain 1 3	1.0	3.0	47.87	4.40	5.7	10.89	36.9	58.8	1e-04 ***
Pretreat:Stain 2 3	2.0	3.0	37.83	4.40	5.7	8.60	26.9	48.8	2e-04 ***
Pretreat:Stain 1 4	1.0	4.0	52.03	4.40	5.7	11.83	41.1	63.0	<2e-16 ***
Pretreat:Stain 2 4	2.0	4.0	35.73	4.40	5.7	8.13	24.8	46.7	3e-04 ***

```

> diff lsmeans(ws.mod3)
Differences of LSMEANS:

```

	Estimate	Standard Error	DF	t-value	Lower CI	Upper CI	p-value
Pretreat 1 - 2	11.4	5.684	4.0	2.01	-4.3644	27.198	0.115
Stain 1 - 2	-4.0	2.058	12.0	-1.94	-8.4847	0.485	0.076 .
Stain 1 - 3	4.5	2.058	12.0	2.19	0.0153	8.985	0.049 *
Stain 1 - 4	3.5	2.058	12.0	1.68	-1.0180	7.951	0.118
Stain 2 - 3	8.5	2.058	12.0	4.13	4.0153	12.985	0.001 **
Stain 2 - 4	7.5	2.058	12.0	3.63	2.9820	11.951	0.004 **
Stain 3 - 4	-1.0	2.058	12.0	-0.50	-5.5180	3.451	0.625
Pretreat:Stain 1 1 - 2 1	7.4	6.218	5.7	1.20	-8.0087	22.875	0.280
Pretreat:Stain 1 1 - 1 2	-6.2	2.911	12.0	-2.14	-12.5756	0.109	0.053 .
Pretreat:Stain 1 1 - 2 2	5.7	6.218	5.7	0.91	-9.7754	21.109	0.399
Pretreat:Stain 1 1 - 1 3	3.2	2.911	12.0	1.10	-3.1423	9.542	0.293
Pretreat:Stain 1 1 - 2 3	13.2	6.218	5.7	2.13	-2.2087	28.675	0.080 .
Pretreat:Stain 1 1 - 1 4	-1.0	2.911	12.0	-0.33	-7.3089	5.376	0.746
Pretreat:Stain 1 1 - 2 4	15.3	6.218	5.7	2.47	-0.1087	30.775	0.051 .
Pretreat:Stain 2 1 - 1 2	-13.7	6.218	5.7	-2.20	-29.1087	1.775	0.073 .
Pretreat:Stain 2 1 - 2 2	-1.8	2.911	12.0	-0.61	-8.1089	4.576	0.555
Pretreat:Stain 2 1 - 1 3	-4.2	6.218	5.7	-0.68	-19.6754	11.209	0.523
Pretreat:Stain 2 1 - 2 3	5.8	2.911	12.0	1.99	-0.5423	12.142	0.070 .
Pretreat:Stain 2 1 - 1 4	-8.4	6.218	5.7	-1.35	-23.8421	7.042	0.228
Pretreat:Stain 2 1 - 2 4	7.9	2.911	12.0	2.71	1.5577	14.242	0.019 *
Pretreat:Stain 1 2 - 2 2	11.9	6.218	5.7	1.91	-3.5421	27.342	0.107
Pretreat:Stain 1 2 - 1 3	9.4	2.911	12.0	3.24	3.0911	15.776	0.007 **
Pretreat:Stain 1 2 - 2 3	19.5	6.218	5.7	3.13	4.0246	34.909	0.022 **
Pretreat:Stain 1 2 - 1 4	5.3	2.911	12.0	1.81	-1.0756	11.609	0.096 .
Pretreat:Stain 1 2 - 2 4	21.6	6.218	5.7	3.47	6.1246	37.009	0.015 *
Pretreat:Stain 2 2 - 1 3	-2.5	6.218	5.7	-0.40	-17.9087	12.975	0.706
Pretreat:Stain 2 2 - 2 3	7.6	2.911	12.0	2.60	1.2244	13.909	0.023 *
Pretreat:Stain 2 2 - 1 4	-6.6	6.218	5.7	-1.07	-22.0754	8.809	0.330
Pretreat:Stain 2 2 - 2 4	9.7	2.911	12.0	3.32	3.3244	16.009	0.006 **
Pretreat:Stain 1 3 - 2 3	10.0	6.218	5.7	1.61	-5.4087	25.475	0.161
Pretreat:Stain 1 3 - 1 4	-4.2	2.911	12.0	-1.43	-10.5089	2.176	0.178
Pretreat:Stain 1 3 - 2 4	12.1	6.218	5.7	1.95	-3.3087	27.575	0.102
Pretreat:Stain 2 3 - 1 4	-14.2	6.218	5.7	-2.28	-29.6421	1.242	0.065 .
Pretreat:Stain 2 3 - 2 4	2.1	2.911	12.0	0.72	-4.2423	8.442	0.484
Pretreat:Stain 1 4 - 2 4	16.3	6.218	5.7	2.62	0.8579	31.742	0.042 *

```

> rand(ws.mod3)
Analysis of Random effects Table:

```

	Chi.sq	Chi.DF	p.value
Pretreat:WP_unit	13.4	1	3e-04 ***

Example – Observational Study of Axon Densities of Optic Nerves

In this study, samples of $n = 12$ normal and Alzheimer's patients were obtained and mean axon densities ($2000 \mu\text{m}^2$) were measured in their left and right eyes. In this analysis, group (normal/Alzheimer's) acted as the Whole Plot factor, with $a = 2$ levels. The subjects (nested within group) are the Whole Plot units, with $n = 12$ subjects per group. The eyes (left/right) are the Sub Plot factor, with $b = 2$ levels. The data are given below in tabular form along with relevant means.

Normal				Alzheimer's			
Subject	Right	Left	Mean	Subject	Right	Left	Mean
1	673	766	719.5	13	538	377	457.5
2	899	956	927.5	14	583	555	569.0
3	616	605	610.5	15	696	298	497.0
4	749	858	803.5	16	568	583	575.5
5	1078	1017	1047.5	17	649	700	674.5
6	978	861	919.5	18	284	458	371.0
7	706	569	637.5	19	862	746	804.0
8	1005	991	998.0	20	848	774	811.0
9	1420	1258	1339.0	21	716	698	707.0
10	1003	997	1000.0	22	508	563	535.5
11	818	982	900.0	23	378	374	376.0
12	761	701	731.0	24	621	633	627.0
Mean	892.167	880.083	886.125		604.250	563.250	583.750
Overall	748.208	721.667	734.938				

The Sums of Squares and F-tests are computed below.

$$SS_A = 2(12) \left[(886.125 - 734.983)^2 + (583.750 - 734.983)^2 \right] = 1097167.69 \quad df_A = 2 - 1 \quad MS_A = 1097167.69$$

$$SS_{WPErr} = 2 \left[(719.5 - 886.125)^2 + \dots + (627.0 - 583.750)^2 \right] = 1392055.6 \quad df_{WPErr} = 2(12 - 1) = 22 \quad MS_{WPErr} = 63275.25$$

$$SS_B = 2(12) \left[(748.208 - 734.983)^2 + (721.667 - 734.983)^2 \right] = 8453.52 \quad df_B = 2 - 1 = 1 \quad MS_B = 8453.52$$

$$SS_{AB} = 12 \left[(892.167 - 886.125 - 748.208 + 734.938)^2 + \dots + (563.250 - 583.750 - 721.667 + 734.938)^2 \right] = 2508.52$$

$$df_{AB} = (2 - 1)(2 - 1) = 1 \quad MS_{AB} = 2508.52$$

$$SS_{SPErr} = \left[(673 - 719.5 - 892.167 + 886.125)^2 + \dots + (633 - 627.0 - 563.250 + 583.750)^2 \right] = 167889.46$$

$$df_{SPErr} = 2(2 - 1)(12 - 1) = 22 \quad MS_{SPErr} = 7631.34$$

$$H_0^A : \alpha_1 = \alpha_2 = 0 \quad F_A = \frac{1097167.69}{63275.25} = 17.34 \quad F_{.95;1,22} = 4.30 \quad P(F_{1,22} \geq 17.34) = .0004$$

$$H_0^B : \beta_1 = \beta_2 = 0 \quad F_B = \frac{8453.52}{7631.34} = 1.108 \quad F_{.95;1,22} = 4.30 \quad P(F_{1,22} \geq 1.108) = .3039$$

$$H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{22} = 0 \quad F_{AB} = \frac{2508.52}{7631.34} = 0.329 \quad F_{.95;1,22} = 4.30 \quad P(F_{1,22} \geq 0.329) = .5721$$

The Analysis of Variance is given below in Tabular form.

Source	df	SS	MS	F	F(.95)	P-value
Group	1	1097167.69	1097167.69	17.340	4.301	0.0004
WP Error	22	1392055.63	63275.26			
Eye	1	8453.52	8453.52	1.108	4.301	0.3040
GroupxEye	1	2508.52	2508.52	0.329	4.301	0.5722
SP Error	22	167889.46	7631.34			
Total	47	2668074.81				

The estimated variance components, means, standard errors and formulas for confidence intervals for mean differences are computed below.

$$\hat{\sigma}^2 = 7631.34 \quad \hat{\sigma}_\gamma^2 = \frac{63275.26 - 7631.34}{2} = 27821.96$$

Whole Plot Factor:

$$\hat{V}\{\bar{Y}_{i..}\} = \frac{63275.26}{2(12)} = 2636.47 \quad \hat{SE}\{\bar{Y}_{i..}\} = \sqrt{2636.47} = 51.35$$

$$\hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{2(63275.26)}{2(12)} = 5272.94 \quad \hat{SE}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \sqrt{5272.94} = 72.62$$

95% CI for $\alpha_1 - \alpha_2$: $(886.125 - 583.750) \pm 2.074(72.62) \equiv 302.375 \pm 150.614$

Sub Plot Factor:

$$\hat{V}\{\bar{Y}_{.j.}\} = \frac{63275.26 + (2-1)(7631.34)}{2(2)(12)} = 1477.22 \quad \hat{SE}\{\bar{Y}_{.j.}\} = \sqrt{1477.2} = 38.43$$

$$\hat{V}\{\bar{Y}_{.j.} - \bar{Y}_{.j'.}\} = \frac{2(7631.34)}{2(12)} = 635.95 \quad \hat{SE}\{\bar{Y}_{.j.} - \bar{Y}_{.j'.}\} = \sqrt{635.95} = 25.22$$

95% CI for $\beta_1 - \beta_2$: $(748.208 - 721.667) \pm 2.074(25.22) \equiv 26.541 \pm 52.31$

Simple Effects:

$$\hat{V}\{\bar{Y}_{ij.}\} = \frac{63275.26 + (2-1)(7631.34)}{2(12)} = 2954.44 \quad \hat{SE}\{\bar{Y}_{ij.}\} = \sqrt{2954.44} = 54.35$$

1) Two simple effects @ same level of Whole Plot:

$$\hat{V}\{\bar{Y}_{ij.} - \bar{Y}_{ij'.}\} = \frac{2(7631.34)}{12} = 1271.89 \quad \hat{SE}\{\bar{Y}_{ij.} - \bar{Y}_{ij'.}\} = \sqrt{1271.89} = 35.66$$

95% CI for $(\alpha\beta)_{i1} - (\alpha\beta)_{i2}$: $(\bar{y}_{i1.} - \bar{y}_{i2.}) \pm 2.074(35.66) \equiv (\bar{y}_{ij.} - \bar{y}_{ij'.}) \pm 73.97$

2) Two simple effects @ different levels of Whole Plot ($i \neq i', \forall j, j'$):

$$\hat{V}\{\bar{Y}_{ij.} - \bar{Y}_{i'j'.}\} = \frac{2[63275.26 + (2-1)(7631.34)]}{2(12)} = 5908.88 \quad \hat{SE}\{\bar{Y}_{ij.} - \bar{Y}_{i'j'.}\} = \sqrt{5908.88} = 76.87$$

95% CI for $(\alpha\beta)_{ij} - (\alpha\beta)_{i'j'}$: $(\bar{y}_{ij.} - \bar{y}_{i'j'.}) \pm 2.052(76.87) \equiv (\bar{y}_{ij.} - \bar{y}_{i'j'.}) \pm 157.74$

Satterthwaite's Approximate df: $\nu^* = \frac{(63275.26 + (2-1)(7631.34))^2}{\left(\frac{(63275.26)^2}{2(12-1)} + \frac{((2-1)7631.34)^2}{2(2-1)(12-1)}\right)} = \frac{(70906.6)^2}{\left(\frac{(63275.26)^2 + (7631.34)^2}{22}\right)} = 27.23$

Note that both examples had large variation among Whole Plot units, which is common in practice. The Wood Stain study had only 3 Whole Plot units per Whole Plot treatment, while the Alzheimer's Eye Axon study had 12 Whole Plot units per Whole Plot treatment. This leads to higher power to detect Whole Plot effects in the second study. The R Program and Output are given below.

R Program

```
alz.eyes <- read.csv("http://www.stat.ufl.edu/~winner/data/alzheimers_eyes.csv",
header=T)
attach(alz.eyes); names(alz.eyes)

subject <- factor(subject)
alz_grp <- factor(alz_grp, levels=1:2, labels=c("Nor", "Alz"))
eye <- factor(eye, levels=1:2, labels=c("R", "L"))

alzeyes.mod1 <- aov(axondens ~ alz_grp + alz_grp:subject + eye + alz_grp:eye)
anova(alzeyes.mod1)

library(lmerTest)

alzeyes.mod2 <- lmer(axondens ~ alz_grp*eye + (1|alz_grp:subject))
summary(alzeyes.mod2)
anova(alzeyes.mod2)
lsmmeans(alzeyes.mod2)
diff1smmeans(alzeyes.mod2)
rand(alzeyes.mod2)
```

R Output

Analysis of Variance Table

Response: axondens

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
alz_grp	1	1097168	1097168	143.7713	4.037e-11	***
eye	1	8454	8454	1.1077	0.3040	
alz_grp:subject	22	1392056	63275	8.2915	2.812e-06	***
alz_grp:eye	1	2509	2509	0.3287	0.5722	

> summary(alzeyes.mod2)

Random effects:

Groups	Name	Variance	Std.Dev.
alz_grp:subject	(Intercept)	27822	166.80
Residual		7631	87.36

Number of obs: 48, groups: alz_grp:subject, 24

Fixed effects:

	Estimate	Std. Error	df	t value	Pr(> t)	
(Intercept)	892.17	54.35	27.23	16.414	1.33e-15	***
alz_grpAlz	-287.92	76.87	27.23	-3.746	0.000855	***
eyeL	-12.08	35.66	22.00	-0.339	0.737962	
alz_grpAlz:eyeL	-28.92	50.44	22.00	-0.573	0.572233	

> anova(alzeyes.mod2)

Analysis of Variance Table of type 3 with Satterthwaite approximation for degrees of freedom

	Sum Sq	Mean Sq	NumDF	DenDF	F.value	Pr(>F)
alz_grp	132324	132324	1	22	17.3396	0.0004041 ***
eye	8454	8454	1	22	1.1077	0.3039977
alz_grp:eye	2509	2509	1	22	0.3287	0.5722325

> lsmmeans(alzeyes.mod2)

Least Squares Means table:

	alz_grp	eye	Estimate	Standard Error	DF	t-value	Lower CI	Upper CI	p-value		
alz_grp	Nor	2.0	NA	886.1	51.4	22.0	17.3	780	993	<2e-16 ***	
alz_grp	Alz	1.0	NA	583.8	51.4	22.0	11.4	477	690	<2e-16 ***	
eye	R	NA	2.0	748.2	38.4	27.2	19.5	669	827	<2e-16 ***	
eye	L	NA	1.0	721.7	38.4	27.2	18.8	643	800	<2e-16 ***	
alz_grp:eye	Nor	R	2.0	2.0	892.2	54.4	27.2	16.4	781	1004	<2e-16 ***
alz_grp:eye	Alz	R	1.0	2.0	604.2	54.4	27.2	11.1	493	716	<2e-16 ***
alz_grp:eye	Nor	L	2.0	1.0	880.1	54.4	27.2	16.2	769	992	<2e-16 ***
alz_grp:eye	Alz	L	1.0	1.0	563.2	54.4	27.2	10.4	452	675	<2e-16 ***

Continued below.

```

> diff1smeans(alzeyes.mod2)
Differences of LSMEANS:
      Estimate Standard Error    DF t-value Lower CI Upper CI p-value
alz_grp Nor - Alz          302.4      72.6   22.0    4.16   151.8   453.0 4e-04 ***
eye R - L                26.5      25.2   22.0    1.05   -25.8    78.8 0.304
alz_grp:eye Nor R - Alz R    287.9      76.9   27.2    3.75   130.3   445.6 9e-04 ***
alz_grp:eye Nor R - Nor L    12.1      35.7   22.0    0.34   -61.9    86.0 0.738
alz_grp:eye Nor R - Alz L    328.9      76.9   27.2    4.28   171.3   486.6 2e-04 ***
alz_grp:eye Alz R - Nor L   -275.8      76.9   27.2   -3.59  -433.5  -118.2 0.001 **
alz_grp:eye Alz R - Alz L     41.0      35.7   22.0    1.15   -33.0   115.0 0.263
alz_grp:eye Nor L - Alz L    316.8      76.9   27.2    4.12   159.2   474.5 3e-04 ***

> rand(alzeyes.mod2)
Analysis of Random effects Table:
      Chi.sq Chi.DF p.value
alz_grp:subject    21     1 4e-06 ***

```

A special case of Split-Plot Designs run as Completely Randomized Designs are **Repeated Measures Designs**. In these cases, subjects (Whole Plot units) are assigned at random to Whole-Plot Treatments, and then observed at multiple points in time (Sub-Plot “treatment”). One problem that occurs in practice is that the covariance (and correlation) between measurements within the same subject tend to decrease as time points get further away. This phenomenon is inconsistent with the structure described here, where we assume the covariance and correlation of any two measurements made on the Whole-Plot units are as follow.

$$j \neq j': \text{COV}\{Y_{ijk}, Y_{ij'k}\} = \sigma_\gamma^2 \Rightarrow \text{CORR}\{Y_{ijk}, Y_{ij'k}\} = \frac{\text{COV}\{Y_{ijk}, Y_{ij'k}\}}{\sqrt{V\{Y_{ijk}\}V\{Y_{ij'k}\}}} = \frac{\sigma_\gamma^2}{\sigma_\gamma^2 + \sigma^2}$$

We will return to Repeated Measures Designs in Chapter 12.

The design described above is easily extended to factorial treatment structures at the Whole-Plot and Sub-Plot levels. For instance, suppose we have the Whole-Plot structure is a 2-Way Factorial with factors A and B, and Whole-Plot units are assigned at random to the *ab* combinations of A and B. Further, the Sub-Plot structure is a 2-Way Factorial with factors C and D. If there are no interactions between the Sub-Plot factors and the Whole-Plot units, then we have the following model, assuming A, B, C, and D are fixed factors.

$$Y_{ijklm} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \lambda_{m(ij)} + \gamma_k + \delta_l + (\gamma\delta)_{kl} + (\alpha\gamma)_{ik} + (\alpha\delta)_{il} + (\alpha\gamma\delta)_{ikl} + (\beta\gamma)_{jk} + (\beta\delta)_{jl} + (\beta\gamma\delta)_{jkl} + (\alpha\beta\gamma\delta)_{ijkl} + \varepsilon_{ijklm} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c; l = 1, \dots, d; m = 1, \dots, n$$

When Factors C and D are Independent of Whole-Plot Units:

$$\text{COV}\{Y_{ijklm}, Y_{i'j'k'l'm'}\} = \begin{cases} \sigma_\lambda^2 + \sigma^2 & i = i', j = j', k = k', l = l', m = m' \\ \sigma_\lambda^2 & i = i', j = j', m = m'; k \neq k' \text{ and/or } l \neq l' \\ 0 & \text{otherwise} \end{cases}$$

For this model, we would have the following Analysis of Variance Table.

Source	df	Error Term	Error_df
A	a-1	MS_WPErr	ab(n-1)
B	b-1	MS_WPErr	ab(n-1)
AB	(a-1)(b-1)	MS_WPErr	ab(n-1)
WPError	ab(n-1)		
C	c-1	MS_SPErr	ab(cd-1)(n-1)
D	d-1	MS_SPErr	ab(cd-1)(n-1)
CD	(c-1)(d-1)	MS_SPErr	ab(cd-1)(n-1)
AC	(a-1)(c-1)	MS_SPErr	ab(cd-1)(n-1)
AD	(a-1)(d-1)	MS_SPErr	ab(cd-1)(n-1)
ACD	(a-1)(c-1)(d-1)	MS_SPErr	ab(cd-1)(n-1)
BC	(b-1)(c-1)	MS_SPErr	ab(cd-1)(n-1)
BD	(b-1)(d-1)	MS_SPErr	ab(cd-1)(n-1)
BCD	(b-1)(c-1)(d-1)	MS_SPErr	ab(cd-1)(n-1)
ABCD	(a-1)(b-1)(c-1)(d-1)	MS_SPErr	ab(cd-1)(n-1)
SPError	ab(cd-1)(n-1)		
Total	abcdn-1		

12.2. Split-Plot in a Randomized Block Design

In many experiments, the Split-Plot experiment is conducted as a Randomized Block Design. The blocks may be different days where the experiment is run, or different locations in an agricultural setting. In this case, the Whole-Plot treatments are randomly assigned to the a “larger” units within the blocks and the Sub-Plot treatments are assigned to the b “smaller” subunits within the larger (Whole-Plot) units. Here we consider the cases where there is a single Whole-Plot factor and a single Sub-Plot factor. We will consider the analysis where the blocks (aka replicates) are random and all combinations of fixed and random Whole-Plot and Sub-Plot factors. The models are given below.

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \gamma_k + (\alpha\gamma)_{ik} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c$$

$$\text{Whole-Plot Factor: Fixed: } \sum_{i=1}^a \alpha_i = 0 \quad \text{Random: } \alpha_i \sim NID(0, \sigma_\alpha^2)$$

$$\text{Blocks: } \beta_j \sim NID(0, \sigma_\beta^2) \quad \text{WP/Block Interaction: } (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2)$$

$$\text{Sub-Plot Factor: Fixed: } \sum_{j=1}^c \gamma_k = 0 \quad \text{Random: } \gamma_k \sim NID(0, \sigma_\gamma^2)$$

$$\text{WP/SP Interaction: Fixed: } \sum_{i=1}^a (\alpha\gamma)_{ik} = \sum_{j=1}^c (\alpha\gamma)_{ik} = 0 \quad \text{Random: } (\alpha\gamma)_{ik} \sim NID(0, \sigma_{\alpha\gamma}^2)$$

$$\text{Error: } \varepsilon_{ijk} \sim NID(0, \sigma^2) \quad \text{All random effects assumed to be independent.}$$

The Sums of Squares are computed as usual. Note that the error term and its Sums of Squares is the sum of those for Sub-Plot/Block and the Whole-Plot/Sub-Plot/Block Interactions. The Expected Mean Squares and F-tests are derived below. First given is the case where both Whole-Plot and Sub-Plot factors are fixed.

$$E\{Y_{ijk}\} = \mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik}$$

$$\text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 & i=i' \ j=j' \ k=k' \\ \sigma_\beta^2 + \sigma_{\alpha\beta}^2 & i=i' \ j=j' \ k \neq k' \\ \sigma_\beta^2 & i \neq i' \ j=j' \ \forall k, k' \\ 0 & j \neq j' \ \forall i, i', k, k' \end{cases}$$

$$V\left\{\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c Y_{ijk}\right\} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c V\{Y_{ijk}\} + 2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{c-1} \sum_{k'=k+1}^c \text{COV}\{Y_{ijk}, Y_{ijk'}\} + 2 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{k'=1}^c \text{COV}\{Y_{ijk}, Y_{i'jk'}\} +$$

$$+ 2 \sum_{i=1}^a \sum_{i'=1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^c \sum_{k'=1}^c \text{COV}\{Y_{ijk}, Y_{i'j'k'}\}$$

$$= abc(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) + abc(c-1)(\sigma_\beta^2 + \sigma_{\alpha\beta}^2) + a(a-1)bc^2\sigma_\beta^2 + a^2b(b-1)c^2(0)$$

$$= a^2bc^2\sigma_\beta^2 + abc^2\sigma_{\alpha\beta}^2 + abc\sigma^2$$

$$\Rightarrow V\{\bar{Y}_{\dots}\} = \frac{a^2bc^2\sigma_\beta^2 + abc^2\sigma_{\alpha\beta}^2 + abc\sigma^2}{(abc)^2} = \frac{1}{b}\sigma_\beta^2 + \frac{1}{ab}\sigma_{\alpha\beta}^2 + \frac{1}{abc}\sigma^2$$

$$V\{\bar{Y}_{i..}\} = \frac{1}{b}\sigma_\beta^2 + \frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{bc}\sigma^2 \quad V\{\bar{Y}_{.j.}\} = \sigma_\beta^2 + \frac{1}{a}\sigma_{\alpha\beta}^2 + \frac{1}{ac}\sigma^2 \quad V\{\bar{Y}_{..k}\} = \frac{1}{b}\sigma_\beta^2 + \frac{1}{ab}\sigma_{\alpha\beta}^2 + \frac{1}{ab}\sigma^2$$

$$V\{\bar{Y}_{ij.}\} = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{1}{c}\sigma^2 \quad V\{\bar{Y}_{i.k}\} = \frac{1}{b}(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2) \quad V\{\bar{Y}_{.jk}\} = \sigma_\beta^2 + \frac{1}{a}\sigma_{\alpha\beta}^2 + \frac{1}{a}\sigma^2$$

$$E\{\bar{Y}_{\dots}^2\} = \left(\frac{1}{abc}\right)^2 [a^2bc^2\sigma_\beta^2 + abc^2\sigma_{\alpha\beta}^2 + abc\sigma^2] + \mu^2 \quad E\{\bar{Y}_{i..}^2\} = \left(\frac{1}{bc}\right)^2 [bc^2\sigma_\beta^2 + bc^2\sigma_{\alpha\beta}^2 + bc\sigma^2] + (\mu + \alpha_i)^2$$

$$E\{\bar{Y}_{.j.}^2\} = \left(\frac{1}{ac}\right)^2 [a^2c^2\sigma_\beta^2 + ac^2\sigma_{\alpha\beta}^2 + ac\sigma^2] + \mu^2 \quad E\{\bar{Y}_{..k}^2\} = \left(\frac{1}{ab}\right)^2 [a^2b\sigma_\beta^2 + ab\sigma_{\alpha\beta}^2 + ab\sigma^2] + (\mu + \gamma_k)^2$$

$$E\{\bar{Y}_{ij.}^2\} = \left(\frac{1}{c}\right)^2 [c^2\sigma_\beta^2 + c^2\sigma_{\alpha\beta}^2 + c\sigma^2] + (\mu + \alpha_i)^2 \quad E\{\bar{Y}_{i.k}^2\} = \left(\frac{1}{b}\right)^2 [b\sigma_\beta^2 + b\sigma_{\alpha\beta}^2 + b\sigma^2] + (\mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik})^2$$

$$E\{\bar{Y}_{.jk}^2\} = \left(\frac{1}{a}\right)^2 [a^2\sigma_\beta^2 + a\sigma_{\alpha\beta}^2 + a\sigma^2] + (\mu + \gamma_k)^2 \quad E\{Y_{ijk}^2\} = [\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2] + (\mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik})^2$$

$$E\{MS_{\text{BLK}}\} = ac\sigma_\beta^2 + c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{\text{BLK}} = b-1$$

$$E\{MS_{\text{WP}}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 + bc \frac{\sum_{i=1}^a \alpha_i^2}{a-1} \quad df_{\text{WP}} = a-1$$

$$E\{MS_{\text{BLK} \times \text{WP}}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{\text{BLK} \times \text{WP}} = (a-1)(b-1)$$

$$E\{MS_{\text{SP}}\} = \sigma^2 + ab \frac{\sum_{k=1}^c \gamma_k^2}{c-1} \quad df_{\text{SP}} = c-1$$

$$E\{MS_{\text{WP} \times \text{SP}}\} = \sigma^2 + b \frac{\sum_{i=1}^a \sum_{k=1}^c (\alpha\gamma)_{ik}^2}{(a-1)(c-1)} \quad df_{\text{WP} \times \text{SP}} = (a-1)(c-1)$$

$$E\{MS_{\text{ERR}}\} = \sigma^2 \quad df_{\text{ERR}} = a(b-1)(c-1)$$

The model structure described above leads to the following tests, estimators, and inferences concerning the means. Note that if the Block Main Effect and/or Block/Whole-Plot interaction estimates are negative

$\left(\hat{\sigma}_\beta^2 < 0 \text{ and/or } \hat{\sigma}_{\alpha\beta}^2 < 0 \right)$, then the **lmerTest** package in R removes the term(s) from the model and pools their sums of squares and degrees of freedom with the Error term.

Tests for Whole-Plot, Sub-Plot, and Interaction Effects:

$$\text{Whole-Plot Trt Effects: } H_0 : \alpha_1 = \dots = \alpha_a = 0 \quad F_{\text{WP}} = \frac{MS_{\text{WP}}}{MS_{\text{BLK} \times \text{WP}}} \quad P_{\text{WP}} = P\left(F_{a-1, (a-1)(b-1)} \geq F_{\text{WP}}\right)$$

$$\text{Sub-Plot Trt Effects: } H_0 : \gamma_1 = \dots = \gamma_c = 0 \quad F_{\text{SP}} = \frac{MS_{\text{SP}}}{MS_{\text{ERR}}} \quad P_{\text{SP}} = P\left(F_{c-1, a(b-1)(c-1)} \geq F_{\text{SP}}\right)$$

$$\text{WP} \times \text{SP Interaction: } H_0 : (\alpha\gamma)_{ik} = 0 \quad \forall i, k \quad F_{\text{WP} \times \text{SP}} = \frac{MS_{\text{WP} \times \text{SP}}}{MS_{\text{ERR}}} \quad P_{\text{WP} \times \text{SP}} = P\left(F_{(a-1)(c-1), a(b-1)(c-1)} \geq F_{\text{WP} \times \text{SP}}\right)$$

Estimators of Variance Components:

$$E\{MS_{\text{BLK}}\} = ac\sigma_\beta^2 + c\sigma_{\alpha\beta}^2 + \sigma^2 \quad E\{MS_{\text{BLK} \times \text{WP}}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 \quad E\{MS_{\text{ERR}}\} = \sigma^2$$

$$\Rightarrow \hat{\sigma}^2 = MS_{\text{ERR}} \quad \hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{\text{BLK} \times \text{WP}} - MS_{\text{ERR}}}{c} \quad \hat{\sigma}_\beta^2 = \frac{MS_{\text{BLK}} - MS_{\text{BLK} \times \text{WP}}}{ac}$$

Point and Interval Estimators for Whole-Plot Means and Differences of Means:

$$E\{\bar{Y}_{i..}\} = \mu + \alpha_i \quad V\{\bar{Y}_{i..}\} = \frac{1}{b}\sigma_\beta^2 + \frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{bc}\sigma^2$$

$$\Rightarrow \hat{V}\{\bar{Y}_{i..}\} = \frac{(MS_{\text{BLK}} - MS_{\text{BLK} \times \text{WP}}) + a(MS_{\text{BLK} \times \text{WP}} - MS_{\text{ERR}}) + aMS_{\text{ERR}}}{abc} = \frac{MS_{\text{BLK}} + (a-1)MS_{\text{BLK} \times \text{WP}}}{abc}$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \alpha_i): \quad \bar{y}_{i..} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{\text{BLK}} + (a-1)MS_{\text{BLK} \times \text{WP}}}{abc}}$$

$$v^* = \frac{[MS_{\text{BLK}} + (a-1)MS_{\text{ERR}}]^2}{\left[\frac{[MS_{\text{BLK}}]^2}{b-1} + \frac{[(a-1)MS_{\text{ERR}}]^2}{a(b-1)(c-1)}\right]}$$

$$E\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = (\mu + \alpha_i) - (\mu + \alpha_{i'}) = \alpha_i - \alpha_{i'} \quad V\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = V\{\bar{Y}_{i..}\} + V\{\bar{Y}_{i'..}\} - 2\text{COV}\{\bar{Y}_{i..}, \bar{Y}_{i'..}\}$$

$$\text{COV}\{Y_{i..}, Y_{i'..}\} = \text{COV}\left\{\sum_{j=1}^b \sum_{k=1}^c Y_{ijk}, \sum_{j=1}^b \sum_{k=1}^c Y_{i'jk}\right\} = 2 \sum_{j=1}^b \sum_{k=1}^{c-1} \sum_{k'=k+1}^c \text{COV}\{Y_{ijk}, Y_{i'jk'}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^c \sum_{k'=1}^c \text{COV}\{Y_{ijk}, Y_{i'j'k'}\} =$$

$$= bc^2\sigma_\beta^2 + b(b-1)c^2(0) = bc^2\sigma_\beta^2 \quad \Rightarrow \text{COV}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{1}{b^2c^2}(bc^2\sigma_\beta^2) = \frac{1}{b}\sigma_\beta^2$$

$$\Rightarrow V\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = 2 \left[\frac{1}{b}\sigma_\beta^2 + \frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{bc}\sigma^2 - \frac{1}{b}\sigma_\beta^2 \right] = \frac{2}{b} \left[\sigma_{\alpha\beta}^2 + \frac{1}{c}\sigma^2 \right]$$

$$\Rightarrow \hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{2MS_{\text{BLK} \times \text{WP}}}{bc}$$

$$(1-\alpha)100\% \text{ CI for } (\alpha_i - \alpha_{i'}): \quad (\bar{y}_{i..} - \bar{y}_{i'..}) \pm t_{1-\alpha/2; (a-1)(b-1)} \sqrt{\frac{2MS_{\text{BLK} \times \text{WP}}}{bc}}$$

Point and Interval Estimators for Sub-Plot Treatment Means and Differences of Means:

$$E\{\bar{Y}_{\bullet\bullet k}\} = \mu + \gamma_k \quad V\{\bar{Y}_{\bullet\bullet k}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma^2}{ab}$$

$$\Rightarrow \hat{V}\{\bar{Y}_{\bullet\bullet k}\} = \frac{(MS_{\text{BLK}} - MS_{\text{BLK} \times \text{WP}}) + (MS_{\text{BLK} \times \text{WP}} - MS_{\text{ERR}}) + cMS_{\text{ERR}}}{abc} = \frac{MS_{\text{BLK}} + (c-1)MS_{\text{ERR}}}{abc}$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \gamma_k): \quad \bar{y}_{\bullet\bullet k} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{\text{BLK}} + (c-1)MS_{\text{ERR}}}{abc}}$$

$$v^* = \frac{[MS_{\text{BLK}} + (c-1)MS_{\text{ERR}}]^2}{\left[\frac{[MS_{\text{BLK}}]^2}{b-1} + \frac{[(c-1)MS_{\text{ERR}}]^2}{a(b-1)(c-1)} \right]}$$

$$E\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = \left(\mu + \frac{1}{ab} \sum_{i=1}^a \alpha_i + \gamma_k + \frac{1}{ab} \sum_{i=1}^a (\alpha\gamma)_{ik} \right) - \left(\mu + \frac{1}{ab} \sum_{i=1}^a \alpha_i + \gamma_{k'} + \frac{1}{ab} \sum_{i=1}^a (\alpha\gamma)_{ik'} \right) = \gamma_k - \gamma_{k'}$$

$$V\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = V\{\bar{Y}_{\bullet\bullet k}\} + V\{\bar{Y}_{\bullet\bullet k'}\} - 2\text{COV}\{\bar{Y}_{\bullet\bullet k}, \bar{Y}_{\bullet\bullet k'}\}$$

$$\text{COV}\{Y_{\bullet\bullet k}, Y_{\bullet\bullet k'}\} = \text{COV}\left\{ \sum_{i=1}^a \sum_{j=1}^b Y_{ijk}, \sum_{i=1}^a \sum_{j=1}^b Y_{ijk'} \right\} = \sum_{i=1}^a \sum_{j=1}^b \text{COV}\{Y_{ijk}, Y_{ijk'}\} +$$

$$+ 2 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^b \text{COV}\{Y_{ijk}, Y_{i'jk'}\} + 2 \sum_{i=1}^a \sum_{i'=1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{i'j'k'}\} =$$

$$= ab[\sigma_\beta^2 + \sigma_{\alpha\beta}^2] + a(a-1)b\sigma_\beta^2 + a^2b(b-1)(0) = a^2b\sigma_\beta^2 + ab\sigma_{\alpha\beta}^2$$

$$\Rightarrow \text{COV}\{\bar{Y}_{\bullet\bullet k}, \bar{Y}_{\bullet\bullet k'}\} = \left(\frac{1}{a^2b^2} \right) [a^2b\sigma_\beta^2 + ab\sigma_{\alpha\beta}^2] = \frac{1}{b}\sigma_\beta^2 + \frac{1}{ab}\sigma_{\alpha\beta}^2$$

$$\Rightarrow V\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = \frac{2}{a^2b^2} [a^2b\sigma_\beta^2 + ab\sigma_{\alpha\beta}^2 + ab\sigma^2 - a^2b\sigma_\beta^2 - ab\sigma_{\alpha\beta}^2] = \frac{2\sigma^2}{ab}$$

$$\Rightarrow \hat{V}\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = \frac{2MS_{\text{ERR}}}{ab}$$

$$(1-\alpha)100\% \text{ CI for } (\gamma_k - \gamma_{k'}): \quad (\bar{y}_{\bullet\bullet k} - \bar{y}_{\bullet\bullet k'}) \pm t_{1-\alpha/2; a(b-1)(c-1)} \sqrt{\frac{2MS_{\text{ERR}}}{ab}}$$

Finally, consider the case when the Whole-Plot and Sub-Plot factors have a significant interaction. We can compare Sub-Plot factor levels within specific levels of the Whole-Plot and compare Whole-Plot factor levels within specific Sub-Plot levels. These types of comparisons are referred to as **slices**.

Comparing Sub-Plot Treatment Levels Within the Same Whole-Plot Treatment:

$$E\{\bar{Y}_{i\bullet k}\} = \mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik} \quad V\{\bar{Y}_{i\bullet k}\} = \frac{1}{b}(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2)$$

$$\Rightarrow \hat{V}\{\bar{Y}_{i\bullet k}\} = \frac{(MS_{BLK} - MS_{BLK \times WP}) + a(MS_{BLK \times WP} - MS_{ERR}) + acMS_{ERR}}{abc} = \frac{MS_{BLK} + (a-1)MS_{BLK \times WP} + a(c-1)MS_{ERR}}{abc}$$

$$(1-\alpha)100\% \text{ CI for } \mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik} : \bar{y}_{i\bullet k} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{BLK} + (a-1)MS_{BLK \times WP} + a(c-1)MS_{ERR}}{abc}}$$

$$v^* = \frac{[MS_{BLK} + (a-1)MS_{BLK \times WP} + a(c-1)MS_{ERR}]^2}{\left[\frac{[MS_{BLK}]^2}{b-1} + \frac{[(a-1)MS_{BLK \times WP}]^2}{(a-1)(b-1)} + \frac{[a(c-1)MS_{ERR}]^2}{a(b-1)(c-1)} \right]}$$

$$E\{\bar{Y}_{i\bullet k} - \bar{Y}_{i\bullet k'}\} = [\mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik}] + [\mu + \alpha_i + \gamma_{k'} + (\alpha\gamma)_{ik'}] = (\gamma_k - \gamma_{k'}) + ((\alpha\gamma)_{ik} - (\alpha\gamma)_{ik'})$$

$$V\{\bar{Y}_{i\bullet k} - \bar{Y}_{i\bullet k'}\} = V\{\bar{Y}_{i\bullet k}\} + V\{\bar{Y}_{i\bullet k'}\} - 2\text{COV}\{\bar{Y}_{i\bullet k}, \bar{Y}_{i\bullet k'}\}$$

$$\text{COV}\{Y_{i\bullet k}, Y_{i\bullet k'}\} = \sum_{j=1}^b \text{COV}\{Y_{ijk}, Y_{ijk'}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{ij'k'}\} = b[\sigma_\beta^2 + \sigma_{\alpha\beta}^2] + b(b-1)(0)$$

$$\Rightarrow \text{COV}\{\bar{Y}_{i\bullet k}, \bar{Y}_{i\bullet k'}\} = \frac{1}{b^2}[b\sigma_\beta^2 + b\sigma_{\alpha\beta}^2] = \frac{1}{b}[\sigma_\beta^2 + \sigma_{\alpha\beta}^2]$$

$$\Rightarrow V\{\bar{Y}_{i\bullet k} - \bar{Y}_{i\bullet k'}\} = \frac{2}{b}[\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 - \sigma_\beta^2 - \sigma_{\alpha\beta}^2] = \frac{2\sigma^2}{b} \Rightarrow \hat{V}\{\bar{Y}_{i\bullet k} - \bar{Y}_{i\bullet k'}\} = \frac{2MS_{ERR}}{b}$$

$$(1-\alpha)100\% \text{ CI for } (\gamma_k - \gamma_{k'}) + ((\alpha\gamma)_{ik} - (\alpha\gamma)_{ik'}) : (\bar{y}_{i\bullet k} - \bar{y}_{i\bullet k'}) \pm t_{1-\alpha/2; a(b-1)(c-1)} \sqrt{\frac{2MS_{ERR}}{b}}$$

Comparing Whole-Plot Treatment Levels Within the Same Sub-Plot Treatment:

$$E\{\bar{Y}_{i\bullet k} - \bar{Y}_{i'\bullet k}\} = [\mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik}] + [\mu + \alpha_{i'} + \gamma_k + (\alpha\gamma)_{i'k}] = (\alpha_i - \alpha_{i'}) + ((\alpha\gamma)_{ik} - (\alpha\gamma)_{i'k})$$

$$V\{\bar{Y}_{i\bullet k} - \bar{Y}_{i'\bullet k}\} = V\{\bar{Y}_{i\bullet k}\} + V\{\bar{Y}_{i'\bullet k}\} - 2\text{COV}\{\bar{Y}_{i\bullet k}, \bar{Y}_{i'\bullet k}\}$$

$$\text{COV}\{Y_{i\bullet k}, Y_{i'\bullet k}\} = \sum_{j=1}^b \text{COV}\{Y_{ijk}, Y_{i'jk}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{i'j'k}\} = b[\sigma_\beta^2] + b(b-1)(0)$$

$$\Rightarrow \text{COV}\{\bar{Y}_{i\bullet k}, \bar{Y}_{i'\bullet k}\} = \frac{1}{b^2}[b\sigma_\beta^2] = \frac{1}{b}[\sigma_\beta^2]$$

$$\Rightarrow V\{\bar{Y}_{i\bullet k} - \bar{Y}_{i'\bullet k}\} = \frac{2}{b}[\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2 - \sigma_\beta^2] = \frac{2(\sigma_{\alpha\beta}^2 + \sigma^2)}{b} \Rightarrow \hat{V}\{\bar{Y}_{i\bullet k} - \bar{Y}_{i'\bullet k}\} = \frac{2[MS_{BLK \times WP} + (c-1)MS_{ERR}]}{bc}$$

$$(1-\alpha)100\% \text{ CI for } (\alpha_i - \alpha_{i'}) + ((\alpha\gamma)_{ik} - (\alpha\gamma)_{i'k}) : (\bar{y}_{i\bullet k} - \bar{y}_{i'\bullet k}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2[MS_{BLK \times WP} + (c-1)MS_{ERR}]}{bc}}$$

$$v^* = \frac{[MS_{BLK \times WP} + (c-1)MS_{ERR}]^2}{\left[\frac{[MS_{BLK \times WP}]^2}{(a-1)(b-1)} + \frac{[(c-1)MS_{ERR}]^2}{a(b-1)(c-1)} \right]}$$

Example – Chymosin for Skim Mozzarella Cheese

A study was conducted measuring various chemical and sensory properties of Chymosin treated part-skim Mozzarella cheese aged at varying amounts of time (Moynihan, *et al* (2014)). The experiment was conducted as a Split-Plot Design with the Whole-Plot factor having $a = 4$ levels (High/Low level Bovine Calf Chymosin and High/Low Camel Chymosin). The labels for these treatments are HBCC, LBCC, HCC, and LCC, respectively. The Sub-Plot factor was Ripening time with $c = 4$ levels (14, 28, 56, and 84 days). The experiment was conducted in $b = 3$ days of cheesemaking (blocks). One measurement assessed was Blister Quantity of melted cheese. Data were simulated to match the treatment cell means and the Analysis of Variance, and are given below.

Trt	Time	Block	Trt*Time	Trt*Block	Y	Trt_Mn	Time_Mn	Blk_Mn	Tr*Ti_Mn	Tr*Bl_Mn	All_Mn
1	1	1	11	11	11.3670	10.0250	7.9100	10.7966	8.7700	12.0238	9.0100
1	2	1	12	11	12.3855	10.0250	8.5025	10.7966	10.2800	12.0238	9.0100
1	3	1	13	11	11.3486	10.0250	9.1850	10.7966	9.3000	12.0238	9.0100
1	4	1	14	11	12.9940	10.0250	10.4425	10.7966	11.7500	12.0238	9.0100
1	1	2	11	12	8.2528	10.0250	7.9100	8.5494	8.7700	9.5849	9.0100
1	2	2	12	12	9.6265	10.0250	8.5025	8.5494	10.2800	9.5849	9.0100
1	3	2	13	12	9.4045	10.0250	9.1850	8.5494	9.3000	9.5849	9.0100
1	4	2	14	12	11.0558	10.0250	10.4425	8.5494	11.7500	9.5849	9.0100
1	1	3	11	13	6.6902	10.0250	7.9100	7.6840	8.7700	8.4663	9.0100
1	2	3	12	13	8.8280	10.0250	8.5025	7.6840	10.2800	8.4663	9.0100
1	3	3	13	13	7.1469	10.0250	9.1850	7.6840	9.3000	8.4663	9.0100
1	4	3	14	13	11.2001	10.0250	10.4425	7.6840	11.7500	8.4663	9.0100
2	1	1	21	21	11.5682	10.0525	7.9100	10.7966	8.7300	12.1389	9.0100
2	2	1	22	21	12.2921	10.0525	8.5025	10.7966	9.5500	12.1389	9.0100
2	3	1	23	21	11.6615	10.0525	9.1850	10.7966	10.3400	12.1389	9.0100
2	4	1	24	21	13.0339	10.0525	10.4425	10.7966	11.5900	12.1389	9.0100
2	1	2	21	22	8.1313	10.0525	7.9100	8.5494	8.7300	9.3154	9.0100
2	2	2	22	22	8.3870	10.0525	8.5025	8.5494	9.5500	9.3154	9.0100
2	3	2	23	22	10.1418	10.0525	9.1850	8.5494	10.3400	9.3154	9.0100
2	4	2	24	22	10.6013	10.0525	10.4425	8.5494	11.5900	9.3154	9.0100
2	1	3	21	23	6.4905	10.0525	7.9100	7.6840	8.7300	8.7032	9.0100
2	2	3	22	23	7.9708	10.0525	8.5025	7.6840	9.5500	8.7032	9.0100
2	3	3	23	23	9.2167	10.0525	9.1850	7.6840	10.3400	8.7032	9.0100
2	4	3	24	23	11.1348	10.0525	10.4425	7.6840	11.5900	8.7032	9.0100
3	1	1	31	31	10.4932	8.3700	7.9100	10.7966	7.5500	10.5617	9.0100
3	2	1	32	31	11.2653	8.3700	8.5025	10.7966	8.0800	10.5617	9.0100
3	3	1	33	31	11.5261	8.3700	9.1850	10.7966	8.6900	10.5617	9.0100
3	4	1	34	31	8.9623	8.3700	10.4425	10.7966	9.1600	10.5617	9.0100
3	1	2	31	32	6.0880	8.3700	7.9100	8.5494	7.5500	7.8250	9.0100
3	2	2	32	32	7.2212	8.3700	8.5025	8.5494	8.0800	7.8250	9.0100
3	3	2	33	32	7.7073	8.3700	9.1850	8.5494	8.6900	7.8250	9.0100
3	4	2	34	32	10.2834	8.3700	10.4425	8.5494	9.1600	7.8250	9.0100
3	1	3	31	33	6.0687	8.3700	7.9100	7.6840	7.5500	6.7233	9.0100
3	2	3	32	33	5.7535	8.3700	8.5025	7.6840	8.0800	6.7233	9.0100
3	3	3	33	33	6.8366	8.3700	9.1850	7.6840	8.6900	6.7233	9.0100
3	4	3	34	33	8.2342	8.3700	10.4425	7.6840	9.1600	6.7233	9.0100
4	1	1	41	41	6.8920	7.5925	7.9100	10.7966	6.5900	8.4621	9.0100
4	2	1	42	41	6.7532	7.5925	8.5025	10.7966	6.1000	8.4621	9.0100
4	3	1	43	41	9.1379	7.5925	9.1850	10.7966	8.4100	8.4621	9.0100
4	4	1	44	41	11.0652	7.5925	10.4425	10.7966	9.2700	8.4621	9.0100
4	1	2	41	42	6.5720	7.5925	7.9100	8.5494	6.5900	7.4721	9.0100
4	2	2	42	42	6.6207	7.5925	8.5025	8.5494	6.1000	7.4721	9.0100
4	3	2	43	42	7.3662	7.5925	9.1850	8.5494	8.4100	7.4721	9.0100
4	4	2	44	42	9.3296	7.5925	10.4425	8.5494	9.2700	7.4721	9.0100
4	1	3	41	43	6.3059	7.5925	7.9100	7.6840	6.5900	6.8433	9.0100
4	2	3	42	43	4.9261	7.5925	8.5025	7.6840	6.1000	6.8433	9.0100
4	3	3	43	43	8.7259	7.5925	9.1850	7.6840	8.4100	6.8433	9.0100
4	4	3	44	43	7.4151	7.5925	10.4425	7.6840	9.2700	6.8433	9.0100

The Analysis of Variance and F-tests are given below.

$$\begin{aligned}
 SS_{TOT} &= (11.3670 - 9.0100)^2 + \dots + (7.4151 - 9.0100)^2 = 222.9132 & df_{TOT} &= 4(3)(4) - 1 = 47 \\
 SS_{BLK} &= 4(4) \left[(10.7966 - 9.0100)^2 + (8.5494 - 9.0100)^2 + (7.6840 - 9.0100)^2 \right] = 82.6002 & df_{BLK} &= 3 - 1 = 2 \\
 SS_{WP} &= 3(4) \left[(10.0250 - 9.0100)^2 + \dots + (7.5925 - 9.0100)^2 \right] = 54.4313 & df_{WP} &= 4 - 1 = 3 \\
 SS_{BLK \times WP} &= 4 \left[(12.0238 - 10.0250 - 10.7966 + 9.0100)^2 + \dots + (6.8433 - 7.5925 - 7.6860 + 9.0100)^2 \right] = 7.3200 & df_{BLK \times WP} &= (4-1)(3-1) = 6 \\
 SS_{SP} &= 4(3) \left[(7.9100 - 9.0100)^2 + \dots + (10.4425 - 9.0100)^2 \right] = 42.6028 & df_{SP} &= 4 - 1 = 3 \\
 SS_{WP \times SP} &= 3 \left[(8.7700 - 10.0250 - 7.9100 + 9.0100)^2 + \dots + (9.2700 - 7.5925 - 10.4425 + 9.0100)^2 \right] = 10.7589 & df_{WP \times SP} &= (4-1)(4-1) = 9 \\
 SS_{ERR} &= 222.9132 - 82.6002 - 54.4313 - 7.3200 - 42.6028 - 1.8635 = 10.7589 & df_{ERR} &= 4(3-1)(4-1) = 24
 \end{aligned}$$

Source	df	SS	MS	F	F(.95)	P-value
Block	2	82.6002	41.3001			
WP_Trtr	3	54.4313	18.1438	14.8719	4.7571	0.0035
WP*Block	6	7.3200	1.2200			
SP_Trtr	3	42.6028	14.2010	13.5247	3.0088	0.0000
WP*SP	9	10.7589	1.1954	1.1385	2.3002	0.3754
Error	24	25.2000	1.0500			
Total	47	222.9132				

There are significant main effects for both the Whole-Plot and Sub-Plot factors. There is no evidence of an interaction between Chymosin treatment and Ripening time. We compute parameter estimates and confidence intervals here.

$$\hat{\sigma}^2 = 1.0500 \quad \hat{\sigma}_{\alpha\beta}^2 = \frac{1.2200 - 1.0500}{4} = 0.0425 \quad \hat{\sigma}_{\beta}^2 = \frac{41.3001 - 1.2200}{4(4)} = 2.0500$$

$$\hat{V}\{\bar{Y}_{i..}\} = \frac{41.3001 + (4-1)(1.2200)}{4(3)(4)} = 0.9367 \quad \hat{SE}\{\bar{Y}_{i..}\} = \sqrt{0.9367} = 0.9678$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \alpha_i): \bar{y}_{i..} \pm 3.726(0.9623) \equiv \bar{y}_{i..} \pm 3.5855$$

$$v^* = \frac{[41.3001 + (4-1)(1.2200)]^2}{\left[\frac{[41.3001]^2}{3-1} + \frac{[(4-1)(1.2200)]^2}{4(3-1)(4-1)} \right]} = 2.3640 \quad t_{.975; 2.3640} = 3.726$$

$$\hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{2(1.2200)}{3(4)} = 0.2033 \quad \hat{SE}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \sqrt{0.2033} = 0.4509$$

$$95\% \text{ CI for } (\alpha_i - \alpha_{i'}): (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 2.447(0.4509) \equiv (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 1.1034$$

$$\hat{V}\{\bar{Y}_{..k}\} = \frac{41.3001 + (4-1)1.0500}{4(3)(4)} = 0.9260 \quad \hat{SE}\{\bar{Y}_{..k}\} = \sqrt{0.9260} = 0.9623$$

$$95\% \text{ CI for } (\mu + \gamma_k): \bar{y}_{..k} \pm 3.787(0.9623) \equiv \bar{y}_{..k} \pm 3.6443$$

$$v^* = \frac{[41.3001 + (4-1)(1.0500)]^2}{\left[\frac{[41.3001]^2}{3-1} + \frac{[(4-1)(1.0500)]^2}{4(3-1)(4-1)} \right]} = 2.3156 \quad t_{.975; 2.3156} = 3.787$$

$$\hat{V}\{\bar{Y}_{..k} - \bar{Y}_{..k'}\} = \frac{2(1.0500)}{4(3)} = 0.1750 \quad \hat{SE}\{\bar{Y}_{..k} - \bar{Y}_{..k'}\} = \sqrt{0.1750} = 0.4183$$

$$95\% \text{ CI for } (\gamma_k - \gamma_{k'}): (\bar{y}_{..k} - \bar{y}_{..k'}) \pm 2.064(0.4183) \equiv (\bar{y}_{..k} - \bar{y}_{..k'}) \pm 0.8634$$

Although the Chymosin/Ripening Time Interaction is not significant, we will compute the standard errors and set-up Confidence Intervals for the Simple Effects as described above.

$$\hat{V}\{\bar{Y}_{i\bullet k}\} = \frac{41.3001 + (4-1)(1.2200) + 4(4-1)1.0500}{4(3)(4)} = 1.1992 \quad \hat{SE}\{\bar{Y}_{i\bullet k}\} = \sqrt{1.1992} = 1.0951$$

$$95\% \text{ CI for } \mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik}: \bar{y}_{i\bullet k} \pm 2.821(1.0951) \equiv \bar{y}_{i\bullet k} \pm 3.0893$$

$$v^* = \frac{[41.3001 + (4-1)(1.2200) + 4(4-1)1.0500]^2}{\left[\frac{[41.3001]^2}{3-1} + \frac{[(4-1)(1.2200)]^2}{(4-1)(3-1)} + \frac{[4(4-1)1.0500]^2}{4(3-1)(4-1)} \right]} = 3.8449 \quad t_{.975;3.8449} = 2.821$$

Comparing Sub-Plot Treatment Levels Within the Same Whole-Plot Treatment:

$$\hat{V}\{\bar{Y}_{i\bullet k} - \bar{Y}_{i\bullet k'}\} = \frac{2(1.0500)}{3} = 0.7000 \quad \hat{SE}\{\bar{Y}_{i\bullet k} - \bar{Y}_{i\bullet k'}\} = \sqrt{0.7000} = 0.8367$$

$$95\% \text{ CI for } (\gamma_k - \gamma_{k'}) + ((\alpha\gamma)_{ik} - (\alpha\gamma)_{ik'}): (\bar{y}_{i\bullet k} - \bar{y}_{i\bullet k'}) \pm 2.064(0.8367) \equiv (\bar{y}_{i\bullet k} - \bar{y}_{i\bullet k'}) \pm 1.7269$$

Comparing Whole-Plot Treatment Levels Within the Same Sub-Plot Treatment:

$$\hat{V}\{\bar{Y}_{i\bullet k} - \bar{Y}_{i' \bullet k}\} = \frac{2[1.2200 + (4-1)(1.0500)]}{3(4)} = 0.7283 \quad \hat{SE}\{\bar{Y}_{i\bullet k} - \bar{Y}_{i' \bullet k}\} = \sqrt{0.7283} = 0.8534$$

$$95\% \text{ CI for } (\alpha_i - \alpha_{i'}) + ((\alpha\gamma)_{ik} - (\alpha\gamma)_{i'k}): (\bar{y}_{i\bullet k} - \bar{y}_{i' \bullet k}) \pm 2.045(0.8534) \equiv (\bar{y}_{i\bullet k} - \bar{y}_{i' \bullet k}) \pm 1.7452$$

$$v^* = \frac{[MS_{\text{BLK} \times \text{WP}} + (c-1)MS_{\text{ERR}}]^2}{\left[\frac{[MS_{\text{BLK} \times \text{WP}}]^2}{(a-1)(b-1)} + \frac{[(c-1)MS_{\text{ERR}}]^2}{a(b-1)(c-1)} \right]} = 28.87 \quad t_{.975;29} = 2.045$$

The R program and partial output are given below.

R Program

```
ccheese <- read.csv("http://www.stat.ufl.edu/~winner/data/camel_cheese.csv",
header=T)
attach(ccheese); names(ccheese)

c.trt <- factor(c.trt)
c.time <- factor(c.time)
c.blk <- factor(c.blk)

ccheese.mod1 <- aov(blister ~ c.trt*c.blk + c.time + c.trt:c.time)
anova(ccheese.mod1)

library(lmerTest)

ccheese.mod2 <- lmer(blister ~ c.trt*c.time + (1|c.blk) + (1|c.trt:c.blk))
summary(ccheese.mod2)
anova(ccheese.mod2)
lsmmeans(ccheese.mod2)
diff1smmeans(ccheese.mod2)
rand(ccheese.mod2)
```

Partial R Output

```

> anova(ccheese.mod1)
Analysis of Variance Table

Response: blister
      Df Sum Sq Mean Sq F value    Pr(>F)
c.trt   3  54.431  18.144  17.2798 3.420e-06 ***
c.blk   2  82.600  41.300  39.3334 2.663e-08 ***
c.time  3  42.603  14.201  13.5247 2.269e-05 ***
c.trt:c.blk  6   7.320   1.220   1.1619   0.3588
c.trt:c.time  9  10.759   1.195   1.1385   0.3754
Residuals 24  25.200   1.050

> summary(ccheese.mod2)

Random effects:
Groups      Name      Variance Std.Dev.
c.trt:c.blk (Intercept) 0.0425  0.2062
c.blk      (Intercept) 2.5050  1.5827
Residual                  1.0500  1.0247

> anova(ccheese.mod2)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value    Pr(>F)
c.trt  46.847  15.6155     3     6  14.8719  0.003478 **
c.time  42.603  14.2010     3    24  13.5247  2.269e-05 ***
c.trt:c.time 10.759  1.1954     9    24   1.1385  0.375426

> lsmeans(ccheese.mod2)
Least Squares Means table:
      c.trt c.time Estimate Standard Error DF t-value Lower CI Upper CI p-value
c.trt  1      NA  10.025      0.968  2.4  10.36  6.42  13.63  0.005 **
c.trt  2      NA  10.053      0.968  2.4  10.39  6.45  13.66  0.005 **
c.trt  3      NA   8.370      0.968  2.4   8.65  4.76  11.98  0.008 **
c.trt  4      NA   7.593      0.968  2.4   7.84  3.99  11.20  0.010 **
c.time  1      NA   7.910      0.962  2.3   8.22  4.27  11.55  0.009 **
c.time  2      NA   8.502      0.962  2.3   8.84  4.86  12.15  0.008 **
c.time  3      NA   9.185      0.962  2.3   9.54  5.54  12.83  0.007 **
c.time  4      NA  10.443      0.962  2.3  10.85  6.80  14.09  0.005 **
c.trt:c.time 1 1  1.0  1.0  8.770  1.095  3.8  8.01  5.68  11.86  0.002 **
c.trt:c.time 4 4  4.0  4.0  9.270  1.095  3.8  8.47  6.18  12.36  0.001 **

> difflsmeans(ccheese.mod2)
Differences of LSMEANS:
      Estimate Standard Error DF t-value Lower CI Upper CI p-value
c.trt 1 - 2      0.0      0.4509  6.0  -0.06  -1.1309  1.0759  0.953
c.trt 3 - 4      0.8      0.4509  6.0   1.72  -0.3259  1.8809  0.135
c.time 1 - 2     -0.6      0.4183 24.0  -1.42  -1.4559  0.2709  0.170
c.time 3 - 4     -1.3      0.4183 24.0  -3.01  -2.1209  -0.3941  0.006 **
c.trt:c.time 1 1 - 2 1  0.0      0.8534 28.9   0.05  -1.7058  1.7858  0.963
c.trt:c.time 3 4 - 4 4 -0.1      0.8534 28.9  -0.13  -1.8558  1.6358  0.898

> rand(ccheese.mod2)
Analysis of Random effects Table:
      Chi.sq Chi.DF p.value
c.blk  10.7210     1  0.001 **
c.trt:c.blk  0.0557     1  0.813

```

Two of the responses reported in the study had negative estimates for variance components. One variable (Hardness of Melted Cheese) had a negative estimate of $\sigma_{\alpha\beta}^2$, the other variable (Adhesiveness of Mass) had a negative estimate of σ_{β}^2 . Once these terms are removed from the model, the Expected Mean Squares are as follow. The F-tests for Whole-Plot and Sub-Plot main effects and Interaction will use the “adjusted” error terms and their corresponding “adjusted” degrees of freedom.

$$\sigma_{\alpha\beta}^2 = 0:$$

$$E\{MS_{\text{BLK}}\} = ac\sigma_{\beta}^2 + \sigma^2 \quad df_{\text{BLK}} = b-1 \quad E\{MS_{\text{WP}}\} = \sigma^2 + bc \frac{\sum_{i=1}^a \alpha_i^2}{a-1} \quad df_{\text{WP}} = a-1$$

$$E(MS_{\text{BLK} \times \text{WP}}) = \sigma^2 \quad df_{\text{BLK} \times \text{WP}} = (a-1)(b-1) \quad E(MS_{\text{ERR}}) = \sigma^2 \quad df_{\text{ERR}} = a(b-1)(c-1)$$

$$MS_{\text{ERR}^*} = \frac{SS_{\text{BLK} \times \text{WP}} + SS_{\text{ERR}}}{(a-1)(b-1) + a(b-1)(c-1)} = \frac{SS_{\text{BLK} \times \text{WP}} + SS_{\text{ERR}}}{(b-1)(ac-1)} \quad df_{\text{ERR}^*} = (b-1)(ac-1)$$

$$H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad F_A = \frac{MS_{\text{WP}}}{MS_{\text{ERR}^*}} \quad P_A = P(F_{a-1, (b-1)(ac-1)} \geq F_A)$$

$$H_0^B : \beta_1 = \dots = \beta_b = 0 \quad F_B = \frac{MS_{\text{SP}}}{MS_{\text{ERR}^*}} \quad P_B = P(F_{b-1, (b-1)(ac-1)} \geq F_B)$$

$$H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{ab} = 0 \quad F_{AB} = \frac{MS_{\text{WP} \times \text{SP}}}{MS_{\text{ERR}^*}} \quad P_{AB} = P(F_{(a-1)(b-1), (b-1)(ac-1)} \geq F_{AB})$$

$$\sigma_{\beta}^2 = 0:$$

$$E\{MS_{\text{BLK}}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{\text{BLK}} = b-1 \quad E\{MS_{\text{WP}}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 + bc \frac{\sum_{i=1}^a \alpha_i^2}{a-1} \quad df_{\text{WP}} = a-1$$

$$E(MS_{\text{BLK} \times \text{WP}}) = c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{\text{BLK} \times \text{WP}} = (a-1)(b-1)$$

$$MS_{\text{BLK} \times \text{WP}^*} = \frac{SS_{\text{BLK}} + SS_{\text{BLK} \times \text{WP}}}{(b-1) + (a-1)(b-1)} = \frac{SS_{\text{BLK}} + SS_{\text{BLK} \times \text{WP}}}{a(b-1)} \quad df_{\text{BLK} \times \text{WP}^*} = a(b-1)$$

$$H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad F_A = \frac{MS_{\text{WP}}}{MS_{\text{BLK} \times \text{WP}^*}} \quad P_A = P(F_{a-1, a(b-1)} \geq F_A)$$

For the Chymosin Hardness data, we obtain the following ANOVA table.

Source	df	SS	MS	F	F(.95)	P-value
Block	2	1.3980	0.6990			
WP_Tr1	3	11.6320	3.8773	68.0232	4.7571	0.0001
WP*Block	6	0.3420	0.0570			
SP_Tr1	3	11.8250	3.9417	29.6311	3.0088	0.0000
WP*SP	9	1.8635	0.2071	1.5565	2.3002	0.1851
Error	24	3.1926	0.1330			
Total	47	30.2531	0.6437			

For this analysis, we compute a negative estimate for $\sigma_{\alpha\beta}^2$: $\hat{\sigma}_{\alpha\beta}^2 = \frac{0.0570 - 0.1330}{4} = -0.0190$. Combining the Block/Whole-Plot Interaction with the error term gives the following results.

$$MS_{ERR^*} = \frac{0.3420 + 3.1926}{(3-1)(4(4)-1)} = \frac{3.5346}{30} = 0.1178 \quad df_{ERR^*} = 30$$

$$H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad F_A = \frac{3.8773}{0.1178} = 32.9143 \quad P_A = P(F_{3,30} \geq 32.9143) = .0000$$

$$H_0^B : \beta_1 = \dots = \beta_b = 0 \quad F_B = \frac{3.9417}{0.1178} = 33.2317 \quad P_B = P(F_{3,30} \geq 33.2317) = .0000$$

$$H_0^{AB} : (\alpha\beta)_{11} = \dots = (\alpha\beta)_{ab} = 0 \quad F_{AB} = \frac{0.2071}{0.1178} = 1.7581 \quad P_{AB} = P(F_{9,30} \geq 1.7581) = .1189$$

The R Program and output, based on the **lmerTest** package are given below.

R Program

```
ccheese <- read.csv("http://www.stat.ufl.edu/~winner/data/camel_cheese.csv",
header=T)
attach(ccheese); names(ccheese)

c.trt <- factor(c.trt)
c.time <- factor(c.time)
c.blk <- factor(c.blk)

library(lmerTest)

ccheese.mod2 <- lmer(hardness ~ c.trt*c.time + (1|c.blk) + (1|c.trt:c.blk))
summary(ccheese.mod2)
anova(ccheese.mod2)
```

R Output

```
> summary(ccheese.mod2)

Random effects:
Groups      Name      Variance Std.Dev.
c.trt:c.blk (Intercept) 0.00000  0.0000
c.blk      (Intercept) 0.03632  0.1906
Residual                            0.11782  0.3432

> anova(ccheese.mod2)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value    Pr(>F)
c.trt    11.6320  3.8773     3    30  32.909 1.286e-09 ***
c.time    11.8250  3.9417     3    30  33.455 1.066e-09 ***
c.trt:c.time  1.8635  0.2071     9    30   1.757  0.1191
```

For the Chymosin Adhesiveness of Mass data, we obtain the following ANOVA table.

Source	df	SS	MS	F	F(.95)	P-value
Block	2	0.2740	0.1370			
WP_Trt	3	18.9358	6.3119	17.2929	4.7571	0.0023
WP*Block	6	2.1900	0.3650			
SP_Trt	3	22.8941	7.6314	45.1494	3.0088	0.0000
WP*SP	9	7.2357	0.8040	4.7565	2.3002	0.0011
Error	24	4.0566	0.1690			
Total	47	55.5862				

This leads to a negative estimate of σ_{β}^2 : $\hat{\sigma}_{\beta}^2 = \frac{0.1370 - 0.3650}{4(4)} = -0.0143$. Combining the Block and

Block/Whole-Plot sums of squares leads to the following test for Whole-Plot effects.

$$MS_{\text{BLK} \times \text{WP}^*} = \frac{0.2740 + 2.1900}{4(3-1)} = \frac{2.4640}{8} = 0.308 \quad df_{\text{BLK} \times \text{WP}^*} = 8$$

$$H_0^A : \alpha_1 = \dots = \alpha_a = 0 \quad F_A = \frac{6.3119}{0.308} = 20.4932 \quad P_A = P(F_{3,8} \geq 20.4932) = .0004$$

The R Program and output, based on the **lmerTest** package are given below.

R Program

```
ccheese <- read.csv("http://www.stat.ufl.edu/~winner/data/camel_cheese.csv",
header=T)
attach(ccheese); names(ccheese)

c.trt <- factor(c.trt)
c.time <- factor(c.time)
c.blk <- factor(c.blk)

library(lmerTest)

ccheese.mod2 <- lmer(adhesive ~ c.trt*c.time + (1|c.blk) + (1|c.trt:c.blk))
summary(ccheese.mod2)
anova(ccheese.mod2)
```

R Output

```
> summary(ccheese.mod2)

Random effects:
Groups      Name          Variance Std.Dev.
c.trt:c.blk (Intercept) 0.03474 0.1864
c.blk      (Intercept) 0.00000 0.0000
Residual                            0.16903 0.4111

> anova(ccheese.mod2)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom

```

	Sum Sq	Mean Sq	NumDF	DenDF	F.value	Pr(>F)	
c.trt	10.3916	3.4639	3	8	20.493	0.0004121	***
c.time	22.8941	7.6314	3	24	45.149	5.057e-10	***
c.trt:c.time	7.2357	0.8040	9	24	4.757	0.0010573	**

Consider cases where one or both of the Whole-Plot and Sub-Plot factors are Random. We consider first the case where the Whole-Plot factor is fixed, and the Sub-Plot factor is random. Then we reverse it to where the Whole-Plot factor is random, and the Sub-Plot factor is fixed. Finally, we conclude with the case where both factors are random.

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \gamma_k + (\alpha\gamma)_{ik} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c$$

$$\sum_{i=1}^a \alpha_i = 0 \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2) \quad \gamma_k \sim NID(0, \sigma_\gamma^2)$$

$$(\alpha\gamma)_{ik} \sim N(0, \sigma_{\alpha\gamma}^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma_\varepsilon^2) \quad \{\beta_j\} \perp \{(\alpha\beta)_{ij}\} \perp \{\gamma_k\} \perp \{(\alpha\gamma)_{ik}\} \perp \{\varepsilon_{ijk}\}$$

Expected Mean Squares:

$$E\{MS_{BLK}\} = ac\sigma_\beta^2 + c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{BLK} = b-1$$

$$E\{MS_{WP}\} = c\sigma_{\alpha\beta}^2 + b\sigma_{\alpha\gamma}^2 + \sigma^2 + bc \frac{\sum_{i=1}^a \alpha_i^2}{a-1} \quad df_{WP} = a-1$$

$$E\{MS_{BLK \times WP}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{BLK \times WP} = (a-1)(b-1)$$

$$E\{MS_{SP}\} = b\sigma_{\alpha\gamma}^2 + ab\sigma_\gamma^2 + \sigma^2 \quad df_{SP} = c-1$$

$$E\{MS_{WP \times SP}\} = b\sigma_{\alpha\gamma}^2 + \sigma^2 \quad df_{WP \times SP} = (a-1)(c-1)$$

$$E\{MS_{ERR}\} = \sigma^2 \quad df_{ERR} = a(b-1)(c-1)$$

$$\hat{\sigma}^2 = MS_{ERR} \quad \hat{\sigma}_{\alpha\gamma}^2 = \frac{MS_{WP \times SP} - MS_{ERR}}{b} \quad \hat{\sigma}_\gamma^2 = \frac{MS_{SP} - MS_{WP \times SP}}{ab}$$

$$\hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{BLK \times WP} - MS_{ERR}}{c} \quad \hat{\sigma}_\beta^2 = \frac{MS_{BLK} - MS_{BLK \times WP}}{ac}$$

Test for Whole-Plot Treatment Effects:

$$H_0 : \alpha_1 = \dots = \alpha_a = 0 \quad H_A : \text{Not all } \alpha_i = 0$$

$$\left[E(MS_{WP}) + E(MS_{ERR}) \right] - \left[E(MS_{BLK \times WP}) + E(MS_{WP \times SP}) \right] =$$

$$= E(MS_{WP}) - \left[E(MS_{BLK \times WP}) + E(MS_{WP \times SP}) - E(MS_{ERR}) \right] = bc \frac{\sum_{i=1}^a \alpha_i^2}{a-1}$$

$$\text{Test Statistic: } F_{WP} = \frac{MS_{WP}}{MS_{BLK \times WP} + MS_{WP \times SP} - MS_{ERR}}$$

Numerator and Approximate Denominator Degrees of Freedom:

$$v_1 = a-1 \quad v_2 = \frac{(MS_{BLK \times WP} + MS_{WP \times SP} - MS_{ERR})^2}{\frac{(MS_{BLK \times WP})^2}{(a-1)(b-1)} + \frac{(MS_{WP \times SP})^2}{(a-1)(c-1)} + \frac{(-MS_{ERR})^2}{a(b-1)(c-1)}}$$

Testing for Sub-Plot and Interaction Effects:

$$H_0^C : \sigma_\gamma^2 = 0 \quad H_A^C : \sigma_\gamma^2 > 0 \quad F_{SP} = \frac{MS_{SP}}{MS_{WP \times SP}} \quad P_{SP} = P(F_{c-1, (a-1)(c-1)} \geq F_{SP})$$

$$H_0^{AC} : \sigma_{\alpha\gamma}^2 = 0 \quad H_A^{AC} : \sigma_{\alpha\gamma}^2 > 0 \quad F_{WP \times SP} = \frac{MS_{WP \times SP}}{MS_{ERR}} \quad P_{WP \times SP} = P(F_{(a-1)(c-1), a(b-1)(c-1)} \geq F_{WP \times SP})$$

The covariance structure and variances of Whole-Plot means and their differences are given here.

$$\text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_\gamma^2 + \sigma_{\alpha\gamma}^2 + \sigma^2 & i = i', j = j', k = k' \\ \sigma_\beta^2 + \sigma_{\alpha\beta}^2 & i = i', j = j', k \neq k' \\ \sigma_\gamma^2 + \sigma_{\alpha\gamma}^2 & i = i', j \neq j', k = k' \\ \sigma_\beta^2 + \sigma_\gamma^2 & i \neq i', j = j', k = k' \\ \sigma_\gamma^2 & i \neq i', j \neq j', k = k' \\ \sigma_\beta^2 & i \neq i', j = j', k \neq k' \\ 0 & \forall i, i', j \neq j', k \neq k' \end{cases}$$

$$V\{\bar{Y}_{i\bullet\bullet}\} = \frac{1}{b^2c^2} \times$$

$$\left[\sum_{j=1}^b \sum_{k=1}^c V\{Y_{ijk}\} + 2 \sum_{j=1}^b \sum_{k=1}^{c-1} \sum_{k'=k+1}^c \text{COV}\{Y_{ijk}, Y_{ijk'}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^c \text{COV}\{Y_{ijk}, Y_{ij'k}\} + 4 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^{c-1} \sum_{k'=k+1}^c \text{COV}\{Y_{ijk}, Y_{ij'k'}\} \right]$$

$$= \frac{1}{b^2c^2} \left[bc(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_\gamma^2 + \sigma_{\alpha\gamma}^2 + \sigma^2) + bc(c-1)(\sigma_\beta^2 + \sigma_{\alpha\beta}^2) + b(b-1)c(\sigma_\gamma^2 + \sigma_{\alpha\gamma}^2) + b(b-1)c(c-1)(0) \right]$$

$$= \frac{1}{b} \sigma_\beta^2 + \frac{1}{b} \sigma_{\alpha\beta}^2 + \frac{1}{c} \sigma_\gamma^2 + \frac{1}{c} \sigma_{\alpha\gamma}^2 + \frac{1}{bc} \sigma^2$$

$$\hat{V}\{\bar{Y}_{i\bullet\bullet}\} = \frac{(MS_{\text{BLK}} - MS_{\text{BLK} \times \text{WP}}) + a(MS_{\text{BLK} \times \text{WP}} - MS_{\text{ERR}}) + (MS_{\text{SP}} - MS_{\text{WP} \times \text{SP}}) + a(MS_{\text{WP} \times \text{SP}} - MS_{\text{ERR}}) + aMS_{\text{ERR}}}{abc}$$

$$= \frac{MS_{\text{BLK}} + (a-1)MS_{\text{BLK} \times \text{WP}} + MS_{\text{SP}} + (a-1)MS_{\text{WP} \times \text{SP}} - aMS_{\text{ERR}}}{abc}$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \alpha_i): \bar{y}_{i\bullet\bullet} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{\text{BLK}} + (a-1)MS_{\text{BLK} \times \text{WP}} + MS_{\text{SP}} + (a-1)MS_{\text{WP} \times \text{SP}} - aMS_{\text{ERR}}}{abc}}$$

$$v^* = \frac{[MS_{\text{BLK}} + (a-1)MS_{\text{BLK} \times \text{WP}} + MS_{\text{SP}} + (a-1)MS_{\text{WP} \times \text{SP}} - aMS_{\text{ERR}}]^2}{\left[\frac{[MS_{\text{BLK}}]^2}{b-1} + \frac{[(a-1)MS_{\text{BLK} \times \text{WP}}]^2}{(a-1)(b-1)} + \frac{[MS_{\text{SP}}]^2}{c-1} + \frac{[(a-1)MS_{\text{WP} \times \text{SP}}]^2}{(a-1)(c-1)} + \frac{[-aMS_{\text{ERR}}]^2}{a(b-1)(c-1)} \right]}$$

$$i \neq i': \text{COV}\{\bar{Y}_{i\bullet\bullet}, \bar{Y}_{i'\bullet\bullet}\} = \frac{1}{b^2c^2} \times$$

$$\left[\sum_{j=1}^b \sum_{k=1}^c \text{COV}\{Y_{ijk}, Y_{i'jk}\} + 2 \sum_{j=1}^b \sum_{k=1}^{c-1} \sum_{k'=k+1}^c \text{COV}\{Y_{ijk}, Y_{i'jk'}\} + 2 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^c \text{COV}\{Y_{ijk}, Y_{i'j'k}\} + 4 \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^{c-1} \sum_{k'=k+1}^c \text{COV}\{Y_{ijk}, Y_{i'j'k'}\} \right]$$

$$= \frac{1}{b^2c^2} \left[bc(\sigma_\beta^2 + \sigma_\gamma^2) + bc(c-1)\sigma_\beta^2 + b(b-1)c\sigma_\gamma^2 + b(b-1)c(c-1)(0) \right] = \frac{1}{b} \sigma_\beta^2 + \frac{1}{c} \sigma_\gamma^2$$

$$\Rightarrow V\{\bar{Y}_{i\bullet\bullet} - \bar{Y}_{i'\bullet\bullet}\} = 2 \left(\frac{1}{b} \sigma_\beta^2 + \frac{1}{b} \sigma_{\alpha\beta}^2 + \frac{1}{c} \sigma_\gamma^2 + \frac{1}{c} \sigma_{\alpha\gamma}^2 + \frac{1}{bc} \sigma^2 \right) - 2 \left(\frac{1}{b} \sigma_\beta^2 + \frac{1}{c} \sigma_\gamma^2 \right) = 2 \left(\frac{1}{b} \sigma_{\alpha\beta}^2 + \frac{1}{c} \sigma_{\alpha\gamma}^2 + \frac{1}{bc} \sigma^2 \right)$$

$$\Rightarrow \hat{V}\{\bar{Y}_{i\bullet\bullet} - \bar{Y}_{i'\bullet\bullet}\} = 2 \left(\frac{(MS_{\text{BLK} \times \text{WP}} - MS_{\text{ERR}}) + (MS_{\text{WP} \times \text{SP}} - MS_{\text{ERR}}) + MS_{\text{ERR}}}{bc} \right) = 2 \left(\frac{MS_{\text{BLK} \times \text{WP}} + MS_{\text{WP} \times \text{SP}} - MS_{\text{ERR}}}{bc} \right)$$

$$(1-\alpha)100\% \text{ CI for } (\alpha_i - \alpha_{i'}): (\bar{y}_{i\bullet\bullet} - \bar{y}_{i'\bullet\bullet}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2(MS_{\text{BLK} \times \text{WP}} + MS_{\text{WP} \times \text{SP}} - MS_{\text{ERR}})}{bc}}$$

$$v^* = \frac{[MS_{\text{BLK} \times \text{WP}} + MS_{\text{WP} \times \text{SP}} - MS_{\text{ERR}}]^2}{\left[\frac{[MS_{\text{BLK} \times \text{WP}}]^2}{(a-1)(b-1)} + \frac{[MS_{\text{WP} \times \text{SP}}]^2}{(a-1)(c-1)} + \frac{[-MS_{\text{ERR}}]^2}{a(b-1)(c-1)} \right]}$$

Example – Tournament Round Effects in Ladies Professional Golf Association (LPGA)

Most of the professional golf tournaments in the United States consist of 4 rounds, that are played on Thursday through Sunday, weather permitting. To test whether there are Round effects (1,2,3, and 4), we consider the following quasi-experiment. We take a sample of tournaments from a given season (this dataset is from the 2003 LPGA season). We also take a sample of golfers who competed in each of the tournaments. The tournaments act as blocks, and vary due to course difficulty and weather conditions over the 4 day event. It is impossible to construct a Completely Randomized Design for the Round/Golfer factorial structure within blocks. That is, each golfer completes Round 1 on Thursday, Round 2 on Friday, Round 3 on Saturday, and Round 4 on Sunday. Thus, Round will be the Whole-Plot (fixed) factor and Golfer will be the Sub-Plot (random) factor. The data is based on $a = 4$ Rounds, $b = 8$ Tournaments, and $c = 6$ Golfers, for a combined $N = 192$ observations, which are given below in tabular form.

Golfer	Tourney	Round	Score	Golfer	Tourney	Round	Score	Golfer	Tourney	Round	Score
Beth Daniel	2	1	70	Grace Park	2	1	67	Lorena Ochoa	2	1	71
Beth Daniel	2	2	69	Grace Park	2	2	67	Lorena Ochoa	2	2	70
Beth Daniel	2	3	65	Grace Park	2	3	67	Lorena Ochoa	2	3	64
Beth Daniel	2	4	68	Grace Park	2	4	65	Lorena Ochoa	2	4	66
Beth Daniel	7	1	70	Grace Park	7	1	67	Lorena Ochoa	7	1	66
Beth Daniel	7	2	72	Grace Park	7	2	68	Lorena Ochoa	7	2	69
Beth Daniel	7	3	73	Grace Park	7	3	69	Lorena Ochoa	7	3	72
Beth Daniel	7	4	76	Grace Park	7	4	71	Lorena Ochoa	7	4	69
Beth Daniel	16	1	69	Grace Park	16	1	68	Lorena Ochoa	16	1	72
Beth Daniel	16	2	69	Grace Park	16	2	75	Lorena Ochoa	16	2	74
Beth Daniel	16	3	69	Grace Park	16	3	69	Lorena Ochoa	16	3	73
Beth Daniel	16	4	68	Grace Park	16	4	67	Lorena Ochoa	16	4	72
Beth Daniel	19	1	74	Grace Park	19	1	74	Lorena Ochoa	19	1	74
Beth Daniel	19	2	71	Grace Park	19	2	65	Lorena Ochoa	19	2	65
Beth Daniel	19	3	67	Grace Park	19	3	71	Lorena Ochoa	19	3	77
Beth Daniel	19	4	76	Grace Park	19	4	70	Lorena Ochoa	19	4	74
Beth Daniel	22	1	69	Grace Park	22	1	71	Lorena Ochoa	22	1	73
Beth Daniel	22	2	69	Grace Park	22	2	72	Lorena Ochoa	22	2	69
Beth Daniel	22	3	71	Grace Park	22	3	68	Lorena Ochoa	22	3	69
Beth Daniel	22	4	70	Grace Park	22	4	70	Lorena Ochoa	22	4	77
Beth Daniel	26	1	69	Grace Park	26	1	67	Lorena Ochoa	26	1	72
Beth Daniel	26	2	71	Grace Park	26	2	73	Lorena Ochoa	26	2	69
Beth Daniel	26	3	74	Grace Park	26	3	67	Lorena Ochoa	26	3	68
Beth Daniel	26	4	72	Grace Park	26	4	69	Lorena Ochoa	26	4	69
Beth Daniel	27	1	70	Grace Park	27	1	70	Lorena Ochoa	27	1	73
Beth Daniel	27	2	69	Grace Park	27	2	69	Lorena Ochoa	27	2	73
Beth Daniel	27	3	67	Grace Park	27	3	73	Lorena Ochoa	27	3	71
Beth Daniel	27	4	70	Grace Park	27	4	69	Lorena Ochoa	27	4	69
Beth Daniel	31	1	75	Grace Park	31	1	76	Lorena Ochoa	31	1	76
Beth Daniel	31	2	72	Grace Park	31	2	75	Lorena Ochoa	31	2	76
Beth Daniel	31	3	68	Grace Park	31	3	69	Lorena Ochoa	31	3	76
Beth Daniel	31	4	72	Grace Park	31	4	69	Lorena Ochoa	31	4	75
Candie Kung	2	1	71	Karrie Webb	2	1	66	Se Ri Pak	2	1	65
Candie Kung	2	2	73	Karrie Webb	2	2	67	Se Ri Pak	2	2	68
Candie Kung	2	3	72	Karrie Webb	2	3	68	Se Ri Pak	2	3	68
Candie Kung	2	4	73	Karrie Webb	2	4	75	Se Ri Pak	2	4	64
Candie Kung	7	1	72	Karrie Webb	7	1	70	Se Ri Pak	7	1	69
Candie Kung	7	2	70	Karrie Webb	7	2	71	Se Ri Pak	7	2	69
Candie Kung	7	3	74	Karrie Webb	7	3	68	Se Ri Pak	7	3	70
Candie Kung	7	4	71	Karrie Webb	7	4	67	Se Ri Pak	7	4	72
Candie Kung	16	1	72	Karrie Webb	16	1	72	Se Ri Pak	16	1	69
Candie Kung	16	2	74	Karrie Webb	16	2	72	Se Ri Pak	16	2	75
Candie Kung	16	3	69	Karrie Webb	16	3	71	Se Ri Pak	16	3	68
Candie Kung	16	4	74	Karrie Webb	16	4	73	Se Ri Pak	16	4	69
Candie Kung	19	1	73	Karrie Webb	19	1	67	Se Ri Pak	19	1	69
Candie Kung	19	2	71	Karrie Webb	19	2	72	Se Ri Pak	19	2	69
Candie Kung	19	3	69	Karrie Webb	19	3	70	Se Ri Pak	19	3	69
Candie Kung	19	4	73	Karrie Webb	19	4	71	Se Ri Pak	19	4	72
Candie Kung	22	1	71	Karrie Webb	22	1	72	Se Ri Pak	22	1	70
Candie Kung	22	2	67	Karrie Webb	22	2	70	Se Ri Pak	22	2	71
Candie Kung	22	3	66	Karrie Webb	22	3	65	Se Ri Pak	22	3	67
Candie Kung	22	4	70	Karrie Webb	22	4	73	Se Ri Pak	22	4	68
Candie Kung	26	1	74	Karrie Webb	26	1	67	Se Ri Pak	26	1	71
Candie Kung	26	2	69	Karrie Webb	26	2	73	Se Ri Pak	26	2	64
Candie Kung	26	3	66	Karrie Webb	26	3	70	Se Ri Pak	26	3	71
Candie Kung	26	4	74	Karrie Webb	26	4	68	Se Ri Pak	26	4	70
Candie Kung	27	1	75	Karrie Webb	27	1	72	Se Ri Pak	27	1	69
Candie Kung	27	2	69	Karrie Webb	27	2	73	Se Ri Pak	27	2	68
Candie Kung	27	3	76	Karrie Webb	27	3	69	Se Ri Pak	27	3	69
Candie Kung	27	4	76	Karrie Webb	27	4	71	Se Ri Pak	27	4	73
Candie Kung	31	1	82	Karrie Webb	31	1	73	Se Ri Pak	31	1	73
Candie Kung	31	2	75	Karrie Webb	31	2	75	Se Ri Pak	31	2	70
Candie Kung	31	3	77	Karrie Webb	31	3	73	Se Ri Pak	31	3	72
Candie Kung	31	4	69	Karrie Webb	31	4	72	Se Ri Pak	31	4	73

The means by Golfer, Tournament, and Round are given below, followed by the ANOVA table.

Daniel	70.4375	Tourney1	68.2917	Round1	70.9792
Kung	72.0938	Tourney2	70.2083	Round2	70.5417
Park	69.5398	Tourney3	70.9583	Round3	69.875
Webb	70.5000	Tourney4	70.9583	Round4	70.9167
Ochoa	71.3438	Tourney5	69.9167		
Pak	69.5000	Tourney6	69.8750		
		Tourney7	70.9583		
		Tourney8	73.4583	Overall	70.5781

Source	df	SS	MS	F	df1	df2	F(.95)	P-value
Tourney (BLK)	7	360.6198	51.5171					
Round (WP)	3	37.0156	12.3385	1.4668	3	10.6424	3.7083	0.2820
Tourney*Round (BLKxWP)	21	198.6927	9.4616					
Golfer (SP)	5	161.2969	32.2594	4.8690	5	140	2.2789	0.0004
Round*Golfer (WPxSP)	15	83.6406	5.5760	0.8416	15	140	1.7384	0.6302
Error	140	927.5625	6.6254					
Total	191	1768.8281						

The calculations for the approximate F-test for Round Effects are given below, as well as variance component estimates.

$$\text{Test Statistic: } F_{WP} = \frac{12.3385}{9.4616 + 5.5760 - 6.6254} = \frac{12.3385}{8.4122} = 1.4667$$

Numerator and Approximate Denominator Degrees of Freedom:

$$v_1 = 4 - 1 = 3 \quad v_2 = \frac{(9.4616 + 5.5760 - 6.6254)^2}{\frac{(9.4616)^2}{(4-1)(8-1)} + \frac{(5.5760)^2}{(4-1)(6-1)} + \frac{(-6.6254)^2}{4(8-1)(6-1)}} = \frac{70.7651}{6.6493} = 10.6425$$

$$F_{.95;3,10.6425} = 3.6275 \quad P(F_{3,10.6425} \geq 1.4667) = .2788$$

$$\hat{\sigma}^2 = 6.6254 \quad \hat{\sigma}_{\alpha\gamma}^2 = \frac{5.5760 - 6.6254}{8} < 0 \quad \hat{\sigma}_{\gamma}^2 = \frac{32.2594 - 6.6254}{4(8)} = 0.8011$$

$$\hat{\sigma}_{\alpha\beta}^2 = \frac{9.4616 - 6.6254}{6} = 2.8362 \quad \hat{\sigma}_{\beta}^2 = \frac{51.5171 - 9.4616}{4(6)} = 1.7523$$

Similar to the Hardness and Adhesiveness responses for the Chymosin dataset, we obtain a negative estimate for the Round/Golfer (Whole-Plot/Sub-Plot) interaction. When we set that variance component to zero, we obtain the following Expected Mean Squares and F-test for Round Effects. Note that this also changes the variance of Round means, as well as differences and contrasts among Round means.

$$\sigma_{\alpha\gamma}^2 = 0:$$

$$E\{MS_{WP}\} = c\sigma_{\alpha\beta}^2 + b\sigma_{\alpha\gamma}^2 + \sigma^2 + bc \frac{\sum_{i=1}^a \alpha_i^2}{a-1} = c\sigma_{\alpha\beta}^2 + \sigma^2 + bc \frac{\sum_{i=1}^a \alpha_i^2}{a-1} \quad df_{WP} = a-1$$

$$E\{MS_{BLK \times WP}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{BLK \times WP} = (a-1)(b-1)$$

$$H_0^A: \alpha_1 = \dots = \alpha_a = 0 \quad F_A = \frac{MS_{WP}}{MS_{BLK \times WP}} \quad P_A = P(F_{a-1, (a-1)(b-1)} \geq F_A)$$

$$\text{LPGA Data: } F_A = \frac{12.3385}{9.4616} = 1.3041 \quad P_A = P(F_{3,21} \geq 1.3041) = .2994$$

$$E\{MS_{SP}\} = b\sigma_{\alpha\gamma}^2 + ab\sigma_{\gamma}^2 + \sigma^2 = ab\sigma_{\gamma}^2 + \sigma^2 \quad df_{SP} = c-1$$

$$E\{MS_{WP \times SP}\} = b\sigma_{\alpha\gamma}^2 + \sigma^2 = \sigma^2 \quad df_{WP \times SP} = (a-1)(c-1)$$

$$E\{MS_{ERR}\} = \sigma^2 \quad df_{ERR} = a(b-1)(c-1)$$

$$\hat{\sigma}^2 = MS_{ERR^*} = \frac{SS_{WP \times SP} + SS_{ERR}}{(a-1)(c-1) + a(b-1)(c-1)} = \frac{SS_{WP \times SP} + SS_{ERR}}{(ab-1)(c-1)} = \frac{83.6406 + 927.5625}{(4(8)-1)(6-1)} = \frac{1011.2031}{155} = 6.5239$$

$$\hat{\sigma}_{\gamma}^2 = \frac{32.2594 - 6.5239}{4(8)} = 0.8042 \quad \hat{\sigma}_{\alpha\beta}^2 = \frac{9.4616 - 6.5239}{6} = 0.4896$$

$$V\{\bar{Y}_{i..}\} = \frac{1}{b}\sigma_{\beta}^2 + \frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{c}\sigma_{\gamma}^2 + \frac{1}{c}\sigma_{\alpha\gamma}^2 + \frac{1}{bc}\sigma^2 = \frac{1}{b}\sigma_{\beta}^2 + \frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{c}\sigma_{\gamma}^2 + \frac{1}{bc}\sigma^2$$

$$\hat{V}\{\bar{Y}_{i..}\} = \frac{(MS_{BLK} - MS_{BLK \times WP}) + a(MS_{BLK \times WP} - MS_{ERR^*}) + (MS_{SP} - MS_{ERR^*}) + aMS_{ERR^*}}{abc} =$$

$$= \frac{MS_{BLK} + (a-1)MS_{BLK \times WP} + MS_{SP} - MS_{ERR^*}}{abc} = \frac{51.5171 + (4-1)(9.4616) + 32.2594 - 6.5239}{4(8)(6)} =$$

$$= \frac{105.6374}{192} = 0.5502 \quad \hat{SE}\{\bar{Y}_{i..}\} = \sqrt{0.5502} = 0.7418$$

$$95\% \text{ CI for } (\mu + \alpha_i): \bar{y}_{i..} \pm 2.102(0.7418) \equiv \bar{y}_{i..} \pm 1.5593 \quad (t_{.975; 17.8286} = 2.102)$$

$$v^* = \frac{[51.5171 + (4-1)(9.4616) + 32.2594 - 6.5239]^2}{\left[\frac{[51.5171]^2}{8-1} + \frac{[(4-1)(9.4616)]^2}{(4-1)(8-1)} + \frac{[32.2594]^2}{6-1} + \frac{[-6.5239]^2}{(4(8)-1)(6-1)} \right]} = \frac{11159.2603}{625.9194} = 17.8286$$

$$V\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = 2\left(\frac{1}{b}\sigma_{\beta}^2 + \frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{c}\sigma_{\gamma}^2 + \frac{1}{c}\sigma_{\alpha\gamma}^2 + \frac{1}{bc}\sigma^2\right) - 2\left(\frac{1}{b}\sigma_{\beta}^2 + \frac{1}{c}\sigma_{\gamma}^2\right) =$$

$$2\left(\frac{1}{b}\sigma_{\beta}^2 + \frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{c}\sigma_{\gamma}^2 + \frac{1}{bc}\sigma^2\right) - 2\left(\frac{1}{b}\sigma_{\beta}^2 + \frac{1}{c}\sigma_{\gamma}^2\right) = 2\left(\frac{1}{b}\sigma_{\alpha\beta}^2 + \frac{1}{bc}\sigma^2\right)$$

$$\hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = 2\left(\frac{(MS_{BLK \times WP} - MS_{ERR^*}) + MS_{ERR^*}}{bc}\right) = 2\left(\frac{MS_{BLK \times WP}}{bc}\right) = 2\left(\frac{9.4616}{8(6)}\right) = 0.3942$$

$$\hat{SE}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \sqrt{0.3942} = 0.6279 \quad df_{BLK \times WP} = 21 \quad t_{.975; 21} = 2.080$$

$$95\% \text{ CI for } (\alpha_i - \alpha_{i'}): (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 2.080(0.6279) \equiv (\bar{y}_{i..} - \bar{y}_{i'..}) \pm 1.3060$$

The R Program and Output are given below.

R Program

```
lpga <- read.fwf("http://www.stat.ufl.edu/~winner/consult/lpgasplt.dat",
  width=c(24,3,3,5),col.names=c("golfer","tourney","round","score"))
attach(lpга)

tourney <- factor(tourney); round <- factor(round); golfer <- factor(golfer)

lpga.mod1 <- aov(score ~ tourney*round + golfer + round:golfer)
anova(lpга.mod1)

library(lmerTest)

lpga.mod2 <- lmer(score ~ round + (1|tourney) + (1|tourney:round) +
  (1|golfer) + (1|round:golfer))
summary(lpга.mod2)
anova(lpга.mod2)
lsmeans(lpга.mod2)
diff(lsmeans(lpга.mod2))
rand(lpга.mod2)
```

R Output

```
> anova(lpга.mod1)
Analysis of Variance Table

Response: score
      Df Sum Sq Mean Sq F value    Pr(>F)
tourney  7 360.62  51.517  7.7756 6.178e-08 ***
round    3  37.02  12.339  1.8623 0.1387742
golfer   5 161.30  32.259  4.8690 0.0003883 ***
tourney:round 21 198.69  9.462  1.4281 0.1148814
round:golfer 15  83.64   5.576  0.8416 0.6301785
Residuals 140 927.56   6.625

> summary(lpга.mod2)
Linear mixed model fit by REML t-tests use Satterthwaite approximations to
degrees of freedom [merModLmerTest]
Formula: score ~ round + (1 | tourney) + (1 | tourney:round) + (1 | golfer) +
(1 | round:golfer)

REML criterion at convergence: 931.9

Scaled residuals:
   Min       1Q   Median       3Q      Max
-2.28490 -0.60768 -0.02712  0.67492  2.61663

Random effects:
 Groups      Name          Variance Std.Dev.
tourney:round (Intercept)  0.4896   0.6997
round:golfer  (Intercept)  0.0000   0.0000
tourney      (Intercept)  1.7523   1.3238
golfer       (Intercept)  0.8042   0.8968
Residual    (Intercept)  6.5239   2.5542

> anova(lpга.mod2)
Analysis of Variance Table of type 3 with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value Pr(>F)
round 25.523  8.5076     3     21  1.3041 0.2994
> lsmeans(lpга.mod2)
Least Squares Means table:
      round Estimate Standard Error   DF t-value Lower CI Upper CI p-value
round 1  1.0  70.979      0.742 17.8  95.690    69.4    72.5 <2e-16
round 2  2.0  70.542      0.742 17.8  95.100    69.0    72.1 <2e-16
round 3  3.0  69.875      0.742 17.8  94.200    68.3    71.4 <2e-16
round 4  4.0  70.917      0.742 17.8  95.610    69.4    72.5 <2e-16
```

```

> diff1smeans(lpga.mod2)
Differences of LSMEANS:
      Estimate Standard Error   DF t-value Lower CI Upper CI p-value
round 1 - 2      0.4      0.6279 21.0    0.70   -0.868   1.743   0.49
round 1 - 3      1.1      0.6279 21.0    1.76   -0.202   2.410   0.09
round 1 - 4      0.1      0.6279 21.0    0.10   -1.243   1.368   0.92
round 2 - 3      0.7      0.6279 21.0    1.06   -0.639   1.972   0.30
round 2 - 4     -0.4      0.6279 21.0   -0.60   -1.681   0.931   0.56
round 3 - 4     -1.0      0.6279 21.0   -1.66   -2.347   0.264   0.11

```

```

---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

```

> rand(lpga.mod2)
Analysis of Random effects Table:
      Chi.sq Chi.DF p.value
tourney      9.06e+00      1 0.003 **
tourney:round 1.40e+00      1 0.236
golfer       6.77e+00      1 0.009 **
round:golfer  1.14e-13      1 1.000

```

An alternative mixed effects model would be if the Whole-Plot effects are random and the Sub-Plot effects are fixed. The structure of this model would be as follows.

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \gamma_k + (\alpha\gamma)_{ik} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c$$

$$\alpha_i \sim NID(0, \sigma_\alpha^2) \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2)$$

$$\sum_{k=1}^c \gamma_k = 0 \quad (\alpha\gamma)_{ik} \sim N(0, \sigma_{\alpha\gamma}^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \quad \{\alpha_i\} \perp \{\beta_j\} \perp \{(\alpha\beta)_{ij}\} \perp \{(\alpha\gamma)_{ik}\} \perp \{\varepsilon_{ijk}\}$$

$$E\{Y_{ijk}\} = \mu + \gamma_k \quad \text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_{\alpha\gamma}^2 + \sigma^2 & i = i', j = j', k = k' \\ \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 & i = i', j = j', k \neq k' \\ \sigma_\alpha^2 + \sigma_{\alpha\gamma}^2 & i = i', j \neq j', k = k' \\ \sigma_\alpha^2 & i = i', j \neq j', k \neq k' \\ \sigma_\beta^2 & i \neq i', j = j', \forall k, k' \\ 0 & i \neq i', j \neq j', \forall k, k' \end{cases}$$

$$E\{MS_{\text{BLK}}\} = ac\sigma_\beta^2 + c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{\text{BLK}} = b - 1$$

$$E\{MS_{\text{WP}}\} = bc\sigma_\alpha^2 + c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{\text{WP}} = a - 1$$

$$E\{MS_{\text{BLK} \times \text{WP}}\} = c\sigma_{\alpha\beta}^2 + \sigma^2 \quad df_{\text{BLK} \times \text{WP}} = (a - 1)(b - 1)$$

$$E\{MS_{\text{SP}}\} = b\sigma_{\alpha\gamma}^2 + \sigma^2 + ab \frac{\sum_{k=1}^c \gamma_k^2}{c - 1} \quad df_{\text{SP}} = c - 1$$

$$E\{MS_{\text{WP} \times \text{SP}}\} = b\sigma_{\alpha\gamma}^2 + \sigma^2 \quad df_{\text{WP} \times \text{SP}} = (a - 1)(c - 1)$$

$$E\{MS_{\text{ERR}}\} = \sigma^2 \quad df_{\text{ERR}} = a(b - 1)(c - 1)$$

$$H_0^c: \gamma_1 = \dots = \gamma_c = 0 \quad F_C = \frac{MS_{\text{SP}}}{MS_{\text{WP} \times \text{SP}}} \quad P_C = P(F_{c-1, (a-1)(c-1)} \geq F_C)$$

$$\hat{\sigma}^2 = MS_{\text{ERR}} \quad \hat{\sigma}_{\alpha\gamma}^2 = \frac{MS_{\text{WP} \times \text{SP}} - MS_{\text{ERR}}}{b} \quad \hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{\text{BLK} \times \text{WP}} - MS_{\text{ERR}}}{c}$$

$$\hat{\sigma}_\alpha^2 = \frac{MS_{\text{WP}} - MS_{\text{BLK} \times \text{WP}}}{bc} \quad \hat{\sigma}_\beta^2 = \frac{MS_{\text{BLK}} - MS_{\text{BLK} \times \text{WP}}}{ac}$$

The variance structure of the Sub-Plot means and their differences along with forms of their confidence intervals are given below.

$$\begin{aligned}
V\{\bar{Y}_{\bullet\bullet k}\} &= \frac{1}{a^2 b^2} \times \\
&\left[\sum_{i=1}^a \sum_{j=1}^b V\{Y_{ijk}\} + 2 \sum_{i=1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{ij'k}\} + 2 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^b \text{COV}\{Y_{ijk}, Y_{i'jk}\} + 4 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{i'j'k}\} \right] \\
&= \frac{1}{a^2 b^2} \left[ab(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_{\alpha\gamma}^2 + \sigma^2) + ab(b-1)(\sigma_\alpha^2 + \sigma_{\alpha\gamma}^2) + a(a-1)b(\sigma_\beta^2) + a(a-1)b(b-1)(0) \right] \\
&= \frac{1}{a} \sigma_\alpha^2 + \frac{1}{b} \sigma_\beta^2 + \frac{1}{ab} \sigma_{\alpha\beta}^2 + \frac{1}{a} \sigma_{\alpha\gamma}^2 + \frac{1}{ab} \sigma^2 \\
\hat{V}\{\bar{Y}_{\bullet\bullet k}\} &= \frac{(MS_{WP} - MS_{BLK \times WP}) + (MS_{BLK} - MS_{BLK \times WP}) + (MS_{BLK \times WP} - MS_{ERR}) + c(MS_{WP \times SP} - MS_{ERR}) + cMS_{ERR}}{abc} \\
&= \frac{MS_{WP} + MS_{BLK} - MS_{BLK \times WP} + cMS_{WP \times SP} - MS_{ERR}}{abc} \\
(1-\alpha)100\% \text{ CI for } (\mu + \gamma_k): & \quad \bar{y}_{\bullet\bullet k} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{WP} + MS_{BLK} - MS_{BLK \times WP} + cMS_{WP \times SP} - MS_{ERR}}{abc}} \\
v^* &= \frac{[MS_{WP} + MS_{BLK} - MS_{BLK \times WP} + cMS_{WP \times SP} - MS_{ERR}]^2}{\left[\frac{[MS_{WP}]^2}{a-1} + \frac{[MS_{BLK}]^2}{b-1} + \frac{[-MS_{BLK \times WP}]^2}{(a-1)(b-1)} + \frac{[cMS_{WP \times SP}]^2}{(a-1)(c-1)} + \frac{[-MS_{ERR}]^2}{a(b-1)(c-1)} \right]} \\
k \neq k': \text{ COV}\{\bar{Y}_{\bullet\bullet k}, \bar{Y}_{\bullet\bullet k'}\} &= \frac{1}{a^2 b^2} \times \\
&\left[\sum_{i=1}^a \sum_{j=1}^b \text{COV}\{Y_{ijk}, Y_{ij'k'}\} + 2 \sum_{i=1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{ij'k'}\} + 2 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^b \text{COV}\{Y_{ijk}, Y_{i'jk'}\} + 4 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \text{COV}\{Y_{ijk}, Y_{i'j'k'}\} \right] \\
&= \frac{1}{a^2 b^2} \left[ab(\sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2) + ab(b-1)\sigma_\alpha^2 + a(a-1)b\sigma_\beta^2 + a(a-1)b(b-1)(0) \right] = \frac{1}{a} \sigma_\alpha^2 + \frac{1}{b} \sigma_\beta^2 + \frac{1}{ab} \sigma_{\alpha\beta}^2 \\
\Rightarrow V\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} &= 2 \left(\frac{1}{a} \sigma_\alpha^2 + \frac{1}{b} \sigma_\beta^2 + \frac{1}{ab} \sigma_{\alpha\beta}^2 + \frac{1}{a} \sigma_{\alpha\gamma}^2 + \frac{1}{ab} \sigma^2 \right) - 2 \left(\frac{1}{a} \sigma_\alpha^2 + \frac{1}{b} \sigma_\beta^2 + \frac{1}{ab} \sigma_{\alpha\beta}^2 \right) = 2 \left(\frac{1}{a} \sigma_{\alpha\gamma}^2 + \frac{1}{ab} \sigma^2 \right) \\
\Rightarrow \hat{V}\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} &= 2 \left(\frac{(MS_{WP \times SP} - MS_{ERR}) + MS_{ERR}}{ab} \right) = 2 \left(\frac{MS_{WP \times SP}}{ab} \right) \\
(1-\alpha)100\% \text{ CI for } (\gamma_k - \gamma_{k'}): & \quad (\bar{y}_{\bullet\bullet k} - \bar{y}_{\bullet\bullet k'}) \pm t_{1-\alpha/2; (a-1)(c-1)} \sqrt{\frac{2MS_{WP \times SP}}{ab}}
\end{aligned}$$

The case where both the Whole-Plot and Sub-Plot factors are random is given below in terms of the Variance/Covariance structure of the data and the Expected Mean Squares. Estimates and tests are constructed exactly as in the previously described cases.

$$\begin{aligned}
Y_{ijk} &= \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \gamma_k + (\alpha\gamma)_{ik} + \varepsilon_{ijk} \quad i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c \\
\alpha_i &\sim NID(0, \sigma_\alpha^2) \quad \beta_j \sim NID(0, \sigma_\beta^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2) \\
\gamma_k &\sim NID(0, \sigma_\gamma^2) \quad (\alpha\gamma)_{ik} \sim N(0, \sigma_{\alpha\gamma}^2) \quad \varepsilon_{ijk} \sim NID(0, \sigma^2) \\
\{\alpha_i\} &\perp \{\beta_j\} \perp \{(\alpha\beta)_{ij}\} \perp \{\gamma_k\} \perp \{(\alpha\gamma)_{ik}\} \perp \{\varepsilon_{ijk}\}
\end{aligned}$$

$$\text{COV}\{Y_{ijk}, Y_{i'j'k'}\} = \begin{cases} \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_\gamma^2 + \sigma_{\alpha\gamma}^2 + \sigma^2 & i = i', j = j', k = k' \\ \sigma_\alpha^2 + \sigma_\beta^2 + \sigma_{\alpha\beta}^2 & i = i', j = j', k \neq k' \\ \sigma_\alpha^2 + \sigma_\gamma^2 + \sigma_{\alpha\gamma}^2 & i = i', j \neq j', k = k' \\ \sigma_\beta^2 + \sigma_\gamma^2 & i \neq i', j = j', k = k' \\ \sigma_\alpha^2 & i = i', j \neq j', k \neq k' \\ \sigma_\beta^2 & i \neq i', j = j', k \neq k' \\ \sigma_\gamma^2 & i \neq i', j \neq j', k = k' \\ 0 & i \neq i', j \neq j', k \neq k' \end{cases}$$

$$E\{MS_{\text{BLK}}\} = ac\sigma_b^2 + c\sigma_{ab}^2 + \sigma^2 \quad df_{\text{BLK}} = b-1$$

$$E\{MS_{\text{WP}}\} = bc\sigma_a^2 + c\sigma_{ab}^2 + b\sigma_{ac}^2 + \sigma^2 \quad df_{\text{WP}} = a-1$$

$$E\{MS_{\text{BLK} \times \text{WP}}\} = c\sigma_{ab}^2 + \sigma^2 \quad df_{\text{BLK} \times \text{WP}} = (a-1)(b-1)$$

$$E\{MS_{\text{SP}}\} = ab\sigma_c^2 + b\sigma_{ac}^2 + \sigma^2 \quad df_{\text{SP}} = c-1$$

$$E\{MS_{\text{WP} \times \text{SP}}\} = b\sigma_{ac}^2 + \sigma^2 \quad df_{\text{WP} \times \text{SP}} = (a-1)(c-1)$$

$$E\{MS_{\text{ERR}}\} = \sigma^2 \quad df_{\text{ERR}} = a(b-1)(c-1)$$

11.3. Split-Split Plot in a Randomized Block Design

The split-plot design can be extended to a third stage of randomization in a direct extension of the standard split-plot. Here we consider the case where all treatment factors are fixed, and the blocks are random. The model is given below.

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \gamma_k + (\alpha\gamma)_{ik} + \varepsilon_{ijk}^* + \delta_l + (\alpha\delta)_{il} + (\gamma\delta)_{kl} + (\alpha\gamma\delta)_{ikl} + \varepsilon_{ijkl}^{**}$$

$$i = 1, \dots, a; j = 1, \dots, b; k = 1, \dots, c; l = 1, \dots, d$$

$$\sum_{i=1}^a \alpha_i = \sum_{k=1}^c \gamma_k = \sum_{l=1}^d \delta_l = \sum_{i,k} (\alpha\gamma)_{ik} = \sum_{i,l} (\alpha\delta)_{il} = \sum_{k,l} (\gamma\delta)_{kl} = \sum_{i,k,l} (\alpha\gamma\delta)_{ikl}$$

$$\beta_j \sim NID(0, \sigma_\beta^2) \quad (\alpha\beta)_{ij} \sim NID(0, \sigma_{\alpha\beta}^2)$$

$$\varepsilon_{ijk}^* = (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} \sim NID(0, \sigma_2^2)$$

$$\varepsilon_{ijkl}^{**} = (\beta\delta)_{jl} + (\alpha\beta\delta)_{ijl} + (\beta\gamma\delta)_{jkl} + (\alpha\beta\gamma\delta)_{ijkl} \sim NID(0, \sigma_3^2)$$

$$\{\beta_j\} \perp \{(\alpha\beta)_{ij}\} \perp \{\varepsilon_{ijk}^*\} \perp \{\varepsilon_{ijkl}^{**}\}$$

The covariance structure, variances of means, and Expected Mean squares are given below, where Factor A is the Whole-Plot factor, Factor B is the Block (or Replicate Factor), Factor C is the Sub-Plot Factor, and Factor D is the Sub-Sub-Plot Factor.

$$E\{Y_{ijkl}\} = \mu + \alpha_i + \gamma_k + (\alpha\gamma)_{ik} + \delta_l + (\alpha\delta)_{il} + (\gamma\delta)_{kl} + (\alpha\gamma\delta)_{ikl}$$

$$\text{COV}\{Y_{ijkl}, Y_{i'j'k'l'}\} = \begin{cases} \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_2^2 + \sigma_3^2 & i=i', j=j', k=k', l=l' \\ \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_2^2 & i=i', j=j', k=k', l \neq l' \\ \sigma_\beta^2 + \sigma_{\alpha\beta}^2 & i=i', j=j', k \neq k', \forall l, l' \\ \sigma_\beta^2 & i \neq i', j=j', \forall k, k', l, l' \\ 0 & j \neq j', \forall i, i', k, k', l, l' \end{cases}$$

$$V\left\{\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^d Y_{ijkl}\right\} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^d V\{Y_{ijkl}\} + 2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{l=1}^{d-1} \sum_{l'=l+1}^d \text{COV}\{Y_{ijkl}, Y_{ijk'l'}\} + 2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{c-1} \sum_{k'=k+1}^c \sum_{l=1}^d \sum_{l'=1}^d \text{COV}\{Y_{ijkl}, Y_{ijk'l'}\} +$$

$$2 \sum_{i=1}^{a-1} \sum_{i'=i+1}^a \sum_{j=1}^b \sum_{k=1}^c \sum_{k'=k+1}^c \sum_{l=1}^d \sum_{l'=1}^d \text{COV}\{Y_{ijkl}, Y_{i'jk'l'}\} + 2 \sum_{i=1}^a \sum_{i'=1}^a \sum_{j=1}^{b-1} \sum_{j'=j+1}^b \sum_{k=1}^c \sum_{k'=1}^c \sum_{l=1}^d \sum_{l'=1}^d \text{COV}\{Y_{ijkl}, Y_{i'j'k'l'}\}$$

$$= abcd(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_2^2 + \sigma_3^2) + abcd(d-1)(\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_2^2) + abc(c-1)d^2(\sigma_\beta^2 + \sigma_{\alpha\beta}^2) + a(a-1)bc^2d^2\sigma_\beta^2 + a^2b(b-1)c^2d^2(0)$$

$$= a^2bc^2d^2\sigma_\beta^2 + abc^2d^2\sigma_{\alpha\beta}^2 + abcd^2\sigma_2^2 + abcd\sigma_3^2$$

$$\Rightarrow V\{\bar{Y}_{\dots}\} = \frac{a^2bc^2d^2\sigma_\beta^2 + abc^2d^2\sigma_{\alpha\beta}^2 + abcd^2\sigma_2^2 + abcd\sigma_3^2}{(abcd)^2} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{abc} + \frac{\sigma_3^2}{abcd}$$

$$V\{\bar{Y}_{i\dots}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{bc} + \frac{\sigma_3^2}{bcd} \quad V\{\bar{Y}_{\cdot j\dots}\} = \sigma_\beta^2 + \frac{\sigma_{\alpha\beta}^2}{a} + \frac{\sigma_2^2}{ac} + \frac{\sigma_3^2}{ac}$$

$$V\{\bar{Y}_{\dots k\dots}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{ab} + \frac{\sigma_3^2}{abd} \quad V\{\bar{Y}_{\dots l}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{abc} + \frac{\sigma_3^2}{abc}$$

$$V\{\bar{Y}_{ij\dots}\} = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma_2^2}{c} + \frac{\sigma_3^2}{cd} \quad V\{\bar{Y}_{i\cdot k\dots}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{b} + \frac{\sigma_3^2}{bd} \quad V\{\bar{Y}_{i\dots l}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{bc} + \frac{\sigma_3^2}{bc}$$

$$V\{\bar{Y}_{\cdot jk\dots}\} = \sigma_\beta^2 + \frac{\sigma_{\alpha\beta}^2}{a} + \frac{\sigma_2^2}{a} + \frac{\sigma_3^2}{ad} \quad V\{\bar{Y}_{\cdot j\cdot l}\} = \sigma_\beta^2 + \frac{\sigma_{\alpha\beta}^2}{a} + \frac{\sigma_2^2}{ac} + \frac{\sigma_3^2}{ac} \quad V\{\bar{Y}_{\dots kl}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{ab} + \frac{\sigma_3^2}{ab}$$

$$V\{\bar{Y}_{ijk\dots}\} = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma_2^2 + \frac{\sigma_3^2}{d} \quad V\{\bar{Y}_{ij\cdot l}\} = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \frac{\sigma_2^2}{c} + \frac{\sigma_3^2}{c}$$

$$V\{\bar{Y}_{i\cdot kl}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{b} + \frac{\sigma_3^2}{b} \quad V\{\bar{Y}_{\cdot jkl}\} = \sigma_\beta^2 + \frac{\sigma_{\alpha\beta}^2}{a} + \frac{\sigma_2^2}{a} + \frac{\sigma_3^2}{a}$$

$$E\{MS_{\text{BLK}}\} = acd\sigma_\beta^2 + cd\sigma_{\alpha\beta}^2 + d\sigma_2^2 + \sigma_3^2 \quad df_{\text{BLK}} = b-1$$

$$E\{MS_{\text{WP}}\} = cd\sigma_{\alpha\beta}^2 + d\sigma_2^2 + \sigma_3^2 + bcd \frac{\sum_{i=1}^a \alpha_i^2}{a-1} \quad df_{\text{WP}} = a-1$$

$$E\{MS_{\text{BLK} \times \text{WP}}\} = cd\sigma_{\alpha\beta}^2 + d\sigma_2^2 + \sigma_3^2 \quad df_{\text{BLK} \times \text{WP}} = (a-1)(b-1)$$

$$E\{MS_{\text{SP}}\} = d\sigma_2^2 + \sigma_3^2 + \frac{abd \sum_{k=1}^c \gamma_k^2}{c-1} \quad df_{\text{SP}} = c-1$$

$$E\{MS_{\text{WP} \times \text{SP}}\} = d\sigma_2^2 + \sigma_3^2 + \frac{bd \sum_{i=1}^a \sum_{k=1}^c (\alpha\gamma)_{ik}^2}{(a-1)(c-1)} \quad df_{\text{WP} \times \text{SP}} = (a-1)(c-1)$$

$$E\{MS_{\text{ERR2}}\} = d\sigma_2^2 + \sigma_3^2 \quad df_{\text{ERR2}} = a(b-1)(c-1)$$

$$E\{MS_{\text{SSP}}\} = \sigma_3^2 + \frac{abcd \sum_{l=1}^d \delta_l^2}{d-1} \quad df_{\text{SSP}} = d-1$$

$$E\{MS_{\text{WP} \times \text{SSP}}\} = \sigma_3^2 + \frac{bc \sum_{i=1}^a \sum_{l=1}^d (\alpha\delta)_{il}^2}{(a-1)(d-1)} \quad df_{\text{WP} \times \text{SSP}} = (a-1)(d-1)$$

$$E\{MS_{\text{SP} \times \text{SSP}}\} = \sigma_3^2 + \frac{ab \sum_{k=1}^c \sum_{l=1}^d (\gamma\delta)_{kl}^2}{(c-1)(d-1)} \quad df_{\text{SP} \times \text{SSP}} = (c-1)(d-1)$$

$$E\{MS_{\text{WP} \times \text{SP} \times \text{SSP}}\} = \sigma_3^2 + \frac{b \sum_{i=1}^a \sum_{k=1}^c \sum_{l=1}^d (\alpha\gamma\delta)_{ikl}^2}{(a-1)(c-1)(d-1)} \quad df_{\text{WP} \times \text{SP} \times \text{SSP}} = (a-1)(c-1)(d-1)$$

$$E\{MS_{\text{ERR3}}\} = \sigma_3^2 \quad df_{\text{ERR3}} = ac(b-1)(d-1)$$

Thus the Whole-Plot, Sub-Plot, and Whole-Plot/Sub-Plot factors and interactions are tested as in the standard Split-Plot analysis. The Sub-Sub-Plot, and its interactions with the Whole-Plot and Sub-Plot are tested versus the Error3 Mean Square, which makes use of the sum of the following sums of squares and degrees of freedom.

$$SS_{ERR3} = SS_{BLK \times SSP} + SS_{BLK \times WP \times SSP} + SS_{BLK \times SP \times SSP} + SS_{BLK \times WP \times SP \times SSP}$$

$$df_{ERR3} = df_{BLK \times SSP} + df_{BLK \times WP \times SSP} + df_{BLK \times SP \times SSP} + df_{BLK \times WP \times SP \times SSP} =$$

$$(b-1)(d-1) + (a-1)(b-1)(d-1) + (b-1)(c-1)(d-1) + (a-1)(b-1)(c-1)(d-1) = ac(b-1)(d-1)$$

Estimates and inferences concerning variance components and comparisons of treatment means are similar to those for the Split-Plot, with the main results given below.

Tests for Whole-Plot, Sub-Plot, Sub-Plot, and Interaction Effects:

Whole-Plot Trt Effects: $H_0 : \alpha_1 = \dots = \alpha_a = 0$ $F_{WP} = \frac{MS_{WP}}{MS_{BLK \times WP}}$ $P_{WP} = P(F_{a-1, (a-1)(b-1)} \geq F_{WP})$

Sub-Plot Trt Effects: $H_0 : \gamma_1 = \dots = \gamma_c = 0$ $F_{SP} = \frac{MS_{SP}}{MS_{ERR2}}$ $P_{SP} = P(F_{c-1, a(b-1)(c-1)} \geq F_{SP})$

WP \times SP Interaction: $H_0 : (\alpha\gamma)_{ik} = 0 \forall i, k$ $F_{WP \times SP} = \frac{MS_{WP \times SP}}{MS_{ERR2}}$ $P_{WP \times SP} = P(F_{(a-1)(c-1), a(b-1)(c-1)} \geq F_{WP \times SP})$

Sub-Sub-Plot Trt Effects: $H_0 : \delta_1 = \dots = \delta_d = 0$ $F_{SSP} = \frac{MS_{SSP}}{MS_{ERR3}}$ $P_{SSP} = P(F_{d-1, ac(b-1)(d-1)} \geq F_{SSP})$

WP \times SSP Interaction: $H_0 : (\alpha\delta)_{il} = 0 \forall i, l$ $F_{WP \times SSP} = \frac{MS_{WP \times SSP}}{MS_{ERR3}}$ $P_{WP \times SSP} = P(F_{(a-1)(d-1), ac(b-1)(d-1)} \geq F_{WP \times SSP})$

SP \times SSP Interaction: $H_0 : (\gamma\delta)_{kl} = 0 \forall k, l$ $F_{SP \times SSP} = \frac{MS_{SP \times SSP}}{MS_{ERR3}}$ $P_{SP \times SSP} = P(F_{(c-1)(d-1), ac(b-1)(d-1)} \geq F_{SP \times SSP})$

WP \times SP \times SSP Interaction: $H_0 : (\alpha\gamma\delta)_{ikl} = 0 \forall i, k, l$ $F_{WP \times SP \times SSP} = \frac{MS_{WP \times SP \times SSP}}{MS_{ERR3}}$

$P_{WP \times SP \times SSP} = P(F_{(a-1)(c-1)(d-1), ac(b-1)(d-1)} \geq F_{WP \times SP \times SSP})$

Estimators of Variance Components:

$$E\{MS_{BLK}\} = acd\sigma_\beta^2 + cd\sigma_{\alpha\beta}^2 + d\sigma_2^2 + \sigma_3^2 \quad E\{MS_{BLK \times WP}\} = cd\sigma_{\alpha\beta}^2 + d\sigma_2^2 + \sigma_3^2$$

$$E\{MS_{ERR2}\} = d\sigma_2^2 + \sigma_3^2 \quad E\{MS_{ERR3}\} = \sigma_3^2$$

$$\Rightarrow \hat{\sigma}_3^2 = MS_{ERR3} \quad \hat{\sigma}_2^2 = \frac{MS_{ERR2} - MS_{ERR3}}{d} \quad \hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{BLK \times WP} - MS_{ERR2}}{cd} \quad \hat{\sigma}_\beta^2 = \frac{MS_{BLK} - MS_{BLK \times WP}}{acd}$$

Point and Interval Estimators for Whole-Plot Means and Differences of Means:

$$E\{\bar{Y}_{i\dots}\} = \mu + \alpha_i \quad V\{\bar{Y}_{i\dots}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{bc} + \frac{\sigma_3^2}{bcd}$$

$$\Rightarrow \hat{V}\{\bar{Y}_{i\dots}\} = \frac{(MS_{BLK} - MS_{BLK \times WP}) + a(MS_{BLK \times WP} - MS_{ERR2}) + a(MS_{ERR2} - MS_{ERR3}) + aMS_{ERR3}}{abcd} = \frac{MS_{BLK} + (a-1)MS_{BLK \times WP}}{abcd}$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \alpha_i): \quad \bar{y}_{i\dots} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{BLK} + (a-1)MS_{BLK \times WP}}{abcd}}$$

$$v^* = \frac{[MS_{BLK} + (a-1)MS_{BLK \times WP}]^2}{\left[\frac{[MS_{BLK}]^2}{b-1} + \frac{[(a-1)MS_{BLK \times WP}]^2}{a(b-1)(c-1)} \right]}$$

$$E\{\bar{Y}_{i\dots} - \bar{Y}_{i'\dots}\} = (\mu + \alpha_i) - (\mu + \alpha_{i'}) = \alpha_i - \alpha_{i'} \quad V\{\bar{Y}_{i\dots} - \bar{Y}_{i'\dots}\} = V\{\bar{Y}_{i\dots}\} + V\{\bar{Y}_{i'\dots}\} - 2\text{COV}\{\bar{Y}_{i\dots}, \bar{Y}_{i'\dots}\}$$

$$\text{COV}\{\bar{Y}_{i\dots}, \bar{Y}_{i'\dots}\} = \frac{1}{b^2 c^2 d^2} (bc^2 d^2 \sigma_\beta^2) = \frac{\sigma_\beta^2}{b}$$

$$\Rightarrow V\{\bar{Y}_{i\dots} - \bar{Y}_{i'\dots}\} = 2 \left[\frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{bc} + \frac{\sigma_3^2}{bcd} - \frac{\sigma_\beta^2}{b} \right] = \frac{2}{b} \left[\sigma_{\alpha\beta}^2 + \frac{\sigma_2^2}{c} + \frac{\sigma_3^2}{cd} \right]$$

$$\Rightarrow \hat{V}\{\bar{Y}_{i\dots} - \bar{Y}_{i'\dots}\} = \frac{2MS_{BLK \times WP}}{bcd}$$

$$(1-\alpha)100\% \text{ CI for } (\alpha_i - \alpha_{i'}): \quad (\bar{y}_{i\dots} - \bar{y}_{i'\dots}) \pm t_{1-\alpha/2; (a-1)(b-1)} \sqrt{\frac{2MS_{BLK \times WP}}{bcd}}$$

Point and Interval Estimators for Sub-Plot Treatment Means and Differences of Means:

$$E\{\bar{Y}_{\bullet\bullet k}\} = \mu + \gamma_k \quad V\{\bar{Y}_{\bullet\bullet k}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{ab} + \frac{\sigma_3^2}{abd}$$

$$\Rightarrow \hat{V}\{\bar{Y}_{\bullet\bullet k}\} = \frac{(MS_{BLK} - MS_{BLK \times WP}) + (MS_{BLK \times WP} - MS_{ERR2}) + c(MS_{ERR2} - MS_{ERR3}) + cMS_{ERR3}}{abcd} = \frac{MS_{BLK} + (c-1)MS_{ERR2}}{abcd}$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \gamma_k): \quad \bar{y}_{\bullet\bullet k} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{BLK} + (c-1)MS_{ERR2}}{abcd}} \quad v^* = \frac{[MS_{BLK} + (c-1)MS_{ERR2}]^2}{\left[\frac{[MS_{BLK}]^2}{b-1} + \frac{[(c-1)MS_{ERR2}]^2}{a(b-1)(c-1)} \right]}$$

$$E\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = \gamma_k - \gamma_{k'} \quad V\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = V\{\bar{Y}_{\bullet\bullet k}\} + V\{\bar{Y}_{\bullet\bullet k'}\} - 2\text{COV}\{\bar{Y}_{\bullet\bullet k}, \bar{Y}_{\bullet\bullet k'}\}$$

$$\text{COV}\{\bar{Y}_{\bullet\bullet k}, \bar{Y}_{\bullet\bullet k'}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} \quad V\{\bar{Y}_{\bullet\bullet k}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{ab} + \frac{\sigma_3^2}{abd}$$

$$\Rightarrow V\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = 2 \left[\frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{ab} + \frac{\sigma_3^2}{abd} - \frac{\sigma_\beta^2}{b} - \frac{\sigma_{\alpha\beta}^2}{ab} \right] = 2 \left(\frac{\sigma_2^2}{ab} + \frac{\sigma_3^2}{abd} \right) \Rightarrow \hat{V}\{\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet k'}\} = \frac{2MS_{ERR2}}{abd}$$

$$(1-\alpha)100\% \text{ CI for } (\gamma_k - \gamma_{k'}): \quad (\bar{y}_{\bullet\bullet k} - \bar{y}_{\bullet\bullet k'}) \pm t_{1-\alpha/2; a(b-1)(c-1)} \sqrt{\frac{2MS_{ERR2}}{abd}}$$

Point and Interval Estimators for Sub-Sub-Plot Means and Differences of Means:

$$E\{\bar{Y}_{\dots l}\} = \mu + \delta_l \quad V\{\bar{Y}_{\dots l}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{abc} + \frac{\sigma_3^2}{abc}$$

$$\Rightarrow \hat{V}\{\bar{Y}_{\dots l}\} = \frac{(MS_{BLK} - MS_{BLK \times WP}) + (MS_{BLK \times WP} - MS_{ERR2}) + (MS_{ERR2} - MS_{ERR3}) + dMS_{ERR3}}{abcd} = \frac{MS_{ERR3}}{abc}$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \delta_l): \quad \bar{y}_{\dots l} \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{MS_{ERR3}}{abc}}$$

$$E\{\bar{Y}_{\dots l} - \bar{Y}_{\dots l'}\} = \delta_l - \delta_{l'} \quad V\{\bar{Y}_{\dots l} - \bar{Y}_{\dots l'}\} = V\{\bar{Y}_{\dots l}\} + V\{\bar{Y}_{\dots l'}\} - 2\text{COV}\{\bar{Y}_{\dots l}, \bar{Y}_{\dots l'}\}$$

$$\text{COV}\{\bar{Y}_{\dots l} - \bar{Y}_{\dots l'}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{abc}$$

$$\Rightarrow V\{\bar{Y}_{\dots l} - \bar{Y}_{\dots l'}\} = 2\left[\frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{abc} + \frac{\sigma_3^2}{abc} - \frac{\sigma_\beta^2}{b} - \frac{\sigma_{\alpha\beta}^2}{ab} - \frac{\sigma_2^2}{abc}\right] = 2\left[\frac{\sigma_3^2}{abc}\right] \Rightarrow \hat{V}\{\bar{Y}_{\dots l} - \bar{Y}_{\dots l'}\} = \frac{2MS_{ERR3}}{abc}$$

$$(1-\alpha)100\% \text{ CI for } (\delta_l - \delta_{l'}): \quad (\bar{y}_{\dots l} - \bar{y}_{\dots l'}) \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{2MS_{ERR3}}{abc}}$$

Comparing Treatment Effects within Levels of Other Factors when Interaction is Present

Level of Sub-Sub-Plot Factor Within Same Level of Whole-Plot Factor: $\bar{Y}_{i\bullet\bullet} - \bar{Y}_{i\bullet\bullet'}$

$$V\{\bar{Y}_{i\bullet\bullet}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{bc} + \frac{\sigma_3^2}{bc} \quad \text{COV}\{\bar{Y}_{i\bullet\bullet}, \bar{Y}_{i\bullet\bullet'}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{bc} \quad V\{\bar{Y}_{i\bullet\bullet} - \bar{Y}_{i\bullet\bullet'}\} = \frac{2\sigma_3^2}{bc} \quad \hat{V}\{\bar{Y}_{i\bullet\bullet} - \bar{Y}_{i\bullet\bullet'}\} = \frac{2MS_{ERR3}}{bc}$$

$$(1-\alpha)100\% \text{ CI for } ((\delta_i + (\alpha\delta)_{i\bullet}) - (\delta_{i'} + (\alpha\delta)_{i\bullet'})): \quad (\bar{y}_{i\bullet\bullet} - \bar{y}_{i\bullet\bullet'}) \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{2MS_{ERR3}}{bc}}$$

Levels of Sub-Sub-Plot Factor Within Same Level of Sub-Plot Factor: $\bar{Y}_{\bullet\bullet kl} - \bar{Y}_{\bullet\bullet k'l'}$

$$V\{\bar{Y}_{\bullet\bullet kl}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{ab} + \frac{\sigma_3^2}{ab} \quad \text{COV}\{\bar{Y}_{\bullet\bullet kl}, \bar{Y}_{\bullet\bullet k'l'}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} + \frac{\sigma_2^2}{ab} \quad V\{\bar{Y}_{\bullet\bullet kl} - \bar{Y}_{\bullet\bullet k'l'}\} = \frac{2\sigma_3^2}{ab} \quad \hat{V}\{\bar{Y}_{\bullet\bullet kl} - \bar{Y}_{\bullet\bullet k'l'}\} = \frac{2MS_{ERR3}}{ab}$$

$$(1-\alpha)100\% \text{ CI for } ((\delta_i + (\gamma\delta)_{kl}) - (\delta_{i'} + (\gamma\delta)_{k'l'})): \quad (\bar{y}_{\bullet\bullet kl} - \bar{y}_{\bullet\bullet k'l'}) \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{2MS_{ERR3}}{ab}}$$

Levels of Sub-Sub-Plot Factor Within Same Levels of Whole-Plot and Sub-Plot Factors: $\bar{Y}_{i\bullet kl} - \bar{Y}_{i\bullet k'l'}$

$$V\{\bar{Y}_{i\bullet kl}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{b} + \frac{\sigma_3^2}{b} \quad \text{COV}\{\bar{Y}_{i\bullet kl}, \bar{Y}_{i\bullet k'l'}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{b} \quad V\{\bar{Y}_{i\bullet kl} - \bar{Y}_{i\bullet k'l'}\} = \frac{2\sigma_3^2}{b} \quad \hat{V}\{\bar{Y}_{i\bullet kl} - \bar{Y}_{i\bullet k'l'}\} = \frac{2MS_{ERR3}}{b}$$

$$(1-\alpha)100\% \text{ CI for } ((\delta_i + (\alpha\delta)_{i\bullet} + (\gamma\delta)_{kl} + (\alpha\gamma\delta)_{ikl}) - (\delta_{i'} + (\alpha\delta)_{i\bullet'} + (\beta\delta)_{k'l'} + (\alpha\gamma\delta)_{i'k'l'})): \quad (\bar{y}_{i\bullet kl} - \bar{y}_{i\bullet k'l'}) \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{2MS_{ERR3}}{b}}$$

Levels of Sub-Plot Factor Within Same or Different Levels of Sub-Sub-Plot Factors: $\bar{Y}_{\bullet\bullet kl} - \bar{Y}_{\bullet\bullet k'l'}$

$$\text{COV}\{\bar{Y}_{\bullet\bullet kl}, \bar{Y}_{\bullet\bullet k'l'}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{ab} \quad V\{\bar{Y}_{\bullet\bullet kl} - \bar{Y}_{\bullet\bullet k'l'}\} = \frac{2(\sigma_2^2 + \sigma_3^2)}{ab} \quad \hat{V}\{\bar{Y}_{\bullet\bullet kl} - \bar{Y}_{\bullet\bullet k'l'}\} = \frac{2(MS_{ERR2} + (d-1)MS_{ERR3})}{abd}$$

$$(1-\alpha)100\% \text{ CI for } ((\gamma_k + (\gamma\delta)_{kl}) - (\gamma_{k'} + (\gamma\delta)_{k'l'})): \quad (\bar{y}_{\bullet\bullet kl} - \bar{y}_{\bullet\bullet k'l'}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2(MS_{ERR2} + (d-1)MS_{ERR3})}{abd}}$$

$$v^* = \frac{(MS_{ERR2} + (d-1)MS_{ERR3})^2}{\left[\frac{(MS_{ERR2})^2}{a(b-1)(c-1)} + \frac{((d-1)MS_{ERR3})^2}{ac(b-1)(d-1)}\right]}$$

Levels of Sub-Plot Factor Within Same Levels of Whole Plot and Sub-Sub-Plot Factors: $\bar{Y}_{i\bullet kl} - \bar{Y}_{i\bullet k'l}$

$$\text{COV}\{\bar{Y}_{i\bullet kl}, \bar{Y}_{i\bullet k'l}\} = \frac{\sigma_\beta^2}{b} + \frac{\sigma_{\alpha\beta}^2}{b} \quad V\{\bar{Y}_{i\bullet kl} - \bar{Y}_{i\bullet k'l}\} = \frac{2(\sigma_2^2 + \sigma_3^2)}{b} \quad \hat{V}\{\bar{Y}_{i\bullet kl} - \bar{Y}_{i\bullet k'l}\} = \frac{2(MS_{\text{ERR}2} + (d-1)MS_{\text{ERR}3})}{bd}$$

$$(1-\alpha)100\% \text{ CI for } ((\gamma_k + (\gamma\delta)_{kl}) - (\gamma_{k'} + (\gamma\delta)_{k'l'})) : (\bar{y}_{\bullet\bullet kl} - \bar{y}_{\bullet\bullet k'l'}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2(MS_{\text{ERR}2} + (d-1)MS_{\text{ERR}3})}{bd}}$$

Levels of Whole-Plot Factor Within Same or Different Levels of Sub-Sub-Plot Factor: $\bar{Y}_{i\bullet\bullet l} - \bar{Y}_{i'\bullet\bullet l'}$

$$\text{COV}\{\bar{Y}_{i\bullet\bullet l}, \bar{Y}_{i'\bullet\bullet l'}\} = \frac{\sigma_\beta^2}{b} \quad V\{\bar{Y}_{i\bullet\bullet l} - \bar{Y}_{i'\bullet\bullet l'}\} = 2\left[\frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{bc} + \frac{\sigma_3^2}{bc}\right] \quad \hat{V}\{\bar{Y}_{i\bullet\bullet l} - \bar{Y}_{i'\bullet\bullet l'}\} = \frac{2(MS_{\text{BLK}\times\text{WP}} + (d-1)MS_{\text{ERR}3})}{bcd}$$

$$(1-\alpha)100\% \text{ CI for } ((\alpha_i + (\alpha\delta)_{il}) - (\alpha_{i'} + (\alpha\delta)_{i'l'})) : (\bar{y}_{i\bullet\bullet l} - \bar{y}_{i'\bullet\bullet l'}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2(MS_{\text{BLK}\times\text{WP}} + (d-1)MS_{\text{ERR}3})}{bcd}}$$

$$v^* = \frac{(MS_{\text{BLK}\times\text{WP}} + (d-1)MS_{\text{ERR}3})^2}{\left[\frac{(MS_{\text{BLK}\times\text{WP}})^2}{(a-1)(b-1)} + \frac{((d-1)MS_{\text{ERR}3})^2}{ac(b-1)(d-1)}\right]}$$

Levels of Whole-Plot Factor Within Same or Different Levels of Sub-Plot and Sub-Sub-Plot Factors: $\bar{Y}_{i\bullet kl} - \bar{Y}_{i'\bullet k'l'}$

$$\text{COV}\{\bar{Y}_{i\bullet kl}, \bar{Y}_{i'\bullet k'l'}\} = \frac{\sigma_\beta^2}{b} \quad V\{\bar{Y}_{i\bullet kl} - \bar{Y}_{i'\bullet k'l'}\} = 2\left[\frac{\sigma_{\alpha\beta}^2}{b} + \frac{\sigma_2^2}{b} + \frac{\sigma_3^2}{b}\right] \quad \hat{V}\{\bar{Y}_{i\bullet kl} - \bar{Y}_{i'\bullet k'l'}\} = \frac{2(MS_{\text{BLK}\times\text{WP}} + (c-1)MS_{\text{ERR}2} + c(d-1)MS_{\text{ERR}3})}{bcd}$$

$$(1-\alpha)100\% \text{ CI for } ((\alpha_i + (\alpha\gamma)_{ik} + (\alpha\delta)_{il} + (\alpha\gamma\delta)_{ikl}) - (\alpha_{i'} + (\alpha\gamma)_{i'k'} + (\alpha\delta)_{i'l'} + (\alpha\gamma\delta)_{i'k'l'})) :$$

$$(\bar{y}_{i\bullet kl} - \bar{y}_{i'\bullet k'l'}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2(MS_{\text{BLK}\times\text{WP}} + (c-1)MS_{\text{ERR}2} + c(d-1)MS_{\text{ERR}3})}{bcd}}$$

$$v^* = \frac{(MS_{\text{BLK}\times\text{WP}} + (c-1)MS_{\text{ERR}2} + c(d-1)MS_{\text{ERR}3})^2}{\left[\frac{(MS_{\text{BLK}\times\text{WP}})^2}{(a-1)(b-1)} + \frac{((c-1)MS_{\text{ERR}2})^2}{a(b-1)(c-1)} + \frac{(c(d-1)MS_{\text{ERR}3})^2}{ac(b-1)(d-1)}\right]}$$

Example – Foil Lidding for Contact Lens Packaging

A study was conducted to study the effects of 3 factors on the response maximum peeling of contact lens packaging (Ferryanto and Tollefson (2010)). The factors were Set Temperature (400, 430, and 460°F), Seal Pressure (35, 45, 55 psig), and Dwell Time (1.20, 1.60, 2.00 seconds). The experiment was conducted in 2 replicates (blocks). The experiment was conducted as a Split-Split Plot Design, with Temperature as the Whole-Plot factor, Pressure as the Sub-Plot factor, and Dwell Time as the Sub-Sub-Plot factor. The data design and data are given below.

Note that in the first replicate the Whole-Plot units 1-3 were assigned to Temperatures 460, 430, and 400, the Sub-Plot units 1-3 within Whole-Plot unit 1 were assigned to Pressures 35, 45, and 55; and Sub-Sub-Plot units 1-3 within Whole-Plot unit 1 and Sub-Plot unit 1 were assigned to dwell times 2.0, 1.2, and 1.6. The remainder of the design can be determined from the data layout. Below the data are the means for each of the levels of 3 treatment factors and the replicates.

Replicate	TempF	pressure	dwltime	peelmx	Replicate	TempF	pressure	dwltime	peelmx
1	460	35	2	21.6	2	400	45	1.6	12.2
1	460	35	1.2	15.4	2	400	45	1.2	9.3
1	460	35	1.6	18.3	2	400	45	2	14
1	460	45	1.6	19.4	2	400	55	2	14.8
1	460	45	1.2	15.8	2	400	55	1.2	9.6
1	460	45	2	24.2	2	400	55	1.6	12.3
1	460	55	2	27.6	2	400	35	2	13
1	460	55	1.6	21.8	2	400	35	1.2	8.3
1	460	55	1.2	16.9	2	400	35	1.6	10.6
1	430	35	1.6	15.8	2	460	35	2	21
1	430	35	2	17.6	2	460	35	1.6	18.6
1	430	35	1.2	13.5	2	460	35	1.2	16.1
1	430	55	1.2	14.4	2	460	55	1.2	17.1
1	430	55	1.6	16.7	2	460	55	2	29.2
1	430	55	2	20.2	2	460	55	1.6	23.6
1	430	45	1.2	13.9	2	460	45	1.2	17.4
1	430	45	1.6	15.8	2	460	45	1.6	19.9
1	430	45	2	17.7	2	460	45	2	23.7
1	400	35	1.6	11.7	2	430	55	2	20.9
1	400	35	1.2	8.3	2	430	55	1.2	13.9
1	400	35	2	13.3	2	430	55	1.6	16.2
1	400	55	2	14.4	2	430	35	2	17.7
1	400	55	1.2	9.9	2	430	35	1.6	15.9
1	400	55	1.6	12	2	430	35	1.2	13.1
1	400	45	1.2	8.9	2	430	45	1.2	13
1	400	45	2	12.6	2	430	45	1.6	16.4
1	400	45	1.6	11.7	2	430	45	2	19.2

Replicate	Mean	Temp	Mean	Pressure	Mean	DwellTm	Mean
1	15.90	400	11.49	35	14.99	1.2	13.04
2	16.19	430	16.22	45	15.84	1.6	16.05
Overall	16.04	460	20.42	55	17.31	2.0	19.04

The Analysis of Variance is given below. Note that Error1 is the Block/Whole Plot (Rep/Temperature) interaction; Error2 is the sum of the Block/Sub-Plot and Block/Whole-Plot/Sub-Plot interactions; and Error3 is the sum of the Block/Sub-Sub-Plot, Block/Whole-Plot/Sub-Sub-Plot, Block/Sub-Plot/Sub-Sub-Plot, and Block/Whole-Plot/Sub-Plot/Sub-Sub-Plot interactions. All main effects and interactions among the 3 treatment factors are significant.

Source	df	SS	MS	Error df	Error MS	F	F(.95)	Pr(>F)
Rep (B)	1	1.070	1.070	2	0.397	2.695	18.513	0.2423
Temp (A)	2	718.148	359.074	2	0.397	904.806	19.000	0.0011
RT (AB)	2	0.794	0.397					
Press ("C)	2	49.443	24.722	6	0.374	66.022		0.0001
TP (AC)	4	16.432	4.108	6	0.374	10.971		0.0063
RP (BC)	2	1.216	0.608					
RPT (ABC)	4	1.031	0.258					
Dwell (D)	2	323.401	161.701	18	0.284	569.591	3.555	0.0000
TD (AD)	4	21.388	5.347	18	0.284	18.835	2.928	0.0000
PD (CD)	4	12.076	3.019	18	0.284	10.634	2.928	0.0001
TPD (ACD)	8	10.306	1.288	18	0.284	4.538	2.510	0.0037
RD (BD)	2	0.340	0.170					
RTD (ABD)	4	1.826	0.457					
RPD (BCD)	4	0.867	0.217					
RTDP (ABCD)	8	2.076	0.259					
Total	53	1160.413	21.895					
Error1 (AB)	2	0.794	0.397					
Error2 (BC+ABC)	6	2.247	0.374					
Error3 (BD+ABD+BCD+ABCD)	18	5.110	0.284					

The point estimates for variance components, Confidence Intervals for treatment means and differences are given below.

$$\hat{\sigma}_3^2 = MS_{ERR3} = 0.284 \quad \hat{\sigma}_2^2 = \frac{MS_{ERR2} - MS_{ERR3}}{d} = \frac{0.374 - 0.284}{3} = 0.300$$

$$\hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{BLK \times WP} - MS_{ERR2}}{cd} = \frac{0.397 - 0.374}{3(3)} = 0.00256 \quad \hat{\sigma}_\beta^2 = \frac{MS_{BLK} - MS_{BLK \times WP}}{acd} = \frac{1.070 - 0.397}{3(3)(3)} = 0.0249$$

Estimating and Comparing Temperature (Whole-Plot) Means:

$$\hat{SE}\{\bar{Y}_{i\dots}\} = \sqrt{\frac{MS_{BLK} + (a-1)MS_{BLK \times WP}}{abcd}} = \sqrt{\frac{1.070 + (3-1)0.397}{3(2)(3)(3)}} = \sqrt{\frac{1.864}{54}} = 0.1858$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \alpha_i): \bar{y}_{i\dots} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{BLK} + (a-1)MS_{BLK \times WP}}{abcd}} \equiv \bar{y}_{i\dots} \pm 3.707(0.1858) \equiv \bar{y}_{i\dots} \pm 0.6888$$

$$v^* = \frac{[MS_{BLK} + (a-1)MS_{BLK \times WP}]^2}{\left[\frac{MS_{BLK}^2}{b-1} + \frac{[(a-1)MS_{BLK \times WP}]^2}{(a-1)(b-1)}\right]} = \frac{[1.070 + (3-1)0.397]^2}{\left[\frac{1.070^2}{2-1} + \frac{[(3-1)0.397]^2}{(3-1)(2-1)}\right]} = \frac{3.4745}{1.4601} = 2.38 \quad t_{.975; 2.38} = 3.707$$

$$\hat{SE}\{\bar{Y}_{i\dots} - \bar{Y}_{i'\dots}\} = \sqrt{\frac{2MS_{BLK \times WP}}{bcd}} = \sqrt{\frac{2(0.397)}{2(3)(3)}} = 0.2100$$

$$(1-\alpha)100\% \text{ CI for } (\alpha_i - \alpha_{i'}): (\bar{y}_{i\dots} - \bar{y}_{i'\dots}) \pm t_{1-\alpha/2; (a-1)(b-1)} \sqrt{\frac{2MS_{BLK \times WP}}{bcd}} \equiv (\bar{y}_{i\dots} - \bar{y}_{i'\dots}) \pm 4.303(0.2100)$$

$$\equiv (\bar{y}_{i\dots} - \bar{y}_{i'\dots}) \pm 0.9037$$

$$\hat{\sigma}_3^2 = MS_{ERR3} = 0.284 \quad \hat{\sigma}_2^2 = \frac{MS_{ERR2} - MS_{ERR3}}{d} = \frac{0.374 - 0.284}{3} = 0.300$$

$$\hat{\sigma}_{\alpha\beta}^2 = \frac{MS_{BLK \times WP} - MS_{ERR2}}{cd} = \frac{0.397 - 0.374}{3(3)} = 0.00256 \quad \hat{\sigma}_\beta^2 = \frac{MS_{BLK} - MS_{BLK \times WP}}{acd} = \frac{1.070 - 0.397}{3(3)(3)} = 0.0249$$

Estimating and Comparing Pressure (Sub-Plot) Means:

$$\hat{SE}\{\bar{Y}_{\dots k}\} = \sqrt{\frac{MS_{BLK} + (c-1)MS_{ERR2}}{abcd}} = \sqrt{\frac{1.070 + (3-1)0.374}{3(2)(3)(3)}} = \sqrt{\frac{1.818}{54}} = 0.1835$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \gamma_k): \bar{y}_{\dots k} \pm t_{1-\alpha/2; v^*} \sqrt{\frac{MS_{BLK} + (c-1)MS_{ERR2}}{abcd}} \equiv \bar{y}_{\dots k} \pm 3.417(0.1835)$$

$$\equiv \bar{y}_{\dots k} \pm 0.6270$$

$$v^* = \frac{[MS_{BLK} + (c-1)MS_{ERR2}]^2}{\left[\frac{MS_{BLK}^2}{b-1} + \frac{[(c-1)MS_{ERR2}]^2}{a(b-1)(c-1)}\right]} = \frac{[1.818]^2}{\left[\frac{[1.070]^2}{2-1} + \frac{[(3-1)0.374]^2}{3(2-1)(3-1)}\right]} = \frac{3.3051}{1.2382} = 2.67 \quad t_{.975; 2.67} = 3.417$$

$$\hat{SE}\{\bar{Y}_{\dots k} - \bar{Y}_{\dots k'}\} = \sqrt{\frac{2MS_{ERR2}}{abd}} = \sqrt{\frac{2(0.374)}{3(2)(3)}} = 0.2039$$

$$(1-\alpha)100\% \text{ CI for } (\gamma_k - \gamma_{k'}): (\bar{y}_{\dots k} - \bar{y}_{\dots k'}) \pm t_{1-\alpha/2; a(b-1)(c-1)} \sqrt{\frac{2MS_{ERR2}}{abd}} \equiv (\bar{y}_{\dots k} - \bar{y}_{\dots k'}) \pm 2.447(0.2039)$$

$$\equiv (\bar{y}_{\dots k} - \bar{y}_{\dots k'}) \pm 0.4988$$

Estimating and Comparing Dwell Time (Sub-Sub-Plot) Means:

$$\hat{SE}\{\bar{Y}_{\dots l}\} = \sqrt{\frac{MS_{ERR3}}{abc}} = \sqrt{\frac{0.284}{3(2)(3)}} = 0.1256 \quad \hat{SE}\{\bar{Y}_{\dots l} - \bar{Y}_{\dots l'}\} = \sqrt{\frac{2MS_{ERR3}}{abc}} = \sqrt{\frac{2(0.284)}{3(2)(3)}} = 0.1776$$

$$(1-\alpha)100\% \text{ CI for } (\mu + \delta_l): \bar{y}_{\dots l} \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{MS_{ERR3}}{abc}} \equiv \bar{y}_{\dots l} \pm 2.101(0.1256) \equiv \bar{y}_{\dots l} \pm 0.2639$$

$$(1-\alpha)100\% \text{ CI for } (\delta_l - \delta_{l'}): (\bar{y}_{\dots l} - \bar{y}_{\dots l'}) \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{2MS_{ERR3}}{abc}} \equiv (\bar{y}_{\dots l} - \bar{y}_{\dots l'}) \pm 2.101(0.1776)$$

$$\equiv (\bar{y}_{\dots l} - \bar{y}_{\dots l'}) \pm 0.3731$$

The Confidence Intervals for the means and differences between means are given below for the simple effects.

Temp	Mean	LB	UB	Pressure	Mean	LB	UB	DwellTm	Mean	LB	UB
400	11.49	10.806	12.183	35	14.99	14.362	15.616	1.2	13.04	12.781	13.308
430	16.22	15.528	16.905	45	15.84	15.212	16.466	1.6	16.05	15.786	16.314
460	20.42	19.733	21.111	55	17.31	16.679	17.933	2	19.04	18.775	19.303

Temp1	Temp2	MeanDiff	LB	UB
400	430	-4.72	-5.626	-3.819
400	460	-8.93	-9.831	-8.024
430	460	-4.21	-5.109	-3.302
Press1	Press2	MeanDiff	LB	UB
35	45	-0.85	-1.054	-0.646
35	55	-2.32	-2.521	-2.113
45	55	-1.47	-1.671	-1.263
Dwell1	Dwell2	MeanDiff	LB	UB
1.2	1.6	-3.01	-3.379	-2.632
1.2	2.0	-5.99	-6.368	-5.621
1.6	2.0	-2.99	-3.362	-2.616

Interaction effects are considered for four cases. The first compares Dwell Times 1.2 and 2.0 with Temperature at 400. The second compares Dwell Times 1.6 and 2.0 with Temperature at 460 and Pressure at 45. The third compares Pressures 35 and 55 with Dwell Time at 1.6. The fourth compares Temperatures 400 and 430 with Pressure at 45 and Dwell Time at 2.0. These effects are given below, followed by computation of their 95% Confidence Intervals.

T=400	D=1.2	D=1.6	D=2.0	Mean	AllMean	
P=35	8.300	11.150	13.150	10.867	14.989	P=35
P=45	9.100	11.950	13.300	11.450	15.839	P=45
P=55	9.750	12.150	14.600	12.167	17.306	P=55
Mean	9.050	11.750	13.683	11.494	11.494	T=400
T=430	D=1.2	D=1.6	D=2.0	Mean		
P=35	13.300	15.850	17.650	15.600		
P=45	13.450	16.100	18.450	16.000		
P=55	14.150	16.450	20.550	17.050		
Mean	13.633	16.133	18.883	16.217	16.217	T=430
T=460	D=1.2	D=1.6	D=2.0	Mean		
P=35	15.750	18.450	21.300	18.500		
P=45	16.600	19.650	23.950	20.067		
P=55	17.000	22.700	28.400	22.700		
Mean	16.450	20.267	24.550	20.422	20.422	T=460
AllMean	13.044	16.050	19.039		16.044	Overall
	D=1.2	D=1.6	D=2.0			

$$\begin{aligned}
 & \text{Dwell Times 1.2 } (l = 1) \text{ and 2.0 } (l = 3) \text{ with Temp=400 } (i = 1): (\delta_1 + (\alpha\delta)_{11}) - (\delta_3 + (\alpha\delta)_{13}) \\
 & (\bar{y}_{1\bullet\bullet 1} - \bar{y}_{1\bullet\bullet 3}) \pm t_{1-\alpha/2, ac(b-1)(d-1)} \sqrt{\frac{2MS_{ERR3}}{bc}} \equiv (9.050 - 13.683) \pm 2.101 \sqrt{\frac{2(0.284)}{2(3)}} \equiv -4.633 \pm 2.101(0.3077) \\
 & \equiv -4.633 \pm 0.6464 \equiv (-5.279, -3.987)
 \end{aligned}$$

Dwell Times 1.6 ($l = 2$) and 2.0 ($l = 3$) with Temp=460 ($i = 3$) and Press=45 ($k = 2$):

$$\begin{aligned} & (\delta_2 + (\alpha\delta)_{32} + (\gamma\delta)_{22} + (\alpha\gamma\delta)_{322}) - (\delta_3 + (\alpha\delta)_{33} + (\gamma\delta)_{23} + (\alpha\gamma\delta)_{323}) \\ & (\bar{y}_{3\bullet 22} - \bar{y}_{3\bullet 23}) \pm t_{1-\alpha/2; ac(b-1)(d-1)} \sqrt{\frac{2MS_{ERR3}}{b}} \equiv (19.650 - 23.950) \pm 2.101 \sqrt{\frac{2(0.284)}{2}} \equiv -4.300 \pm 2.101(0.5329) \\ & \equiv -4.300 \pm 1.120 \equiv (-5.420, -3.180) \end{aligned}$$

Pressures 35 ($k = 1$) and 55 ($k = 3$) with Dwell Time=1.6 ($l = 2$): $(\gamma_1 + (\gamma\delta)_{12}) - (\gamma_3 + (\gamma\delta)_{32})$

$$\begin{aligned} \bar{y}_{\bullet\bullet 12} &= \frac{11.15 + 15.85 + 18.45}{3} = 15.15 & \bar{y}_{\bullet\bullet 32} &= \frac{12.15 + 16.45 + 22.70}{3} = 17.10 \\ MS_{ERR2} + (d-1)MS_{ERR3} &= 0.374 + (3-1)0.284 = 0.942 \\ & (\bar{y}_{\bullet\bullet 12} - \bar{y}_{\bullet\bullet 32}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2(MS_{ERR2} + (d-1)MS_{ERR3})}{abd}} \equiv (15.150 - 17.100) \pm 2.077 \sqrt{\frac{2(0.942)}{3(2)(3)}} \equiv -1.950 \pm 2.077(0.3235) \\ & \equiv -1.950 \pm 0.672 \equiv (-2.622, -1.278) \end{aligned}$$

$$v^* = \frac{[MS_{ERR2} + (d-1)MS_{ERR3}]^2}{\left[\frac{(MS_{ERR2})^2}{a(b-1)(c-1)} + \frac{((d-1)MS_{ERR3})^2}{ac(b-1)(d-1)} \right]} = \frac{(0.942)^2}{\left[\frac{(0.374)^2}{3(2-1)(3-1)} + \frac{((3-1)0.284)^2}{3(3)(2-1)(3-1)} \right]} = \frac{0.8874}{0.0412} = 21.52 \quad t_{.975; 21.5} = 2.077$$

Temps 400 ($i = 1$) and 430 ($i = 2$) with Press=45 ($k = 2$) and Dwell Time=2.0 ($l = 3$):

$$\begin{aligned} & (\alpha_1 + (\alpha\gamma)_{12} + (\alpha\delta)_{13} + (\alpha\gamma\delta)_{123}) - (\alpha_2 + (\alpha\gamma)_{22} + (\alpha\delta)_{23} + (\alpha\gamma\delta)_{223}) \\ MS_{BLK \times WP} + (c-1)MS_{ERR2} + c(d-1)MS_{ERR3} &= 0.397 + (3-1)0.374 + 3(3-1)0.284 = 0.397 + 0.748 + 1.704 = 2.849 \\ & (\bar{y}_{1\bullet 23} - \bar{y}_{2\bullet 23}) \pm t_{1-\alpha/2; v^*} \sqrt{\frac{2(MS_{BLK \times WP} + (c-1)MS_{ERR2} + c(d-1)MS_{ERR3})}{bcd}} \equiv (13.30 - 18.45) \pm 2.062 \sqrt{\frac{2(2.849)}{2(3)(3)}} \\ & \equiv -5.15 \pm 2.062(0.5626) \equiv -5.15 \pm 1.160 \equiv (-6.310, -4.990) \end{aligned}$$

$$v^* = \frac{[MS_{BLK \times WP} + (c-1)MS_{ERR2} + c(d-1)MS_{ERR3}]^2}{\left[\frac{(MS_{BLK \times WP})^2}{(a-1)(b-1)} + \frac{((c-1)MS_{ERR2})^2}{a(b-1)(c-1)} + \frac{(c(d-1)MS_{ERR3})^2}{ac(b-1)(d-1)} \right]} = \frac{(2.849)^2}{\left[\frac{(0.397)^2}{(3-1)(2-1)} + \frac{((3-1)0.374)^2}{3(2-1)(3-1)} + \frac{(3(3-1)0.284)^2}{3(3)(2-1)(3-1)} \right]} =$$

$$\frac{8.1168}{0.3334} = 24.35 \quad t_{.975; 24.35} = 2.062$$

The R Program and partial Output are given below.

R Program

```
contactlens <- read.csv("E:\\DesignofExp\\contactlens1.csv",header=T)
attach(contactlens); names(contactlens)

replicate <- factor(replicate)
TempF <- factor(TempF)
pressure <- factor(pressure)
dwlttime <- factor(dwlttime)

cl.mod1 <- aov(peelmx ~ replicate*TempF*pressure*dwlttime)
anova(cl.mod1)

library(lmerTest)

cl.mod2 <- lmer(peelmx ~ TempF*pressure*dwlttime + (1|replicate) +
  (1|TempF:replicate)+ (1|replicate:TempF:pressure))
summary(cl.mod2)
anova(cl.mod2)
lsmeans(cl.mod2)
diff1smeans(cl.mod2)
rand(cl.mod2)
```

R Output

```
> anova(cl.mod1)
Analysis of Variance Table

Response: peelmx

          Df Sum Sq Mean Sq F value Pr(>F)
replicate  1  1.07    1.07      0.00 0.959
TempF      2 718.15   359.07    14.14 <0.001
pressure   2  49.44    24.72     1.00 0.375
dwlttime   2 323.40   161.70    6.54 <0.001
replicate:TempF  2  0.79    0.40     0.02 0.881
replicate:pressure  2  1.22    0.61     0.03 0.861
TempF:pressure  4 16.43    4.11     0.17 0.687
replicate:dwlttime  2  0.34    0.17     0.01 0.917
TempF:dwlttime  4 21.39    5.35     0.22 0.937
pressure:dwlttime  4 12.08    3.02     0.12 0.737
replicate:TempF:pressure  4  1.03    0.26     0.01 0.917
replicate:TempF:dwlttime  4  1.83    0.46     0.01 0.917
replicate:pressure:dwlttime  4  0.87    0.22     0.01 0.917
TempF:pressure:dwlttime  8 10.31    1.29     0.05 0.837
replicate:TempF:pressure:dwlttime  8  2.08    0.26     0.01 0.917
Residuals    0  0.00

Warning message:
In anova.lm(cl.mod1) :
  ANOVA F-tests on an essentially perfect fit are unreliable

> summary(cl.mod2)
Linear mixed model fit by REML
t-tests use Satterthwaite approximations to degrees of freedom ['lmerMod']
Formula: peelmx ~ TempF * pressure * dwlttime + (1 | replicate) + (1 |
TempF:replicate) + (1 | replicate:TempF:pressure)

REML criterion at convergence: 65

Scaled residuals:
   Min       1Q   Median       3Q      Max
-1.2730 -0.4708  0.0000  0.4708  1.2730

Random effects:
 Groups              Name              Variance Std.Dev.
replicate:TempF:pressure (Intercept) 0.03019 0.1737
TempF:replicate         (Intercept) 0.00249 0.0499
replicate                (Intercept) 0.02492 0.1579
Residual                0.28389 0.5328
Number of obs: 54, groups: replicate:TempF:pressure, 18; TempF:replicate, 6;
replicate, 2
```

```

> anova(c1.mod2)
Analysis of Variance Table of type III with Satterthwaite
approximation for degrees of freedom

```

	Sum Sq	Mean Sq	NumDF	DenDF	F.value	Pr(>F)	
TempF	513.73	256.864	2	2	904.81	0.0011040	**
pressure	37.49	18.743	2	6	66.02	8.211e-05	***
dwltime	323.40	161.701	2	18	569.59	< 2.2e-16	***
TempF:pressure	12.46	3.115	4	6	10.97	0.0063324	**
TempF:dwltime	21.39	5.347	4	18	18.83	3.049e-06	***
pressure:dwltime	12.08	3.019	4	18	10.63	0.0001331	***
TempF:pressure:dwltime	10.31	1.288	8	18	4.54	0.0036931	**

```

> lsmeans(c1.mod2)
Least Squares Means table:

```

	TempF	pressure	dwltime	Estimate	Standard Error	DF	t-value	Lower CI	Upper CI	p-value
TempF 400	1.0	NA	NA	11.494	0.186	2.4	61.9	10.81	12.18	1e-04
TempF 430	2.0	NA	NA	16.217	0.186	2.4	87.3	15.53	16.91	<2e-16
TempF 460	3.0	NA	NA	20.422	0.186	2.4	109.9	19.73	21.11	<2e-16
pressure 35	NA	1.0	NA	14.989	0.184	2.7	81.7	14.36	15.62	<2e-16
pressure 45	NA	2.0	NA	15.839	0.184	2.7	86.3	15.21	16.47	<2e-16
pressure 55	NA	3.0	NA	17.306	0.184	2.7	94.3	16.68	17.93	<2e-16
dwltime 1.2	NA	NA	1.0	13.044	0.174	2.3	74.9	12.38	13.71	1e-04
dwltime 1.6	NA	NA	2.0	16.050	0.174	2.3	92.2	15.39	16.71	<2e-16
dwltime 2	NA	NA	3.0	19.039	0.174	2.3	109.3	18.38	19.70	<2e-16

```

> diff1smeans(c1.mod2)
Differences of LSMEANS:

```

	Estimate	Standard Error	DF	t-value	Lower CI	Upper CI	p-value
TempF 400 - 430	-4.7	0.210	2.0	-22.49	-5.626	-3.8187	0.002 **
TempF 400 - 460	-8.9	0.210	2.0	-42.52	-9.831	-8.0243	6e-04 ***
TempF 430 - 460	-4.2	0.210	2.0	-20.03	-5.109	-3.3021	0.002 **
pressure 35 - 45	-0.8	0.204	6.0	-4.17	-1.349	-0.3509	0.006 **
pressure 35 - 55	-2.3	0.204	6.0	-11.36	-2.816	-1.8176	<2e-16 ***
pressure 45 - 55	-1.5	0.204	6.0	-7.19	-1.966	-0.9676	4e-04 ***
dwltime 1.2 - 1.6	-3.0	0.178	18.0	-16.92	-3.379	-2.6324	<2e-16 ***
dwltime 1.2 - 2	-6.0	0.178	18.0	-33.75	-6.368	-5.6213	<2e-16 ***
dwltime 1.6 - 2	-3.0	0.178	18.0	-16.83	-3.362	-2.6158	<2e-16 ***
TempF:dwltime 400 1.2 - 400 2	-4.6	0.308	18.0	-15.06	-5.280	-3.9870	<2e-16 ***

```

> rand(c1.mod2)
Analysis of Random effects Table:

```

	chi.sq	chi.DF	p.value
replicate	0.35234	1	0.6
TempF:replicate	0.00256	1	1.0
replicate:TempF:pressure	0.18025	1	0.7

References and Related Sources:

Montgomery, D.C. (2001). *Design and Analysis of Experiments*. 4th edition. Wiley, New York.

Kuehl, R.O. (2000). *Design of Experiments*. 2nd edition. Duxbury, Pacific Grove, CA.

Steel, R.G.D. and Torrie, J.H. (1960). *Principles and Procedures of Statistics*. McGraw-Hill, New York.

Data Sources:

K.J. Potcner and S.M. Kowalski (2004). "How to Analyze a Split-Plot Experiment," *Quality Progress*, Vol. 37, #12, pp. 67-74.

A.C. Moynihan, S. Govindasamy-Lucey, J.J. Jaeggi, M.E. Johnson, J.A. Lucey, P.L.H. McSweeney (2014). "Effect of Camel Chynosin on the Texture, Functionality, and Sensory Properties of Low-Moisture, Part-Skim Mozzarella Cheese," *Journal of Dairy Science*, Vol. 97, #1, pp.85-96.

LPGA Data: www.lpga.com

L. Ferryanto and M. Tollefson (2010). "A Split-Split-Plot Design of Experiments for Foil Lidding of Contact Lens Packages," *Quality Engineering*, Vol. 22, pp. 317-327.

Chapter 12 – Repeated Measures Designs

Repeated Measures (RM) Designs involve experimental units that are observed on multiple occasions or under multiple conditions or treatments. In the case of a RM in a Completely Randomized Design (CRD), units are assigned at random to treatments, then observed at multiple time points. In these studies, units are nested within treatments and the analysis of the 1-Way ANOVA for a CRD is extended to include time main effects and time/treatment interaction effects. Often the time trends for the treatments are modeled using linear or polynomial models. Note the similarity with Random Coefficient Regression models, with the exception that RM models assume individual unit random effects have mean 0, but that measurements on the same unit are correlated.

In other cases, when each subject receives each treatment, the model is like a Randomized Complete Block Design. In these models, again subjects (units) are assumed to have effects that have mean 0, with correlated responses within subjects.

12.1. Repeated Measures in a Completely Randomized Design

This extends the 1-Way ANOVA to measurements at multiple time points. There are g treatments or groups, with n_i units or subjects within treatment i . Each unit or subject is observed/measured on t occasions in a balanced RM design. The Analysis of Variance has the following sources of variation: Treatments, Units nested within Treatments, Time Periods, Treatment/Time interaction, and Error2 (Time by Unit within Treatments interaction). Treatments and Time Periods are treated as fixed effects, while Units are considered random effects. There are three ways to approach the analysis: Split-plot ANOVA, Multivariate Analysis of Variance (MANOVA), and as a mixed linear model with a specific covariance structure for observations within units.

12.1.1. Univariate Split-Plot Method

The Split-plot approach is only appropriate when the within unit measurement display **Compound Symmetry (CS)** or meet the **Huynh-Feldt (HF)** condition. These can be described as follows. First, define Y_{ijk} be the observation on the j^{th} unit within the i^{th} at the k^{th} time point.

$$\mathbf{Y}_{ij} = \begin{bmatrix} Y_{ij1} \\ Y_{ij2} \\ \vdots \\ Y_{ijt} \end{bmatrix} \quad i = 1, \dots, g; j = 1, \dots, n_i \quad \text{CS: } V\{\mathbf{Y}_{ij}\} = \begin{bmatrix} \sigma^2 & \rho\sigma^2 & \dots & \rho\sigma^2 \\ \rho\sigma^2 & \sigma^2 & \dots & \rho\sigma^2 \\ \vdots & \vdots & \ddots & \vdots \\ \rho\sigma^2 & \rho\sigma^2 & \dots & \sigma^2 \end{bmatrix} \quad \text{H-F: } V\{Y_{ijt_1} - Y_{ijt_2}\} = c \quad \forall t_1, t_2$$

Thus, the CS condition implies that the variance of each observation is constant (σ^2), and the covariance between any two observations on the same unit is constant ($\rho\sigma^2$). The Huynh-Feldt condition is less restrictive, only requiring that the variance of the difference between any two measurements on the same unit is constant. The univariate model and Sums of squares are given as follows. To test for Treatment effects, the error term is Units(Trts); the Time and Treatment/Time interaction use Error2 as the error term. In this model, Treatment is referred to as a **Between Subject** factor and Time is a **Within Subject** factor. The model below is based on the Compound Symmetry assumption, which is often not reasonable, especially as the number of time points, t , gets large. This is a result of the fact that measurements closer together in time are more highly correlated than observations further apart in time.

$$Y_{ijk} = \mu + \alpha_i + \beta_{j(i)} + \tau_k + (\alpha\tau)_{ik} + \varepsilon_{jk(i)} \quad i=1, \dots, g; j=1, \dots, n_i; k=1, \dots, t \quad N = n_1 + \dots + n_g$$

$$\sum_{i=1}^g \alpha_i = \sum_{k=1}^t \tau_k = \sum_{i=1}^g (\alpha\tau)_{ik} = \sum_{k=1}^t (\alpha\tau)_{ik} = 0 \quad \beta_{j(i)} \sim NID(0, \sigma_\beta^2) \quad \varepsilon_{jk(i)} \sim N(0, \sigma_\varepsilon^2)$$

$$\text{COV} \left\{ \varepsilon_{jk(i)}, \varepsilon_{j'k'(i')} \right\} = \begin{cases} \sigma^2 = \sigma_\beta^2 + \sigma_\varepsilon^2 & i = i', j = j', k = k' \\ \rho\sigma^2 = \sigma_\beta^2 & i = i', j = j', k \neq k' \\ 0 & i = i', j \neq j', \forall k, k' \\ 0 & i \neq i', \forall j, j', k, k' \end{cases}$$

$$\text{Treatments (A): } SS_A = t \sum_{i=1}^g n_i (\bar{Y}_{i\bullet\bullet} - \bar{Y}_{\bullet\bullet\bullet})^2 \quad df_A = g - 1$$

$$\text{Units w/in Trts (B(A)) (Error1): } SS_{B(A)} = t \sum_{i=1}^g \sum_{j=1}^{n_i} (\bar{Y}_{ij\bullet} - \bar{Y}_{i\bullet\bullet})^2 \quad df_{B(A)} = \sum_{i=1}^g (n_i - 1) = N - g$$

$$\text{Time Periods (T): } SS_T = N \sum_{k=1}^t (\bar{Y}_{\bullet\bullet k} - \bar{Y}_{\bullet\bullet\bullet})^2 \quad df_T = t - 1$$

$$\text{Treatment} \times \text{Time (AT): } SS_{AT} = \sum_{i=1}^g \sum_{k=1}^t n_i (\bar{Y}_{i\bullet k} - \bar{Y}_{i\bullet\bullet} - \bar{Y}_{\bullet\bullet k} + \bar{Y}_{\bullet\bullet\bullet})^2 \quad df_{AT} = (g - 1)(t - 1)$$

$$\text{Time} \times \text{Unit(Trt) (Error2): } SS_{\text{Err2}} = \sum_{i=1}^g \sum_{j=1}^{n_i} \sum_{k=1}^t (Y_{ijk} - \bar{Y}_{ij\bullet} - \bar{Y}_{i\bullet k} + \bar{Y}_{i\bullet\bullet})^2 \quad df_{\text{Err2}} = (N - g)(t - 1)$$

The variances of the various means and Expected Mean Squares are derived below (assuming, but is not necessary that $n_1 = \dots = n_g = n$).

$$V \left\{ \sum_{i=1}^g \sum_{j=1}^n \sum_{k=1}^t Y_{ijk} \right\} = \sum_{i=1}^g \sum_{j=1}^n \sum_{k=1}^t V \{ Y_{ijk} \} + \sum_{i=1}^g \sum_{j=1}^n \sum_{k=1}^{t-1} \sum_{k'=k+1}^t \text{COV} \{ Y_{ijk}, Y_{ijk'} \}$$

$$+ \sum_{i=1}^{g-1} \sum_{i'=i+1}^g \sum_{j=1}^n \sum_{j'=j+1}^n \sum_{k=1}^t \sum_{k'=1}^t \text{COV} \{ Y_{ijk}, Y_{i'j'k'} \} + \sum_{i=1}^g \sum_{i'=1}^g \sum_{j=1}^{n-1} \sum_{j'=j+1}^n \sum_{k=1}^t \sum_{k'=1}^t \text{COV} \{ Y_{ijk}, Y_{i'j'k'} \}$$

$$= gnt [\sigma_\beta^2 + \sigma_\varepsilon^2] + gnt(t-1)\sigma_\beta^2 + g(g-1)n^2t^2(0) + g^2n(n-1)t^2(0)$$

$$\Rightarrow V \{ \bar{Y}_{\bullet\bullet\bullet} \} = \left(\frac{1}{gnt} \right)^2 [gnt^2\sigma_\beta^2 + gnt\sigma_\varepsilon^2] = \frac{\sigma_\beta^2}{gn} + \frac{\sigma_\varepsilon^2}{gnt} \quad \text{For unequal } n_i : gn \equiv N = \sum_{i=1}^g n_i$$

$$V \{ \bar{Y}_{i\bullet\bullet} \} = \frac{\sigma_\beta^2}{n} + \frac{\sigma_\varepsilon^2}{nt} \quad V \{ \bar{Y}_{ij\bullet} \} = \sigma_\beta^2 + \frac{\sigma_\varepsilon^2}{t} \quad V \{ \bar{Y}_{\bullet\bullet k} \} = \frac{\sigma_\beta^2}{gn} + \frac{\sigma_\varepsilon^2}{gn} \quad V \{ \bar{Y}_{i\bullet k} \} = \frac{\sigma_\beta^2}{n} + \frac{\sigma_\varepsilon^2}{n}$$

$$E \{ \bar{Y}_{\bullet\bullet\bullet}^2 \} = \frac{\sigma_\beta^2}{gn} + \frac{\sigma_\varepsilon^2}{gnt} + \mu^2 \quad E \{ \bar{Y}_{i\bullet\bullet}^2 \} = \frac{\sigma_\beta^2}{n} + \frac{\sigma_\varepsilon^2}{nt} + (\mu + \alpha_i)^2 \quad E \{ \bar{Y}_{ij\bullet}^2 \} = \sigma_\beta^2 + \frac{\sigma_\varepsilon^2}{t} + (\mu + \alpha_i)^2$$

$$E \{ \bar{Y}_{\bullet\bullet k}^2 \} = \frac{\sigma_\beta^2}{gn} + \frac{\sigma_\varepsilon^2}{gn} + (\mu + \tau_k)^2 \quad E \{ \bar{Y}_{i\bullet k}^2 \} = \frac{\sigma_\beta^2}{n} + \frac{\sigma_\varepsilon^2}{n} + (\mu + \alpha_i + \tau_k + (\alpha\tau)_{ik})^2$$

$$E \{ Y_{ijk}^2 \} = \sigma_\beta^2 + \sigma_\varepsilon^2 + (\mu + \alpha_i + \tau_k + (\alpha\tau)_{ik})^2$$

$$\begin{aligned} \text{Treatments: } E(MS_A) &= t\sigma_\beta^2 + \sigma_\varepsilon^2 + nt \frac{\sum_{i=1}^g \alpha_i^2}{g-1} & df_A &= g-1 \\ \text{Units (Trts): } E(MS_{B(A)}) &= t\sigma_\beta^2 + \sigma_\varepsilon^2 & df_{B(A)} &= g(n-1) \\ \text{Time: } E(MS_T) &= \sigma_\varepsilon^2 + gn \frac{\sum_{k=1}^t \tau_k^2}{t-1} & df_T &= t-1 \\ \text{Trt} \times \text{Time: } E(MS_{AT}) &= \sigma_\varepsilon^2 + n \frac{\sum_{i=1}^g \sum_{k=1}^t (\alpha\tau)_{ik}^2}{(g-1)(t-1)} & df_{AT} &= (g-1)(t-1) \\ \text{ERROR2: } E(MS_{\text{ERR2}}) &= \sigma_\varepsilon^2 & df_{\text{ERR2}} &= g(n-1)(t-1) \end{aligned}$$

Tests for Fixed effects, variance component estimates and comparisons among Treatment and Time means are given below.

$$\begin{aligned} \text{Treatment Effects: } H_0 : \alpha_1 = \dots = \alpha_g = 0 \\ \text{Test Statistic: } F_A &= \frac{MS_A}{MS_{B(A)}} & P_A &= P(F \geq F_A | F \sim F_{g-1, g(n-1)}) \\ \text{Time Effects: } H_0 : \tau_1 = \dots = \tau_t = 0 \\ \text{Test Statistic: } F_T &= \frac{MS_T}{MS_{\text{ERR2}}} & P_T &= P(F \geq F_T | F \sim F_{t-1, g(n-1)(t-1)}) \\ \text{Treatment/Time Interaction: } H_0 : (\alpha\tau)_{ik} = 0 \forall i, k \\ \text{Test Statistic: } F_{AT} &= \frac{MS_{AT}}{MS_{\text{ERR2}}} & P_{AT} &= P(F \geq F_{AT} | F \sim F_{(g-1)(t-1), g(n-1)(t-1)}) \\ E\{MS_{\text{ERR2}}\} &= \sigma_\varepsilon^2 & E\{MS_{B(A)}\} &= t\sigma_\beta^2 + \sigma_\varepsilon^2 \Rightarrow \hat{\sigma}_\varepsilon^2 = MS_{\text{ERR2}} & \hat{\sigma}_\beta^2 &= \frac{MS_{B(A)} - MS_{\text{ERR2}}}{t} \\ \text{Comparing Treatment Means:} \\ E\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} &= \alpha_i - \alpha_{i'} & V\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} &= 2V\{\bar{Y}_{i..}\} = 2\left[\frac{\sigma_\beta^2}{n} + \frac{\sigma_\varepsilon^2}{nt}\right] & \hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} &= \frac{2MS_{B(A)}}{nt} \\ 95\% \text{ CI for } \alpha_i - \alpha_{i'} : & (\bar{y}_{i..} - \bar{y}_{i'..}) \pm t_{1-\alpha/2; g(n-1)} \sqrt{\frac{2MS_{B(A)}}{nt}} \\ \text{Comparing Time Means:} \\ E\{\bar{Y}_{..k} - \bar{Y}_{..k'}\} &= \tau_k - \tau_{k'} \\ V\{\bar{Y}_{..k} - \bar{Y}_{..k'}\} &= 2V\{\bar{Y}_{..k}\} - 2COV\{\bar{Y}_{..k}, \bar{Y}_{..k'}\} = 2\left[\frac{\sigma_\beta^2}{gn} + \frac{\sigma_\varepsilon^2}{gn}\right] - 2\left(\frac{\sigma_\beta^2}{gn}\right) = \frac{2\sigma_\varepsilon^2}{gn} \\ \hat{V}\{\bar{Y}_{..k} - \bar{Y}_{..k'}\} &= \frac{2MS_{\text{ERR2}}}{gn} & 95\% \text{ CI for } \tau_k - \tau_{k'} : & (\bar{y}_{..k} - \bar{y}_{..k'}) \pm t_{1-\alpha/2; g(n-1)(t-1)} \sqrt{\frac{2MS_{\text{ERR2}}}{gn}} \end{aligned}$$

Comparing Treatments at a Single Time Point:

$$E\{\bar{Y}_{i\bullet k} - \bar{Y}_{i'\bullet k}\} = (\alpha_i - \alpha_{i'}) + ((\alpha\tau)_{ik} - (\alpha\tau)_{i'k})$$

$$V\{\bar{Y}_{i\bullet k} - \bar{Y}_{i'\bullet k}\} = 2V\{\bar{Y}_{i\bullet k}\} = 2\left[\frac{\sigma_\beta^2}{n} + \frac{\sigma_\epsilon^2}{n}\right]$$

$$\hat{V}(\bar{Y}_{i\bullet k} - \bar{Y}_{i'\bullet k}) = \frac{2\left(MS_{B(A)} + (t-1)MS_{ERR2} \right)}{nt}$$

95% CI for $(\alpha_i - \alpha_{i'}) + ((\alpha\tau)_{ik} - (\alpha\tau)_{i'k})$:

$$\left(\bar{y}_{i\bullet k} - \bar{y}_{i'\bullet k} \right) \pm t_{1-\alpha/2;v} \sqrt{\frac{2\left(MS_{B(A)} + (t-1)MS_{ERR2} \right)}{nt}}$$

$$v^* = \frac{\left[(t-1)MS_{ERR2} + MS_{B(A)} \right]^2}{\frac{\left[(t-1)MS_{ERR2} \right]^2}{g(n-1)(t-1)} + \frac{\left[MS_{B(A)} \right]^2}{g(n-1)}}$$

Example: CO₂ Exchange Rates in Plants Under 2 Treatments at 4 Time Points

Results of an experiment comparing $a = 2$ treatment conditions (1=Dry, 2=Wet) for sedum writii plants. There were $n = 3$ plants per treatment, and each plant was observed $t = 4$ time points. The data, relevant means and deviations, and the Sums of Squares are given below. The response is CO₂ exchange rate.

Trt	PlantID	Time	TrtxTime	Y	TrtMn	PlantMn	TimeMn	TrTmMn	AllMn	TrtDv	Plt(Tr)Dv	TmDv	TrTmDv	Err2Dv	TotDv
1	1	1	11	-1.397	-0.8328	-0.8733	-1.6108	-1.7190	-0.8303	-0.0025	-0.0405	-0.7805	-0.1057	0.3625	-0.5667
1	2	1	11	-2.402	-0.8328	-1.5765	-1.6108	-1.7190	-0.8303	-0.0025	-0.7438	-0.7805	-0.1057	0.0607	-1.5717
1	3	1	11	-1.358	-0.8328	-0.0485	-1.6108	-1.7190	-0.8303	-0.0025	0.7843	-0.7805	-0.1057	-0.4233	-0.5277
2	4	1	21	-1.160	-0.8278	-0.6318	-1.6108	-1.5027	-0.8303	0.0025	0.1961	-0.7805	0.1057	0.1466	-0.3297
2	5	1	21	-1.470	-0.8278	-0.7718	-1.6108	-1.5027	-0.8303	0.0025	0.0561	-0.7805	0.1057	-0.0234	-0.6397
2	6	1	21	-1.878	-0.8278	-1.0800	-1.6108	-1.5027	-0.8303	0.0025	-0.2522	-0.7805	0.1057	-0.1232	-1.0477
1	1	2	12	-0.699	-0.8328	-0.8733	-1.0593	-0.3100	-0.8303	-0.0025	-0.0405	-0.2290	0.7518	-0.3485	0.1313
1	2	2	12	-1.201	-0.8328	-1.5765	-1.0593	-0.3100	-0.8303	-0.0025	-0.7438	-0.2290	0.7518	-0.1473	-0.3707
1	3	2	12	0.970	-0.8328	-0.0485	-1.0593	-0.3100	-0.8303	-0.0025	0.7843	-0.2290	0.7518	0.4958	1.8003
2	4	2	22	-1.367	-0.8278	-0.6318	-1.0593	-1.8087	-0.8303	0.0025	0.1961	-0.2290	-0.7518	0.2456	-0.5367
2	5	2	22	-1.617	-0.8278	-0.7718	-1.0593	-1.8087	-0.8303	0.0025	0.0561	-0.2290	-0.7518	0.1356	-0.7867
2	6	2	22	-2.442	-0.8278	-1.0800	-1.0593	-1.8087	-0.8303	0.0025	-0.2522	-0.2290	-0.7518	-0.3812	-1.6117
1	1	3	13	-0.873	-0.8328	-0.8733	-0.6817	-0.8563	-0.8303	-0.0025	-0.0405	0.1486	-0.1722	0.0238	-0.0427
1	2	3	13	-1.502	-0.8328	-1.5765	-0.6817	-0.8563	-0.8303	-0.0025	-0.7438	0.1486	-0.1722	0.0981	-0.6717
1	3	3	13	-0.194	-0.8328	-0.0485	-0.6817	-0.8563	-0.8303	-0.0025	0.7843	0.1486	-0.1722	-0.1219	0.6363
2	4	3	23	-0.410	-0.8278	-0.6318	-0.6817	-0.5070	-0.8303	0.0025	0.1961	0.1486	0.1722	-0.0991	0.4203
2	5	3	23	-0.735	-0.8278	-0.7718	-0.6817	-0.5070	-0.8303	0.0025	0.0561	0.1486	0.1722	-0.2841	0.0953
2	6	3	23	-0.376	-0.8278	-1.0800	-0.6817	-0.5070	-0.8303	0.0025	-0.2522	0.1486	0.1722	0.3832	0.4543
1	1	4	14	-0.524	-0.8328	-0.8733	0.0307	-0.4457	-0.8303	-0.0025	-0.0405	0.8610	-0.4739	-0.0378	0.3063
1	2	4	14	-1.201	-0.8328	-1.5765	0.0307	-0.4457	-0.8303	-0.0025	-0.7438	0.8610	-0.4739	-0.0116	-0.3707
1	3	4	14	0.388	-0.8328	-0.0485	0.0307	-0.4457	-0.8303	-0.0025	0.7843	0.8610	-0.4739	0.0494	1.2183
2	4	4	24	0.410	-0.8278	-0.6318	0.0307	0.5070	-0.8303	0.0025	0.1961	0.8610	0.4739	-0.2931	1.2403
2	5	4	24	0.735	-0.8278	-0.7718	0.0307	0.5070	-0.8303	0.0025	0.0561	0.8610	0.4739	0.1719	1.5653
2	6	4	24	0.376	-0.8278	-1.0800	0.0307	0.5070	-0.8303	0.0025	-0.2522	0.8610	0.4739	0.1212	1.2063
									Source	A	B(A)	T	AT	Err2	Total
									SumSq	0.00015	5.10014	8.55026	4.98347	1.36086	19.9949
									df	1	4	3	3	12	23

Before setting up the Analysis of Variance and the F-tests, we consider how well the data fit the assumption of Compound Symmetry. Below is the matrix containing the variances for the time points on the main diagonal, the covariances of measurements for row k and column k' above the diagonal, and the correlations below the

main diagonal. It is clear that even with this very small sample size, the CS assumption is not reasonable. Also included is the variances of the Time Differences, which is the sum of the Time variances minus twice the covariances. The Huynh-Feldt condition also does not appear reasonable with estimated variances of Time differences ranging from 0.63 to 3.79. Note that the errors used to obtain these variances and covariances are those in the column labeled Err2Dv.

Corr\Cov				
k\k'	1	2	3	4
1	0.5691	0.9987	0.1432	0.2044
2	0.7411	3.1909	-0.1251	1.7001
3	0.3229	-0.1191	0.3458	-0.3824
4	0.2068	0.7265	-0.4963	1.7164
	k	k'	V(k-k')	
	1	2	1.7627	
	1	3	0.6284	
	1	4	1.8767	
	2	3	3.7868	
	2	4	1.5070	
	3	4	2.8268	

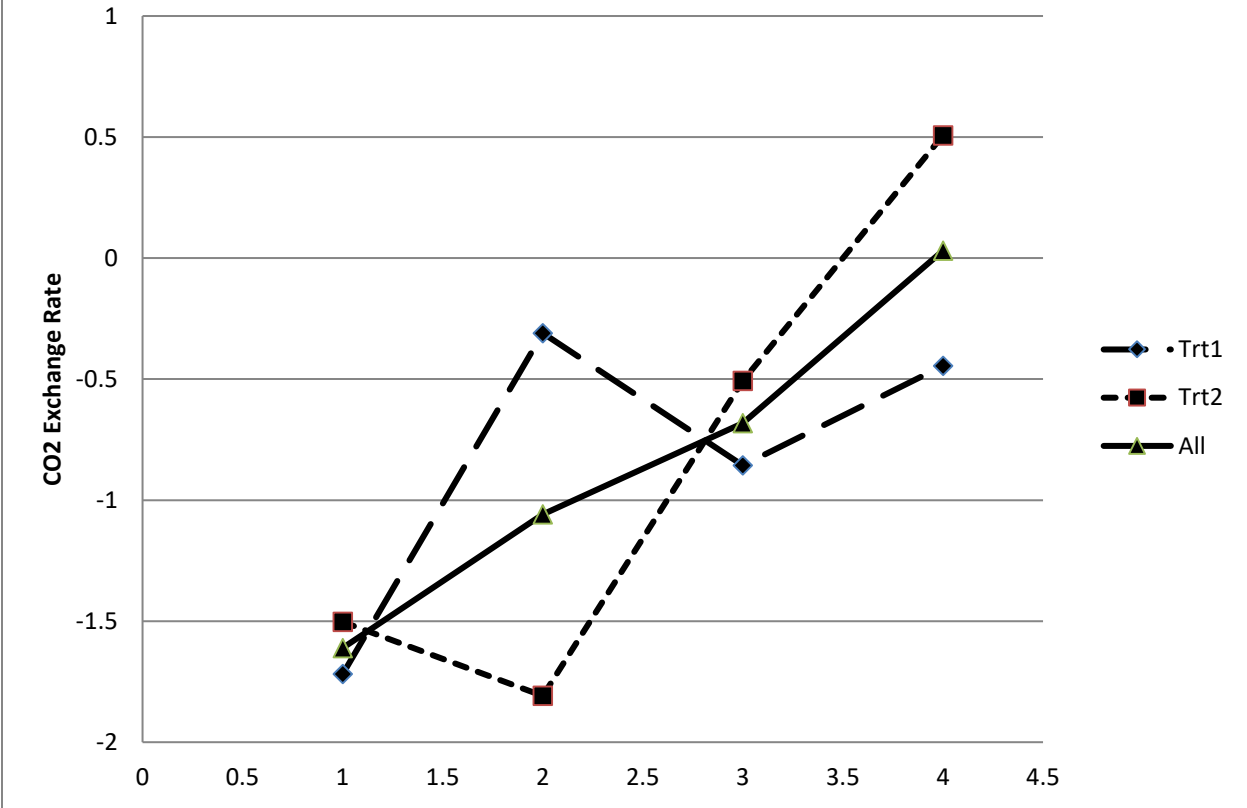
Although the validity of tests and inferences for comparing means is in question, the analysis is conducted as a demonstration of the computations.

Source	SumSq	df	MS	DenomMS	Denomdf	F	F(.95)	P(>F)
A	0.000145	1	0.000145	1.2750344	4	0.0001	7.7086	0.9920
B(A)	5.100138	4	1.275034					
T	8.550264	3	2.850088	0.1134049	12	25.1320	3.4903	0.0000
AT	4.983469	3	1.661156	0.1134049	12	14.6480	3.4903	0.0003
Err2	1.360859	12	0.113405					
Total	19.99487	23						
Trt\Time	1	2	3	4	All			
1	-1.7190	-0.3100	-0.8563	-0.4457	-0.8328			
2	-1.5027	-1.8087	-0.5070	0.5070	-0.8278			
All	-1.6108	-1.0593	-0.6817	0.0307	-0.8303			

There is strong evidence of a Treatment/Time interaction ($F_{AT} = 14.65$, $P_{AT} = .0003$), and a Time main effect ($F_T = 25.13$, $P_T = .0000$). There is no evidence of a Treatment main effect ($F_A = 0.0001$, $P_A = .9920$). Further, the Time (marginal) means tend to be increasing approximately linearly over time. The pattern does not hold within the 2 Treatments. The interaction plot is given below.

$$\hat{\sigma}_\varepsilon^2 = MS_{ERR2} = 0.1134 \quad \hat{\sigma}_\beta^2 = \frac{MS_{B(A)} - MS_{ERR2}}{t} = \frac{1.2750 - 0.1134}{4} = 0.2904$$

CO2 Exchange Rate versus Time by Treatment



Computations to compare Treatment, Time, and Treatment within Time are given below.

$$g = 2 \quad n = 3 \quad t = 4 \quad MS_{B(A)} = 1.2750 \quad df_{B(A)} = 2(3-1) = 4 \quad MS_{ERR2} = 0.1134 \quad df_{ERR2} = 2(3-1)(4-1) = 12$$

Comparing Treatment Means:

$$\hat{V}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \frac{2MS_{B(A)}}{nt} = \frac{2(1.2750)}{3(4)} = 0.2125 \quad \hat{SE}\{\bar{Y}_{i..} - \bar{Y}_{i'..}\} = \sqrt{0.2125} = 0.4610 \quad t_{0.975;4} = 2.7764$$

$$95\% \text{ CI for } \alpha_1 - \alpha_2: (\bar{y}_{..} - \bar{y}_{i'..}) \pm t_{1-\alpha/2;g(n-1)} \sqrt{\frac{2MS_{B(A)}}{nt}} \equiv ((-0.8328) - (-0.8278)) \pm 2.7764(0.4610)$$

$$\equiv -0.005 \pm 1.280 \equiv (-1.285, 1.275)$$

Comparing Time Means:

$$\hat{V}\{\bar{Y}_{..k} - \bar{Y}_{..k'}\} = \frac{2MS_{ERR2}}{gn} = \frac{2(0.1134)}{2(3)} = 0.0378 \quad \hat{SE}\{\bar{Y}_{..k} - \bar{Y}_{..k'}\} = \sqrt{0.0378} = 0.1944 \quad t_{0.975;12} = 2.179$$

$$95\% \text{ CI for } \tau_k - \tau_{k'}: (\bar{y}_{..k} - \bar{y}_{..k'}) \pm t_{1-\alpha/2;g(n-1)(t-1)} \sqrt{\frac{2MS_{ERR2}}{gn}} \equiv (\bar{y}_{..k} - \bar{y}_{..k'}) \pm 2.179(0.1944)$$

$$\equiv (\bar{y}_{..k} - \bar{y}_{..k'}) \pm 0.4236 \quad (\bar{y}_{..1} - \bar{y}_{..2}) = -0.5515 \quad (\bar{y}_{..1} - \bar{y}_{..3}) = -0.9292 \quad (\bar{y}_{..1} - \bar{y}_{..4}) = -1.6415$$

$$(\bar{y}_{..2} - \bar{y}_{..3}) = -0.3777 \quad (\bar{y}_{..2} - \bar{y}_{..4}) = -1.0900 \quad (\bar{y}_{..3} - \bar{y}_{..4}) = -0.7123$$

Comparing Treatments at a Single Time Point:

$$\hat{V}(\bar{Y}_{i.k} - \bar{Y}_{i'.k}) = \frac{2(MS_{B(A)} + (t-1)MS_{ERR2})}{nt} = \frac{2(1.2750 + (4-1)0.1134)}{3(4)} = \frac{2(1.6152)}{12} = 0.2692$$

$$\hat{SE}(\bar{Y}_{i.k} - \bar{Y}_{i'.k}) = \sqrt{0.2692} = 0.5188 \quad t_{.975;6.27} = 2.422$$

95% CI for $(\alpha_i - \alpha_{i'}) + ((\alpha\tau)_{ik} - (\alpha\tau)_{i'k})$:

$$(\bar{y}_{i.k} - \bar{y}_{i'.k}) \pm t_{1-\alpha/2;v^*} \sqrt{\frac{2(MS_{B(A)} + (t-1)MS_{ERR2})}{nt}} \equiv (\bar{y}_{i.k} - \bar{y}_{i'.k}) \pm 2.422(0.5188) \equiv (\bar{y}_{i.k} - \bar{y}_{i'.k}) \pm 1.257$$

$$v^* = \frac{[(t-1)MS_{ERR2} + MS_{B(A)}]^2}{\left[\frac{[(t-1)MS_{ERR2}]^2}{g(n-1)(t-1)} + \frac{[MS_{B(A)}]^2}{g(n-1)} \right]} = \frac{[1.2750 + (4-1)0.1134]^2}{\left[\frac{[(4-1)0.1134]^2}{2(3-1)(4-1)} + \frac{[1.2750]^2}{2(3-1)} \right]} = \frac{2.6089}{0.4161} = 6.27$$

$$(\bar{y}_{1.1} - \bar{y}_{2.1}) = -0.216 \quad (\bar{y}_{1.2} - \bar{y}_{2.2}) = 1.499 \quad (\bar{y}_{1.3} - \bar{y}_{2.3}) = -0.349 \quad (\bar{y}_{1.4} - \bar{y}_{2.4}) = -0.953$$

The time trend can be decomposed into Linear, Quadratic, and Cubic trends making use of orthogonal polynomials. Further the interaction effect can also be decomposed that way. This is an extension of the method used for the 1-Way ANOVA with equally spaced numeric levels. Calculations for the Sums of Squares are given below. Once the contrasts are obtained, the Sums of Squares are computed and then F-tests can be conducted.

Overall Times: $L_m = \sum_{k=1}^t C_{mk} \bar{Y}_{..k} \quad SS_m = \frac{gnL_m^2}{\sum_{k=1}^t C_{mk}^2} \quad m = 1, \dots, t-1$

Times within Trt i : $L_{mi} = \sum_{k=1}^t C_{mk} \bar{Y}_{i.k} \quad SS_{mi} = \frac{nL_{mi}^2}{\sum_{k=1}^t C_{mk}^2} \quad m = 1, \dots, t-1; \quad i = 1, \dots, g$

Treatment \times Time Sum of Squares: $\sum_{i=1}^g SS_{mi} - SS_m$

Time	Trt1	Trt2	All	C1	C2	C3	
1	-1.719	-1.50267	-1.61083	-3	1	-1	
2	-0.31	-1.80867	-1.05933	-1	-1	3	
3	-0.85633	-0.507	-0.68167	1	-1	-3	
4	-0.44567	0.507	0.030667	3	1	1	
							Total SS
	Contrast	Trt1		3.273667	-0.998333	2.912333	
	Contrast	Trt2		7.330667	1.32	-1.89533	
	Contrast	All		5.302167	0.1608333	0.5085	
	SumSq	Trt1		1.607534	0.7475021	1.272253	3.627289
	SumSq	Trt2		8.060801	1.3068	0.538843	9.906444
	SumSq	All		8.433891	0.038801	0.077572	8.550264
	SumSq	TrtxTime		1.234444	2.015501	1.733524	4.983469

This leads to the following partitions of the Time and Treatment/Time interaction Sums of Squares and F-tests.

Source	SumSq	df	MS	F	F(.95)	Pr(>F)
T	8.550264	3	2.850088	25.1320	3.4903	0.0000
T Linear	8.433891	1	8.433891	74.3697	4.7472	0.0000
T Quadratic	0.038801	1	0.038801	0.3421	4.7472	0.5694
T Cubic	0.077572	1	0.077572	0.6840	4.7472	0.4243
AT	4.983469	3	1.661156	14.6480	3.4903	0.0003
AT Linear	1.234444	1	1.234444	10.8853	4.7472	0.0063
AT Quadratic	2.015501	1	2.015501	17.7726	4.7472	0.0012
AT Cubic	1.733524	1	1.733524	15.2861	4.7472	0.0021
Err2	1.360859	12	0.113405			

The Time effect is purely linear, consistent with the plot. The interaction effect is messier as the 2 Treatments appear to differ in terms of all 3 components with respect to Time.

The R Program and Output for the analysis are given below. Note that in co2.mod1 and co2.mod3, Time is treated as a nominal factor, while in co2.mod2, Time is treated as ordinal, and the Time Sum of Squares is partitioned into Linear, Quadratic, and Cubic effects.

R Program

```
sedumwr <-
read.table("http://www.stat.ufl.edu/~winner/data/sedumwr.dat",header=F,
  col.names=c("trt_co2","plantID","time_co2","co2exc"))
attach(sedumwr)

trt_co2 <- factor(trt_co2)
plantID <- factor(plantID)
time_co2n <- factor(time_co2)
time_co2o <- factor(time_co2, ordered=T)

co2.mod1 <- aov(co2exc ~ trt_co2 + trt_co2/plantID + time_co2n +
trt_co2:time_co2n)
summary(co2.mod1)

co2.mod2 <- aov(co2exc ~ trt_co2*time_co2o + Error(plantID))
summary(co2.mod2)
summary(co2.mod2,split=list(time_co2o=list(linear=1, quadratic=2, cubic=3)))

library(lmerTest)

co2.mod3 <- lmer(co2exc ~ trt_co2*time_co2n + (1|trt_co2:plantID))
summary(co2.mod3)
anova(co2.mod3)
lsmeans(co2.mod3)
diff1smeans(co2.mod3)
rand(co2.mod3)
```

Partial R Output

```

> co2.mod1 <- aov(co2exc ~ trt_co2 + trt_co2/plantID + time_co2n + trt_co2:time_co2n)
> summary(co2.mod1)
      Df Sum Sq Mean Sq F value    Pr(>F)
trt_co2      1  0.000  0.0001    0.001 0.972060
time_co2n    3  8.550  2.8501   25.132 1.85e-05 ***
trt_co2:plantID 4  5.100  1.2750   11.243 0.000501 ***
trt_co2:time_co2n 3  4.983  1.6612   14.648 0.000258 ***
Residuals   12  1.361  0.1134
>
> co2.mod2 <- aov(co2exc ~ trt_co2*time_co2o + Error(plantID))
> summary(co2.mod2)

Error: plantID
      Df Sum Sq Mean Sq F value    Pr(>F)
trt_co2      1  0.0  0.0001     0  0.992
Residuals    4  5.1  1.2750

Error: within
      Df Sum Sq Mean Sq F value    Pr(>F)
time_co2o    3  8.550  2.8501   25.13 1.85e-05 ***
trt_co2:time_co2o 3  4.983  1.6612   14.65 0.000258 ***
Residuals   12  1.361  0.1134
---

> summary(co2.mod2,split=list(time_co2o=list(linear=1, quadratic=2, cubic=3)))

Error: plantID
      Df Sum Sq Mean Sq F value    Pr(>F)
trt_co2      1  0.0  0.0001     0  0.992
Residuals    4  5.1  1.2750

Error: within
      Df Sum Sq Mean Sq F value    Pr(>F)
time_co2o    3  8.550  2.850  25.132 1.85e-05 ***
  time_co2o: linear      1  8.434  8.434  74.370 1.73e-06 ***
  time_co2o: quadratic   1  0.039  0.039   0.342 0.569429
  time_co2o: cubic       1  0.078  0.078   0.684 0.424346
trt_co2:time_co2o      3  4.983  1.661  14.648 0.000258 ***
  trt_co2:time_co2o: linear 1  1.234  1.234  10.885 0.006349 **
  trt_co2:time_co2o: quadratic 1  2.016  2.016  17.773 0.001198 **
  trt_co2:time_co2o: cubic   1  1.734  1.734  15.286 0.002073 **
Residuals             12  1.361  0.113

REML criterion at convergence: 29

Scaled residuals:
    Min       1Q   Median       3Q      Max
-1.19848 -0.48268 -0.03538  0.43484  1.67926

Random effects:
 Groups      Name          Variance Std.Dev.
trt_co2:plantID (Intercept) 0.2904  0.5389
Residual                0.1134  0.3368
Number of obs: 24, groups: trt_co2:plantID, 6

Fixed effects:
      Estimate Std. Error    df t value Pr(>|t|)
(Intercept)   -1.7190    0.3669   6.2710 -4.685 0.003007 **
trt_co22       0.2163    0.5189   6.2710  0.417 0.690617
time_co2n2     1.4090    0.2750  12.0000  5.124 0.000251 ***
time_co2n3     0.8627    0.2750  12.0000  3.137 0.008573 **
time_co2n4     1.2733    0.2750  12.0000  4.631 0.000579 ***
trt_co22:time_co2n2 -1.7150    0.3889  12.0000 -4.410 0.000850 ***
trt_co22:time_co2n3  0.1330    0.3889  12.0000  0.342 0.738243
trt_co22:time_co2n4  0.7363    0.3889  12.0000  1.894 0.082633 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Correlation of Fixed Effects:
      (Intr) trt_22 tm_c22 tm_c23 tm_c24 t_22:_22 t_22:_23
trt_co22   -0.707
time_co2n2 -0.375  0.265
time_co2n3 -0.375  0.265  0.500
time_co2n4 -0.375  0.265  0.500  0.500
trt_c22:_22  0.265 -0.375 -0.707 -0.354 -0.354
trt_c22:_23  0.265 -0.375 -0.354 -0.354 -0.707  0.500
trt_c22:_24  0.265 -0.375 -0.354 -0.354 -0.707  0.500  0.500

```

```

> anova(co2.mod3)
Analysis of Variance Table of type III with Satterthwaite
approximation for degrees of freedom
      trt_co2      Sum Sq Mean Sq NumDF DenDF F.value Pr(>F)
trt_co2      0.0000 0.00001      1      4  0.0001 0.992001
time_co2n    8.5503 2.85009      3     12 25.1320 1.846e-05 ***
trt_co2:time_co2n 4.9835 1.66116      3     12 14.6480 0.000258 ***

> lsmeans(co2.mod3)
Least Squares Means table:
      trt_co2 time_co2n Estimate Standard Error DF t-value Lower CI Upper CI p-value
trt_co2 1      1.0      NA      -0.8328      0.3260 4.0 -2.55 -1.738 0.0723 0.063 .
trt_co2 2      2.0      NA      -0.8278      0.3260 4.0 -2.54 -1.733 0.0772 0.064 .
time_co2n 1      NA      1.0      -1.6108      0.2594 6.3 -6.21 -2.239 -0.9826 7e-04 ***
time_co2n 2      NA      2.0      -1.0593      0.2594 6.3 -4.08 -1.688 -0.4311 0.006 **
time_co2n 3      NA      3.0      -0.6817      0.2594 6.3 -2.63 -1.310 -0.0535 0.038 *
time_co2n 4      NA      4.0      0.0307      0.2594 6.3 0.12 -0.598 0.6589 0.910
trt_co2:time_co2n 1 1      1.0      1.0      -1.7190      0.3669 6.3 -4.69 -2.607 -0.8306 0.003 **
trt_co2:time_co2n 2 1      2.0      1.0      -1.5027      0.3669 6.3 -4.10 -2.391 -0.6142 0.006 **
trt_co2:time_co2n 1 2      1.0      2.0      -0.3100      0.3669 6.3 -0.84 -1.198 0.5784 0.429
trt_co2:time_co2n 2 2      2.0      2.0      -1.8087      0.3669 6.3 -4.93 -2.697 -0.9202 0.002 **
trt_co2:time_co2n 1 3      1.0      3.0      -0.8563      0.3669 6.3 -2.33 -1.745 0.0321 0.056 .
trt_co2:time_co2n 2 3      2.0      3.0      -0.5070      0.3669 6.3 -1.38 -1.395 0.3814 0.214
trt_co2:time_co2n 1 4      1.0      4.0      -0.4457      0.3669 6.3 -1.21 -1.334 0.4428 0.268
trt_co2:time_co2n 2 4      2.0      4.0      0.5070      0.3669 6.3 1.38 -0.381 1.3954 0.214

> diff lsmeans(co2.mod3)
Differences of LSMEANS:
      Estimate Standard Error DF t-value Lower CI Upper CI p-value
trt_co2 1 - 2      0.0      0.4610 4.0 -0.01 -1.2848 1.2750 0.992
time_co2n 1 - 2     -0.6      0.1944 12.0 -2.84 -0.9751 -0.1279 0.015 *
time_co2n 1 - 3     -0.9      0.1944 12.0 -4.78 -1.3528 -0.5055 4e-04 ***
time_co2n 1 - 4     -1.6      0.1944 12.0 -8.44 -2.0651 -1.2179 <2e-16 ***
time_co2n 2 - 3     -0.4      0.1944 12.0 -1.94 -0.8013 0.0460 0.076 .
time_co2n 2 - 4     -1.1      0.1944 12.0 -5.61 -1.5136 -0.6664 1e-04 ***
time_co2n 3 - 4     -0.7      0.1944 12.0 -3.66 -1.1360 -0.2887 0.003 **
trt_co2:time_co2n 1 1 - 2 1     -0.2      0.5189 6.3 -0.42 -1.4728 1.0401 0.691
trt_co2:time_co2n 1 2 - 2 2      1.5      0.5189 6.3 2.89 0.2422 2.7551 0.026 *
trt_co2:time_co2n 1 3 - 2 3     -0.3      0.5189 6.3 -0.67 -1.6058 0.9071 0.525
trt_co2:time_co2n 1 4 - 2 4     -1.0      0.5189 6.3 -1.84 -2.2091 0.3038 0.114

> rand(co2.mod3)
Analysis of Random effects Table:
      Chi.sq chi.DF p.value
trt_co2:plantID 10.6      1 0.001 **

```

12.1.2. Matrix Approach – Multivariate Analysis of Variance (MANOVA)

Due to the problems with the Compound Symmetry and Huynh-Feldt (aka Sphericity) assumptions, methods for adjusting tests for Within Subjects factors were developed. These adjustments are based on the extent to which the assumptions are not met, and adjust the degrees of freedom for the F-tests. The two adjustment factors are known as the **Greenhouse-Geisser** (GG) and the **Huynh-Feldt** (H-F) and are produced by most statistical computing packages. The method is described here (see e.g. Kuehl (2000)). The test is called **Mauchly's Test**.

$$\text{Suppose } t = 3: \mathbf{Y}_{ij} = \begin{bmatrix} Y_{ij1} \\ Y_{ij2} \\ Y_{ij3} \end{bmatrix} \Rightarrow \Sigma_{\mathbf{Y}} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_2^2 & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_3^2 \end{bmatrix} \quad i = 1, \dots, g; \quad j = 1, \dots, n_i$$

$$\text{Let } \mathbf{C} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{bmatrix} \quad \mathbf{C}\mathbf{C}' = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\Rightarrow \mathbf{C}\Sigma_{\mathbf{Y}}\mathbf{C}' = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \quad \text{When the Huynh-Feldt condition holds. We can test } H_0: \mathbf{C}\Sigma_{\mathbf{Y}}\mathbf{C}' = \lambda \mathbf{I} \text{ as follows:}$$

1) Obtain the Sample Covariance Matrix (\mathbf{S}_Y), where: $s_{lm} = \frac{\sum_{i=1}^g \sum_{j=1}^n (Y_{ijl} - \bar{Y}_{i \cdot l})(Y_{ijm} - \bar{Y}_{i \cdot m})}{g(n-1)}$ $l = m \Rightarrow s_{ll} = s_l^2$

2) Compute: $W = \frac{(t-1)^{t-1} |\mathbf{CS}_Y \mathbf{C}'|}{(\text{trace}(\mathbf{CS}_Y \mathbf{C}'))^{t-1}}$ $df_w = \frac{t(t-1)}{2} - 1$ $\nu = g(n-1)$ $\gamma = \nu - \frac{2t^2 - 3t + 3}{6(t-1)}$

3) Test Statistic: $-\gamma \ln W$ which under null hypothesis is approximately distributed as $\chi_{df_w}^2$

In general, the k^{th} row of C will be: $\left[\frac{1}{\sqrt{k+k^2}} \quad \dots \quad \frac{1}{\sqrt{k+k^2}} \quad \frac{-k}{\sqrt{k+k^2}} \quad 0 \quad \dots \quad 0 \right]$
 | k terms|

Adjusted Degrees of Freedom:

Let $\mathbf{A} = \mathbf{CS}_Y \mathbf{C}' = \begin{bmatrix} a_{11} & \dots & a_{1,t-1} \\ \vdots & \ddots & \vdots \\ a_{t-1,1} & \dots & a_{t-1,t-1} \end{bmatrix}$

Greenhouse-Geisser $\hat{\varepsilon} = \frac{\left(\sum_{i=1}^{t-1} a_{ii} \right)^2}{(t-1) \sum_{i=1}^{t-1} \sum_{j=1}^{t-1} a_{ij}^2}$ Huynh-Feldt $\tilde{\varepsilon} = \frac{N(t-1) \hat{\varepsilon} - 2}{(t-1) \left(\nu - (t-1) \hat{\varepsilon} \right)}$

where $N = gn$ (Total number of Units) and $\nu = N - g$ (Degrees of freedom for Units(Trts))

Within-Subjects Adjusted Degrees of Freedom:

Greenhouse-Geisser Adjustment:

Time: $df_1 = \hat{\varepsilon}(t-1)$ $df_2 = \hat{\varepsilon} g(n-1)(t-1)$

Time \times Trt: $df_1 = \hat{\varepsilon}(g-1)(t-1)$ $df_2 = \hat{\varepsilon} g(n-1)(t-1)$

Hunh-Feldt Adjustment:

Time: $df_1 = \min(1, \tilde{\varepsilon})(t-1)$ $df_2 = \min(1, \tilde{\varepsilon}) g(n-1)(t-1)$

Time \times Trt: $df_1 = \min(1, \tilde{\varepsilon})(g-1)(t-1)$ $df_2 = \min(1, \tilde{\varepsilon}) g(n-1)(t-1)$

Example: Zylkene for Cat Anxiety

A study compared $g = 2$ treatments (Zylkene ($i=1$) and placebo ($i=2$)) in $N = 34$ cats ($n_1 = n_2 = 17$) over $t = 5$ time points (Beata, *et al* (2007)). The response measured was a clinical global score based on various criteria (where high scores mean less anxiety, and are preferred). The multivariate form of the data is given below.

cat_id	trt	es1	es2	es3	es4	es5	dev_es1	dev_es2	dev_es3	dev_es4	dev_es5	TrtMean	CatMean
2	0	9	9	9	9	9	-0.0588	-1.1765	-1.8824	-2.4118	-2.4118	10.5882	9.0000
4	0	9	9	9	9	9	-0.0588	-1.1765	-1.8824	-2.4118	-2.4118	10.5882	9.0000
6	0	6	6	6	6	6	-3.0588	-4.1765	-4.8824	-5.4118	-5.4118	10.5882	6.0000
12	0	8	12	16	16	16	-1.0588	1.8235	5.1176	4.5882	4.5882	10.5882	13.6000
13	0	9	17	18	19	19	-0.0588	6.8235	7.1176	7.5882	7.5882	10.5882	16.4000
14	0	9	9	9	9	9	-0.0588	-1.1765	-1.8824	-2.4118	-2.4118	10.5882	9.0000
15	0	7	7	11	11	11	-2.0588	-3.1765	0.1176	-0.4118	-0.4118	10.5882	9.4000
17	0	13	13	13	13	13	3.9412	2.8235	2.1176	1.5882	1.5882	10.5882	13.0000
19	0	14	14	14	14	15	4.9412	3.8235	3.1176	2.5882	3.5882	10.5882	14.2000
22	0	6	10	10	9	9	-3.0588	-0.1765	-0.8824	-2.4118	-2.4118	10.5882	8.8000
24	0	2	2	2	2	2	-7.0588	-8.1765	-8.8824	-9.4118	-9.4118	10.5882	2.0000
26	0	12	13	14	16	17	2.9412	2.8235	3.1176	4.5882	5.5882	10.5882	14.4000
27	0	11	11	11	11	11	1.9412	0.8235	0.1176	-0.4118	-0.4118	10.5882	11.0000
28	0	15	15	15	15	15	5.9412	4.8235	4.1176	3.5882	3.5882	10.5882	15.0000
29	0	13	15	14	21	19	3.9412	4.8235	3.1176	9.5882	7.5882	10.5882	16.4000
33	0	5	5	4	4	4	-4.0588	-5.1765	-6.8824	-7.4118	-7.4118	10.5882	4.4000
34	0	6	6	10	10	10	-3.0588	-4.1765	-0.8824	-1.4118	-1.4118	10.5882	8.4000
1	1	8	9	8	9	9	-2.9412	-3.1176	-5.5882	-6.1765	-7.1176	13.5882	8.6000
3	1	9	11	12	13	16	-1.9412	-1.1176	-1.5882	-2.1765	-0.1176	13.5882	12.2000
5	1	10	10	10	10	10	-0.9412	-2.1176	-3.5882	-5.1765	-6.1176	13.5882	10.0000
7	1	14	15	17	18	21	3.0588	2.8824	3.4118	2.8235	4.8824	13.5882	17.0000
8	1	13	13	13	13	13	2.0588	0.8824	-0.5882	-2.1765	-3.1176	13.5882	13.0000
9	1	12	14	17	19	19	1.0588	1.8824	3.4118	3.8235	2.8824	13.5882	16.2000
10	1	5	12	14	15	17	-5.9412	-0.1176	0.4118	-0.1765	0.8824	13.5882	12.6000
11	1	10	12	13	14	14	-0.9412	-0.1176	-0.5882	-1.1765	-2.1176	13.5882	12.6000
16	1	14	14	14	14	14	3.0588	1.8824	0.4118	-1.1765	-2.1176	13.5882	14.0000
18	1	13	14	16	18	18	2.0588	1.8824	2.4118	2.8235	1.8824	13.5882	15.8000
20	1	11	9	16	19	19	0.0588	-3.1176	2.4118	3.8235	2.8824	13.5882	14.8000
21	1	13	13	13	13	12	2.0588	0.8824	-0.5882	-2.1765	-4.1176	13.5882	12.8000
23	1	14	14	19	21	21	3.0588	1.8824	5.4118	5.8235	4.8824	13.5882	17.8000
25	1	8	8	9	12	17	-2.9412	-4.1176	-4.5882	-3.1765	0.8824	13.5882	10.8000
30	1	7	9	8	13	14	-3.9412	-3.1176	-5.5882	-2.1765	-2.1176	13.5882	10.2000
31	1	17	18	19	23	23	6.0588	5.8824	5.4118	7.8235	6.8824	13.5882	20.0000
32	1	8	11	13	14	17	-2.9412	-1.1176	-0.5882	-1.1765	0.8824	13.5882	12.6000
PlacMean	Trt=0	9.0588	10.1765	10.8824	11.4118	11.4118						PlacMean	10.5882
ZyIkMean	Trt=1	10.9412	12.1176	13.5882	15.1765	16.1176						ZyIkMean	13.5882
AllMean		10.0000	11.1471	12.2353	13.2941	13.7647						AllMean	12.0882

The deviation columns represent the deviations between the individual cat measurements and their Treatment means during the corresponding Time periods: $Y_{ijk} - \bar{Y}_{i \cdot k}$.

The following matrices are used to conduct Mauchley's Test, and to compute the G-G and H-F degrees of freedom adjustments for the Within Subjects factors Time and Treatment/Time interaction.

S						C					CSC'				
11.3713	9.4982	9.3971	10.4301	9.2408		0.7071	-0.7071	0.0000	0.0000	0.0000		2.1599	1.2141	1.0150	1.0269
9.4982	11.9449	11.7868	13.0754	12.2665		0.4082	0.4082	-0.8165	0.0000	0.0000		1.2141	3.0104	2.2177	1.9132
9.3971	11.7868	15.1213	16.4081	15.6765		0.2887	0.2887	0.2887	-0.8660	0.0000		1.0150	2.2177	3.6081	2.7778
10.4301	13.0754	16.4081	20.3309	19.3989		0.2236	0.2236	0.2236	0.2236	-0.8944		1.0269	1.9132	2.7778	3.3619
9.2408	12.2665	15.6765	19.3989	19.9963											

CSC'	tr(CSC')	t	t-1	w	df(W)	v	gamma	MauchX2	X2(.95)	P-value
11.6629	12.1404	5	4	0.1374	9	32	30.4167	60.3644	16.9190	0.0000

$$g = 2 \quad n = 17 \quad t = 5 \quad |\mathbf{CS}_Y \mathbf{C}'| = 11.6629 \quad \text{trace}(\mathbf{CS}_Y \mathbf{C}') = 2.1599 + 3.0104 + 3.6081 + 3.3619 = 12.1404$$

$$2) \text{ Compute: } W = \frac{(t-1)^{t-1} |\mathbf{CS}_Y \mathbf{C}'|}{(\text{trace}(\mathbf{CS}_Y \mathbf{C}'))^{t-1}} = \frac{(5-1)^{5-1} (11.6629)}{(12.1404)^{5-1}} = 0.1374 \quad df_w = \frac{t(t-1)}{2} - 1 = \frac{5(5-1)}{2} - 1 = 9$$

$$\nu = g(n-1) = 2(17-1) = 32 \quad \gamma = \nu - \frac{2t^2 - 3t + 3}{6(t-1)} = 32 - \frac{2(5)^2 - 3(5) + 3}{6(5-1)} = 30.4167$$

$$3) \text{ Test Statistic: } -\gamma \ln W = -30.4167 \ln(0.1374) = 60.37 \quad \chi_{95; df_w}^2 = \chi_{95; 9}^2 = 16.9190$$

Adjusted Degrees of Freedom:

$$\text{Let } \mathbf{A} = \mathbf{CS}_Y \mathbf{C}' = \begin{bmatrix} 2.1599 & 1.2141 & 1.0150 & 1.0269 \\ 1.2141 & 3.0104 & 2.2177 & 1.9132 \\ 1.0150 & 2.2177 & 3.6081 & 2.7778 \\ 1.0269 & 1.9132 & 2.7778 & 3.3619 \end{bmatrix}$$

$$\sum_{i=1}^{t-1} a_{ii} = 2.1599 + 3.0104 + 3.6081 + 3.3619 = 12.1404$$

$$\sum_{i=1}^{t-1} \sum_{j=1}^{t-1} a_{ij}^2 = 2.1599^2 + 1.2141^2 + \dots + 2.7778^2 + 3.3619^2 = 77.7560$$

$$\text{Greenhouse-Geisser } \hat{\varepsilon} = \frac{\left(\sum_{i=1}^{t-1} a_{ii} \right)^2}{(t-1) \sum_{i=1}^{t-1} \sum_{j=1}^{t-1} a_{ij}^2} = \frac{12.1404^2}{(5-1)77.7560} = \frac{147.3893}{311.0240} = 0.4739$$

$$\text{Huynh-Feldt } \tilde{\varepsilon} = \frac{N(t-1)\hat{\varepsilon} - 2}{(t-1)(\nu - (t-1)\hat{\varepsilon})} = \frac{34(5-1)0.4739 - 2}{(5-1)(32 - (5-1)0.4739)} = \frac{62.4482}{120.4179} = 0.5186$$

where $N = gn$ (Total number of Units) and $\nu = N - g$ (Degrees of freedom for Units(Trts))

Within-Subjects Adjusted Degrees of Freedom:

Greenhouse-Geisser Adjustment:

$$\text{Time: } df_1 = \hat{\varepsilon}(t-1) = 0.4739(5-1) = 1.8956 \quad df_2 = \hat{\varepsilon}g(n-1)(t-1) = 0.4739(2)(17-1)(5-1) = 60.66$$

$$\text{Time} \times \text{Trt: } df_1 = \hat{\varepsilon}(g-1)(t-1) = 1.8956(2-1) = 1.8956 \quad df_2 = \hat{\varepsilon}g(n-1)(t-1) = 60.66$$

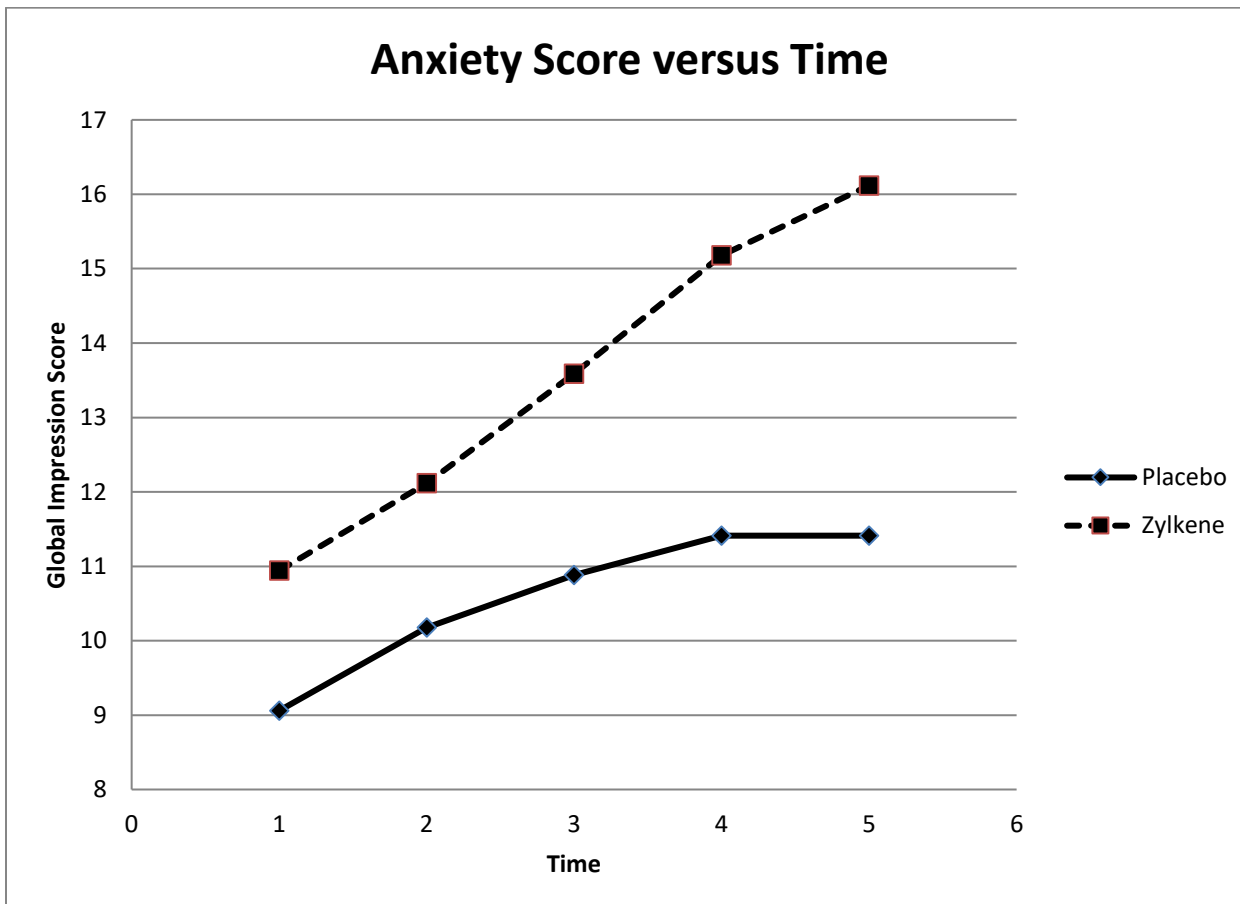
Huynh-Feldt Adjustment:

$$\text{Time: } df_1 = \min\left(1, \tilde{\varepsilon}\right)(t-1) = 0.5186(5-1) = 2.0744 \quad df_2 = \min\left(1, \tilde{\varepsilon}\right)g(n-1)(t-1) = 0.5186(2)(17-1)(5-1) = 66.38$$

$$\text{Time} \times \text{Trt: } df_1 = \min\left(1, \tilde{\varepsilon}\right)(g-1)(t-1) = 2.0728(2-1) = 2.0744 \quad df_2 = \min\left(1, \tilde{\varepsilon}\right)g(n-1)(t-1) = 66.38$$

The original Analysis of Variance based on the Split-Plot analysis, and the G-G and H-F adjustments are given below. There are clearly Treatment and Time Effects, with a significant Time/Treatment interaction. The Time and interaction effects remain significant after the G-G and H-F degrees of freedom adjustments.

Source	df	SS	MS	Error_df	Error_MS	F	F(.95)	P-value
Trts	1	382.5000	382.5000	32	66.6243	5.7412	4.0738	0.0226
Cat(Trt)	32	2131.9765	66.6243					
Time	4	324.1176	81.0294	128	3.0351	26.6974	2.4425	0.0000
Time*Trt	4	50.5882	12.6471	128	3.0351	4.1669	2.4425	0.0033
Error2	128	388.4941	3.0351					
Total	169	3277.6765						
G-G								
Time	1.8956	324.1176	170.9842	60.66	3.0351	26.6974	3.2064	0.0000
Time*Trt	1.8956	50.5882	26.6872	60.66	3.0351	4.1669	3.2064	0.0219
Error2	128	388.4941	3.0351					
H-F								
Time	2.0744	324.1176	156.2465	66.38	3.0351	26.6974	3.0975	0.0000
Time*Trt	2.0744	50.5882	24.3869	66.38	3.0351	4.1669	3.0975	0.0186
Error2	128	388.4941	3.0351					



The R Program and partial Output are given below.

R Program

```
cats.uni <- read.fwf("http://www.stat.ufl.edu/~winner/data/zylkene_uni_cat.dat",
width=c(rep(8,7)),col.names=c("id","weight","age","gender","trt","timepnt","y_cgi"))
attach(cats.uni)
id <- factor(id)
trt <- factor(trt)
timepnt <- factor(timepnt,ordered=T)

cat.mod1 <- aov(y_cgi ~ trt + trt/id + timepnt + trt:timepnt)
summary(cat.mod1)

cat.mod2 <- aov(y_cgi ~ trt*timepnt + Error(id))
summary(cat.mod2)
summary(cat.mod2,split=list(timepnt=list(linear=1, quadratic=2,
cubic=3, quartic=4)))

library(lmerTest)

cat.mod3 <- lmer(y_cgi ~ trt*timepnt + (1|trt:id))
summary(cat.mod3)
anova(cat.mod3)

detach(cats.uni)

#####
cats.multi <- read.fwf("http://www.stat.ufl.edu/~winner/data/cats_anxiety1.dat",
width=c(rep(8,13)), col.names=c("id","weight","age","gender",
"enviro", "origin", "trt_z", "result", "es1", "es2", "es3", "es4", "es5"))

attach(cats.multi)

trt_z <- factor(trt_z)
id <- factor(id)

##### Model with Greenhouse-Geisser and Huynh-Feldt df adjustments

dayLevels <- c(1,2,3,4,5)
dayFactor <- as.factor(dayLevels)
dayFrame <- data.frame(dayFactor)
dayBind <- cbind(es1,es2,es3,es4,es5)
dayModel <- lm(dayBind ~ trt_z)

library(car)
cat.mod5 <- Anova(dayModel, idata=dayFrame, idesign = ~dayFactor)
summary(cat.mod5)
```

Partial R Output

```

> summary(cat.mod1)
      Df Sum Sq Mean Sq F value    Pr(>F)
trt      1  382.5   382.5  126.025 < 2e-16 ***
timepnt  4  324.1   81.0   26.697 4.14e-16 ***
trt:id   32 2132.0   66.6   21.951 < 2e-16 ***
trt:timepnt  4   50.6   12.6   4.167 0.00332 **
Residuals 128  388.5    3.0

```

```

> summary(cat.mod2)
Error: id
      Df Sum Sq Mean Sq F value Pr(>F)
trt      1  382.5   382.5   5.741 0.0226 *
Residuals 32 2132.0   66.6
---
```

```

Error: Within
      Df Sum Sq Mean Sq F value    Pr(>F)
timepnt  4  324.1   81.03  26.697 4.14e-16 ***
trt:timepnt  4   50.6   12.65   4.167 0.00332 **
Residuals 128  388.5    3.04
---
```

```

> summary(cat.mod2,split=list(timepnt=list(linear=1, quadratic=2,
+ cubic=3, quartic=4)))
Error: id
      Df Sum Sq Mean Sq F value Pr(>F)
trt      1  382.5   382.5   5.741 0.0226 *
Residuals 32 2132.0   66.6
---
```

```

Error: Within
      Df Sum Sq Mean Sq F value    Pr(>F)
timepnt      4  324.1   81.0   26.697 4.14e-16 ***
timepnt: linear  1  318.4   318.4 104.891 < 2e-16 ***
timepnt: quadratic  1    4.6    4.6   1.529 0.218523
timepnt: cubic     1    1.0    1.0   0.314 0.576232
timepnt: quartic   1    0.2    0.2   0.055 0.814338
trt:timepnt      4   50.6   12.6   4.167 0.003316 **
trt:timepnt: linear  1   47.4   47.4 15.630 0.000127 ***
trt:timepnt: quadratic  1    2.6    2.6   0.848 0.358874
trt:timepnt: cubic     1    0.6    0.6   0.190 0.663706
trt:timepnt: quartic   1    0.0    0.0   0.000 1.000000
Residuals      128  388.5    3.0

```

```

> summary(cat.mod3)
Linear mixed model fit by REML t-tests use Satterthwaite approximations to degrees of freedom [lmerMod]
Formula: y_cgi ~ trt * timepnt + (1 | trt:id)

REML criterion at convergence: 762.1

Random effects:
Groups Name Variance Std.Dev.
trt:id (Intercept) 12.718 3.566
Residual 3.035 1.742
Number of obs: 170, groups: trt:id, 34

Fixed effects:
      Estimate Std. Error      df t value Pr(>|t|)
(Intercept)  1.059e+01  8.853e-01 3.200e+01 11.960 2.40e-13 ***
trt1         3.000e+00  1.252e+00 3.200e+01  2.396 0.022590 *
timepnt.L    1.879e+00  4.225e-01 1.280e+02  4.446 1.87e-05 ***
timepnt.Q   -6.446e-01  4.225e-01 1.280e+02 -1.525 0.129605
timepnt.C   -3.720e-02  4.225e-01 1.280e+02 -0.088 0.929976
timepnt^4   -7.031e-02  4.225e-01 1.280e+02 -0.166 0.868109
trt1:timepnt.L 2.362e+00  5.976e-01 1.280e+02  3.953 0.000127 ***
trt1:timepnt.Q 5.502e-01  5.976e-01 1.280e+02  0.921 0.358874
trt1:timepnt.C -2.604e-01  5.976e-01 1.280e+02 -0.436 0.663706
trt1:timepnt^4 -6.929e-15  5.976e-01 1.280e+02  0.000 1.000000

```

```

> anova(cat.mod3)
Analysis of Variance Table of type III with Satterthwaite
approximation for degrees of freedom
      Sum Sq Mean Sq NumDF DenDF F.value    Pr(>F)
trt      17.43  17.425    1    32  5.7412  0.022590 *
timepnt  324.12  81.029    4   128 26.6974 4.441e-16 ***
trt:timepnt  50.59  12.647    4   128  4.1669 0.003316 **

```

```

Multivariate Tests: trt_z
Df test stat approx F num Df den Df Pr(>F)
Pillai 1 0.1521191 5.741152 1 32 0.02259 *
Wilks 1 0.8478809 5.741152 1 32 0.02259 *
Hotelling-Lawley 1 0.1794110 5.741152 1 32 0.02259 *
Roy 1 0.1794110 5.741152 1 32 0.02259 *

Univariate Type II Repeated-Measures ANOVA Assuming Sphericity

      SS num Df Error SS den Df      F      Pr(>F)
(Intercept) 24841.3 1 2131.98 32 372.8570 < 2.2e-16 ***
trt_z 382.5 1 2131.98 32 5.7412 0.022590 *
dayFactor 324.1 4 388.49 128 26.6974 4.137e-16 ***
trt_z:dayFactor 50.6 4 388.49 128 4.1669 0.003316 **
---

Mauchly Tests for Sphericity

      Test statistic      p-value
dayFactor 0.13744 1.2302e-09
trt_z:dayFactor 0.13744 1.2302e-09

Greenhouse-Geisser and Huynh-Feldt Corrections
for Departure from Sphericity

      GG eps Pr(>F[GG])
dayFactor 0.47389 8.6e-09 ***
trt_z:dayFactor 0.47389 0.02189 *
---

      HF eps Pr(>F[HF])
dayFactor 0.5028585 3.380776e-09
trt_z:dayFactor 0.5028585 1.969249e-02
>

```

12.1.3. Linear Mixed Effects Models Approach

Researchers have begun using linear mixed effects model software to fit Repeated Measure models with more flexible covariance structures, which has become available more recently. In SAS, Proc Mixed, there are many options for Covariance structures (see Littell, Milliken, Stroup, Wolfinger, and Schabenberger (2016)). These can be used in many practical situations as they demonstrate. In terms of Repeated Measures, there are several structures that can be compared for a given dataset. Littell, Pendergast, and Natarajan (2000) describe fitting a RM model in a pharmaceutical application. Their data set consists on a study with $g = 3$ treatments (2 active drugs and a placebo), $N = 72$ patients, with $n = 24$ patients per treatment with $t = 8$ time points. They consider six covariance structures. First, the model can be written as follows in scalar form, then matrix form, as described previously for the mixed model (with the exception that the error terms within Subjects have a more general covariance structure). The case is given here in terms of g , n , and t . This presumes that the data have been sorted by treatment, subject within treatment, and time within subject within treatment.

$$Y_{ijk} = \mu + \alpha_i + \beta_{j(i)} + \tau_k + (\alpha\tau)_{ik} + \varepsilon_{jk(i)} \quad i = 1, \dots, g; j = 1, \dots, n; k = 1, \dots, t \quad \beta_{j(i)} \sim NID(0, \sigma_\beta^2)$$

$$\begin{aligned}
\mathbf{Y} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{U} + \boldsymbol{\varepsilon} & \mathbf{Y} &= \begin{bmatrix} \mathbf{Y}_{11} \\ \vdots \\ \mathbf{Y}_{gn} \end{bmatrix} & \mathbf{Y}_{ij} &= \begin{bmatrix} Y_{ij1} \\ \vdots \\ Y_{ijt} \end{bmatrix} & \boldsymbol{\beta} &= \begin{bmatrix} \mu \\ \mathbf{a} \\ \boldsymbol{\gamma} \\ (\boldsymbol{\alpha}\boldsymbol{\gamma}) \end{bmatrix} & \boldsymbol{\alpha} &= \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_g \end{bmatrix} & \boldsymbol{\gamma} &= \begin{bmatrix} \gamma_1 \\ \vdots \\ \gamma_t \end{bmatrix} & (\boldsymbol{\alpha}\boldsymbol{\gamma}) &= \begin{bmatrix} (\alpha\delta)_{11} \\ \vdots \\ (\alpha\gamma)_{gt} \end{bmatrix} \\
\mathbf{U} &= \begin{bmatrix} \beta_{1(i)} \\ \vdots \\ \beta_{n(g)} \end{bmatrix} & V\{\mathbf{U}\} &= \sigma_\beta^2 \mathbf{I}_{ng} = \mathbf{G} & \boldsymbol{\varepsilon} &= \begin{bmatrix} \boldsymbol{\varepsilon}_{11} \\ \vdots \\ \boldsymbol{\varepsilon}_{gn} \end{bmatrix} & \boldsymbol{\varepsilon}_{ij} &= \begin{bmatrix} \varepsilon_{ij1} \\ \vdots \\ \varepsilon_{ijt} \end{bmatrix} & V\{\boldsymbol{\varepsilon}_{ij}\} &= \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1t} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{12} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1t} & \sigma_{2t} & \cdots & \sigma_t^2 \end{bmatrix} = \boldsymbol{\Sigma}_{ij} \quad i=1,\dots,g; j=1,\dots,n \\
V\{\boldsymbol{\varepsilon}\} = \mathbf{R} &= \begin{bmatrix} \boldsymbol{\Sigma}_{ij} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Sigma}_{ij} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{\Sigma}_{ij} \end{bmatrix} = \mathbf{I}_{ng} \otimes \boldsymbol{\Sigma}_{ij} \Rightarrow V\{\mathbf{Y}\} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}
\end{aligned}$$

Note that the \mathbf{X} and \mathbf{Z} matrices are not shown, but it should be clear where the 0^s and 1^s would appear in the matrices for this model. Note that \mathbf{X} will be $gnt \times (1+g+t+gt)$ and \mathbf{Z} is $gnt \times gn$. Some commonly used Covariance matrices for \mathbf{Y} include: Simple, Compound Symmetry, Autoregressive of Order 1 (AR(1)), heterogeneous AR(1), and Unstructured. For examples of analyses with these structures using SAS Proc Mixed, see Littell, Pendergast, and Natarajan (2000) and Bagiella, Sloan, and Heitjan (2000).

Assuming $t = 4$ measurements within subjects, these (within subject) Covariance matrices are given below.

$$\begin{aligned}
\text{Simple: } \boldsymbol{\Sigma} &= \begin{bmatrix} \sigma^2 & 0 & 0 & 0 \\ 0 & \sigma^2 & 0 & 0 \\ 0 & 0 & \sigma^2 & 0 \\ 0 & 0 & 0 & \sigma^2 \end{bmatrix} & \text{Compound Symmetry: } \boldsymbol{\Sigma} &= \begin{bmatrix} \sigma^2 + \sigma_\beta^2 & \sigma^2 & \sigma^2 & \sigma^2 \\ \sigma^2 & \sigma^2 + \sigma_\beta^2 & \sigma^2 & \sigma^2 \\ \sigma^2 & \sigma^2 & \sigma^2 + \sigma_\beta^2 & \sigma^2 \\ \sigma^2 & \sigma^2 & \sigma^2 & \sigma^2 + \sigma_\beta^2 \end{bmatrix} \\
\text{Unstructured: } \mathbf{R} &= \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{12} & \sigma_2^2 & \sigma_{12} & \sigma_{24} \\ \sigma_{13} & \sigma_{23} & \sigma_3^2 & \sigma_{34} \\ \sigma_{14} & \sigma_{24} & \sigma_{34} & \sigma_4^2 \end{bmatrix} & \text{AR(1): } \mathbf{R} &= \begin{bmatrix} \sigma^2 & \rho\sigma^2 & \rho^2\sigma^2 & \rho^3\sigma^2 \\ \rho\sigma^2 & \sigma^2 & \rho\sigma^2 & \rho^2\sigma^2 \\ \rho^2\sigma^2 & \rho\sigma^2 & \sigma^2 & \rho\sigma^2 \\ \rho^3\sigma^2 & \rho^2\sigma^2 & \rho\sigma^2 & \sigma^2 \end{bmatrix} \\
\text{Heterogeneous AR(1): } \mathbf{R} &= \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 & \rho^2\sigma_1\sigma_3 & \rho^3\sigma_1\sigma_4 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 & \rho\sigma_2\sigma_3 & \rho^2\sigma_2\sigma_4 \\ \rho^2\sigma_1\sigma_3 & \rho\sigma_2\sigma_3 & \sigma_3^2 & \rho\sigma_3\sigma_4 \\ \rho^3\sigma_1\sigma_4 & \rho^2\sigma_2\sigma_4 & \rho\sigma_3\sigma_4 & \sigma_4^2 \end{bmatrix}
\end{aligned}$$

Example: Zylkene for Cat Anxiety

For the Cat Anxiety data, the following R program and output fits the 5 Covariance structures described above.

R Program

```
cats.uni <- read.csv("http://www.stat.ufl.edu/~winner/data/cat_zyl_uni.csv")
attach(cats.uni); names(cats.uni)

id <- factor(id)
trt <- factor(trt)
timepnt1 <- factor(timepnt,ordered=T)
timepnt <- factor(timepnt, levels=1:5, labels=c("T1","T2","T3","T4","T5"))

library(nlme)

## Simple Covariance Structure (Measurements within cats uncorrelated)
fit.sim <- gls(y ~ trt*timepnt)
summary(fit.sim)
anova(fit.sim)
AIC(fit.sim)
# getVarCov(fit.sim, individual="1",type="conditional")

## Compound Symmetry estimates the 2 variances but separate for ZGZ' and R
fit.cs.g <- gls(y ~ trt*timepnt,
  corr = corCompSymm(, form= ~ 1 | id))
summary(fit.cs.g)
anova(fit.cs.g)
AIC(fit.cs.g)
getVarCov(fit.cs.g, individual="1",type="conditional")

## Unstructured Covariance Structure
fit.un.g <- gls(y ~ trt*timepnt,
  corr = corSymm(form= ~ 1 | id),
  weights = varIdent(form = ~ 1 | timepnt),
  control=lmeControl(maxIter=100, opt="optim"))
summary(fit.un.g)
anova(fit.un.g)
AIC(fit.un.g)
getVarCov(fit.un.g, individual="1",type="conditional")

## AR(1) Covariance Structure
fit.ar1.g <- gls(y ~ trt*timepnt,
  corr = corAR1(, form= ~ 1 | id))
summary(fit.ar1.g)
anova(fit.ar1.g)
AIC(fit.ar1.g)
getVarCov(fit.ar1.g, individual="1",type="conditional")

## Heterogeneous AR(1) Covariance Structure
fit.arh1.g <- gls(y ~ trt*timepnt,
  corr = corAR1(, form= ~ 1 | id),
  weight = varIdent(form = ~ 1 | timepnt),
  control=lmeControl(maxIter=100, opt="optim"))
summary(fit.arh1.g)
anova(fit.arh1.g)
AIC(fit.arh1.g)
getVarCov(fit.arh1.g, individual="1",type="conditional")
```

Partial R Output

```
> fit.sim <- gls(y ~ trt*timepnt)
> summary(fit.sim)
Generalized least squares fit by REML
Model: y ~ trt * timepnt
Data: NULL
      AIC      BIC    logLik
948.7357 982.5626 -463.3678

Residual standard error: 3.968998
Degrees of freedom: 170 total; 160 residual

> anova(fit.sim)
Denom. DF: 160
      numDF  F-value p-value
(Intercept)    1 1576.9324 <.0001
trt             1  24.2812 <.0001
timepnt        4   5.1438 0.0006
trt:timepnt    4   0.8028 0.5250

> AIC(fit.sim)
[1] 948.7357

> fit.cs.g <- gls(y ~ trt*timepnt,
+   corr = corCompSymm(, form= ~ 1 | id))
> summary(fit.cs.g)
Generalized least squares fit by REML
Model: y ~ trt * timepnt
Data: NULL
      AIC      BIC    logLik
782.8744 819.7765 -379.4372
Rho
0.8073306
Residual standard error: 3.968997
Degrees of freedom: 170 total; 160 residual
> anova(fit.cs.g)
Denom. DF: 160
      numDF  F-value p-value
(Intercept)    1 372.8570 <.0001
trt             1   5.7412 0.0177
timepnt        4 26.6974 <.0001
trt:timepnt    4   4.1669 0.0031

> getVarCov(fit.cs.g, individual="1",type="conditional")
Marginal variance covariance matrix
      [,1] [,2] [,3] [,4] [,5]
[1,] 15.753 12.718 12.718 12.718 12.718
[2,] 12.718 15.753 12.718 12.718 12.718
[3,] 12.718 12.718 15.753 12.718 12.718
[4,] 12.718 12.718 12.718 15.753 12.718
[5,] 12.718 12.718 12.718 12.718 15.753
Standard Deviations: 3.969 3.969 3.969 3.969 3.969
```

```

> ## Unstructured Covariance Structure
> summary(fit.un.g)
Generalized least squares fit by REML
Model: y ~ trt * timepnt
Data: NULL
      AIC      BIC    logLik
734.4611 811.3404 -342.2305

Correlation Structure: General
Formula: ~1 | id
Parameter estimate(s):
Correlation:
  1     2     3     4
2 0.815
3 0.717 0.877
4 0.686 0.839 0.936
5 0.613 0.794 0.902 0.962
Variance function:
Structure: Different standard deviations per stratum
Formula: ~1 | timepnt
Parameter estimates:
      T1      T2      T3      T4      T5
1.000000 1.024932 1.153177 1.337170 1.326146

Residual standard error: 3.372119
Degrees of freedom: 170 total; 160 residual

> anova(fit.un.g)
Denom. DF: 160
      numDF  F-value p-value
(Intercept)  1 386.0280 <.0001
trt          1  3.9786 0.0478
timepnt     4  9.7879 <.0001
trt:timepnt  4  2.7233 0.0314

> getVarCov(fit.un.g, individual="1",type="conditional")
Marginal variance covariance matrix
      [,1] [,2] [,3] [,4] [,5]
[1,] 11.3710 9.4985 9.3969 10.430 9.2411
[2,] 9.4985 11.9450 11.7870 13.076 12.2670
[3,] 9.3969 11.7870 15.1220 16.409 15.6770
[4,] 10.4300 13.0760 16.4090 20.332 19.4000
[5,] 9.2411 12.2670 15.6770 19.400 19.9980
Standard Deviations: 3.3721 3.4562 3.8886 4.5091 4.4719

> summary(fit.ar1.g)
Generalized least squares fit by REML
Model: y ~ trt * timepnt
Data: NULL
      AIC      BIC    logLik
728.6384 765.5405 -352.3192

Correlation Structure: AR(1)
Formula: ~1 | id
Parameter estimate(s):
Phi
0.9047053
Residual standard error: 3.963392
Degrees of freedom: 170 total; 160 residual

```

```

> anova(fit.ar1.g)
Denom. DF: 160
      numDF  F-value p-value
(Intercept)    1 369.4090 <.0001
trt             1   6.7869  0.0100
timepnt        4  12.4477 <.0001
trt:timepnt    4   2.0486  0.0901

> getVarCov(fit.ar1.g, individual="1",type="conditional")
Marginal variance covariance matrix
      [,1] [,2] [,3] [,4] [,5]
[1,] 15.708 14.212 12.857 11.632 10.524
[2,] 14.212 15.708 14.212 12.857 11.632
[3,] 12.857 14.212 15.708 14.212 12.857
[4,] 11.632 12.857 14.212 15.708 14.212
[5,] 10.524 11.632 12.857 14.212 15.708
Standard Deviations: 3.9634 3.9634 3.9634 3.9634 3.9634

> summary(fit.arh1.g)
Generalized least squares fit by REML
Model: y ~ trt * timepnt
Data: NULL
      AIC      BIC    logLik
735.5316 784.7343 -351.7658

Correlation Structure: AR(1)
Formula: ~1 | id
Parameter estimate(s):
  Phi
0.9044515
Variance function:
Structure: Different standard deviations per stratum
Formula: ~1 | timepnt
Parameter estimates:
      T1      T2      T3      T4      T5
1.0000000 0.9923661 1.0058430 1.0708572 1.0409322

> anova(fit.arh1.g)
Denom. DF: 160
      numDF  F-value p-value
(Intercept)    1 363.2195 <.0001
trt             1   5.9537  0.0158
timepnt        4  12.4633 <.0001
trt:timepnt    4   2.0559  0.0891

> getVarCov(fit.arh1.g, individual="1",type="conditional")
Marginal variance covariance matrix
      [,1] [,2] [,3] [,4] [,5]
[1,] 14.918 13.390 12.275 11.819 10.391
[2,] 13.390 14.691 13.468 12.968 11.401
[3,] 12.275 13.468 15.093 14.533 12.777
[4,] 11.819 12.968 14.533 17.107 15.040
[5,] 10.391 11.401 12.777 15.040 16.164
Standard Deviations: 3.8624 3.8329 3.8849 4.1361 4.0205

```

Summaries of the models are given below.

For each model, the Variance Structure Based on cat i is: $\Sigma_i = \mathbf{Z}_i \mathbf{G} \mathbf{Z}_i' + \mathbf{R}_i = \sigma_\beta^2 \mathbf{J} + \mathbf{R}_i$

Simple: $\sigma_\beta^2 = 0$, $\hat{\mathbf{R}}_i = \hat{\sigma}^2 \mathbf{I} = 3.9690^2 \mathbf{I}$, $\hat{\Sigma}_i^S = \begin{bmatrix} 15.7530 & 0 & 0 & 0 & 0 \\ 0 & 15.7530 & 0 & 0 & 0 \\ 0 & 0 & 15.7530 & 0 & 0 \\ 0 & 0 & 0 & 15.7530 & 0 \\ 0 & 0 & 0 & 0 & 15.7530 \end{bmatrix}$

Compound Symmetry: $\hat{\sigma}^2 + \hat{\sigma}_\beta^2 = 3.969^2 = 15.753$ $\hat{\sigma}_\beta^2 = 0.80733(15.753) = 12.718$

$\hat{\Sigma}_i^{CS} = \begin{bmatrix} 15.753 & 12.718 & 12.718 & 12.718 & 12.718 \\ 12.718 & 15.753 & 12.718 & 12.718 & 12.718 \\ 12.718 & 12.718 & 15.753 & 12.718 & 12.718 \\ 12.718 & 12.718 & 12.718 & 15.753 & 12.718 \\ 12.718 & 12.718 & 12.718 & 12.718 & 15.753 \end{bmatrix}$

Unstructured: $\hat{\sigma}^2 = 3.372^2 = 11.37$

$\hat{\Sigma}_i^U = \begin{bmatrix} 11.37 & 9.50 & 9.40 & 10.43 & 9.24 \\ 9.50 & 11.95 & 11.79 & 13.08 & 12.27 \\ 9.40 & 11.79 & 15.12 & 16.41 & 15.68 \\ 10.43 & 13.08 & 16.41 & 20.33 & 19.40 \\ 9.24 & 12.27 & 15.68 & 19.40 & 20.00 \end{bmatrix}$

AR(1): $\hat{\sigma}^2 = 3.9634^2 = 15.7508$ $\hat{\rho} = 0.9047$ $\hat{\Sigma}_i^{\text{AR}(1)}$ given in R Output

ARH(1): $\hat{\sigma}_1^2 = [3.862(1.0000)]^2 = 14.918 \dots \hat{\sigma}_5^2 = [3.862(1.0409)]^2 = 16.164$

$\hat{\rho} = 0.9045$ $\hat{\Sigma}_i^{\text{ARH}(1)}$ is the matrix given in R Output

For each model, the main effects of Treatment and Time are significant. For the Compound Symmetry and Unstructured models, the Treatment/Time interaction is significant. For the other models, the interaction is not significant. The AIC values are given below.

$AIC_S = 945.52$ $AIC_{CS} = 784.87$ $AIC_U = 736.46$ $AIC_{AR(1)} = 730.64$ $AIC_{ARH(1)} = 737.53$
 Based on minimized AIC, the model with AR(1) errors presents the “best” fit.

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