

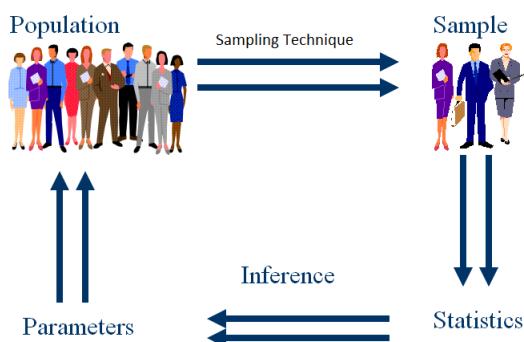
Chapter 1

ST 512 - Review

Readings: Chapters 1-8 as needed

Big ideas in stats:

- Population - all the values, items, or individuals of interest
- Parameter - a (usually) unknown summary value about the population
- Sample - a subset of the population we observe data on
- Statistic - a summary value calculated from the sample observations



Examples of parameters - (true) mean μ , (true) variance σ^2 .

Examples of statistics - sample mean \bar{y} , sample variance $s^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1}$

Inference - Making mathematically sound claims about the population using sample data.

Scales (Types) of Data:

- Qualitative or Categorical - A variable that is described by attributes or labels
Subscales:
Nominal - categories have no ordering (Male, Female)
Ordinal - can order categories (Lickert scale data)
- Quantitative - A variable that is described by numerical measurements where arithmetic can be performed
Subscales:
Discrete - finite or countable finite number of values (# of flowers on a plant, 0, 1, 2, ...)
Continuous - any value in an interval is possible (Temperature, $(-459.67 \text{ deg F}, \infty)$)

Random Variables and Things of Interest:

- Random Variable (RV) - Function that takes in outcomes from an experiment and outputs real numbers, or a numeric outcome to a random process

Things of interest

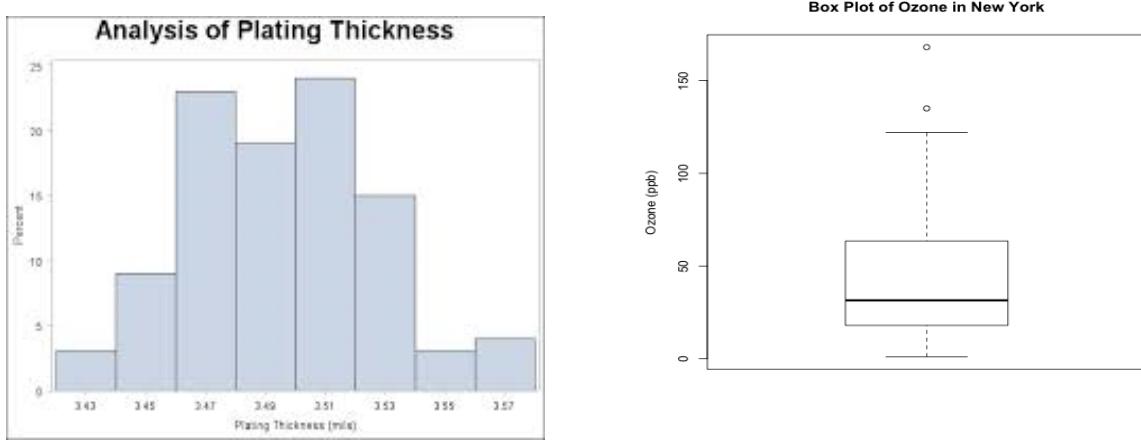
- Distribution - pattern and frequency of observable values
For continuous RVs, visualized with a smooth curve.
- Mean/Median - measures of center of the distribution

Focus on mean: true mean μ , RV sample mean \bar{Y} , observed sample mean \bar{y}
- Standard Deviation, Variance, IQR, Range - measures of spread for the distribution

Focus on SD and Variance: true variance σ^2 , true SD σ , observed sample variance s^2 , observed SD s

Graphical Descriptions of RV's:

- Histogram - Graphs the frequencies or relative frequencies of realizations of a RV
- Boxplot - Uses the Five Number Summary to display the realizations of a RV
Five number summary: \min, Q_1, M, Q_3, \max



Statistics are also RVs. The distribution of a statistic is called a sampling distribution
Central Limit Theorem (CLT):

If a RV Y has a (true) mean μ and (true) variance σ^2 , and a random sample is of size $n \geq 30$ is taken then

$$\bar{Y} \sim N(\mu, \sigma^2/n)$$

Note: If $Y \sim N(\mu, \sigma^2)$ then $\bar{Y} \sim N(\mu, \sigma^2/n)$ for any n .

2 main ways to make inference about a (true) mean, μ :

- When the true SD, σ , is known we looked at the sampling distribution of the statistic

$$Z = \frac{\bar{Y} - \mu}{\sigma/\sqrt{n}} \sim N(0, 1) \quad \text{valid if } \bar{Y} \text{ has a normal distribution}$$

Allows us to form a CI:

And a test statistic: Testing $H_0 : \mu = \mu_0$

$$\bar{y} \pm z_{\alpha/2} \sigma / \sqrt{n}$$

- When the true SD, σ , is unknown we looked at the sampling distribution of the statistic

$$T = \frac{\bar{Y} - \mu}{s/\sqrt{n}} \sim t_{n-1} \quad \text{valid if } \bar{Y} \text{ has a normal distribution, allow for } n \geq 15 \text{ or so in CLT}$$

Allows us to form a CI:

And a test statistic: Testing $H_0 : \mu = \mu_0$

$$\bar{y} \pm t_{(n-1,\alpha/2)} s / \sqrt{n}$$

$$t_{obs} = \frac{\bar{y} - \mu_0}{s / \sqrt{n}}$$

Inference about two (true) means, μ_1 and μ_2 :

- From paired samples, x_1, x_2, \dots, x_n and y_1, y_2, \dots, y_n where difference is normally distributed

$$\text{CI: } (\bar{x} - \bar{y}) \pm t_{(n-1,\alpha/2)} s_{diff} / \sqrt{n}$$

$$\text{HT: } H_0 : \mu_1 = \mu_2, \text{ i.e. } \mu_1 - \mu_2 = 0 \quad t_{obs} = \frac{(\bar{x} - \bar{y}) - 0}{s_{diff} / \sqrt{n}}$$

- Two separate samples from normal populations, x_1, x_2, \dots, x_n and y_1, y_2, \dots, y_n

$$\text{CI: } (\bar{x} - \bar{y}) \pm t_{(\nu,\alpha/2)} \sqrt{s_x^2/n + s_y^2/m} \text{ where } \nu \text{ is an estimate of df}$$

$$\text{HT: } H_0 : \mu_1 = \mu_2, \text{ i.e. } \mu_1 - \mu_2 = 0 \quad t_{obs} = \frac{(\bar{x} - \bar{y}) - 0}{\sqrt{s_x^2/n + s_y^2/m}}$$

Extension to inference about t (true) means, $\mu_1, \mu_2, \dots, \mu_t$:

Balanced One-way ANOVA table (same number of replicates per group)

Source	DF	SS	MS	F-stat	P-value
Treatment	$t - 1$	$n \sum_{i=1}^t (\bar{Y}_{i+} - \bar{Y}_{++})^2$	$\frac{SS(Trt)}{t-1}$	$\frac{MS(Trt)}{MS(E)}$	Use $F(t-1, t(n-1))$
Error	$t(n-1)$	$\sum_{i=1}^t \sum_{j=1}^n (Y_{ij} - \bar{Y}_{i+})^2$	$\frac{SS(E)}{t(n-1)}$		
Total	$nt - 1$	$\sum_{i=1}^t \sum_{j=1}^n (Y_{ij} - \bar{Y}_{++})^2$			

Analysis used for a completely randomized design.

P-value tests $H_0 : \mu_1 = \mu_2 = \dots = \mu_t$ vs $H_A : \text{at least 1 mean differs}$

One Way ANOVA model:

$$Y_{ij} = \mu + \alpha_i + E_{ij}$$

where $i = 1, 2, \dots, t$ and $j = 1, 2, \dots, n$ (total sample size = $nt = N$)

μ = overall mean

α_i = effect from group i

E_{ij} = random error assumed to be iid $N(0, \sigma^2)$

For two quantitative variables measured on the same units, the linear relationship can be investigated:

Simple linear regression model $Y_i = \beta_0 + \beta_1 x_i + E_i$ or use correlation.

For a hypothesis test, the p-value means

probability of observing a test statistic as extreme or more extreme than the one observed, assuming the null hypothesis is true.

For a given a null hypothesis, statistical significance implies

the observed value was unlikely to have occurred by random chance alone (assuming the null hypothesis is true).

For an observed confidence interval (cL, cU) we can say

We are ____% confident the true parameter value is contained in the interval. (**Do not say probability or chance!)

The idea of Confidence means

The procedure used to create the interval has a ____% probability of producing an interval that contains the parameter.

i.e. If the experiment were done repeatedly and an interval made for each sample, ____% of the intervals would contain the parameter value.

Chapter 2

ST 512 - Experiments

Readings: 7.2 and 7.3, pg 244-255

Example: An experiment was run to determine the effects of adding phosphorous (0, 147, 294, 441 kg/m^2) and nitrogen (0, 45, 90, 135 kg/m^2) to the soil of a certain type of grass (a Miscanthus species). The growth of the plant was of interest and at the end of the growing period the plant was dried and the weight recorded with the final measurement being recorded in megagram per hectare ($0.1 kg/m^2$). Four plots of grass were used in total. Within each plot, each combination of phosphorous and nitrogen was observed. A partial data table is given here:

Plot	P	N	Dry yield
1	0	135	1.95
1	0	45	3.51
1	0	90	2.87
1	0	0	2.88
1	294	45	2.37
1	294	0	3.5
1	294	135	3.55
1	294	90	4.4
...

Let's identify (if possible) the response, explanatory variable(s), factor(s), level(s), confounding factor(s), treatment(s), number of replicates, and experimental units.

Sources of Variation in the responses of an experiment:

1. **Treatment effect** - we hope there is an effect due to the variables we control
2. **Identified confounding variables** - We record some variables that are not of interest, but we think may have an effect on the response.
3. **Unidentified sources (Experimental Error or error variation)** -
 - (a) Inherent variability in experimental units - Experimental units are different!
Ex: No two people, paper towels, concrete blocks, or even lab rats are exactly the same.
Consequence: Experimental units respond differently to the same treatment
 - (b) Measurement error - Multiple measurements of a same experimental unit typically contain error.
If the same experimental unit is measured more than once, will the value be the same?
Ex: Blood Pressure, Quality Ratings of food, Break a water sample in two, measure each for bacteria
 - (c) Variations in applying/creating treatments
The treatment is not clearly defined, leaving room for interpretation.
Ex: Two researchers mix concrete, will it come out exactly the same? Ovens don't heat exactly the same, etc.
 - (d) Effects from any other extraneous (or lurking) variables - Extraneous variables are those variables that are not part of the treatment, but may influence the response.

Let's identify these in the previous example.

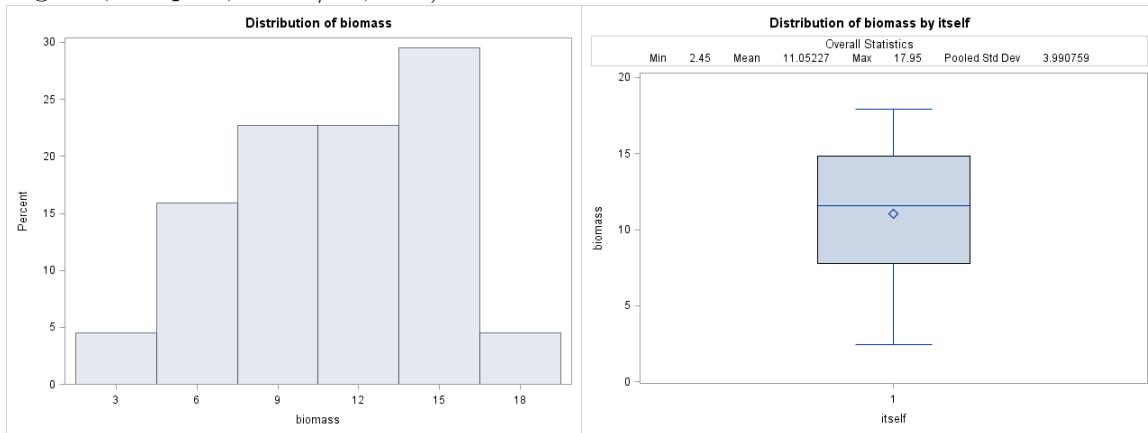
Chapter 3

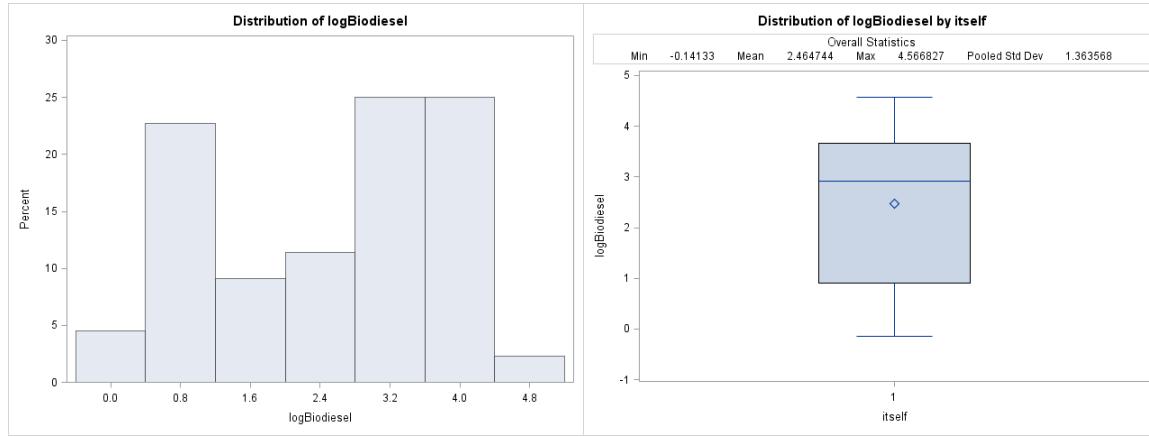
ST 512 - Correlation

Readings for Correlation and SLR: 10.1-10.5 pg 378-420 and 10.7-10.8 pg 425-444 and 8.7 pg 305-311

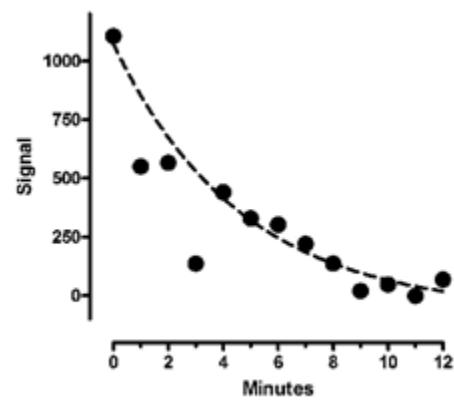
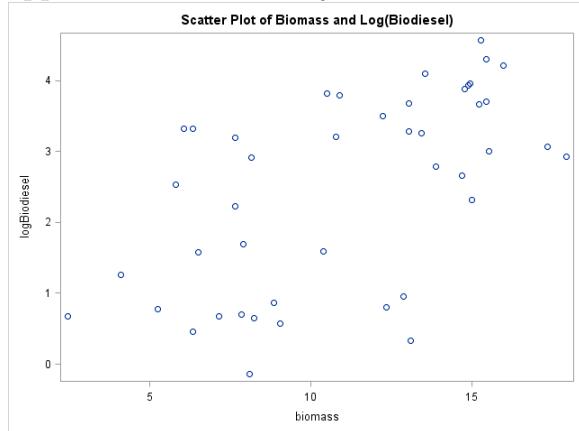
Motivating example: One type of fuel is biodiesel, which comes from plants. An experiment was done to determine how much biodiesel could be generated from a certain type of plant grown in different medias. The final biomass was also recorded on 44 the plants from the experiment. Let's consider these two variables, the log of biodiesel and biomass.

We can look at the distribution of each individually using our univariate methods (histogram, boxplot, mean/sd, etc.)





How can we visually inspect the association between the two? A **Scatter plot** gives a visual approximation of the “joint distribution” between two variables.



Properties of r_{XY}

- r_{XY} is an observed measure of the linear assn. between X and Y in a dataset.
- correlation coefficient is unitless and always between -1 and 1:

$$-1 \leq r_{XY} \leq 1$$

- The closer r_{XY} is to 1, the stronger the positive linear association
- The closer r_{XY} is to -1, the stronger the negative linear association
- The bigger $|r_{XY}|$, the stronger the linear association
- If $|r_{XY}| = 1$, then X and Y are said to be perfectly correlated (relationship is deterministic)

For the log(Biodiesel) (call this Y) and Biomass (call this X) example we can compute the sample correlation coefficient using summary statistics:

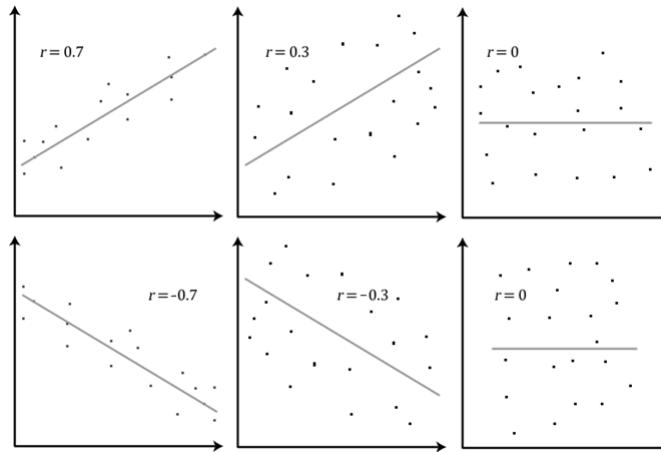
$$\bar{x} = 11.0523, \quad s_X = 3.9908, \quad \bar{y} = 2.4647, \quad s_Y = 1.3636$$

$$s_{XY} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{n - 1} = 3.1485$$

Applying the formula for r_{XY} , we get

$$r_{XY} = \frac{s_{XY}}{s_X s_Y} = \frac{3.1485}{\sqrt{3.9908 \times 1.3636}} = 0.5786$$

Some example scatter plots



An exercise/activity:

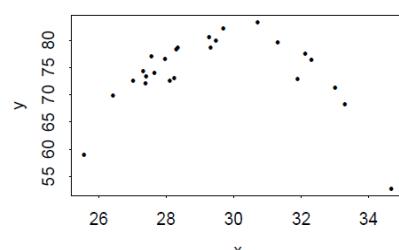
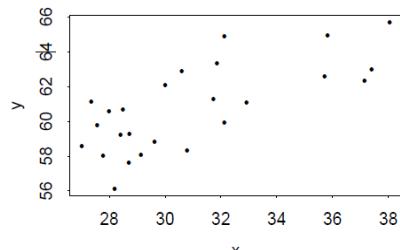
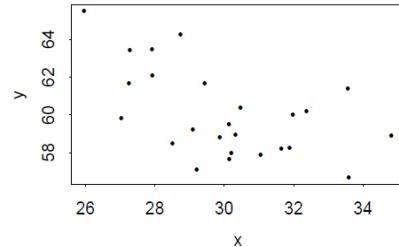
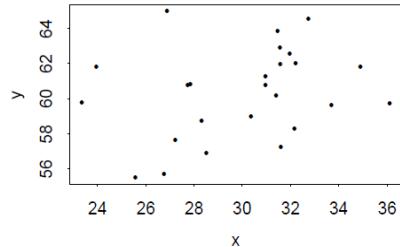
Label the four plots below with the four sample correlation coefficients:

- $r = 0.3$

$$r = 0.7$$

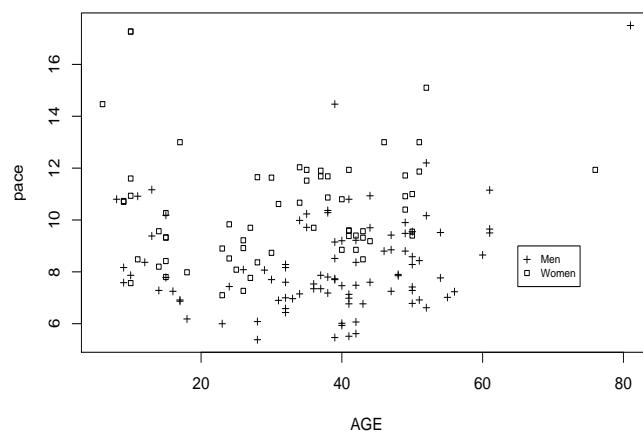
- $r = 0.1$

$$r = -0.6$$



Would it be appropriate to use correlation to summarize the relationship between age and pace in the following scatter plot? Why or why not?

Resolution Run (5k), 1/1/2004



To perform a Hypothesis Test about ρ :

We often want to test the following hypotheses,

$$H_0 : \rho = 0 \quad H_A : \rho \neq 0$$

Assuming H_0 is true, the test statistic is

$$z_{obs} = \left(\frac{1}{2} \sqrt{n-3} \right) \log \frac{1+r}{1-r}$$

and the reference distribution is the standard normal distribution, i.e. reject if $z_{obs} > z_{\alpha/2}$ or if $z_{obs} < z_{1-\alpha/2}$ where z_α satisfies $\alpha = \Pr(Z > z_\alpha)$ with $Z \sim N(0, 1)$.

The p-value is found by finding $2P(Z > |z_{obs}|)$. Why do we multiply by 2?

To find a Confidence Interval for ρ :

An approximate $100(1 - \alpha)\%$ confidence interval for ρ can be obtained by inverting the *Fisher transformation*:

$$\left(\frac{\frac{1+r}{1-r} e^{-2z_{\alpha/2}/\sqrt{n-3}} - 1}{\frac{1+r}{1-r} e^{-2z_{\alpha/2}/\sqrt{n-3}} + 1}, \frac{\frac{1+r}{1-r} e^{2z_{\alpha/2}/\sqrt{n-3}} - 1}{\frac{1+r}{1-r} e^{2z_{\alpha/2}/\sqrt{n-3}} + 1} \right).$$

For the log(Biodiesel) and Biomass example our hypothesis test is:

$$H_0 : \rho = 0 \quad H_A : \rho \neq 0$$

$$\text{giving a test statistic of } z_{obs} = \frac{1}{2} \sqrt{44-3} \log \left(\frac{1+0.5786}{1-0.5786} \right) = 4.228$$

Using an $\alpha = 0.05$ our rejection region is any z_{obs} outside of ± 1.96 .

Our p-value = $2P(Z > 4.228) = 2(0.00001) = 0.00002 < \alpha = 0.05$ so we reject our null hypothesis in favor of the alternative.

What is the interpretation of the p-value=0.00002?

The probability of getting a sample correlation (r) further (in magnitude) from 0 than 0.5786 assuming the true correlation (ρ) is 0 is 0.00002.

The corresponding 95% confidence interval is

$$\left(\frac{\frac{1+0.5786}{1-0.5786} e^{-2*1.96/\sqrt{44-3}} - 1}{\frac{1+0.5786}{1-0.5786} e^{-2*1.96/\sqrt{44-3}} + 1}, \frac{\frac{1+0.5786}{1-0.5786} e^{2*1.96/\sqrt{44-3}} - 1}{\frac{1+0.5786}{1-0.5786} e^{2*1.96/\sqrt{44-3}} + 1} \right) = (0.3401, 0.7471)$$

We can say that we are 95% confident that the true correlation (ρ) is between 0.3401 and 0.7471.

When we say confident, we mean that if we did this experiment repeatedly and made an interval for each experiment, the true correlation would fall in 95% of the intervals created.

How can we get SAS to do this for us?

```
proc corr data=bioexp FISHER(biasadj=NO);
var butterfat temp;
run;
```

Output From Proc Corr for Biomass and Log(Biodiesel) Example

1

The CORR Procedure

2 Variables:	biomass	logBiodiesel
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Covariance Matrix, DF = 43		
	biomass	logBiodiesel
biomass	15.92615751	3.14851427
logBiodiesel	3.14851427	1.85931767

Simple Statistics						
Variable	N	Mean	Std Dev	Sum	Minimum	Maximum
biomass	44	11.05227	3.99076	486.30000	2.45000	17.95000
logBiodiesel	44	2.46474	1.36357	108.44873	-0.14133	4.56683

Pearson Correlation Coefficients, N = 44 Prob > r under H0: Rho=0		
	biomass	logBiodiesel
biomass	1.00000	0.57859 <.0001
logBiodiesel	0.57859 <.0001	1.00000

Pearson Correlation Statistics (Fisher's z Transformation)						
Variable	With Variable	N	Sample Correlation	Fisher's z	95% Confidence Limits	p Value for H0:Rho=0
biomass	logBiodiesel	44	0.57859	0.66035	0.340140 0.747136	<.0001

Note: Significant correlation does NOT imply causation

Famous examples of *spurious correlations*:

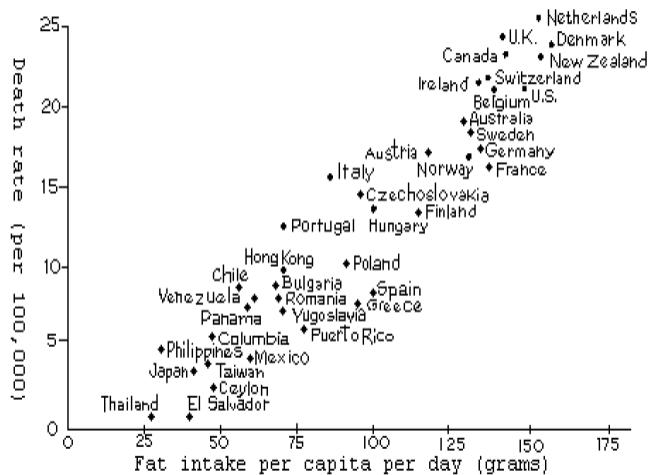
- A study finds a high positive correlation between coffee drinking and coronary heart disease. Newspaper reports say the fragrant essence of the roasted beans of *Coffea arabica* are a menace to public health.
- In a city, if you were to observe the amount of damage and the number of fire engines for enough recent fires, you would likely see a positive and significant correlation among these variables. Obviously, it would be erroneous to conclude that fire engines cause damage.
- *Lurking variable* - a third variable that is responsible for a correlation between two others. (A.k.a. confounding factor.)
An example would be to assess the association between say the reading skills of children and other measurements taken on them, such as shoesize. There may be a statistically significant association between shoe size and reading skills, but that doesn't imply that one causes the other. Rather, both are positively associated with a third variable, *age*.
- Among 50 countries examined in a dietary study, high positive correlation among fat intake and cancer (see figure, next page). This example is taken from from *Statistics* by Freedman, Pisani and Purves.

In countries where people eat lots of fat like the United States rates of breast cancer and colon cancer are high. This correlation is often used to argue that fat in the diet causes cancer. How good is the evidence?

Discussion. If fat in the diet causes cancer, then the points in the diagram should slope up, other things being equal. So the diagram is some evidence for the theory. But the evidence is quite weak, because other things aren't equal. For example, the countries with lots of fat in the diet also have lots of sugar. A plot of colon cancer rates against sugar consumption would look just like figure 8, and nobody thinks that sugar causes colon cancer. As it turns out, fat and sugar are relatively expensive. In rich countries, people can afford to eat fat and sugar rather than starchier grain products. Some aspects of the diet in these countries, or other factors in the life-style, probably do cause certain kinds of cancer and protect against other kinds. So far, epidemiologists can identify only a few of these factors with any real confidence. Fat is not among them.

(p. 152, *Statistics* by Friedman, Pisani, Purves and Adhikari)

Figure 8. Cancer rates plotted against fat in the diet for a sample of countries



Source: K. Carroll. "Experimental evidence of dietary factors and hormone-dependent cancers" Cancer Research vol. 35 (1975) p.3379. Copyright by Cancer Research. Reproduced by permission

Chapter 4

ST 512 - Simple Linear Regression

Readings for Correlation and SLR: 10.1-10.5 pg 378-420 and 10.7-10.8 pg
425-444 and 8.7 pg 305-311

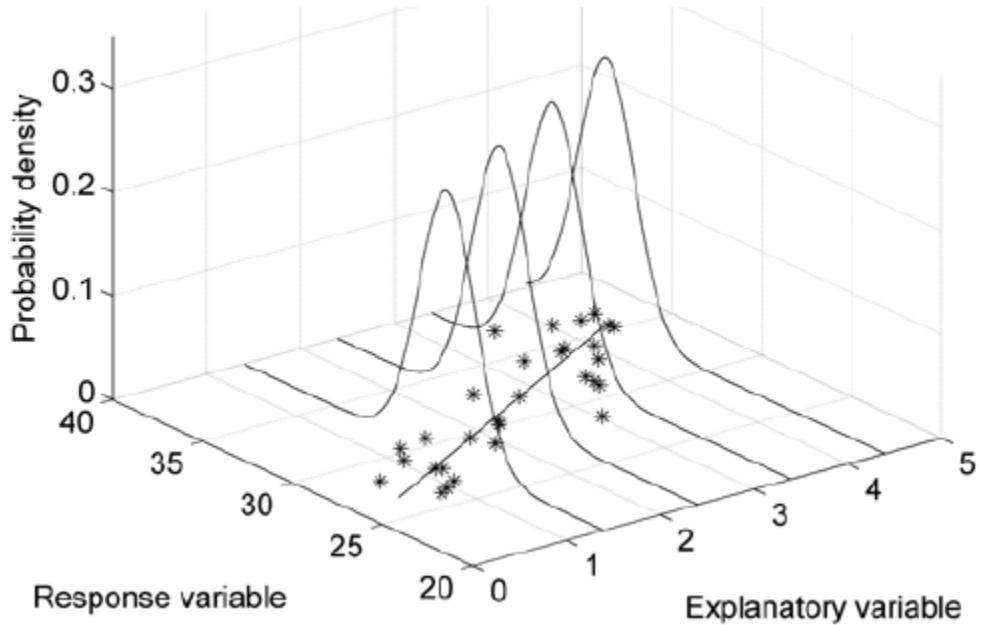
Fit a linear regression model - A probabilistic model for Y conditional on $X = x$:

$$Y_i = \beta_0 + \beta_1 x_i + E_i$$

Definitions:

- Y_i - response (also called dependent variable)
- x_i - explanatory variable (also called independent variable or predictor variable)
- E_i - random error for observation i
- $\beta_0 = E(Y|X = 0)$ - True population intercept (average value of response when $X = 0$)
- β_1 - True population slope (average change in Y per unit increase in x)
- σ^2 - Error variance (variance due to experimental error)

Note: We make the assumption that E_1, \dots, E_n are independent and identically distributed normal random variables with mean 0 and variance σ^2 . We write $E_i \stackrel{iid}{\sim} N(0, \sigma^2)$. This variance is assumed the same for all x , called assumption of **homoskedasticity**.



1. $E(Y|X = x) = \beta_0 + \beta_1 x = \mu(x)$ (The line describes the mean Y for a given X .)
2. $\text{Var}(Y|X = x) = \sigma^2$

For the log(Biodiesel) and Biomass example let's find our fitted line. Recall the summary stats on page 10.

$$\hat{\beta}_1 = s_{XY}/s_X^2 = 3.1485/3.9908^2 = 0.1977$$

$$\hat{\beta}_0 = 2.4647 - 11.0523 * 0.1977 = 0.2797$$

$$\hat{y} = 0.2808 + 0.1977x$$

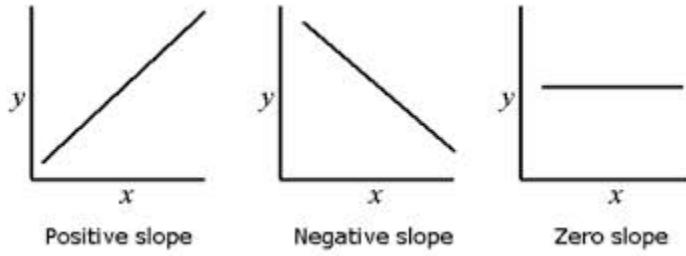
This line can now be used to make predictions for new X values by simply plugging in the x !

Again, we have now have point estimates for our true parameters. How can we make inference (claims about the true values)? Do we have a *significant linear relationship*?

Under the normal distribution assumption on the errors, the RV's $\hat{\beta}_0$ and $\hat{\beta}_1$ follow normal distributions. Thus, we can use this as a basis for inference.

What value of the slope do we test?

- If a linear relationship, Y will tend to change with X (i.e. $\beta_1 \neq 0$)
- If no linear relationship, Y won't tend to change with X (i.e. $\beta_1 = 0$).



Any hypothetical slope, like $H_0 : \beta_1 = \text{slope}_0$ may be tested using the T -statistic below with $df = n - 2$:

$$T = \frac{\hat{\beta}_1 - \text{slope}_0}{\widehat{SE}(\hat{\beta}_1)}$$

and any hypothetical intercept, like $H_0 : \beta_0 = \text{intercept}_0$ may be tested using the T -statistic below with $df = n - 2$:

$$T = \frac{\hat{\beta}_0 - \text{intercept}_0}{\widehat{SE}(\hat{\beta}_0)}$$

Confidence intervals for β_0, β_1
 100(1 - α)% confidence intervals for β_0 and β_1 are given by

$$\hat{\beta}_0 \pm t(n - 2, \alpha/2) \sqrt{MS[E] \left(\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}} \right)}.$$

$$\hat{\beta}_1 \pm t(n - 2, \alpha/2) \sqrt{\frac{MS[E]}{S_{xx}}}.$$

Often we will only care about the test and CI for the slope. The hypothesis test is equivalent to checking if 0 is in the confidence interval. It will depend on the context of the question if testing $\beta_0=0$ makes sense.

Confidence interval for $\mu(x_0) = E(Y|X = x_0)$

The point estimate for $\mu(x_0)$ is simply $\hat{\beta}_0 + \hat{\beta}_1 x_0$. We need to know about the variability of this estimate and we can again use the t-distribution for inference.

$$\text{Var}(\hat{\beta}_0 + \hat{\beta}_1 x_0 | X = x_0) =$$

This yields a confidence interval of the form

$$\hat{\beta}_0 + \hat{\beta}_1 x_0 \pm t(n - 2, \alpha/2) \sqrt{MS[E] \left(\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)}$$

Note: We are attempting to capture the true *mean* at x_0 in this interval.

Prediction interval for a new observation x_0

The point estimate for at x_0 is still $\hat{Y}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0$. However, the variability will change.

$$\text{Var}(\hat{\beta}_0 + \hat{\beta}_1 x_0 + E_{new} | X = x_0) =$$

Thus we can form a PI using

$$\hat{Y}(x_0) \pm t(n - 2, \alpha/2) \sqrt{MS[E] \left(1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)}.$$

Note: In this interval we are attempting to capture the next Y value that takes on x_0 . As this is a much more difficult task, PI's are wider than CI's.

The ANOVA table from simple linear regression

The full ANOVA table for SLR is given below:

Source	Sum of squares	df	Mean Square	F-Ratio
Regression	$SS(R)$	1	$MS(R)$	$MS(R)/MS(E)$
Error	$SS(E)$	$n - 2$	$MS(E)$	
Total	$SS(Tot)$	$n - 1$		

The mean squares represent standardized measures of variation due to the different sources and are given by $SS(\text{source})/df \text{ source}$. Ratios of mean squares often follow an F -distribution and are appropriate for testing different hypotheses of interest.

In this case, to test

$$H_0 : \beta_1 = 0 \quad \text{vs} \quad H_1 : \beta_1 \neq 0$$

$$F = MS(R)/MS(E) \sim F(1, n - 2).$$

That is, the F statistic follows an F -distribution with 1 numerator df and $n - 2$ denominator df. In SLR, this F test is equivalent to the T test we already looked at. The relationship is that $T^2 = F$.

Note: The mean square for error, $MS[E]$, is an unbiased estimator for σ^2 . It is an estimate of the variability due left over once we account for our explanatory variable.

How to get tests in SAS?

For our Biodiesel and Biomass example we can get much of our output from SAS using the following commands:

```
proc reg data=bioexp ;
model logbiodiesel=biomass/clb;
run;
```

Output From Proc Reg for Biomass and Log(Biodiesel) Example

1

The REG Procedure
Model: MODEL1
Dependent Variable: logBiodiesel

Number of Observations Read	44
Number of Observations Used	44

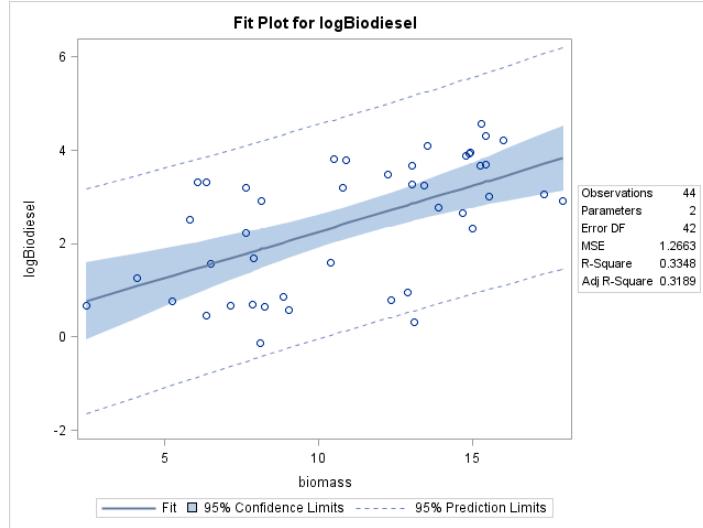
Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	26.76509	26.76509	21.14	<.0001
Error	42	53.18557	1.26632		
Corrected Total	43	79.95066			

Root MSE	1.12531	R-Square	0.3348
Dependent Mean	2.46474	Adj R-Sq	0.3189
Coeff Var	45.65627		

Parameter Estimates						
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t	95% Confidence Limits
Intercept	1	0.27977	0.50463	0.55	0.5822	-0.73862 1.29816
biomass	1	0.19769	0.04300	4.60	<.0001	0.11091 0.28447

Using $\alpha = 0.05$, (1) let's find the CI for the slope by hand, (2) form a CI for the mean log of biodiesel when biomass is 12, and (3) form a PI for a future log biodiesel measurement for a biomass of 12.

SAS will also produce a very nice plot that includes *pointwise* confidence and prediction bands at all points. Notice that the bands get wider the further x_0 is from \bar{x} . Why?

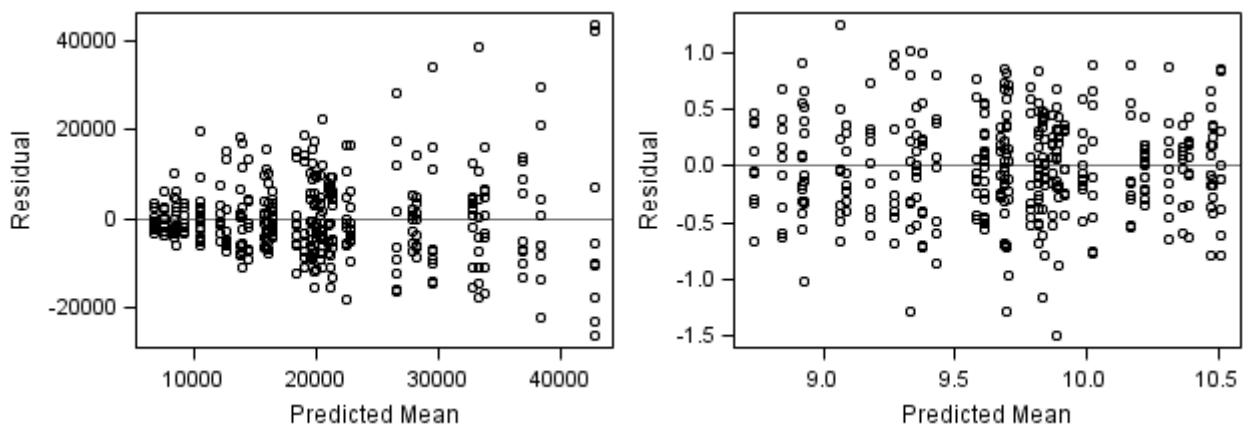


Checking assumptions

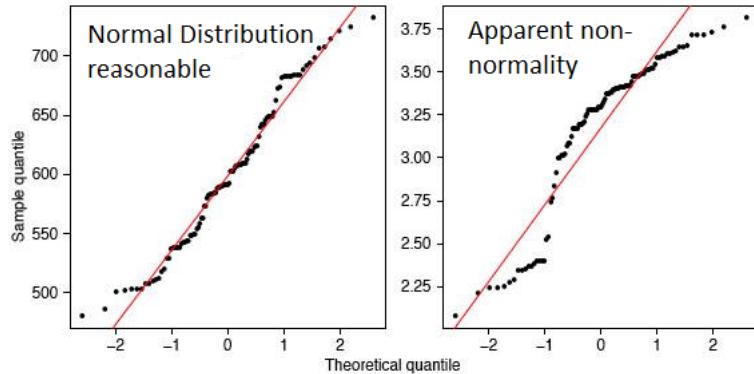
Firstly, we should always inspect a scatter plot to determine if the linear relationship we are assuming in our model is appropriate.

Secondly we can check our assumption of $iidN(0, \sigma^2)$ errors.

- Independence - There is not a check for independence of errors, we simply need to consider whether or not our EU's can be considered independent.
- Constant variance - A residuals vs fitted (predicted) values plot or a residual vs independent variable plot are tools for detecting heteroskedasticity (non-constant variance).



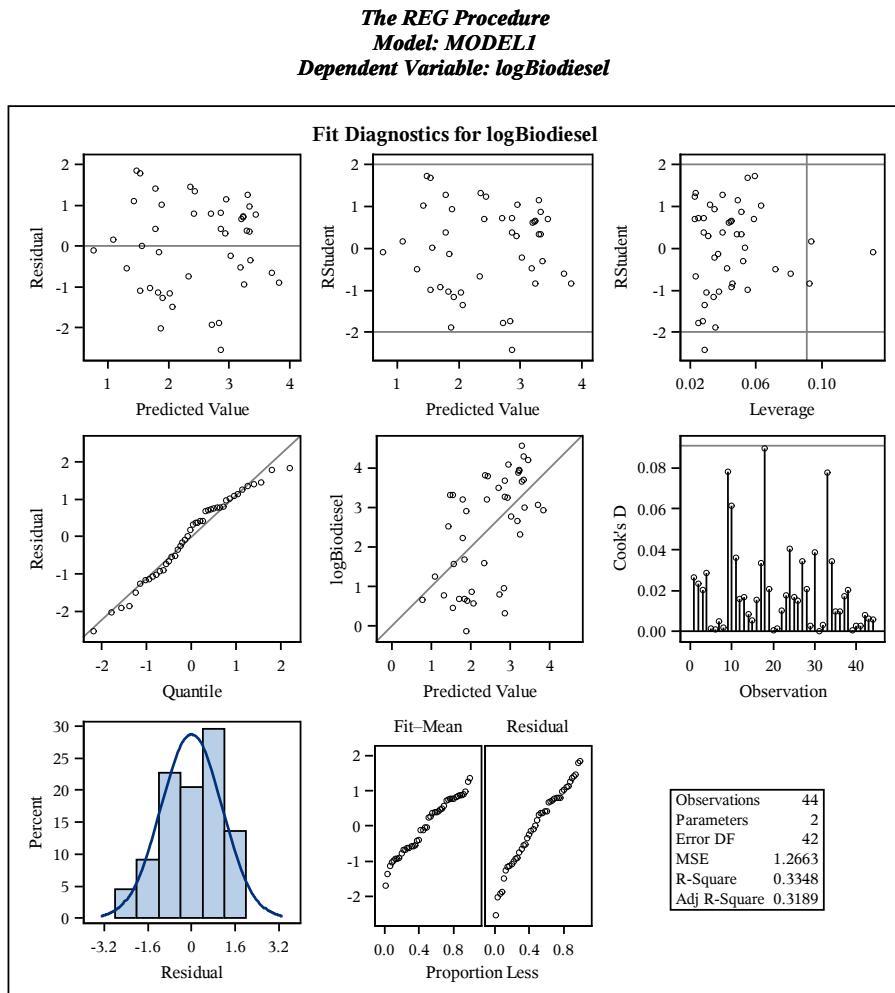
- Normality of errors - A quantile-quantile plot (or qq-plot for short) can be inspected to see if normality is reasonable.

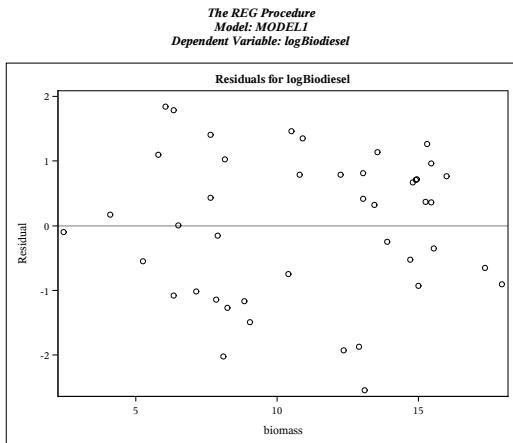


We can inspect the diagnostic plots that SAS produces when the reg procedure is used:

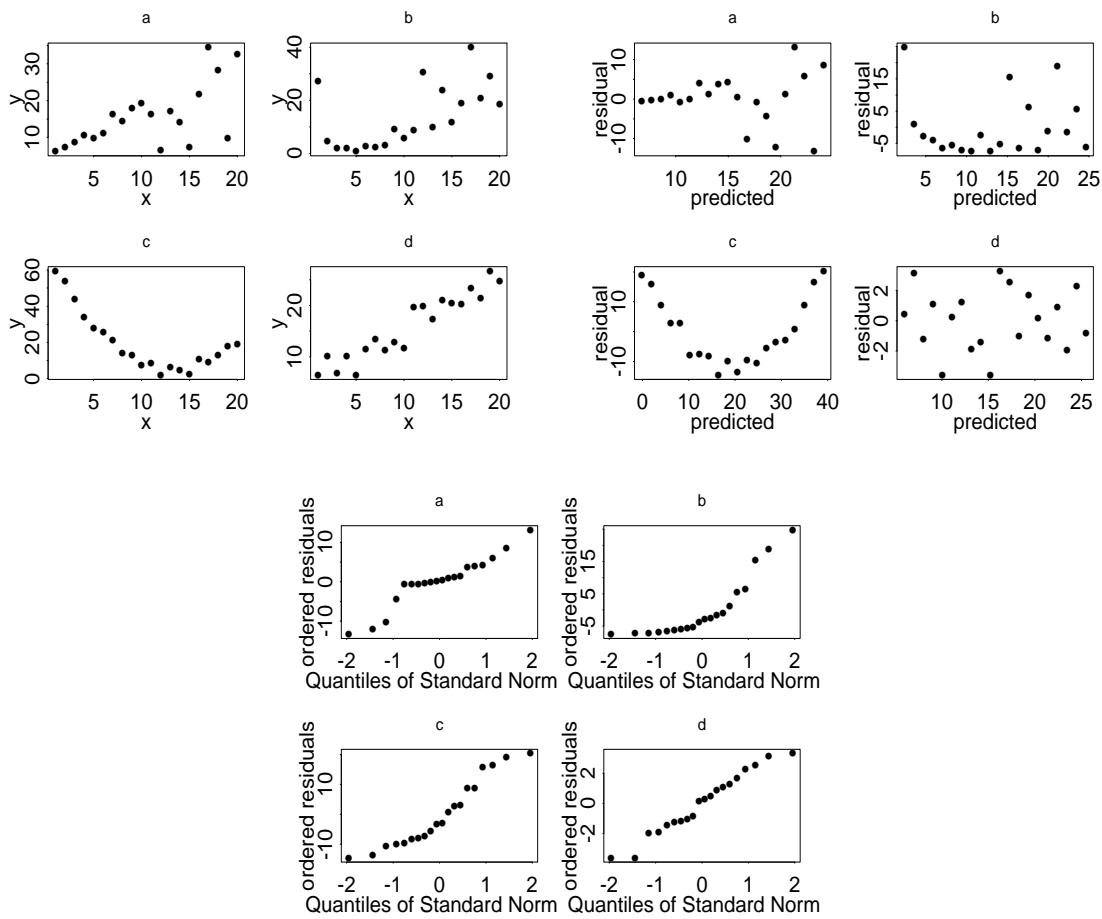
Output From Proc Reg for Biomass and Log(Biodiesel) Example

2





An exercise: Match up letters a,b,c,d with the model violation - Heteroscedasticity, Nonlinearity, Nonnormality, Model fits



Chapter 5

ST 512 - Multiple Linear Regression

Readings: 11.1-11.6 and 11.9-11.11 pg 463 - 515 and 529 - 539

Motivating Example

(Taken from Probability and Statistics, Devore) Soil and sediment adsorption, the extent to which chemicals collect in a condensed form on the surface, is an important characteristic influencing the effectiveness of pesticides and various agricultural chemicals. A study was done on 13 soil samples that measured Y = phosphate adsorption index, X_1 = amount of extractable aluminum, and X_2 = amount of extractable iron. The data are given below:

Adsorption	Aluminum	Iron
4	13	61
18	21	175
14	24	111
18	23	124
26	64	130
26	38	173
21	33	169
30	61	169
28	39	160
36	71	244
65	112	257
62	88	333
40	54	199

MLR model for two quantitative explanatory variables:

For observation i we can use the model

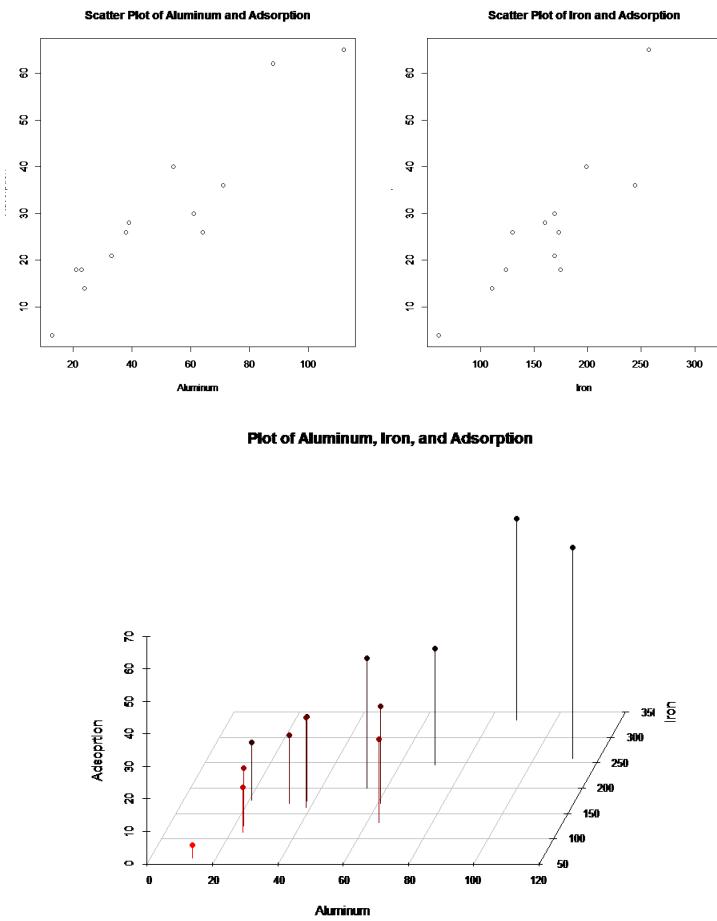
$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + E_i$$

For clarity we can write the model for each subject

$$\begin{aligned}
 Y_1 &= \beta_0 + \beta_1 X_{11} + \beta_2 X_{12} + E_1 \\
 Y_2 &= \beta_0 + \beta_1 X_{21} + \beta_2 X_{22} + E_2 \\
 \vdots &= \vdots \\
 Y_{13} &= \beta_0 + \beta_1 X_{13,1} + \beta_2 X_{13,2} + E_{13}
 \end{aligned}$$

Generally our model is

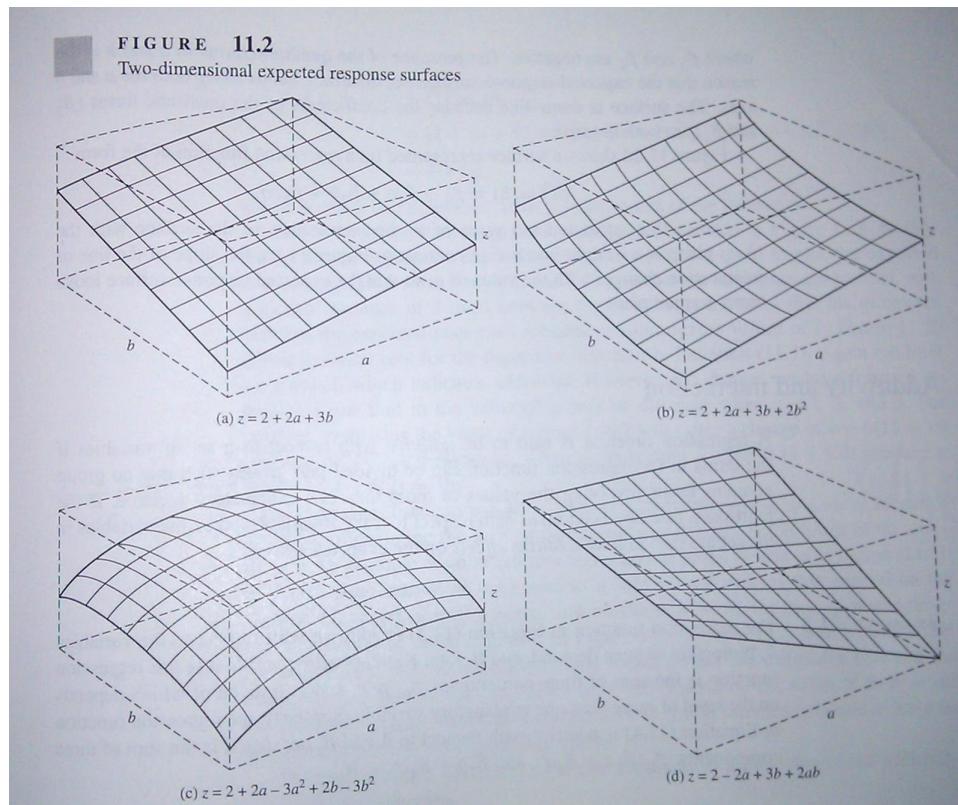
$$Adsorption = \beta_0 + \beta_1 Aluminum + \beta_2 Iron + Experimental\ Error$$



In this case, we don't want to find the best fitting line, but rather the best fitting *plane* (the one that minimizes the squared distances between the plane and the data points). Our hypothesis of interest is that at least one of our variables is useful (i.e. at least one partial slope is truly non-zero). We can then test

$$H_0 : \beta_1 = \beta_2 = 0 \text{ vs } H_A : \text{at least one is non-zero}$$

When we fit an MLR model with p different predictors we are really attempting to find the best 'response surface' of degree p in a $p + 1$ dimensional space. For instance, with one predictor, we are fitting the best line in a 2-d space. The plots below give a number of surfaces that can be fit using two predictors when quadratic or interaction terms are included.



A link to visualizing different surfaces:

http://www.ats.ucla.edu/stat/sas/teach/reg_int/reg_int_cont.htm

Very brief matrix review:

Note: Capital boldface letters are usually used for matrices and boldface lower case letters are usually used for vectors (matrices where the number of rows or the number of columns is 1).

Matrices - rectangular arrays of numbers that have a great many uses. Some matrices, (with *dimension* in parentheses):

$$\begin{aligned}\mathbf{A} &= \begin{pmatrix} 7 & 5 \\ 5 & 2 \\ 3 & 2 \end{pmatrix} \quad (3 \times 2) \\ \mathbf{B} &= \begin{pmatrix} 4 & 2 & 1 \\ 3 & 1 & 1 \end{pmatrix} \quad (2 \times 3) \\ \mathbf{C} &= \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad (2 \times 2) \\ \mathbf{I}_2 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (2 \times 2)\end{aligned}$$

Matrix operations

1. Transposition - swap rows for columns, columns for rows:

$$t(\mathbf{A}) = \mathbf{A}' = \begin{pmatrix} 7 & 5 & 3 \\ 5 & 2 & 2 \end{pmatrix} \quad \text{"transpose of } \mathbf{A}\text{"}$$

2. Addition is elementwise, matrices must have same *dimension*

$$\mathbf{C} + \mathbf{I}_2 = \begin{pmatrix} 1+1 & 1+0 \\ -1+0 & 1+1 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix} \quad (2 \times 2)$$

Subtraction, same deal

$$\mathbf{C} - \mathbf{I}_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (2 \times 2)$$

3. Multiplication requires *conformability*. Element in i^{th} row, j^{th} column of \mathbf{AB} is dot-product of i^{th} row of \mathbf{A} , j^{th} column of \mathbf{B} :

$$\begin{aligned}\mathbf{AB} &= \begin{pmatrix} 7 & 5 \\ 5 & 2 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} 4 & 2 & 1 \\ 3 & 1 & 1 \end{pmatrix} \\ \mathbf{AB} &= \begin{pmatrix} 7 \cdot 4 + 5 \cdot 3, & 7 \cdot 2 + 5 \cdot 1, & 7 \cdot 1 + 5 \cdot 1 \\ 5 \cdot 4 + 2 \cdot 3, & 5 \cdot 2 + 2 \cdot 1, & 5 \cdot 1 + 2 \cdot 1 \\ 3 \cdot 4 + 2 \cdot 3, & 3 \cdot 2 + 2 \cdot 1, & 3 \cdot 1 + 2 \cdot 1 \end{pmatrix} \\ &= \begin{pmatrix} 43 & 19 & 12 \\ 26 & 12 & 7 \\ 18 & 8 & 5 \end{pmatrix}\end{aligned}$$

(The product \mathbf{DE} is not necessarily equal to \mathbf{ED}). The matrices \mathbf{D} and \mathbf{E} are conformable for the product \mathbf{DE} if \mathbf{D} has the same number of columns as \mathbf{E} has rows. Note that in the product of \mathbf{AB} of the matrices given above, $\mathbf{A}(3 \times 2)$ and $\mathbf{B}(2 \times 3)$ are conformable.

\mathbf{I} is reserved for the *identity* matrix, which is *square*, *symmetric*, *diagonal* with 1's along the diagonal and 0's elsewhere:

$$\mathbf{I}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplication of any (conformable) matrix \mathbf{M} by \mathbf{I} gives \mathbf{M} : $\mathbf{AI}_3 = \mathbf{A} = \mathbf{I}_2\mathbf{A}$

4. Inversion. The *inverse* \mathbf{M}^{-1} of a *square* ($r \times r$) matrix \mathbf{M} , if it exists, satisfies $\mathbf{MM}^{-1} = \mathbf{I}_r$ (similar to the reciprocal of real number). A square matrix with an inverse is called *non-singular*.

Inversion can be computationally challenging, but not for (2×2) case:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Find \mathbf{C}^{-1} .

$$\mathbf{C}^{-1} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

The *rank* of a matrix is equal to the number of *linearly independent* rows or columns of the matrix. Vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ are linearly independent if $\sum_i a_i \mathbf{x}_i = 0$ implies $a_1 = a_2 = \dots = a_n = 0$.

Matrix uses: model statements, systems of linear equations, covariance matrices of random vectors,....

Consider two lines $y_1 = 5 - x$, $y_2 = 3 + x$. Do these lines intersect? Where? Write this system of two equations in two unknowns using a matrix:

$$\mathbf{C} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 5 \\ 3 \end{pmatrix}$$

(left-multiply both sides by \mathbf{C}^{-1})

$$\begin{pmatrix} x \\ y \end{pmatrix} = \mathbf{C}^{-1} \begin{pmatrix} 5 \\ 3 \end{pmatrix} = \begin{pmatrix} 1 \\ 4 \end{pmatrix}$$

The lines intersect at the solution, $(x = 1, y = 4)$.

Matrices are cool and very useful!

If we have a random vector (just like a random variable but in vector form, i.e. components yield numeric answers that are random), call it \mathbf{Y} , and a constant vector, call it \mathbf{a} , then

$$E(\mathbf{a}'\mathbf{Y}) = \mathbf{a}'E(\mathbf{Y})$$

$$\text{Var}(\mathbf{a}'\mathbf{Y}) = \mathbf{a}'\text{Var}(\mathbf{Y})\mathbf{a}$$

Understanding matrices if very important as this is how we will look at our models for much of the rest of the class. Also, SAS and other statistical programs use matrices in their calculations and in their output.

Matrix formulation of MLR

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{E}$$

All of the response RVs are placed into the **response vector**:

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}$$

For observation i we can group all of the explanatory variables into a vector

$$\mathbf{x}_i = (1, x_{i1}, x_{i2}, x_{i3}, \dots, x_{ip}).$$

The 1 in the first spot of the vector is for the intercept. If we ‘stack’ these row vectors on top of each other we can make a matrix called the **design matrix**:

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}$$

We also form a column vector corresponding to the regression parameters, called the ‘**beta vector**’:

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$$

and a column vector for the error terms, called the **error vector**:

$$\mathbf{E} = \begin{pmatrix} E_0 \\ E_1 \\ \vdots \\ E_n \end{pmatrix}$$

Now we can see that our MLR model (a system of n equations with $p + 1$ unknowns)

$$\begin{aligned} Y_1 &= \beta_0 + \beta_1 x_{11} + \beta_2 x_{12} + \dots + \beta_p x_{1p} + E_1 \\ Y_2 &= \beta_0 + \beta_1 x_{21} + \beta_2 x_{22} + \dots + \beta_p x_{2p} + E_2 \\ &\vdots = \vdots \\ Y_n &= \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \dots + \beta_p x_{np} + E_n \end{aligned}$$

can be easily rewritten as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{E}$$

Our assumptions on the errors can now be specified as $\mathbf{E} \sim N_n(\mathbf{0}, \sigma^2 \mathbf{I}_n)$ (multivariate normal distribution). $\sigma^2 \mathbf{I}_n$ is called the variance-covariance matrix:

$$Var(\mathbf{E}) = \begin{pmatrix} \sigma^2 & 0 & \dots & 0 \\ 0 & \sigma^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma^2 \end{pmatrix}$$

The diagonals of the matrix give the variances for the E_i 's ($Var(E_1), Var(E_2), \dots, Var(E_n)$) and the off-diagonals (say row i column j) give the covariances between E_i 's and the E_j 's ($Cov(E_i, E_j)$). As the off-diagonals are all 0, our errors are uncorrelated (which for the multivariate normal distribution implies independence).

Let's look at some of these quantities for our adsorption example. We have $n = 13$ and $p = 2$.

$$\mathbf{y} = \begin{pmatrix} 4 \\ 18 \\ 14 \\ 18 \\ 26 \\ 26 \\ 21 \\ 30 \\ 28 \\ 36 \\ 65 \\ 62 \\ 40 \end{pmatrix} \quad \mathbf{X} = \begin{pmatrix} 1 & 13 & 61 \\ 1 & 21 & 175 \\ 1 & 24 & 111 \\ 1 & 23 & 124 \\ 1 & 64 & 130 \\ 1 & 38 & 173 \\ 1 & 33 & 169 \\ 1 & 61 & 169 \\ 1 & 39 & 160 \\ 1 & 71 & 244 \\ 1 & 112 & 257 \\ 1 & 88 & 333 \\ 1 & 54 & 199 \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}$$

The predicted values can be written as

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \mathbf{H}\mathbf{y}$$

and residuals as

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}} = (\mathbf{I} - \mathbf{H})\mathbf{y}$$

- $\hat{\mathbf{y}}$ is called the vector of fitted or predicted values
- $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}$ is called the hat matrix as it ‘places’ the hat on \mathbf{y}
- \mathbf{e} is the vector of residuals

We will still use least squares to select the parameters, which can be written as the minimum of:

$$SS(E) = \sum_{i=1}^n (obs_i - pred_i)^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{i1} - \cdots - \beta_p x_{ip})^2 = \mathbf{e}'\mathbf{e}$$

For the adsorption example, many of these matrices are given below:

$$\begin{aligned} \mathbf{X}'\mathbf{X} &= \begin{pmatrix} 13 & 641 & 2305 \\ 641 & 41831 & 133162 \\ 2305 & 133162 & 467669 \end{pmatrix} & (\mathbf{X}'\mathbf{X})^{-1} &= \begin{pmatrix} 0.633138 & 0.002477 & -0.003826 \\ 0.002477 & 0.000265 & -0.000088 \\ -0.003826 & -0.000088 & 0.000046 \end{pmatrix} \\ \hat{\boldsymbol{\beta}} &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \begin{pmatrix} -7.3507 \\ 0.3490 \\ 0.1127 \end{pmatrix} & \hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} &= \begin{pmatrix} 4.0610 \\ 19.7008 \\ 13.5350 \\ 14.6511 \\ 29.6363 \\ 25.4084 \\ 23.2126 \\ 32.9846 \\ 24.2923 \\ 44.9271 \\ 60.7012 \\ 60.8904 \\ 33.9226 \end{pmatrix} \end{aligned}$$

$$SS(E) = \mathbf{e}'\mathbf{e} = 191.7897 \quad \hat{\sigma}^2 = MS(E) = SS(E)/(n - p - 1) = 191.7897/10 = 19.17897$$

$$\hat{\Sigma} = MS(E)(\mathbf{X}'\mathbf{X})^{-1} = \begin{pmatrix} 12.14294 & 0.04750 & -0.07337 \\ 0.04750 & 0.00508 & -0.00168 \\ -0.07337 & -0.00168 & 0.00088 \end{pmatrix}$$

The parameter estimates and the variance-covariance matrix are very useful for making inference about our intercept and partial slope parameters (done very similarly to SLR). Let's use the above to find the following

1. What is the estimate for β_2 ? What is the interpretation?
2. What is the standard error of $\hat{\beta}_2$?
3. Conduct a test to determine if $\beta_2 = 0$ plausible (technically, after accounting for the linear association between extractable aluminum and adsorption index). Hint: $t(0.025, 10) = 2.228$
4. Estimate the mean adsorption index among the population of ALL soil with extractable aluminum = 100 and extractable iron = 150. Report a standard error for this estimate and a 95% confidence interval and a 95% prediction interval.

Recall that the overall hypotheses we want to test are

$$H_0 : \beta_1 = \beta_2 = 0 \text{ vs } H_A : \text{at least one is non-zero}$$

This is the test done in the ANOVA table given in the output from a MLR model. This is called the **global F-test** as it tests whether at least one of the terms in the model is important for predicting the response.

The ANOVA table for MLR follows the same ideas as in SLR. We are taking the total amount of variation in the response ($SS(Tot)$) and partitioning it into a part due to the model ($SS(R)$) and a part due to experimental error ($SS(E)$). In fact, the formulas for the sums of squares remain the same, only the degrees of freedom and the F -distribution used for finding the p-value change.

The full ANOVA table for MLR is given below:

Source	Sum of squares	df	Mean Square	F-Ratio
Regression	$SS(R)$	p	$MS(R)$	$MS(R)/MS(E)$
Error	$SS(E)$	$n - p - 1$	$MS(E)$	
Total	$SS(Tot)$	$n - 1$		

How to do MLR in SAS?

The following code will produce output appropriate for analysis:

```
proc reg data=adexp ;
model adsorp=aluminum iron/clb;
run;
```

Output From Proc Reg for Adsorption Example

1

The REG Procedure
Model: MODEL1
Dependent Variable: adsorp

Number of Observations Read	14
Number of Observations Used	13
Number of Observations with Missing Values	1

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	3529.90308	1764.95154	92.03	<.0001
Error	10	191.78922	19.17892		
Corrected Total	12	3721.69231			

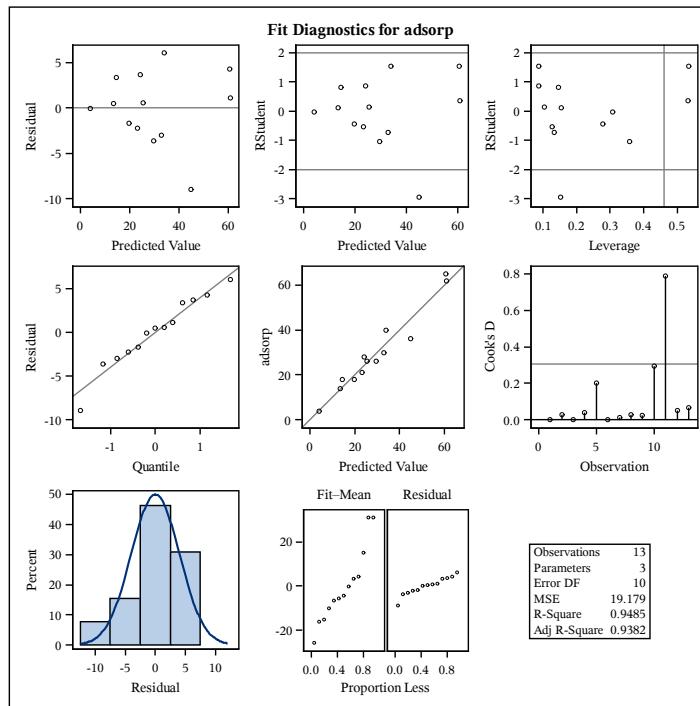
Root MSE	4.37937	R-Square	0.9485
Dependent Mean	29.84615	Adj R-Sq	0.9382
Coeff Var	14.67316		

Parameter Estimates							
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t		95% Confidence Limits
Intercept	1	-7.35066	3.48467	-2.11	0.0611	-15.11498	0.41366
aluminum	1	0.34900	0.07131	4.89	0.0006	0.19012	0.50788
iron	1	0.11273	0.02969	3.80	0.0035	0.04658	0.17889

Output From Proc Reg for Adsorption Example

2

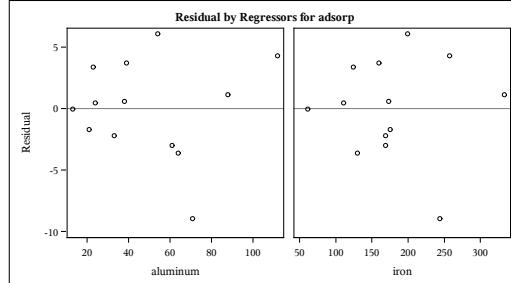
The REG Procedure
Model: MODEL1
Dependent Variable: adsorp



Output From Proc Reg for Adsorption Example

3

The REG Procedure
Model: MODEL1
Dependent Variable: adsorp



A non-additive model example:

A random sample of students taking the same exam:

IQ	Study TIME	GRADE
105	10	75
110	12	79
120	6	68
116	13	85
122	16	91
130	8	79
114	20	98
102	15	76

Consider regressing GRADE on IQ (X_1), TIME(X_2), and TI ($X_1 \times X_2$), where TI = TIME * IQ.
That is, we fit the model:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + E$$

```
proc reg;
model Grade = IQ Time TI;
run;
```

```
The SAS System
The REG Procedure
1

Analysis of Variance

Source          DF      Sum of Squares      Mean Square      F Value      Pr > F
Model           3       610.81033     203.60344      26.22      0.0043
Error           4       31.06467      7.76617
Corrected Total 7       641.87500

Parameter Estimates

Variable      Parameter Estimate      Standard Error      t Value      Pr > |t|
Intercept    1        72.20608    54.07278      1.34      0.2527
IQ           1        -0.13117    0.45530      -0.29      0.7876
Time         1        -4.11107    4.52430      -0.91      0.4149
TI           1        0.05307     0.03858      1.38      0.2410
```

Discussion of the interaction model:

We call the product $TI = Time * IQ$ an "interaction" term. That is, our explanatory variables do not have an independent effect on the response.

$$\widehat{MeanGrade} = 72.21 - 0.13 * IQ - 4.11 * Time + 0.0531 * TI$$

Now if $IQ = 100$ we get

$$\widehat{MeanGrade} = (72.21 - 13.1) + (-4.11 + 5.31) * Time$$

and if $IQ = 120$ we get

$$\widehat{MeanGrade} = (72.21 - 15.7) + (-4.11 + 6.37) * Time.$$

Thus we expect an extra hour of study to increase the grade by 1.20 points for someone with $IQ = 100$ and by 2.26 points for someone with $IQ = 120$ if we use this interaction model.

Generally, we can interpret the (true) β parameters in the model as:

- β_0 - Average value of Grade when IQ and Study Time are 0
- β_1 - Average change in Grade for a unit increase in IQ when Study Time is 0
- β_2 - Average change in Grade for a unit increase in Study Time when IQ is 0
- β_3 - Average change in the slope for IQ (or Study Time) for a given value of Study Time (or IQ).

The interpretation of the interaction 'slope' can be seen by looking at the following:

$$\begin{aligned}\mu(x_1+1, x_2) - \mu(x_1, x_2) &= \beta_0 + \beta_1(x_1+1) + \beta_2x_2 + \beta_3(x_1+1)(x_2) - \beta_0 - \beta_1x_1 - \beta_2x_2 - \beta_3x_1(x_2) \\ &= \beta_1 + \beta_3x_2\end{aligned}$$

So β_3 is the amount the slope for x_1 changes per unit change in x_1 while x_2 is held constant.

Note: The global p-value is significant, but none of our individual terms are. This gives evidence that our model is over-fit. we may want to go back to the simpler "main effects" model.

Model Selection:

x_1, x_2, x_3 denote p independent variables. Consider several models:

1. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1$
 2. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_2 x_2$
 3. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_3 x_3$
 4. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$
 5. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_3 x_3$
 6. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$
 7. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_2 x_2 + \beta_3 x_3$

A is nested in B means model A can be obtained by restricting (e.g. setting to 0) parameter values in model B .

True or false:

- Model 1 nested in Model 4 Model 1 nested in Model 5
 - Model 2 nested in Model 4 Model 4 nested in Model 1
 - Model 3 nested in Model 4 Model 5 nested in Model 4
 - Model 3 nested in Model 7 Model 1 nested in Model 7

A nested in $B \rightarrow A$ called *reduced model*, B called *full model*.

p - number of regression parameters in full model

q - number of regression parameters in reduced model

$p - q$ - number of regression parameters being tested.

Let's get a handle on this notation. Give the extra regression SS terms for comparing some of the nested models on preceding page:

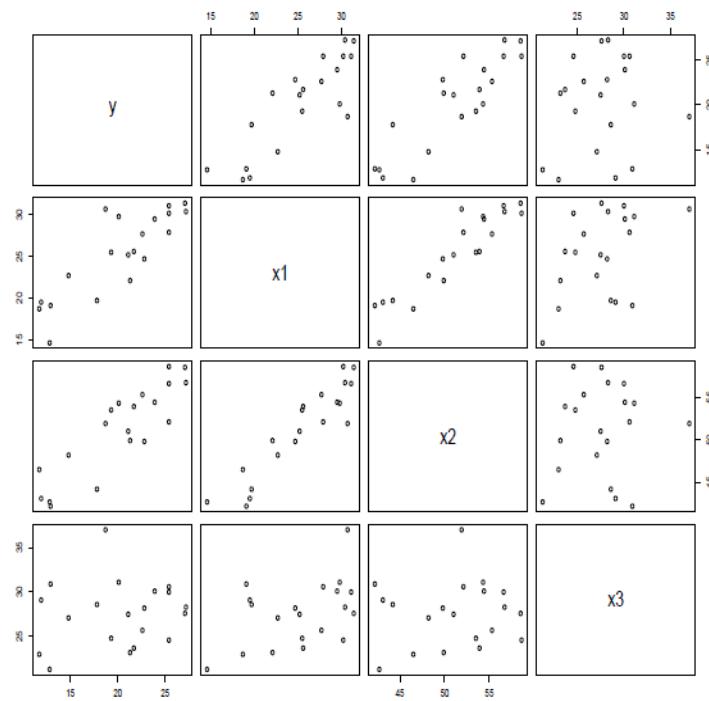
- Model 1 in model 4: $R(\beta_2, \beta_3 | \beta_1)$
 - Model 2 in model 4:
 - Model 3 in model 4:
 - Model 1 in model 5: $R(\beta_3 | \beta_1)$
 - Model 5 in model 4:

An example: How to measure body fat?

For each of $n = 20$ healthy individuals, the following measurements were made: bodyfat percentage y_i , triceps skinfold thickness, x_1 , thigh circumference x_2 , midarm circumference x_3 .

x1	x2	x3	y
19.5	43.1	29.1	11.9
24.7	49.8	28.2	22.8
30.7	51.9	37.0	18.7
29.8	54.3	31.1	20.1
19.1	42.2	30.9	12.9
25.6	53.9	23.7	21.7
31.4	58.5	27.6	27.1
27.9	52.1	30.6	25.4
22.1	49.9	23.2	21.3
25.5	53.5	24.8	19.3
31.1	56.6	30.0	25.4
30.4	56.7	28.3	27.2
18.7	46.5	23.0	11.7
19.7	44.2	28.6	17.8
14.6	42.7	21.3	12.8
29.5	54.4	30.1	23.9
27.7	55.3	25.7	22.6
30.2	58.6	24.6	25.4
22.7	48.2	27.1	14.8
25.2	51.0	27.5	21.1

```
ods graphics on;
proc corr plots=matrix;
var y x1 x2 x3;
run;
```



Pearson Correlation Coefficients, N = 20
 Prob > |r| under H0: Rho=0

	y	x1	x2	x3
y	1.00000	0.84327 <.0001	0.87809 <.0001	0.14244 0.5491
x1	0.84327 <.0001	1.00000	0.92384 <.0001	0.45778 0.0424
x2	0.87809 <.0001	0.92384 <.0001	1.00000	0.08467 0.7227
x3	0.14244 0.5491	0.45778 0.0424	0.08467 0.7227	1.00000

Looking at the scatter plots and the correlation output, marginal associations between y and x_1 and between y and x_2 are highly significant, providing evidence of a strong $r \approx 0.85$ linear association between average bodyfat and triceps skinfold and between average bodyfat and thigh circumference.

Notice the scatter plot between x_1 and x_2 , there is a strong linear relationship. This means that triceps skinfold and thigh circumference are giving some of the same information. This can lead to issues when fitting a model.

Multicollinearity: linear associations among the independent variables; causes problems such as inflated sampling variances for $\hat{\beta}$.

```
proc reg data=bodyfat;
  model y=x1/covb;
  model y=x2/covb;
  model y=x3/covb;
  model y=x1 x2/covb;
  model y=x1 x2 x3/covb;
run;
```

Yields the following output:

Output From Proc Reg for Bodyfat Example

The REG Procedure
Model: MODEL1
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Output From Proc Reg for Bodyfat Example

The REG Procedure
Model: MODEL2
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	352.26980	352.26980	44.30	<.0001
Error	18	143.11970	7.95109		
Corrected Total	19	495.38950			

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	381.96582	381.96582	60.62	<.0001
Error	18	113.42368	6.30132		
Corrected Total	19	495.38950			

Root MSE	2.81977	R-Square	0.7111
Dependent Mean	20.19500	Adj R-Sq	0.6950
Coeff Var	13.96271		

Root MSE	2.51024	R-Square	0.7710
Dependent Mean	20.19500	Adj R-Sq	0.7583
Coeff Var	12.43002		

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	-1.49610	3.31923	-0.45	0.6576
x1	1	0.85719	0.12878	6.66	<.0001

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	-23.63449	5.65741	-4.18	0.0006
x2	1	0.85655	0.11002	7.79	<.0001

Covariance of Estimates		
Variable	Intercept	x1
Intercept	11.01731839	-0.419670565
x1	-0.419670565	0.0165844918

Covariance of Estimates		
Variable	Intercept	x2
Intercept	32.006329324	-0.619332881
x2	-0.619332881	0.0121034372

Output From Proc Reg for Bodyfat Example

The REG Procedure
Model: MODEL3
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Output From Proc Reg for Bodyfat Example

The REG Procedure
Model: MODEL4
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	10.05160	10.05160	0.37	0.5491
Error	18	485.33790	26.96322		
Corrected Total	19	495.38950			

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	385.43871	192.71935	29.80	<.0001
Error	17	109.95079	6.46769		
Corrected Total	19	495.38950			

Root MSE	5.19261	R-Square	0.0203
Dependent Mean	20.19500	Adj R-Sq	-0.0341
Coeff Var	25.71236		

Root MSE	2.54317	R-Square	0.7781
Dependent Mean	20.19500	Adj R-Sq	0.7519
Coeff Var	12.59305		

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	14.68678	9.09593	1.61	0.1238
x3	1	0.19943	0.32663	0.61	0.5491

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	-19.17425	8.36064	-2.29	0.0348
x1	1	0.22235	0.30344	0.73	0.4737
x2	1	0.65942	0.29119	2.26	0.0369

Covariance of Estimates		
Variable	Intercept	x3
Intercept	82.735867956	-2.946694682
x3	-2.946694682	0.1066869907

Covariance of Estimates			
Variable	Intercept	x1	x2
Intercept	69.900312587	1.8469661215	-2.273097628
x1	1.8469661215	0.0920751757	-0.081628463
x2	-2.273097628	-0.081628463	0.0847900309

Output From Proc Reg for Bodyfat Example

5

The REG Procedure
Model: MODEL5
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	396.98461	132.32820	21.52	<.0001
Error	16	98.40489	6.15031		
Corrected Total	19	495.38950			

Root MSE	2.47998	R-Square	0.8014
Dependent Mean	20.19500	Adj R-Sq	0.7641
Coeff Var	12.28017		

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	117.08469	99.78240	1.17	0.2578
x1	1	4.33409	3.01551	1.44	0.1699
x2	1	-2.85685	2.58202	-1.11	0.2849
x3	1	-2.18606	1.59550	-1.37	0.1896

Covariance of Estimates					
Variable	Intercept	x1	x2	x3	
Intercept	9956.5279384	300.1979628	-257.3823153	-158.6704127	
x1	300.1979628	9.0933087788	-7.779145105	-4.7880263	
x2	-257.3823153	-7.779145105	6.6668028532	4.0946155019	
x3	-158.6704127	-4.7880263	4.0946155019	2.545617053	

Question: Why is the global p-value in the last model significant, i.e. at least one predictor is useful, but the individual tests are all nonsignificant?

In the bodyfat data, consider comparing the simple model that Y depends only on x_1 (triceps) versus the full model that it depends on all three.

$$\begin{aligned} \text{Model } A : \mu(x_1, x_2, x_3) &= \beta_0 + \beta_1 x_1 \\ \text{Model } B : \mu(x_1, x_2, x_3) &= \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 \end{aligned}$$

or the null hypothesis

$$H_0 : \beta_2 = \beta_3 = 0 \quad \text{vs} \quad H_1 : \beta_2, \beta_3 \text{ not both 0}$$

after accounting for x_1 . Our F statistic can be used

$$F = \frac{(396.9 - 352.3)/2}{6.15} = \frac{22.3}{6.15} = 3.64$$

How many df for numerator and denominator?

The 95th percentile is $F(0.05, \quad, \quad) = 3.63$.

Our conclusion about the hypotheses?

That is, after accounting for the linear dependence between triceps and bodyfat, there is still some linear association between mean bodyfat and at least one of x_2, x_3 (thigh,midarm).

To get the nested model F -ratio in SAS:

```
proc reg data=bodyfat;
  model y=x1 x2 x3;
  test x2=0,x3=0;
run;
```

Full mode vs only Triceps

4

The REG Procedure
Model: MODEL1

Test 1 Results for Dependent Variable y				
Source	DF	Mean Square	F Value	Pr > F
Numerator	2	22.35741	3.64	0.0500
Denominator	16	6.15031		

However, we saw in the previous output that a model with all three variables is no good. This is due to the multicollinearity. We will now very briefly look at a few automated model selection techniques.

Using proc reg to perform variable selection:

We'll discuss three hypothesis testing methods for selecting variables (there are many other ways to accomplish this we won't discuss).

1. Forward Selection - Start with nothing and work forward.

- (a) Begin with a model with only β_0
- (b) Calculate $R(\beta_i|\beta_0)$ for all possible predictors and find p-values for each
- (c) Take most significant p-value less than a cutoff (say 0.3), add predictor into model.
- (d) Say β_j was added in the last step, repeat above process with added predictor. That is, calculate $R(\beta_i|\beta_0, \beta_j)$ for all other predictors, etc.
- (e) Stop when no predictors are below the cutoff or if the full model is selected.

2. Backward Selection - Start with everything and work backward.

- (a) Start with full model.
- (b) Locate variable with largest p-value greater than a cutoff (say 0.1), remove that variable.
- (c) Repeat until all p-values are less than the cut off or the null model (intercept only model) is chosen.

3. Subset Selection - Compute all possible models, pick best.

- (a) Compare each of the models using a criterion.
- (b) Choose model that minimizes that criterion. Possible criteria include:
 - $Adjusted R^2 = 1 - \frac{n-1}{n-p-1}(1 - R^2)$ (takes into account the addition of more predictors)
 - Mallow's C_P , AIC, AICc, or BIC (all take into account the model complexity, not just how well the model fits the data)

How to do these model selection methods in SAS?

```
proc reg data=bodyfat plots=none;
  model y=x1 x2 x3/selection=cp ;
  model y=x1 x2 x3/selection=forward SLentry=0.3;
  model y=x1 x2 x3/selection=backward SLstay=0.1;
  model y=x1 x2 x3/selection=adjrsq;
run;
```

Variable Selection Methods on Bodyfat Example

The REG Procedure
Model: MODEL1
Dependent Variable: y

C(p) Selection Method

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Variable Selection Methods on Bodyfat Example

The REG Procedure
Model: MODEL2
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Forward Selection: Step 1

Variable x2 Entered: R-Square = 0.7710 and C(p) = 2.4420

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	381.96582	381.96582	60.62	<.0001
Error	18	113.42368	6.30132		
Corrected Total	19	495.38950			

Variable	Parameter Estimate	Standard Error	Type II SS	F Value	Pr > F
Intercept	-23.63449	5.65741	109.97344	17.45	0.0006
x2	0.85655	0.11002	381.96582	60.62	<.0001

Bounds on condition number: 1, 1

No other variable met the 0.3000 significance level for entry into the model.

Summary of Forward Selection							
Step	Variable Entered	Number Vars In	Partial R-Square	Model R-Square	C(p)	F Value	Pr > F
1	x2	1	0.7710	0.7710	2.4420	60.62	<.0001

Variable Selection Methods on Bodyfat Example

The REG Procedure
Model: MODEL3
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Backward Elimination: Step 0

All Variables Entered: R-Square = 0.8014 and C(p) = 4.0000

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	396.98461	132.32820	21.52	<.0001
Error	16	98.40489	6.15031		
Corrected Total	19	495.38950			

Variable	Parameter Estimate	Standard Error	Type II SS	F Value	Pr > F
Intercept	117.08469	99.78240	8.46816	1.38	0.2578
x1	4.33409	3.01551	12.70489	2.07	0.1699
x2	-2.85685	2.58202	7.52928	1.22	0.2849
x3	-2.18606	1.59550	11.54590	1.88	0.1896

Bounds on condition number: 708.84, 4133.4

Backward Elimination: Step 1

Variable x2 Removed: R-Square = 0.7862 and C(p) = 3.2242

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	389.45533	194.72767	31.25	<.0001
Error	17	105.93417	6.23142		
Corrected Total	19	495.38950			

Variable Selection Methods on Bodyfat Example

The REG Procedure
Model: MODEL3
Dependent Variable: y

Backward Elimination: Step 1

Variable	Parameter Estimate	Standard Error	Type II SS	F Value	Pr > F
Intercept	6.79163	4.48829	14.26834	2.29	0.1486
x1	1.00058	0.12823	379.40373	60.89	<.0001
x3	-0.43144	0.17662	37.18554	5.97	0.0258

Bounds on condition number: 1.2651, 5.0605

All variables left in the model are significant at the 0.1000 level.

Summary of Backward Elimination							
Step	Variable Removed	Number Vars In	Partial R-Square	Model R-Square	C(p)	F Value	Pr > F
1	x2	2	0.0152	0.7862	3.2242	1.22	0.2849

The REG Procedure
Model: MODEL4
Dependent Variable: y

Adjusted R-Square Selection Method

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Number in Model	Adjusted R-Square	R-Square	Variables in Model
3	0.7641	0.8014	x1 x2 x3
2	0.7610	0.7862	x1 x3
1	0.7583	0.7710	x2
2	0.7519	0.7781	x1 x2
2	0.7493	0.7757	x2 x3
1	0.6950	0.7111	x1
1	-.0341	0.0203	x3

Types of Sums of Squares

Given that we have 4 predictors, $X_1 - X_4$ we really can have a number of tests based on nested models for $\beta_4 = 0$ (or for any other β for that matter). Let's write them down in terms of extra regression sums of squares:

$R(\beta_4|\beta_0)$ (SLR test)

$R(\beta_4|\beta_0, \beta_1)$ (test after accounting for X_1)

$R(\beta_4|\beta_0, \beta_2)$ (test after accounting for X_2)

$R(\beta_4|\beta_0, \beta_3)$ (test after accounting for X_3)

$R(\beta_4|\beta_0, \beta_1, \beta_2)$ (test after accounting for X_1 and X_2)

$R(\beta_4|\beta_0, \beta_1, \beta_3)$ (test after accounting for X_1 and X_3)

$R(\beta_4|\beta_0, \beta_2, \beta_3)$ (test after accounting for X_2 and X_3)

$R(\beta_4|\beta_0, \beta_1, \beta_2, \beta_3)$ (test after accounting for X_1 , X_2 , and X_3)

Some of these tests can be easily found using different types of sums of squares.

The tests given for the parameter estimates are all type III tests and this is the test usually done to determine if a slope term has significance. However, type I tests are very useful for model building. For example, if we wanted to look at building a model for the bodyfat example and we thought the order of importance for the variables was X_1 (triceps), X_3 (midarm), and X_2 (thigh), we could get sequential tests for these models using type I sums of squares.

In SAS proc reg use the following code:

```
proc reg data=bodyfat;
  model y=x1 x3 x2/ss1; *Note the order of variables is important for Type I;
run;
```

Sequential tests for bodyfat example

1

The REG Procedure
Model: MODEL1
Dependent Variable: y

Number of Observations Read	21
Number of Observations Used	20
Number of Observations with Missing Values	1

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	396.98461	132.32820	21.52	<.0001
Error	16	98.40489	6.15031		
Corrected Total	19	495.38950			

Root MSE	2.47998	R-Square	0.8014
Dependent Mean	20.19500	Adj R-Sq	0.7641
Coeff Var	12.28017		

Parameter Estimates						
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t	Type I SS
Intercept	1	117.08469	99.78240	1.17	0.2578	8156.76050
x1	1	4.33409	3.01551	1.44	0.1699	352.26980
x3	1	-2.18606	1.59550	-1.37	0.1896	37.18554
x2	1	-2.85685	2.58202	-1.11	0.2849	7.52928

Let's label the Type I SS in terms of extra regression sums of squares (R notation).

Note: we will soon use proc glm for our model analysis and this gives even better output for type I sums of squares. (The tests given for type I sums of squares use the *full model* MS(E) rather than the full model MS(E) up to that point. This test still works because MS(E) from each model is an unbiased estimate of σ^2 . The tests using the different MS(E) terms could give different results, but will usually agree.

```
proc glm data=bodyfat;
  model y=x1 x3 x2;
run;
```

Sequential tests for bodyfat example using GLM

2

The GLM Procedure

Dependent Variable: y

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	396.9846118	132.3282039	21.52	<.0001
Error	16	98.4048882	6.1503055		
Corrected Total	19	495.3895000			

R-Square	Coeff Var	Root MSE	y Mean
0.801359	12.28017	2.479981	20.19500

Source	DF	Type I SS	Mean Square	F Value	Pr > F
x1	1	352.2697968	352.2697968	57.28	<.0001
x3	1	37.1855371	37.1855371	6.05	0.0257
x2	1	7.5292779	7.5292779	1.22	0.2849

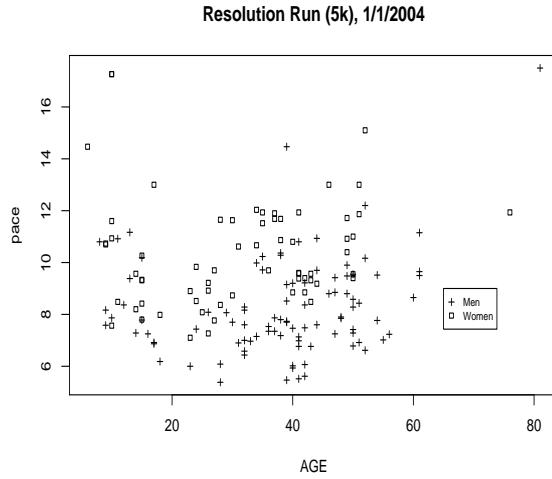
Source	DF	Type III SS	Mean Square	F Value	Pr > F
x1	1	12.70489278	12.70489278	2.07	0.1699
x3	1	11.54590217	11.54590217	1.88	0.1896
x2	1	7.52927788	7.52927788	1.22	0.2849

Parameter	Estimate	Standard Error	t Value	Pr > t
Intercept	117.0846948	99.78240295	1.17	0.2578
x1	4.3340920	3.01551136	1.44	0.1699
x3	-2.1860603	1.59549900	-1.37	0.1896
x2	-2.8568479	2.58201527	-1.11	0.2849

A linear regression example with a quadratic explanatory variable:

Data was collected on 5 kilometer run times. The variables collected were age, sex, and pace.

Obs	age	sex	race	pace
1	28	M	16.6833	5.38333
2	39	M	16.9500	5.46667
3	41	M	17.1333	5.51667
4	42	M	17.4000	5.61667
(abbreviated)
157	52	F	46.8833	15.1000
158	10	F	53.6000	17.2667
159	10	F	53.6167	17.2667
160	81	M	54.3167	17.5000



Quadratic model for pace (Y) as a function of age (x):

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + E_i \quad \text{for } i = 1, \dots, 160$$

where $E_i \stackrel{iid}{\sim} N(0, \sigma^2)$.

Question: What does σ^2 represent in the model?

Question: What do the parameters mean, i.e. what is their interpretation?

We may want to compare this model with a SLR model

$$Y_i = \beta_0 + \beta_1 x_i + E_i \text{ for } i = 1, \dots, 160$$

Question: How can we compare the two models?

```
/* age2 defined in data step as age*age */
PROC REG;
  MODEL pace=age;
  MODEL pace=age age2/ss1 covb;
RUN;
```

Model: MODEL1
Analysis of Variance

Source	DF	Sum of		F Value	Pr > F
		Squares	Mean Square		
Model	1	1.09650	1.09650	0.22	0.6396
Error	158	786.99821	4.98100		
Corrected Total	159	788.09472			

Root MSE	2.23182	R-Square	0.0014
Dependent Mean	9.12063	Adj R-Sq	-0.0049

Variable	DF	Parameter		t Value	Pr > t
		Estimate	Standard Error		
Intercept	1	8.92271	0.45724	19.51	<.0001
age	1	0.00564	0.01203	0.47	0.6396

Model: MODEL2
Analysis of Variance

Source	DF	Sum of		F Value	Pr > F
		Squares	Mean Square		
Model	2	113.64500	56.82250	13.23	<.0001
Error	157	674.44972	4.29586		
Corrected Total	159	788.09472			

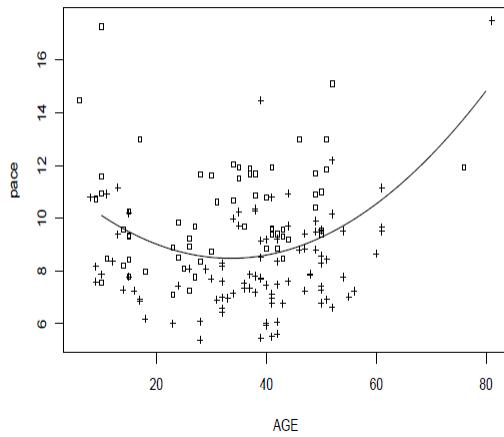
Root MSE	2.07265	R-Square	0.1442
Dependent Mean	9.12063	Adj R-Sq	0.1333

Variable	DF	Parameter	Standard	t Value	Pr > t	Type I SS
		Estimate	Error			
Intercept	1	11.78503	0.70216	16.78	<.0001	13310
age	1	-0.19699	0.04113	-4.79	<.0001	1.09650
age2	1	0.00294	0.00057380	5.12	<.0001	112.54850

Covariance of Estimates

Variable	Intercept	age	age2
Intercept	0.4930258	-0.0265145	0.0003209
age	-0.0265145	0.0016921	-0.0000227
age2	0.0003209	-0.0000227	0.0000003

Resolution Run (5k), 1/1/2004



Fitted models are:

$$\text{Model 1: } \hat{\mu}(x) = 8.923 + 0.0056age$$

$$\text{Model 2: } \hat{\mu}(age) = 11.785 - 0.197age + 0.00294age^2$$

$$\begin{aligned}
F &= \frac{R(\beta_2|\beta_0, \beta_1)}{MS(E)_{full}} \\
&= \frac{(SS(R)_{full} - SS(R)_{red})/1}{MS(E)_{full}} \\
&= \frac{(113.6 - 1.1)/1}{4.3} \\
&= \frac{(SS(E)_{red} - SS(E)_{full})/1}{MS(E)_{full}} \\
&= \frac{(787.0 - 674.4)/1}{4.3} = 26.2 \\
&= \left(\frac{\hat{\beta}_2}{SE} \right)^2 = (5.12)^2
\end{aligned}$$

with $F(0.05, 1, 157) = 3.90$. Since $26.2 \gg 3.9$, we reject that the linear model is appropriate when compared to the quadratic model. This is the same test as the t-test for age2!

Chapter 6

ST 512 - Extra Correlation and Regression Questions

Problems with worked out solutions.

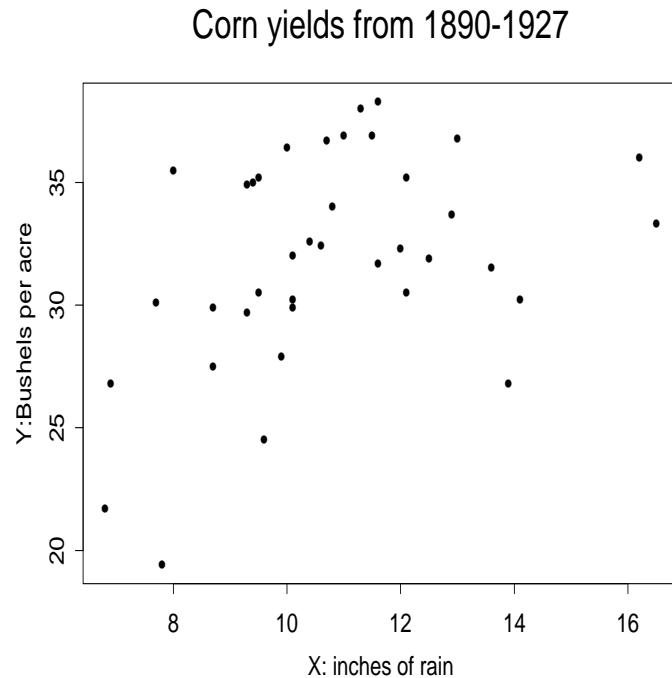
An example: The association between corn yield and rainfall:

Yields y (in bushels/acre) on corn raised in six midwestern states from 1890 to 1927 recorded with rainfall x (inches/yr).

$$y_1, \dots, y_{38} \quad \text{and} \quad x_1, \dots, x_{38}.$$

Year	1890	1891	1892	1893	1894	1895	1896	1897	1898	1899
Yield	24.5	33.7	27.9	27.5	21.7	31.9	36.8	29.9	30.2	32
Rainfall	9.6	12.9	9.9	8.7	6.8	12.5	13	10.1	10.1	10.1
Year	1900	1901	1902	1903	1904	1905	1906	1907	1908	1909
Yield	34	19.4	36	30.2	32.4	36.4	36.9	31.5	30.5	32.3
Rainfall	10.8	7.8	16.2	14.1	10.6	10	11.5	13.6	12.1	12
Year	1910	1911	1912	1913	1914	1915	1916	1917	1918	1919
Yield	34.9	30.1	36.9	26.8	30.5	33.3	29.7	35	29.9	35.2
Rainfall	9.3	7.7	11	6.9	9.5	16.5	9.3	9.4	8.7	9.5
Year	1920	1921	1922	1923	1924	1925	1926	1927		
Yield	38.3	35.2	35.5	36.7	26.8	38	31.7	32.6		
Rainfall	11.6	12.1	8	10.7	13.9	11.3	11.6	10.4		

A *scatter plot* provides a visual for inspecting the association between Y and X .



From the scatter plot, the form of the association appears to be linear or slightly quadratic, the strength is weak to moderate, and the direction is positive.

A correlation analysis was done and a SLR model was fit using SAS yielding the following (partial) output:

```
proc corr data=corn cov;           proc reg data=corn;
var yield rain;                  model yield=rain;
run;                                run;
```

2 Variables:		yield rain
Covariance Matrix, DF = 37		
	yield	rain
yield	19.04190612	3.98025605
rain	3.98025605	5.13217639

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	114.21474	114.21474	6.97	0.0122
Error	36	590.33578	16.39822		
Corrected Total	37	704.55053			

Simple Statistics						
Variable	N	Mean	Std Dev	Sum	Minimum	Maximum
yield	38	31.91579	4.36370	1213	19.40000	38.30000
rain	38	10.78421	2.26543	409.80000	6.80000	16.50000

--	--	--	--	--	--	--

Use the output to

1. Find the value of the correlation coefficient.
2. Find the 95% confidence interval for the population correlation, ρ . Interpret the interval you found.
3. Without conducting a hypothesis test, use the confidence interval to make a conclusion about the hypotheses $H_0 : \rho = 0$ vs $H_A : \rho \neq 0$.
4. Find the fitted line for the SLR with yield as the response and rainfall as the predictor.
5. Use the summary statistics to create 95% confidence intervals for β_1 and β_0 . Note: $t(38, 0.025) = 2.024$.
6. Find a 95% confidence interval for the true mean yield for corn from the six states for a rainfall of 14 inches.
7. Suppose the rainfall collected for a year was 14 inches but the yield of the corn from the six states was not recorded. Find a 95% prediction interval for the yield of the corn from that year.

Solutions:

1. From the output we have

$$\begin{aligned}\bar{x} &= 10.78, & s_X^2 &= 5.13 & s_X &= 2.27 \\ \bar{y} &= 31.92, & s_Y^2 &= 19.04 & s_Y &= 4.36 \\ s_{XY} &= 3.98\end{aligned}$$

Applying the formula for r , we get

$$r = \frac{s_{XY}}{s_X s_Y} = \frac{3.98}{\sqrt{5.13 \times 19.04}} = 0.40$$

2. With $r = 0.40$, $n = 38$, and $z_{\alpha/2} = 1.96$, a 95% interval is given by

$$\left(\frac{\frac{1+0.4}{1-0.4} e^{-2*1.96/\sqrt{38-3}} - 1}{\frac{1+0.4}{1-0.4} e^{-2*1.96/\sqrt{38-3}} + 1}, \frac{\frac{1+0.4}{1-0.4} e^{2*1.96/\sqrt{38-3}} - 1}{\frac{1+0.4}{1-0.4} e^{2*1.96/\sqrt{38-3}} + 1} \right) = (0.09, 0.64).$$

We are 95% confident that the true correlation between corn yield and rainfall is between 0.09 and 0.64.

3. Since there is a one-to-one correspondence between a two-sided HT at the 0.05 level and a $100(1 - \alpha)\%$ CI, we would reject $H_0 : \rho = 0$ as 0 is not in the interval.

4. To find the fitted least squares line:

$$\begin{aligned}
\hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\
&= \frac{3.98}{5.13} = 0.776 (\text{ bushels per acre } \div \text{ inches per year}) \\
\text{or } &= r_{xy} \frac{s_y}{s_x} \\
&= (0.40) \sqrt{\frac{19.04}{5.13}} \\
&= 0.771 (\text{of } f \text{ due to rounding}) \\
\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\
&= 31.92 - 0.776(10.78) \\
&= 23.555 \text{ bushels per acre}
\end{aligned}$$

yielding the least squares line of

$$\hat{y} = 23.555 + (0.776)x.$$

5. To find confidence intervals for the regression parameters:

For β_1 , note that

$$S_{xx} = (n - 1)s_x^2 = 5.13(38 - 1) = 189.81$$

and we can estimate σ^2 using the $MS(E) = 16.40$. Thus, a 95% CI for β_1 is given by

$$0.776 \pm 2.024 \sqrt{\frac{16.40}{189.81}} = (0.181, 1.371)$$

We are 95% confident the true value of the slope lies in this interval. For $\hat{\beta}_0$,

$$23.555 \pm 2.024 \sqrt{16.40 \left(\frac{1}{38} + \frac{(10.78)^2}{189.81} \right)} = (17.052, 30.058)$$

6. First we can find the point estimate

$$\hat{\mu}(14) = 23.555 + 0.776 * 14 = 34.419$$

The standard error of this mean estimate is

$$\sqrt{16.40 \left(\frac{1}{38} + \frac{(14 - 10.78)^2}{189.81} \right)} = 1.125$$

Thus, a 95% CI for the mean corn yield for 14 inches of rain is

$$34.419 \pm 2.024 * 1.125 = (32.142, 36.696)$$

We are 95% confident that the true mean corn yield for all years with 14 inches of rain is between 32.142 and 36.696 bushels per acre.

7. A 95% prediction interval is then

$$34.419 \pm 2.024 \sqrt{16.40 \left(1 + \frac{1}{38} + \frac{(14 - 10.78)^2}{189.81} \right)} = (25.898, 42.940)$$

We are 95% confident that a year that has 14 inches of rain will have a yield between 2.898 and 42.940 bushels per acre.

Looking at the scatter plot, there may be a quadratic relationship. We can fit a linear regression model with rainfall and rainfall squared as predictors to investigate this. Use the following SAS output to conduct a LOF test for the SLR model.

```
data corn; proc reg data=corn;
set corn; model yield= rain rain2/ss1;
rain2=rain*rain; run;
```

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	209.02175	104.51087	7.38	0.0021
Error	35	495.52878	14.15797		
Corrected Total	37	704.55053			

Root MSE	3.76271	R-Square	0.2967
Dependent Mean	31.91579	Adj R-Sq	0.2565
Coeff Var	11.78948		

Parameter Estimates						
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t	Type I SS
Intercept	1	-5.01467	11.44158	-0.44	0.6639	38707
rain	1	6.00428	2.03895	2.94	0.0057	114.21474
rain2	1	-0.22936	0.08864	-2.59	0.0140	94.80700

The F statistic for the LOF test can be written as

$$F = \frac{\frac{SS(R)_f - SS(R)_r}{p-q}}{MS(E)_f} = \frac{\frac{209.02 - 114.21}{2-1}}{14.16} = 6.70$$

We compare this to the critical value from the appropriate F distribution: $F(1, 35, 0.05) = 4.12$

Therefore, we reject $H_0 : \beta_2 = 0$ in favor of $H_A : \beta_2 \neq 0$.

Note: This test statistic of 6.70 is equivalent to the t-test squared $(-2.59)^2$ since we only have 1 numerator degree of freedom.

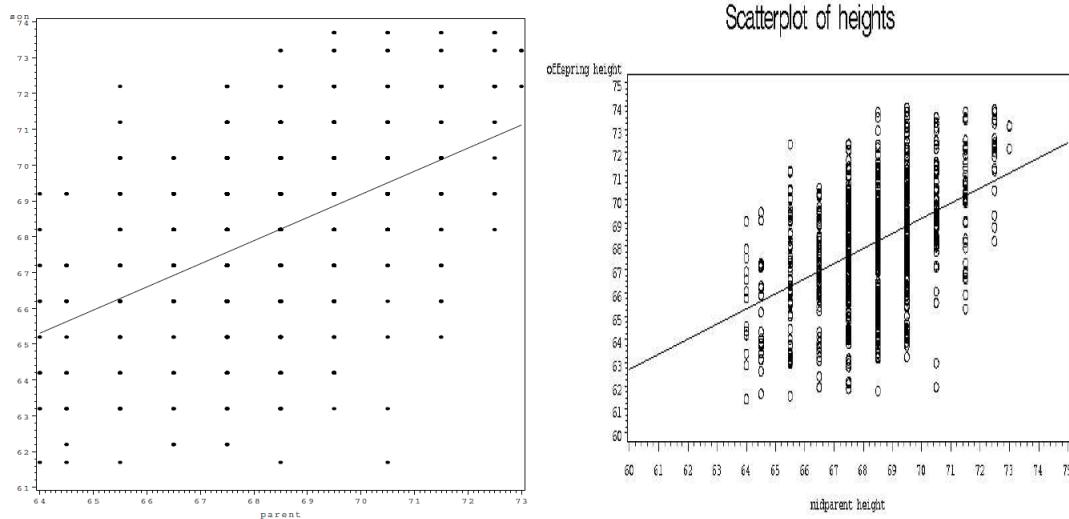
A couple random questions:

1. What type of data is needed to run a MLR model?
2. An industrial quality control expert takes 200 hourly measurements on an industrial furnace which is under control and finds that a 95% confidence interval for the mean temperature is (500.35, 531.36). As a result he tells management that the process should be declared out of control whenever hourly measurements fall outside this interval and, of course, is later fired for incompetence. (Why and what should he have done?)

Solutions:

1. The data situation needed for a MLR model is p quantitative predictors and 1 quantitative response measured on the same individuals (i.e. units).
2. The interval found is for the **mean** temperature. The interval is not trying to capture a single new observation. The interval that should have been found is a prediction interval. This interval will be much wider as it is much more difficult to predict a new value as opposed to predicting the true mean.

The classical regression example - The association between height of adults and their parents



```
/*
| Stigler , History of Statistics pg. 285 gives Galton's famous data |
| on heights of sons (columns,Y) and average parents' height (rows,X) |
| scaled to represent a male height (essentially sons' heights versus |
| fathers' heights).      Taken from Dickey's website.           |
\-----*/
```

61.7	62.2	63.2	64.2	65.2	66.2	67.2	68.2	69.2	70.2	71.2	72.2	73.2	73.7
73.0	0	0	0	0	0	0	0	0	0	0	1	3	0
72.5	0	0	0	0	0	0	1	2	1	2	7	2	4
71.5	0	0	0	0	1	3	4	3	5	10	4	9	2
70.5	1	0	1	0	1	1	3	12	18	14	7	4	3
69.5	0	0	1	16	4	17	27	20	33	25	20	11	4
68.5	1	0	7	11	16	25	31	34	48	21	18	4	3
67.5	0	3	5	14	15	36	38	28	38	19	11	4	0
66.5	0	3	3	5	2	17	17	14	13	4	0	0	0
65.5	1	0	9	5	7	11	11	7	7	5	2	1	0
64.5	1	1	4	4	1	5	5	0	2	0	0	0	0
64.0	1	0	2	4	1	2	2	1	1	0	0	0	0

Many questions we could answer using this dataset: Note: $t(927, 0.025) \approx t(926, 0.025) = 1.963$

- Suppose we ignore midparent height x . Consider estimating the mean $\mu_Y = E(Y)$. Recall a method for obtaining a confidence interval for the mean height of the sons in the population from which these data were randomly sampled. Use summary statistics in the output that follows to complete this naive analysis.

For the rest of the problems, consider a linear regression between the sons' heights and the midparent height. Let Y_1, \dots, Y_n denote the sons' heights. Given their average parent height, $X = x_i$,

$$Y_i = \beta_0 + \beta_1 x_i + E_i \quad \text{for } i = 1, \dots, n (n = 928).$$

where E_1, \dots, E_n are *iid* Normal with mean 0 and variance σ^2 .

Output is given on the following pages, use it to answer the following:

2. What is the meaning, in words, of β_1 ?
3. True/false: (a) β_1 is a statistic (b) β_1 is a parameter (c) β_1 is unknown.
4. What is the observed value of $\hat{\beta}_1$?
5. True/false: (a) $\hat{\beta}_1$ is a statistic (b) $\hat{\beta}_1$ is a parameter (c) $\hat{\beta}_1$ is unknown.
6. Is $\hat{\beta}_1 = \beta_1$?
7. How much does $\hat{\beta}_1$ vary about β_1 from sample to sample? (Provide an estimate of the standard error, as well as an expression indicating how it was computed.)
8. What is a region of plausible values for β_1 suggested by the data? (i.e. a CI)
9. What is the line that best fits these data, using the criterion that smallest sum of squared residuals is "best?"
10. How much of the observed variation in the heights of sons (the y -axis) is explained by this "best" line?
11. Give an expression in terms of the parameters of the model for the true average height of sons with midparent height $x = 68$.
12. What is the estimated average height of sons whose midparent height is $x = 68$?
13. Is this the true average height in the whole population of sons whose midparent height is $x = 68$?
14. What is the estimated standard deviation among the population of sons whose parents have midparent height $x = 68$?
15. What is the estimated standard deviation among the population of sons whose parents have midparent height $x = 72$? Bigger, smaller, or the same as that for $x = 68$?
16. What is the estimated standard error of the estimated average height for sons with midparent height $x = 68$, i.e. $\hat{\mu}(68) = \hat{\beta}_0 + 68\hat{\beta}_1$? Provide an expression for this standard error.
17. Is the estimated standard error of $\hat{\mu}(72)$ bigger, smaller, or the same as that for $\hat{\mu}(68)$?

18. What quantity can you use to describe or characterize the linear association between height and midparent height in the whole population? Is this a parameter or a statistic?
19. Is the observed linear association between son's height and midparent height strong?
To answer, report the value of r and the p-value from the appropriate test.
20. Define $\mu_Y, \sigma_Y, \mu_X, \sigma_X, \rho$. Parameters or statistics?
21. What are plausible values for ρ suggested by the data? (i.e. form a CI)
22. Is $E_1, \dots, E_{928} \stackrel{iid}{\sim} N(0, \sigma^2)$ a reasonable assumption?
23. Based **solely** on this study, can we conclude that larger parents cause larger sons?

Code that produced this output available on web.

Galton Height Data Output

1

The CORR Procedure

2 Variables:	son	parent
---------------------	-----	--------

Covariance Matrix, DF = 927		
	son	parent
son	6.340028724	2.064614487
parent	2.064614487	3.194560689

Simple Statistics						
Variable	N	Mean	Std Dev	Sum	Minimum	Maximum
son	928	68.08847	2.51794	63186	61.70000	73.70000
parent	928	68.30819	1.78733	63390	64.00000	73.00000

Pearson Correlation Coefficients, N = 928 Prob > r under H0: Rho=0		
	son	parent
son	1.00000	0.45876 <.0001
parent	0.45876 <.0001	1.00000

Pearson Correlation Statistics (Fisher's z Transformation)						
Variable	With Variable	N	Sample Correlation	Fisher's z	95% Confidence Limits	p Value for H0:Rho=0
son	parent	928	0.45876	0.49574	0.406407 0.508115	<.0001

Galton Height Data Output

2

The REG Procedure
Model: MODEL1
Dependent Variable: son

Number of Observations Read	930
Number of Observations Used	928
Number of Observations with Missing Values	2

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	1236.93401	1236.93401	246.84	<.0001
Error	926	4640.27261	5.01109		
Corrected Total	927	5877.20663			

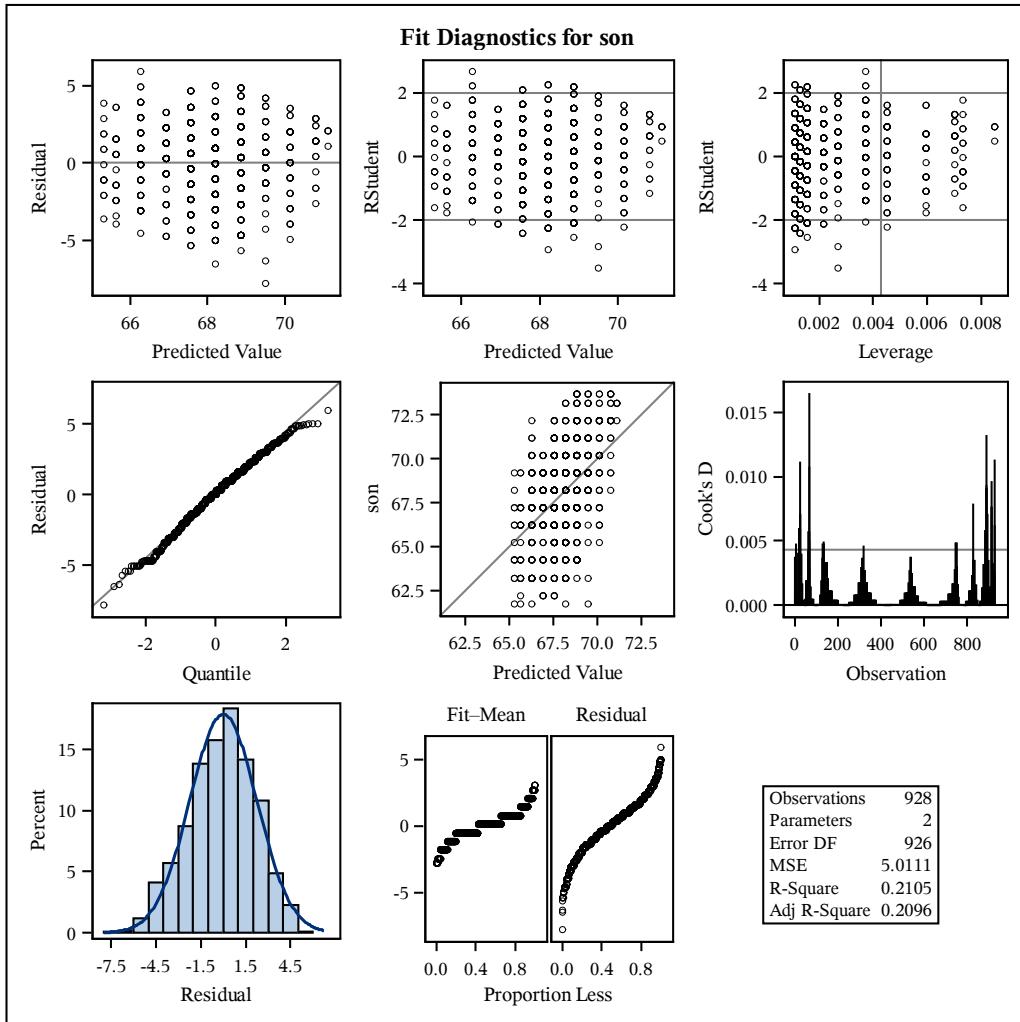
Root MSE	2.23855	R-Square	0.2105
Dependent Mean	68.08847	Adj R-Sq	0.2096
Coeff Var	3.28770		

Parameter Estimates						
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t	95% Confidence Limits
Intercept	1	23.94153	2.81088	8.52	<.0001	18.42510 29.45796
parent	1	0.64629	0.04114	15.71	<.0001	0.56556 0.72702

Galton Height Data Output

3

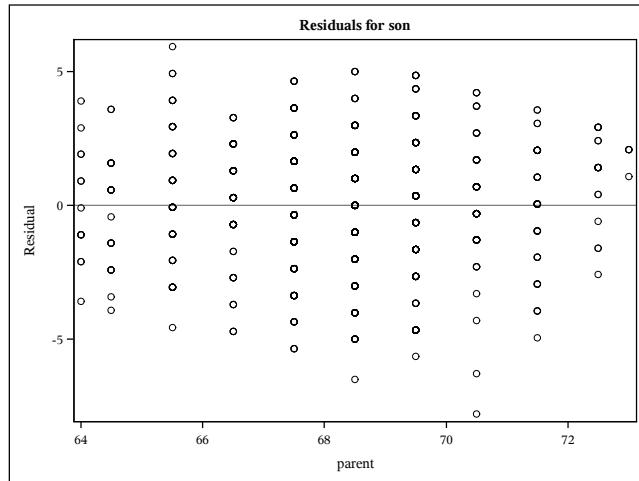
The REG Procedure
Model: MODEL1
Dependent Variable: son



Galton Height Data Output

4

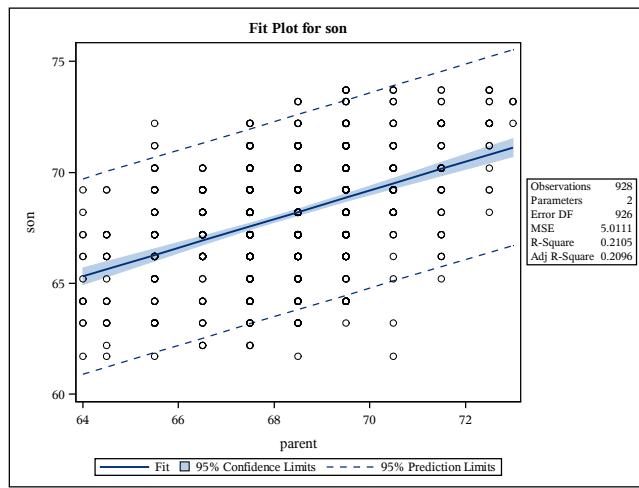
The REG Procedure
Model: MODEL1
Dependent Variable: son



Galton Height Data Output

5

The REG Procedure
Model: MODEL1
Dependent Variable: son



Galton Height Data Output

6

Obs	parent	son	yhat	stdmean	cilow	cishigh	pilow	pihigh	r
1	68	.	67.8893	0.07457	67.7429	68.0356	63.4936	72.2849	.
2	72	.	70.4745	0.16871	70.1434	70.8056	66.0688	74.8801	.

Answers to questions from simple linear regression:

1. A CI for a mean when the true standard deviation is unknown is

$$\bar{y} \pm t(n - 1, \alpha/2)s/\sqrt{n} = 68.09 \pm 1.963 * 2.52/\sqrt{928} = (67.928, 68.252)$$

2. Change in average son's height (inches) per one inch increase in midparent height.

3. β_1 is an unknown parameter.

4. $\hat{\beta}_1 = 0.65$ son inches/midparent inch.

5. $\hat{\beta}_1 = 0.65$ is an observed value of a statistic.

6. β_1 is the slope of the population mean, $\hat{\beta}_1$ is the slope from the SLR of the observed data. $\hat{\beta}_1 = \beta_1$ is very unlikely.

7. $\widehat{SE}(\hat{\beta}_1) = \sqrt{MS[E]/S_{xx}} = 0.041$.

8. Add and subtract 1.963 times the SE to get $(0.566, 0.727)$

9. $y = 23.942 + 0.646x$

10. $r^2 = 21.05\%$

11. $\mu(68) = \beta_0 + 68\beta_1$

12. $\hat{\mu}(68) = \hat{\beta}_0 + 68\hat{\beta}_1 = 67.889$

13. Probably not! $\mu(68) = \beta_0 + 68\beta_1$ is unknown and $\hat{\mu}(68)$ is only an estimate.

14. This question is asking for the square root of the estimate of variation due to experimental error or $\hat{\sigma} = \sqrt{MS[E]} = 2.24$.

15. Same as the previous question as an assumption on our model is that the errors have the same variance (and hence square root) at every point on the line. (Assumption of homoskedasticity.)

16. $SE(\hat{\beta}_0 + 68\hat{\beta}_1) = 0.075$. Expressions given by

$$\begin{aligned}\widehat{SE}(\hat{\mu}(68)) &= \sqrt{MS[E] \left(\frac{1}{n} + \frac{(68 - \bar{x})^2}{\sum(x_i - \bar{x})^2} \right)} \\ &= \sqrt{(1, 68)' MS[E] (X'X)^{-1} (1, 68)}\end{aligned}$$

X a (928×2) design matrix.

17. $\widehat{SE}(\hat{\mu}(72)) > \widehat{SE}(\hat{\mu}(68))$ as it is further from \bar{x} , where we have the most information about our data.

18. ρ , which is the population correlation coefficient (a parameter).

19. $r = 0.459$, moderate, positive. P-value < 0.0001 , there is a significant linear relationship.
20. These are all parameters and describe the mean and standard deviation of the sons' heights, the mean and standard deviation of the midparent's heights, and the correlation between them.
21. The confidence interval is

$$\left(\frac{\frac{1+r}{1-r}e^{-2z/\sqrt{n-3}} - 1}{\frac{1+r}{1-r}e^{-2z/\sqrt{n-3}} + 1}, \frac{\frac{1+r}{1-r}e^{2z/\sqrt{n-3}} - 1}{\frac{1+r}{1-r}e^{2z/\sqrt{n-3}} + 1} \right)$$

or $(0.406, 0.508)$.

22. Residuals reasonably symmetric, no heavy tails. Model fit is ok.
23. Based on this study alone, no. This is an observational study as no midparent heights were assigned by the researchers. However, if science and genetics are brought in, a causal relationship might be inferred.

Recall the example about a random sample of students taking the same exam:

IQ	TIME	GRADE
105	10	75
110	12	79
120	6	68
116	13	85
122	16	91
130	8	79
114	20	98
102	15	76

Consider the additive regression model for the GRADE of subject i , Y_i , in which the mean of Y_i is a linear function of IQ and Time ($X_{i1} = \text{IQ}$ and $X_{i2} = \text{TIME}$) for subjects $i = 1, \dots, 8$:

$$Y = \beta_0 + \beta_1 \text{IQ} + \beta_2 \text{TIME} + \text{error}$$

or

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + E_i$$

Let's write out the model in matrix form:

$$\mathbf{y} = \begin{pmatrix} 75 \\ 79 \\ 68 \\ 85 \\ 91 \\ 79 \\ 98 \\ 76 \end{pmatrix} \quad \mathbf{X} = \begin{pmatrix} 1 & 105 & 10 \\ 1 & 110 & 12 \\ 1 & 120 & 6 \\ 1 & 116 & 13 \\ 1 & 122 & 16 \\ 1 & 130 & 8 \\ 1 & 114 & 20 \\ 1 & 102 & 15 \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}$$

$$\mathbf{X}'\mathbf{X} = \begin{pmatrix} 8 & 919 & 100 \\ 919 & 106165 & 11400 \\ 100 & 11400 & 1394 \end{pmatrix}$$

$$(\mathbf{X}'\mathbf{X})^{-1} = \begin{pmatrix} 28.90 & -0.23 & -0.22 \\ -0.23 & 0.0018 & 0.0011 \\ -0.22 & 0.0011 & 0.0076 \end{pmatrix}$$

$$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \begin{pmatrix} 0.74 \\ 0.47 \\ 2.10 \end{pmatrix}$$

$$SS(E) = \mathbf{e}'\mathbf{e} = (\mathbf{Y} - \hat{\mathbf{Y}})'(\mathbf{Y} - \hat{\mathbf{Y}}) = 45.8, \quad \mathbf{e}'\mathbf{e}/df = 9.15$$

$$\widehat{\Sigma} = MS(E)(\mathbf{X}'\mathbf{X})^{-1} = \begin{pmatrix} 264.45 & -2.07 & -2.05 \\ -2.07 & 0.017 & 0.010 \\ -2.05 & 0.010 & 0.070 \end{pmatrix}$$

Some questions to answer:

1. What is the estimate for β_1 ? Interpretation?
2. What is the standard error of $\hat{\beta}_1$?
3. Is $\beta_1 = 0$ plausible, while controlling for possible linear associations between Test Score and Study time? ($t(0.025, 5) = 2.57$)
4. Estimate the mean grade among the population of ALL students with $IQ = 113$ who study $TIME = 14$ hours.
5. Report a standard error for this mean.
6. Report a 95% confidence interval for this mean.
7. What is the estimate of the error variance?

Some answers:

1. $\hat{\beta}_1 = 0.47$ (second element of $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$, estimated average exam points per IQ point for students studying the same amount)
2. $\sqrt{0.017} = 0.13$ (square root of middle element of $\hat{\Sigma}$)
3. $H_0 : \beta_1 = 0$, T-statistic: $t = (\hat{\beta}_1 - 0)/SE(\hat{\beta}_1)$
Observed value is $t = .47/\sqrt{0.017} = .47/.13 = 3.6 > 2.57$ (“ $\hat{\beta}_1$ differs significantly from 0.”)
4. Unknown population mean: $\theta = \beta_0 + \beta_1(113) + \beta_1(14)$
Estimate : $\hat{\theta} = (1, 113, 14) * \hat{\beta} = 83.6$
5. $\text{Var}((1, 113, 14) * \hat{\beta}) = (1, 113, 14)\widehat{\text{Var}}(\hat{\beta})(1, 113, 14)'$
or $(1, 113, 14)\hat{\Sigma}(1, 113, 14)' = 1.3$ or $SE(\hat{\theta}) = \sqrt{1.3} = 1.14$
6. $\hat{\theta} \pm t(0.025, 5)SE(\hat{\theta})$ or $83.6 \pm 2.57(1.14)$ or $(80.7, 86.6)$
7. The estimate of the error variance is the $MS(E) = 9.15$

Continuing this example, consider this sequence of analyses:

1. Regress GRADE on IQ.
2. Regress GRADE on IQ and TIME.
3. Regress GRADE on TIME IQ TI where TI = TIME*IQ.

ANOVA (Grade on IQ)					
SOURCE	DF	SS	MS	F	p-value
IQ	1	15.9393	15.9393	0.153	0.71
Error	6	625.935	104.32		

It appears that IQ has nothing to do with grade, but we did not look at study time.

Looking at the *multiple* regression we get

The REG Procedure						
Analysis of Variance						
Source	DF	Sum of		Mean Square	F Value	Pr > F
		Squares	Mean Square			
Model	2	596.11512	298.05756	32.57	0.0014	
Error	5	45.75988	9.15198			
Corrected Total	7	641.87500				

Variable	DF	Parameter		Standard		Pr > t
		Estimate	Error	t Value	Pr > t	
Intercept	1	0.73655	16.26280	0.05	0.9656	
IQ	1	0.47308	0.12998	3.64	0.0149	
Time	1	2.10344	0.26418	7.96	0.0005	

Now the test for dependence on IQ is significant $p = 0.0149$. Why? This is a slightly different test. This is testing if IQ is important after taking into account the linear relationship between Grade and Time.

Now recall when we fit the interaction model we found the following (here type I SS are included):

Parameter Estimates						
Variable	DF	Parameter		Standard		
		Estimate	Error	t Value	Pr > t	Type I SS
Intercept	1	72.20608	54.07278	1.34	0.2527	52975
IQ	1	-0.13117	0.45530	-0.29	0.7876	15.93930
Time	1	-4.11107	4.52430	-0.91	0.4149	580.17582
TI	1	0.05307	0.03858	1.38	0.2410	14.69521

This model now appears to be over-fit as the type III tests (tests done after accounting for all other variables in the model) are all non-significant.

We can perform a LOF test to see if the interaction model or the MLR model is preferred. We can find $SS(R)_f$ by summing the type I SS,

$$SS(R)_f = 15.939 + 580.176 + 14.695 = 610.8103$$

The $SS(R)_r$ can be found by subtracting off the TI type I SS from $SS(R)_f$ or by adding all type I SS except TI giving

$$SS(R)_r = 610.8103 - 14.695 = 596.115$$

Now the numerator of our LOF statistic is

$$\frac{610.8103 - 596.115}{3 - 2} = \frac{14.695}{1} = 14.7$$

(Note this is the type I SS for TI !). Our LOF stat is then

$$F = 14.7 / 7.766 = 1.893$$

(MSE found from output in earlier notes.) Comparing this to $F(1, 4, 0.05) = 7.709$ we fail to reject H_0 in favor of H_A . That is, the additive model is adequate.

A random sample of $n = 31$ trees is drawn from a population of trees. On each tree, indexed by i , three variables are measured:

- x_{i1} : “girth”, tree diameter in inches
- x_{i2} : “height” (in feet)
- Y_i : volume of timber, in cubic feet.

Given x_1 and x_2 , a MLR model for these data is given by

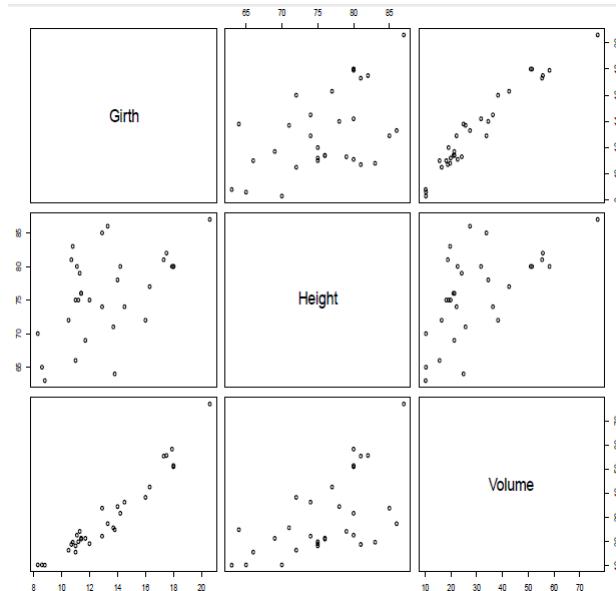
$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + E_i \text{ for } i = 1, \dots, n$$

where errors are assumed iid normal w/ constant variance σ^2 .

For trees with x_1, x_2 the model for mean volume is

$$\mu(x_1, x_2) = E(Y|x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2.$$

A scatterplot matrix



Consider all trees with girth $x_{01} = 15$ in and height $x_{02} = 80$ ft .

- Estimate the mean volume among these trees, along with a standard error and 95% confidence interval. Note : $t(28, 0.025) = 2.048$
- Obtain a 95% prediction interval of y_0 , the volume from an individual tree sampled from this population of 80 footers, with girth 15 inches.

SAS generates $\hat{\beta}$ and $\widehat{Var}(\hat{\beta}) = MSE * (X'X)^{-1}$

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	7684.16251	3842.08126	254.97	<.0001
Error	28	421.92136	15.06862		
Corrected Total	30	8106.08387			
Root MSE		3.88183	R-Square	0.9480	
Dependent Mean		30.17097	Adj R-Sq	0.9442	
Coeff Var		12.86612			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	-57.98766	8.63823	-6.71	<.0001
Girth	1	4.70816	0.26426	17.82	<.0001
Height	1	0.33925	0.13015	2.61	0.0145

Covariance of Estimates

Variable	Intercept	Girth	Height
Intercept	74.6189461	0.4321713812	-1.050768886
Girth	0.4321713812	0.0698357838	-0.017860301
Height	-1.050768886	-0.017860301	0.0169393298

Recall: Let \mathbf{W} denote a $p \times 1$ random vector with mean $\boldsymbol{\mu}_{\mathbf{W}}$ and covariance matrix $\boldsymbol{\Sigma}_{\mathbf{W}}$. Suppose \mathbf{a} is a $p \times 1$ (fixed) vector of coefficients. Then

$$\boxed{\begin{aligned} E(\mathbf{a}'\mathbf{W}) &= \mathbf{a}'\boldsymbol{\mu}_{\mathbf{W}} \\ \text{Var}(\mathbf{a}'\mathbf{W}) &= \mathbf{a}'\boldsymbol{\Sigma}_{\mathbf{W}}\mathbf{a}. \end{aligned}}$$

1. Consider all trees with Girth 15 and Height 80 To estimate mean volume among these trees, along with an estimated standard error, take $\mathbf{x}'_0 = (1, 15, 80)$ and consider

$$\hat{\mu}(\mathbf{x}_0) = \mathbf{x}'_0 \hat{\boldsymbol{\beta}}$$

$$E(\mathbf{x}'_0 \hat{\boldsymbol{\beta}}) = \mathbf{x}'_0 \boldsymbol{\beta}$$

$$\text{Var}(\mathbf{x}'_0 \hat{\boldsymbol{\beta}}) = \mathbf{x}'_0 \hat{\boldsymbol{\Sigma}} \mathbf{x}_0$$

Substitution of $\hat{\boldsymbol{\beta}}$ and $\hat{\boldsymbol{\Sigma}} = \text{MSE}(\mathbf{X}'\mathbf{X})^{-1}$ gives the estimates:

$$\begin{aligned} \hat{\mu}(\mathbf{x}_0) &= (1, 15, 80) \begin{pmatrix} -58.0 \\ 4.71 \\ 0.34 \end{pmatrix} \\ &= 39.8 \\ \widehat{\text{Var}}(\hat{\mu}(\mathbf{x}_0)) &= (1, 15, 80) \begin{pmatrix} 74.62 & 0.43 & -1.05 \\ 0.43 & 0.070 & -0.018 \\ -1.05 & -0.018 & 0.017 \end{pmatrix} \begin{pmatrix} 1 \\ 15 \\ 80 \end{pmatrix} \\ &= 0.72 \\ \widehat{SE}(\hat{\mu}(\mathbf{x}_0)) &= \sqrt{0.72} = 0.849 \end{aligned}$$

Thus, a 95% CI is given by

$$39.8 \pm 2.048 * 0.849 = (38.061, 41.539)$$

2. 95% Prediction limits? Same idea but we add and subtract $t(.025, 28)\sqrt{.72 + \text{MS}(E)}$.

Chapter 7

ST 512 - General Linear Models

Readings: 12.1-12.6 pg 540 - 583

A general linear model:

Models which can include both qualitative and/or quantitative explanatory variables are called general linear models or GLMs. (Again, the ‘linearity’ pertains to the parameters, not the explanatory variables.)

How to write qualitative variables in a GLM format?

ANOVA (Analysis of Variance, i.e. comparing mean squares) revisited:

The One-Way ANOVA model is used when we wish to compare the means of t different groups. (One-Way corresponds to having only one factor of interest.)

Often a completely randomized experimental design will be analyzed using an ANOVA model.

One form of the One-Way ANOVA model is

$$Y_{ij} = \mu + \tau_i + E_{ij}$$

- E_{ij} are i.i.d. $N(0, \sigma^2)$
- $i = 1, \dots, t$ describes the treatment group
- $j = 1, \dots, n_i$ represents the number of observations we have in treatment group i .

We will consider ‘balanced’ designs for now, where $n_i = n$, same number of replicates for each treatment. Total number of observations = $N = nt$

Unknown parameters:

- μ - overall population mean (avg of treatment population means)
- τ_i - difference between (population) mean for treatment i and μ
- σ^2 - (population) variance within a given treatment group (constant across groups)

Goals of One-Way ANOVA: Determine

1. if all treatment means are equal.
2. if treatment means not equal, which means differ from each other.

One-Way ANOVA example:

An experiment was done to determine if there was a difference between antibiotic types in terms of their binding fraction in bovines. There were $N=20$ bovines that were randomly assigned to one of $t=5$ types of antibiotics (the levels of the factor, since only one factor these levels are also the treatments), yielding $n=4$ replicates for each treatment. The data given here, labeled in terms of the One-Way ANOVA format:

Binding Fraction (Y)	Antibiotic	True Trt Mean	Sample Mean
$Y_{11} = 29.6$	Penicillin G	$\mu + \tau_1$	$\bar{y}_{1+} = 28.6$
$Y_{12} = 24.3$	Penicillin G		
$Y_{13} = 28.5$	Penicillin G		
$Y_{14} = 32.0$	Penicillin G		
$Y_{21} = 27.3$	Tetracyclin	$\mu + \tau_2$	$\bar{y}_{2+} = 31.4$
$Y_{22} = 32.6$	Tetracyclin		
$Y_{23} = 30.8$	Tetracyclin		
$Y_{24} = 34.8$	Tetracyclin		
$Y_{31} = 5.8$	Streptomycin	$\mu + \tau_3$	$\bar{y}_{3+} = 7.8$
$Y_{32} = 6.2$	Streptomycin		
$Y_{33} = 11.0$	Streptomycin		
$Y_{34} = 8.3$	Streptomycin		
$Y_{41} = 21.6$	Erythromycin	$\mu + \tau_4$	$\bar{y}_{4+} = 19.1$
$Y_{42} = 17.4$	Erythromycin		
$Y_{43} = 18.3$	Erythromycin		
$Y_{44} = 19.0$	Erythromycin		
$Y_{51} = 29.2$	Chloramphenicol	$\mu + \tau_5$	$\bar{y}_{5+} = 27.8$
$Y_{52} = 32.8$	Chloramphenicol		
$Y_{53} = 25.0$	Chloramphenicol		
$Y_{54} = 24.2$	Chloramphenicol		
$\bar{y}_{++} = 22.9$			

Goal: Test if the population means for these 5 treatments are plausibly equal.
If so, which treatment means differ significantly?

Modeling the binding fraction experiment:

One-Way ANOVA model is appropriate:

$$Y_{ij} = \mu + \tau_i + E_{ij}$$

for $i = 1, \dots, 5$ and $j = 1, \dots, 4$, where E_{ij} are i.i.d. $N(0, \sigma^2)$ errors.

To test $H_0 : \tau_1 = \tau_2 = \dots = \tau_5 = 0$, we just carry out One-Way ANOVA table and look at global p-value.

Table for balanced one-way ANOVA:

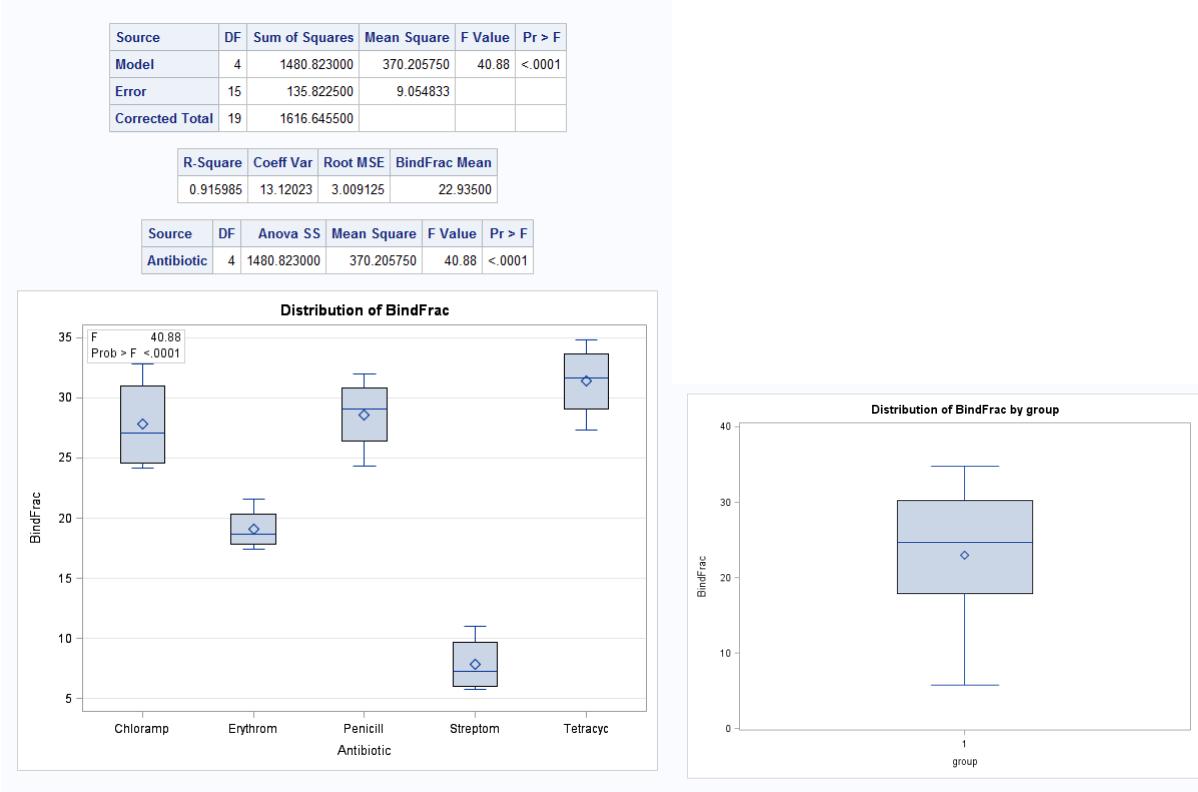
Source	DF	SS	MS	F
Treatments	$t - 1$	$SS(T)$	$MS(T) = \frac{SS(T)}{(t-1)}$	$F = \frac{MS(T)}{MS(E)}$
Error	$t(n - 1)$	$SS(E)$	$MS(E) = \frac{SS(E)}{(N-t)}$	
Total	$nt - 1$	$SS(TOT)$		

where

$$\begin{aligned} SS(T) &= \sum_{i=1}^t \sum_{j=1}^n (\bar{y}_{i+} - \bar{y}_{++})^2 = n \sum_{i=1}^t (\bar{y}_{i+} - \bar{y}_{++})^2 \\ SS(E) &= \sum_{i=1}^t \sum_{j=1}^n (y_{ij} - \bar{y}_{i+})^2 \\ SS(Tot) &= \sum_{i=1}^t \sum_{j=1}^n (y_{ij} - \bar{y}_{++})^2 \end{aligned}$$

Note: $SS(T)$ is also called $SS(\text{Between})$ and $SS(E)$ is also called $SS(\text{Within})$.

For our example,



Conclusion about treatment means begin equal?

Parameter estimates:

- $\hat{\mu} = \bar{y}_{++}$
- $\hat{\tau}_i = \bar{y}_{i+} - \bar{y}_{++}$ and standard errors of treatment means are $\sqrt{\frac{MS(E)}{n}}$
- To compare treatment means we look at $\hat{\tau}_i - \hat{\tau}_j = \bar{y}_{i+} - \bar{y}_{j+}$ with SE = $\sqrt{\frac{2MS(E)}{n}}$

Matrix formulation of the GLM representation of the One-way ANOVA model:
 (will allow us to make inference just as we've done previously!)

$$\mathbf{y} = \begin{pmatrix} 29.6 \\ 24.3 \\ 28.5 \\ 32.0 \\ 27.3 \\ 32.6 \\ 30.8 \\ 34.8 \\ 5.8 \\ 6.2 \\ 11.0 \\ 8.3 \\ 21.6 \\ 17.4 \\ 18.3 \\ 19.0 \\ 29.2 \\ 32.8 \\ 25.0 \\ 24.2 \end{pmatrix} \quad \mathbf{X} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix}$$

SAS proc glm code and output are given below:

```
proc glm data=binding;
class antibiotic;
model bindfrac=antibiotic/solution inverse;
run;
```

The GLM Procedure							
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F		
Model	4	1480.823000	370.205750	40.88	<.0001		
Error	15	135.822500	9.054833				
Corrected Total	19	1616.645500					
R-Square	Coeff Var	Root MSE	BindFrac Mean				
0.915985	13.12023	3.009125	22.93500				
Source	DF	Type I SS	Mean Square	F Value	Pr > F		
Antibiotic	4	1480.823000	370.205750	40.88	<.0001		
Source	DF	Type III SS	Mean Square	F Value	Pr > F		
Antibiotic	4	1480.823000	370.205750	40.88	<.0001		
Parameter		Estimate	Standard Error	t Value	Pr > t 		
Intercept		31.37500000	B	1.50456251	20.85	<.0001	
Antibiotic Chloramp		-3.57500000	B	2.12777270	-1.68	0.1136	
Antibiotic Erythrom		-12.30000000	B	2.12777270	-5.78	<.0001	
Antibiotic Penicill		-2.77500000	B	2.12777270	-1.30	0.2118	
Antibiotic Streptom		-23.55000000	B	2.12777270	-11.07	<.0001	
Antibiotic Tetracyc		0.00000000	B	.	.	.	
X'X Generalized Inverse (g2)							
	Intercept	Dummy001	Dummy002	Dummy003	Dummy004	Dummy005	BindFrac
Intercept	0.25	-0.25	-0.25	-0.25	-0.25	0	31.375
Dummy001	-0.25	0.5	0.25	0.25	0.25	0	-3.575
Dummy002	-0.25	0.25	0.5	0.25	0.25	0	-12.3
Dummy003	-0.25	0.25	0.25	0.5	0.25	0	-2.775
Dummy004	-0.25	0.25	0.25	0.25	0.5	0	-23.55
Dummy005	0	0	0	0	0	0	0
BindFrac	31.375	-3.575	-12.3	-2.775	-23.55	0	135.8225

Estimates of the β 's still found by

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \begin{pmatrix} 27.8 \\ 0.8 \\ 3.6 \\ -20.0 \\ -8.7 \end{pmatrix}$$

Estimates for the five treatment means obtained by using combinations from the $\hat{\boldsymbol{\beta}}$ vector

$$\mu(x_1, x_2, x_3, x_4) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4$$

$$\text{Trt 1 estimate} = \hat{\mu}(1, 0, 0, 0) = \hat{\beta}_0 + \hat{\beta}_1 = 28.6$$

$$\text{Trt 2 estimate} = \hat{\mu}(0, 1, 0, 0) = \hat{\beta}_0 + \hat{\beta}_2 = 31.4$$

$$\text{Trt 3 estimate} = \hat{\mu}(0, 0, 1, 0) = \hat{\beta}_0 + \hat{\beta}_3 = 7.8$$

$$\text{Trt 4 estimate} = \hat{\mu}(0, 0, 0, 1) = \hat{\beta}_0 + \hat{\beta}_4 = 19.1$$

$$\text{Trt 5 estimate} = \hat{\mu}(0, 0, 0, 0) = \hat{\beta}_0 = 27.8$$

For standard errors of the $\hat{\beta}$'s we still have our variance-covariance matrix $\hat{\Sigma} = MS(E)(\mathbf{X}'\mathbf{X})^{-1}$

$$\hat{\Sigma} = MS(E)(\mathbf{X}'\mathbf{X})^{-1} = \begin{pmatrix} 2.3 & -2.3 & -2.3 & -2.3 & -2.3 \\ & 4.5 & 2.3 & 2.3 & 2.3 \\ & & 4.5 & 2.3 & 2.3 \\ & & & 4.5 & 2.3 \\ & & & & 4.5 \end{pmatrix}$$

Note the pattern, what is the reason for it?

To get SE's of our treatment mean estimates we can use vectors: Let $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ be defined by

$$\mathbf{a}^T = (1, 1, 0, 0, 0), \mathbf{b}^T = (1, 0, 1, 0, 0), \mathbf{c}^T = (1, 0, 0, 1, 0), \mathbf{d}^T = (1, 0, 0, 0, 1).$$

Then

$$\begin{aligned} \hat{\mu}(1, 0, 0, 0) &= \hat{\beta}_0 + \hat{\beta}_1 = \mathbf{a}^T \hat{\beta} \\ \hat{\mu}(0, 1, 0, 0) &= \hat{\beta}_0 + \hat{\beta}_2 = \mathbf{b}^T \hat{\beta} \\ \hat{\mu}(0, 0, 1, 0) &= \hat{\beta}_0 + \hat{\beta}_3 = \mathbf{c}^T \hat{\beta} \\ \hat{\mu}(0, 0, 0, 1) &= \hat{\beta}_0 + \hat{\beta}_4 = \mathbf{d}^T \hat{\beta} \\ \hat{\mu}(0, 0, 0, 0) &= \hat{\beta}_0 = \hat{\beta}_0 \end{aligned}$$

and for a balanced design the variances are all the same and are given by

$$\mathbf{a}'\hat{\Sigma}\mathbf{a} = \mathbf{b}'\hat{\Sigma}\mathbf{b} = \mathbf{c}'\hat{\Sigma}\mathbf{c} = \mathbf{d}'\hat{\Sigma}\mathbf{d} = \widehat{\text{Var}}(\hat{\beta}_0) = \widehat{\text{Var}}(\hat{\beta}_0 + \hat{\beta}_j) = 2.3$$

so the estimated SE for any sample treatment mean is $\sqrt{2.3} = 1.5$.

Recall from one-way ANOVA that

$$\widehat{SE}(\bar{y}_{i+}) = \sqrt{\frac{MS(E)}{n}} = \sqrt{\frac{9.1}{4}} = \sqrt{2.3} = 1.5$$

and that for differences between treatment means

$$\widehat{SE}(\bar{y}_{i+} - \bar{y}_{j+}) = \sqrt{\frac{2MS(E)}{n}} = \sqrt{4.5} = 2.1$$

Now we have a framework to use both quantitative and categorical explanatory variables at the same time!

A general linear model for 5k times of men AND women:

Using $X_1 = \text{Age}$, we fit a quadratic model $\mu(x_1) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$ for to predict the mean pace for runners. Consider modeling gender (a categorical variable) as well.

Let x_3 be defined by

$$x_3 = \begin{cases} 1 & \text{female} \\ 0 & \text{male} \end{cases}$$

Some candidate models:

1. The ‘null’ model:

$$\mu(x_1, x_3) = \beta_0$$

2. The One-Way ANOVA model in GLM form:

$$\mu(x_1, x_3) = \beta_0 + \beta_3 x_3$$

3. The SLR model using Age:

$$\mu(x_1, x_3) = \beta_0 + \beta_1 x_1$$

4. The MLR model quadratic in Age:

$$\mu(x_1, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$$

5. A GLM that allows for different intercepts for our parabolas:

$$\mu(x_1, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_3$$

This model has intercept β_0 for males ($x_3 = 0$) and intercept $\beta_0 + \beta_3$ for females ($x_3 = 1$).

$$\text{Equation for males: } \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$$

$$\text{Equation for females: } (\beta_0 + \beta_3) + \beta_1 x_1 + \beta_2 x_1^2$$

6. A GLM that allows for different intercepts and for different shapes of the parabolas:

$$\mu(x_1, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_3 + \beta_4 x_1 x_3 + \beta_5 x_1^2 x_3$$

Intercepts as in the previous model. ‘Linear’ term for males is β_1 and is $\beta_1 + \beta_4$ for females. ‘Quadratic’ term for males is β_2 and is $\beta_2 + \beta_5$ for females.

$$\text{Equation for males: } \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$$

$$\text{Equation for females: } (\beta_0 + \beta_3) + (\beta_1 + \beta_4)x_1 + (\beta_2 + \beta_5)x_1^2$$

We can fit these models in proc glm using the following code: (Note: each model must be done in a separate proc glm statement)

```
proc glm;
class sex;
title 'Model 2';
model pace=sex;
title 'Model 3';
model pace=age;
title 'Model 4';
model pace=age age*age;
title 'Model 5';
model pace=age age*age sex;
title 'Model 6';
model pace=age age*age sex sex*age*age;
run;
```

Model 2

2

The GLM Procedure

Dependent Variable: pace

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	170.7413698	170.7413698	43.70	<.0001
Error	158	617.3533455	3.9072997		
Corrected Total	159	788.0947153			

R-Square	Coeff Var	Root MSE	pace Mean
0.216651	21.67274	1.976689	9.120625

Source	DF	Type I SS	Mean Square	F Value	Pr > F
sex	1	170.7413698	170.7413698	43.70	<.0001

Source	DF	Type III SS	Mean Square	F Value	Pr > F
sex	1	170.7413698	170.7413698	43.70	<.0001

Parameter	Estimate		Standard Error	t Value	Pr > t
Intercept	8.266140351	B	0.20280402	40.76	<.0001
sex F	2.103346829	B	0.31818512	6.61	<.0001
sex M	0.000000000	B	.	.	.

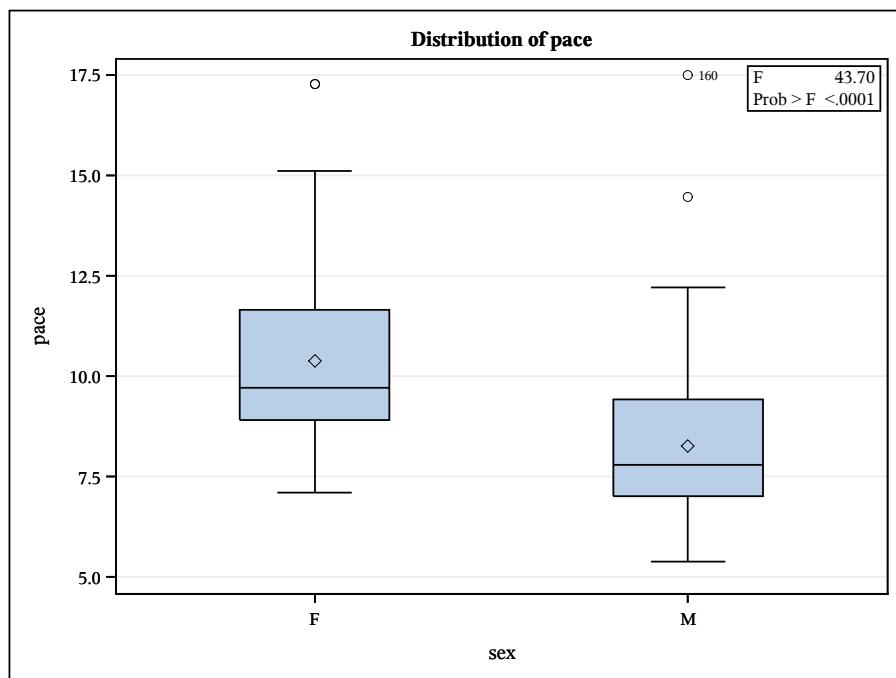
Note: The X'X matrix has been found to be singular, and a generalized inverse was used to solve the normal equations. Terms whose estimates are followed by the letter 'B' are not uniquely estimable.

Model 2

3

The GLM Procedure

Dependent Variable: pace



Model 3

5

The GLM Procedure

Dependent Variable: pace

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	1.0965043	1.0965043	0.22	0.6396
Error	158	786.9982110	4.9810013		
Corrected Total	159	788.0947153			

R-Square	Coeff Var	Root MSE	pace Mean
0.001391	24.46999	2.231816	9.120625

Source	DF	Type I SS	Mean Square	F Value	Pr > F
age	1	1.09650427	1.09650427	0.22	0.6396

Source	DF	Type III SS	Mean Square	F Value	Pr > F
age	1	1.09650427	1.09650427	0.22	0.6396

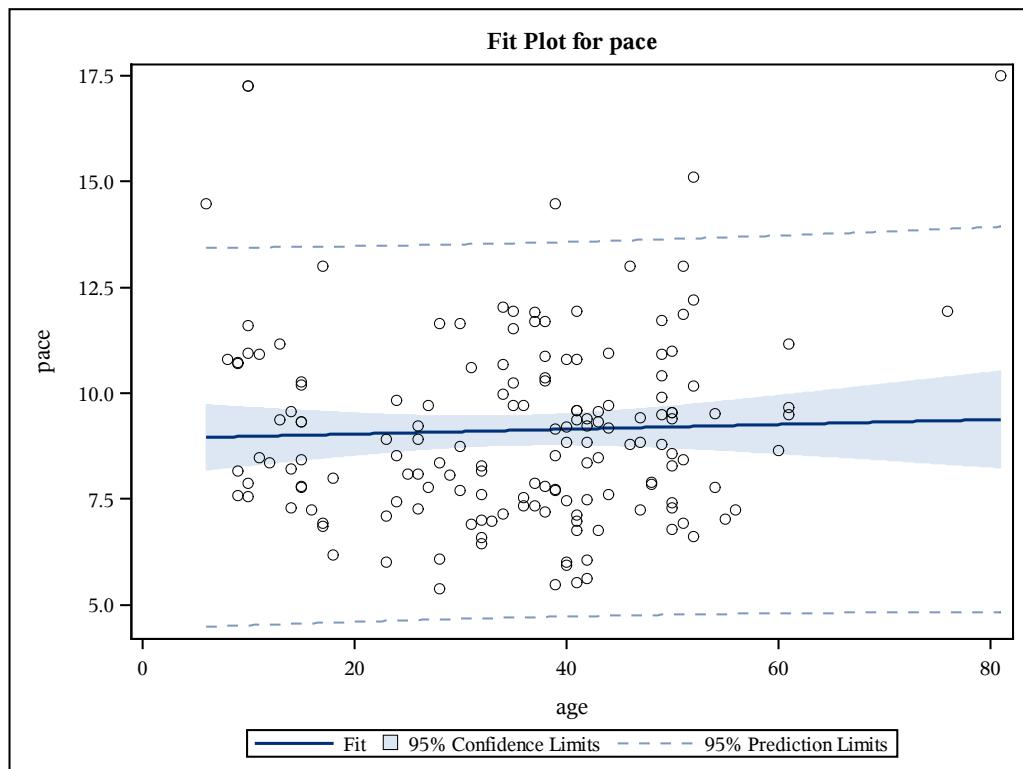
Parameter	Estimate	Standard Error	t Value	Pr > t
Intercept	8.922709126	0.45724042	19.51	<.0001
age	0.005643654	0.01202856	0.47	0.6396

Model 3

6

The GLM Procedure

Dependent Variable: pace



Model 4

8

The GLM Procedure

Dependent Variable: pace

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	113.6450003	56.8225001	13.23	<.0001
Error	157	674.4497150	4.2958581		
Corrected Total	159	788.0947153			

R-Square	Coeff Var	Root MSE	pace Mean
0.144202	22.72482	2.072645	9.120625

Source	DF	Type I SS	Mean Square	F Value	Pr > F
age	1	1.0965043	1.0965043	0.26	0.6141
age*age	1	112.5484960	112.5484960	26.20	<.0001

Source	DF	Type III SS	Mean Square	F Value	Pr > F
age	1	98.5223939	98.5223939	22.93	<.0001
age*age	1	112.5484960	112.5484960	26.20	<.0001

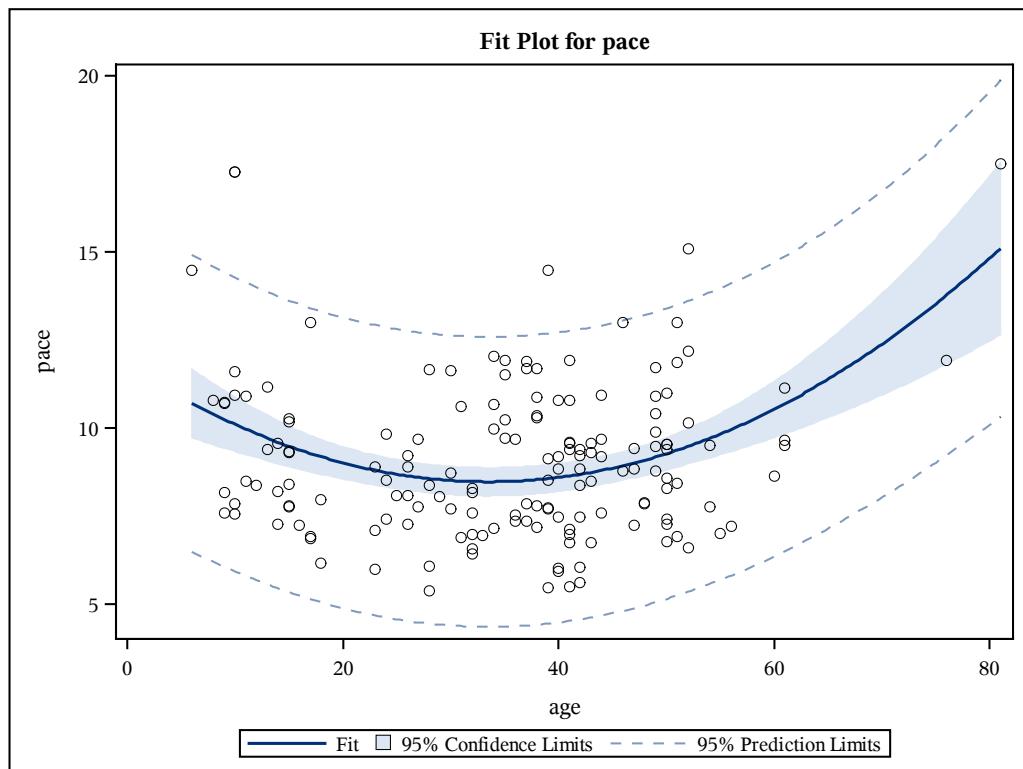
Parameter	Estimate	Standard Error	t Value	Pr > t
Intercept	11.78503486	0.70215799	16.78	<.0001
age	-0.19699301	0.04113470	-4.79	<.0001
age*age	0.00293699	0.00057380	5.12	<.0001

Model 4

9

The GLM Procedure

Dependent Variable: pace



Model 5

11

The GLM Procedure

Dependent Variable: pace

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	290.3485074	96.7828358	30.33	<.0001
Error	156	497.7462079	3.1906808		
Corrected Total	159	788.0947153			

R-Square	Coeff Var	Root MSE	pace Mean
0.368418	19.58471	1.786248	9.120625

Source	DF	Type I SS	Mean Square	F Value	Pr > F
age	1	1.0965043	1.0965043	0.34	0.5586
age*age	1	112.5484960	112.5484960	35.27	<.0001
sex	1	176.7035071	176.7035071	55.38	<.0001

Source	DF	Type III SS	Mean Square	F Value	Pr > F
age	1	73.9438080	73.9438080	23.17	<.0001
age*age	1	102.7473738	102.7473738	32.20	<.0001
sex	1	176.7035071	176.7035071	55.38	<.0001

Parameter	Estimate		Standard Error	t Value	Pr > t
Intercept	10.18316690	B	0.64227743	15.85	<.0001
age	-0.17145849		0.03561638	-4.81	<.0001
age*age	0.00280792		0.00049481	5.67	<.0001
sex F	2.19792213	B	0.29534621	7.44	<.0001
sex M	0.00000000	B	.	.	.

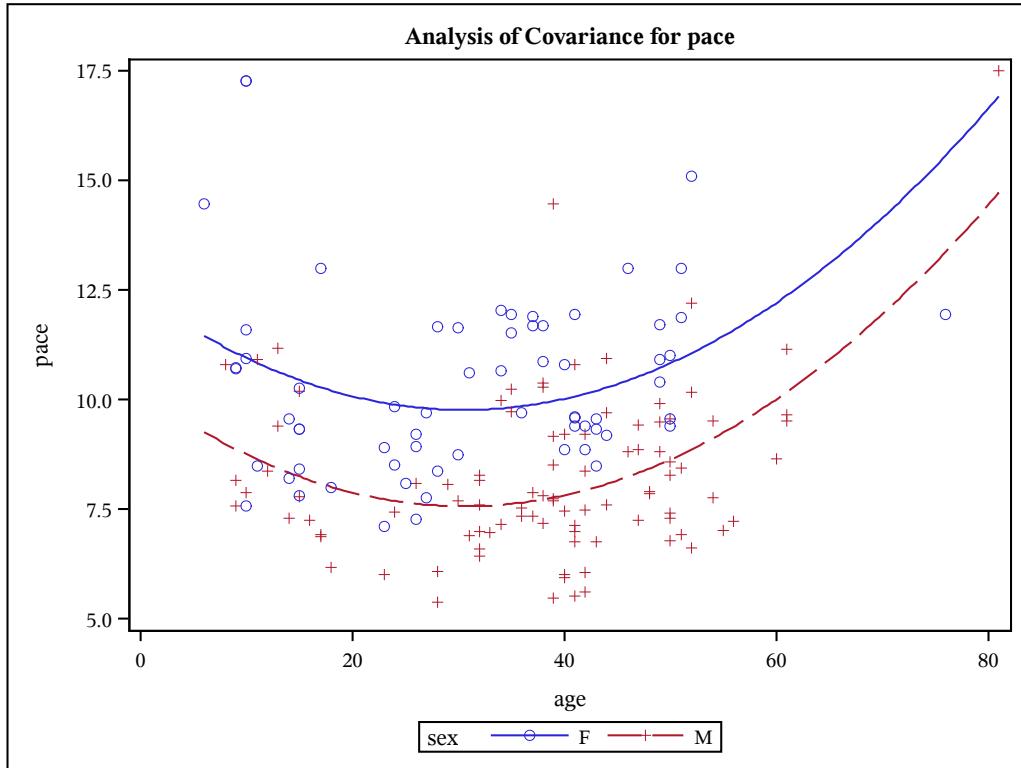
Note: The X'X matrix has been found to be singular, and a generalized inverse was used to solve the normal equations. Terms whose estimates are followed by the letter 'B' are not uniquely estimable.

Model 5

12

The GLM Procedure

Dependent Variable: pace



Model 6

14

The GLM Procedure

Dependent Variable: pace

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	5	293.5282772	58.7056554	18.28	<.0001
Error	154	494.5664380	3.2114704		
Corrected Total	159	788.0947153			

R-Square	Coeff Var	Root MSE	pace Mean
0.372453	19.64841	1.792058	9.120625

Source	DF	Type I SS	Mean Square	F Value	Pr > F
age	1	1.0965043	1.0965043	0.34	0.5599
age*age	1	112.5484960	112.5484960	35.05	<.0001
sex	1	176.7035071	176.7035071	55.02	<.0001
age*sex	1	0.0057235	0.0057235	0.00	0.9664
age*age*sex	1	3.1740464	3.1740464	0.99	0.3217

Source	DF	Type III SS	Mean Square	F Value	Pr > F
age	1	66.02141759	66.02141759	20.56	<.0001
age*age	1	87.52232536	87.52232536	27.25	<.0001
sex	1	3.34259172	3.34259172	1.04	0.3092
age*sex	1	2.85593189	2.85593189	0.89	0.3471
age*age*sex	1	3.17404636	3.17404636	0.99	0.3217

Parameter	Estimate	Standard Error	t Value	Pr > t
Intercept	10.60848468	B	0.88640608	11.97 <.0001
age	-0.19985505	B	0.04841621	-4.13 <.0001
age*age	0.00320665	B	0.00064628	4.96 <.0001
sex F	1.25727925	B	1.23237262	1.02 0.3092
sex M	0.00000000	B	.	.
age*sex F	0.06882008	B	0.07297821	0.94 0.3471
age*sex M	0.00000000	B	.	.

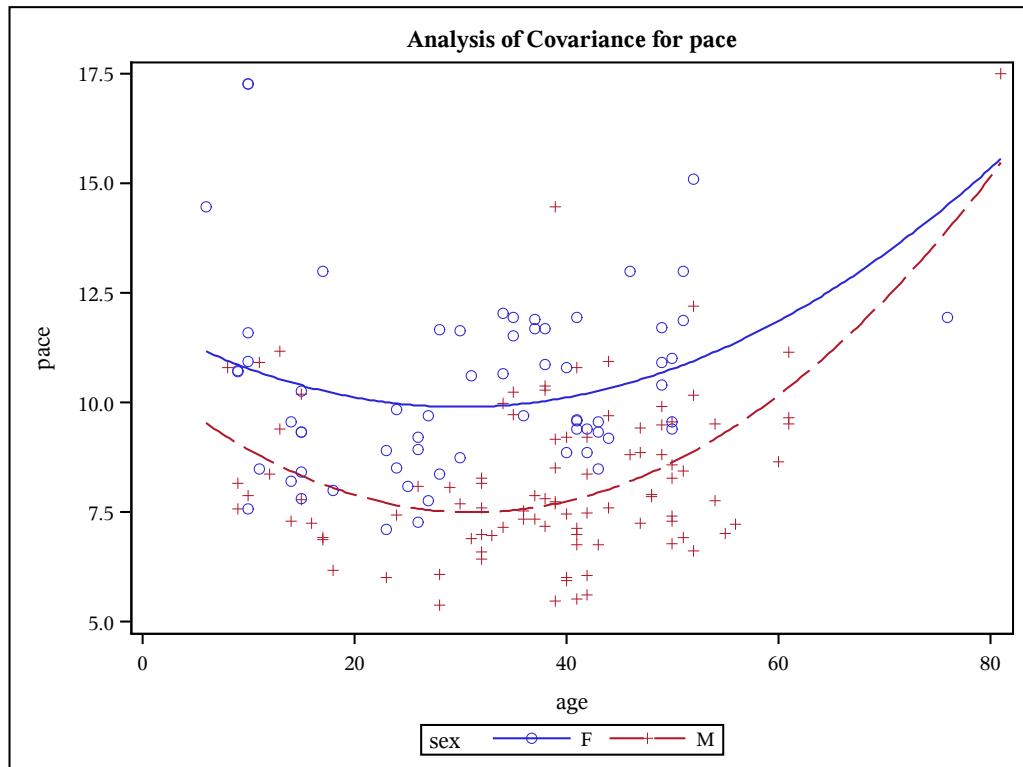
Model 6

15

The GLM Procedure**Dependent Variable: pace**

Parameter	Estimate	Standard Error	t Value	Pr > t	
age*age*sex F	-0.00102594	B	0.00103197	-0.99	0.3217
age*age*sex M	0.00000000	B	.	.	.

Note: The X'X matrix has been found to be singular, and a generalized inverse was used to solve the normal equations. Terms whose estimates are followed by the letter 'B' are not uniquely estimable.



Analysis of covariance, ANCOVA or ACOVA:

Recall the three principles of experimental design:

- Randomization
- Replication
- Error Reducing Methods

One method of error reduction we looked at was blocking. Here we split up the EUs and then randomize treatments to each block. In this way, every treatment occurs in each block and the block effects cancel out.

We are not always able to block, sometimes we don't have the value of the covariate until after the experiment is done. A similar method that will account for these types of covariates is called Analysis of CoVariance (ANCOVA).

Associations between covariates z and the main response variable of interest y can be used to reduce unexplained variation σ^2 .

An nutrition example:

A nutrition scientist conducted an experiment to evaluate the effects of four vitamin supplements on the weight gain of laboratory animals. The experiment was conducted in a completely randomized design with $N = 20$ animals randomized to $a = 4$ supplement groups, each with sample size $n \equiv 5$. The response variable of interest is weight gain, but calorie intake z was measured concomitantly as couldn't separate EUs by this at the beginning.

Diet	$y(g)$	Diet	y	Diet	y	Diet	y
1	48	2	65	3	79	4	59
1	67	2	49	3	52	4	50
1	78	2	37	3	63	4	59
1	69	2	75	3	65	4	42
1	53	2	63	3	67	4	34
1	$\bar{y}_{1+} = 63.0$	2	$\bar{y}_{2+} = 57.4$	3	$\bar{y}_{3+} = 65.2$	4	$\bar{y}_{4+} = 48.8$
1	$s_1 = 12.3$	2	$s_2 = 14.3$	3	$s_3 = 9.7$	4	$s_4 = 10.9$

Q: Is there evidence of a vitamin supplement effect?

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	797.800000	265.933333	1.82	0.1836
Error	16	2334.400000	145.900000		
Corrected Total	19	3132.200000			

P-value < 0.05, fail to reject H_0 . There is no evidence of a diet effect.

Calorie intake z was measured concomitantly:

Diet	y	z									
1	48	350	2	65	400	3	79	510	4	59	530
1	67	440	2	49	450	3	52	410	4	50	520
1	78	440	2	37	370	3	63	470	4	59	520
1	69	510	2	73	530	3	65	470	4	42	510
1	53	470	2	63	420	3	67	480	4	34	430

Q: How and why could these new data be incorporated into analysis?

A: A GLM can take into account both types of variables! The method of ANCOVA can be used to reduce unexplained variation.

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_z z_i + E_i \quad \text{for } i = 1, \dots, 20$$

where x_{ij} is an indicator variable for subject i receiving vitamin supplement j :

$$x_{ij} = \begin{cases} 1 & \text{subject } i \text{ receives supplement } j \\ 0 & \text{else} \end{cases}$$

and errors $E_i \stackrel{iid}{\sim} N(0, \sigma^2)$.

Which Diet is being used as the baseline?

Diet 4

Proceeding with MLR analysis of this GLM:

```
proc glm data=diets;
class diet;
model gain = diet caloric;
run;
```

The GLM Procedure

Dependent Variable: gain

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	4	1951.680373	487.920093	6.20	0.0038
Error	15	1180.519627	78.701308		
Corrected Total	19	3132.200000			

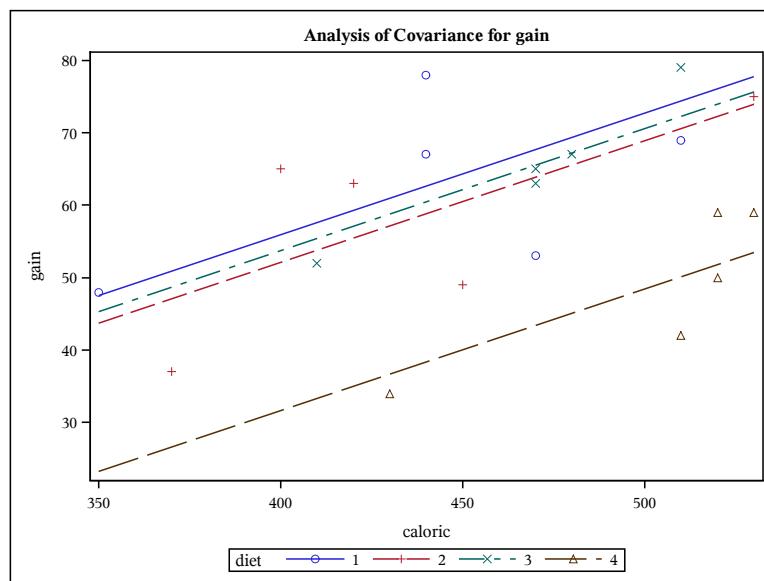
R-Square	Coeff Var	Root MSE	gain Mean
0.623102	15.11308	8.871376	58.70000

Source	DF	Type I SS	Mean Square	F Value	Pr > F
diet	3	797.800000	265.933333	3.38	0.0463
caloric	1	1153.880373	1153.880373	14.66	0.0016

Source	DF	Type III SS	Mean Square	F Value	Pr > F
diet	3	1537.071659	512.357220	6.51	0.0049
caloric	1	1153.880373	1153.880373	14.66	0.0016

The GLM Procedure

Dependent Variable: gain



How can we estimate the mean weight gains for diet, taking into account the caloric intake?

Adjusted vs unadjusted means:

The sample mean weight gains for the four diets and for the caloric intake for each diet group were

Level of diet	N	gain		caloric	
		Mean	Std Dev	Mean	Std Dev
1	5	63.0000000	12.2678441	442.000000	58.9067059
2	5	57.8000000	14.8727940	434.000000	61.0737259
3	5	65.2000000	9.6540147	468.000000	36.3318042
4	5	48.8000000	10.8949530	502.000000	40.8656335

The means for each diet are ‘unadjusted’ means. According to our analysis, caloric intake has a significant effect on weight gain. However, each diet group had a different mean amount of caloric intake. What does this imply?

Unadjusted means do not make any adjustment for the facts that

1. caloric intake may vary by diet (presumably by chance, not because of diet)
2. weight gain depends on caloric intake

Adjusted means or **lsmeans** (least squares means) will estimate mean weight gains at a common value of our caloric intake (our covariate z). The value often used for comparison is \bar{z} , the sample mean of the covariate.

Here, $\bar{z} = (442 + 434 + 468 + 502)/4 = 461.5$. The adjusted means are then just (the sub a is to differentiate unadjusted means and adjusted means)

$$\begin{aligned}\bar{y}_{1,a} &= \hat{\beta}_0 + \hat{\beta}_1 + \hat{\beta}_z(461.5) \\ \bar{y}_{2,a} &= \hat{\beta}_0 + \hat{\beta}_2 + \hat{\beta}_z(461.5) \\ \bar{y}_{3,a} &= \hat{\beta}_0 + \hat{\beta}_3 + \hat{\beta}_z(461.5) \\ \bar{y}_{4,a} &= \hat{\beta}_0 + \hat{\beta}_z(461.5)\end{aligned}$$

To get SAS to report the estimated regression parameter vector $\hat{\beta}$, use the **solution** option in the model statement. The default parametrization is the one we've adopted here where β_0 is the mean of the last level of the classification treatment factor:

Parameter	Estimate	Standard Error	t Value	Pr > t
Intercept	-35.66310108	B	22.41252629	-1.59 0.1324
diet 1	24.29519136	B	6.19932022	3.92 0.0014
diet 2	20.44121688	B	6.35678835	3.22 0.0058
diet 3	22.12060844	B	5.80625371	3.81 0.0017
diet 4	0.00000000	B	.	.
caloric	0.16825319		0.04394140	3.83 0.0016

Substitution of $\hat{\beta}$ into the expressions for adjusted means yields

$$\begin{aligned}\bar{y}_{1,a} &= -35.7 + 24.3 + 0.17(461.5) = 66.3 \\ \bar{y}_{2,a} &= -35.7 + 20.4 + 0.17(461.5) = 62.4 \\ \bar{y}_{3,a} &= -35.7 + 22.1 + 0.17(461.5) = 64.1 \\ \bar{y}_{4,a} &= -35.7 + 0.17(461.5) = 42.0\end{aligned}$$

These means are better for comparisons between diets as the effect of caloric intake (which affects weight gain) is constant across all the diets. Thus, we are removing its effect.

To get proc glm to produce the estimates (above), unadjusted means (above), $(\mathbf{X}^T \mathbf{X})^{-1}$ matrix (below), adjusted means with standard errors (below), and CI's (below):

```
proc glm data=diets;
class diet;
model gain = diet caloric/solution inverse;
means diet;
lsmeans diet/stderr cl;
run;
```

X'X Generalized Inverse (g2)							
	Intercept	diet 1	diet 2	diet 3	diet 4	caloric	gain
Intercept	6.3826300294	-0.938959764	-1.037487733	-0.618743867	0	-0.012315996	-35.66310108
diet 1	-0.938959764	0.4883218842	0.3000981354	0.2500490677	0	0.0014720314	24.295191364
diet 2	-1.037487733	0.3000981354	0.5134445535	0.2567222767	0	0.0016683023	20.441216879
diet 3	-0.618743867	0.2500490677	0.2567222767	0.4283611384	0	0.0008341511	22.12060844
diet 4	0	0	0	0	0	0	0
caloric	-0.012315996	0.0014720314	0.0016683023	0.0008341511	0	0.0000245339	0.1682531894
gain	-35.66310108	24.295191364	20.441216879	22.12060844	0	0.1682531894	1180.5196271

The $(\mathbf{X}^T \mathbf{X})^{-1}$ matrix is found by removing the row/column with 0's and ignoring the row/column for the response.

diet	gain LSMEAN	Standard Error	Pr > t
1	66.2809372	4.0588750	<.0001
2	62.4269627	4.1473443	<.0001
3	64.1063543	3.9776677	<.0001
4	41.9857458	4.3482563	<.0001

diet	gain LSMEAN	95% Confidence Limits	
1	66.280937	57.629650	74.932224
2	62.426963	53.587108	71.266818
3	64.106354	55.628156	72.584552
4	41.985746	32.717657	51.253835

We can now look at all pairwise differences of the lsmeans to see which levels differ significantly.

ANCOVA - What did we just do? We used our covariate to reduce the unexplained variation in our response, allowing a clearer picture of our treatment differences.

Huge assumptions of ANCOVA - We assume the treatment *does not* affect the covariate. In this example, we assume the diets are not causing the animals to have different caloric intake (i.e. do not cause them to eat more or less). (We also need to do our usual assumption checking.)

We can inspect this assumption. Let our covariate be our response and conduct an ANOVA using the diets as our treatments. The global p-value will test if the caloric intake means differ significantly for each diet. We hope to see no significance here!

```
proc anova data=diets;
class diet;
model caloric = diet;
run;
```

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	14095.00000	4698.33333	1.84	0.1798
Error	16	40760.00000	2547.50000		
Corrected Total	19	54855.00000			

No evidence that treatment affects covariate.

Chapter 8

ST 512 - Contrasts and Multiple Comparisons

Readings: 9.1-9.5 326-360

Consider the traditional balanced One-Way ANOVA model. That is, we have a *continuous* response, Y , and a *qualitative or categorical* predictor which we call our **factor**. This factor has t *levels* (also the *treatments* in this case) and our interest lies in whether or not the mean response differs between the treatments.

The parametrization of the One-way ANOVA model we have looked at is

$$Y_{ij} = \mu + \tau_i + E_{ij}, \quad i = 1, 2, \dots, t, \quad j = 1, \dots, n_i,$$

$E_{ij} \sim N(0, \sigma^2)$ (balanced implies n_i is the same for all levels). The (true) treatment mean for treatment i is given by $\mu + \tau_i = \mu_i$.

Consider the bovine antibiotic/binding percentage example from earlier. Let

$$\begin{aligned}\mu_1 &= \mu + \tau_1 = \text{mean of Chloramphenicol treatment} \\ \mu_2 &= \mu + \tau_2 = \text{mean of Erythromycin treatment} \\ \mu_3 &= \mu + \tau_3 = \text{mean of Penicillin G treatment} \\ \mu_4 &= \mu + \tau_4 = \text{mean of Streptomycin treatment} \\ \mu_5 &= \mu + \tau_5 = \text{mean of Tetracyclin treatment}\end{aligned}$$

There were four observations at each treatment level. Recall the p-value for testing the global hypothesis that

$$H_0 : \tau_1 = \tau_2 = \tau_3 = \tau_4 = \tau_5 = 0 \quad vs \quad H_A : \text{At least 1 differs}$$

which is equivalent to testing

$$H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4 = \mu_5 = 0 \quad vs \quad H_A : \text{At least 1 differs}$$

was < 0.0001 implying we should reject H_0 in favor of H_A . That is, at the 5% significance level there is enough evidence to conclude the mean for at least one of the antibiotics differs.

Given the answer to the previous question, the next logical question to answer is: ‘Which treatment means are different?’ Suppose we want first inspect the difference between the Cholramphenicol (μ_1) and Erythromycin treatment means (μ_2). In terms of μ_1 and μ_2 , how can we write this question as a null and alternative hypotheses?

This is an example of a **linear combination** of treatment means. In general, a linear combination of treatment means takes the form

For the bovine experiment, which of the following are linear combinations of treatment means?

- $\theta_6 = 4\mu_1 + 3\mu_2 - 7\mu_5$
- $\theta_7 = 3\mu_1\mu_4 + 2\mu_3$
- $\theta_8 = \mu_1 + \mu_2 + \mu_3 + \mu_4 + \mu_5$
- $\theta_9 = \mu_1^2 + 3\mu_2 + 1$

If the coefficients of the linear combination sum to zero (i.e. $c_1 + c_2 + \dots + c_t = 0$), the linear combination is called a **contrast**.

Is our linear combination $\mu_1 - \mu_2 = 0$ a contrast? How about any of θ_6 through θ_9 ?

If we want to do inference about a linear combination of treatment means we need an estimator of θ , call it $\hat{\theta}$ and we will also need a measure of variability, say $\hat{SE}(\hat{\theta})$.

An estimator is given by substitution of the sample means:

$$\hat{\theta} = c_1 \bar{Y}_{1+} + c_2 \bar{Y}_{2+} + \dots + c_t \bar{Y}_{t+}$$

Use the output from the code that follows to estimate the following linear combinations:

$$\theta_1 = \mu_1 \quad \hat{\theta}_1 = \bar{y}_{1+} = \underline{\hspace{10cm}}$$

$$\theta_2 = \mu_2 \quad \hat{\theta}_2 = \bar{y}_{2+} = \underline{\hspace{10cm}}$$

$$\theta_3 = \mu_3 \quad \hat{\theta}_3 = \bar{y}_{3+} = \underline{\hspace{10cm}}$$

$$\theta_4 = \mu_4 \quad \hat{\theta}_4 = \bar{y}_{4+} = \underline{\hspace{10cm}}$$

$$\theta_5 = \mu_5 \quad \hat{\theta}_5 = \bar{y}_{5+} = \underline{\hspace{10cm}}$$

What is the relationship between the $\hat{\beta}$ estimates (from the '/solution' option) and these means again?

```

proc glm data=binding;
class antibiotic;
model bindfrac=antibiotic/solution;
means antibiotic;
run;

```

Parameter	Estimate		Standard Error	t Value	Pr > t
Intercept	31.37500000	B	1.50456251	20.85	<.0001
Antibiotic Chloramp	-3.57500000	B	2.12777270	-1.68	0.1136
Antibiotic Erythrom	-12.30000000	B	2.12777270	-5.78	<.0001
Antibiotic Penicill	-2.77500000	B	2.12777270	-1.30	0.2118
Antibiotic Streptom	-23.55000000	B	2.12777270	-11.07	<.0001
Antibiotic Tetracyc	0.00000000	B	.	.	.

Level of Antibiotic	N	BindFrac	
		Mean	Std Dev
Chloramp	4	27.8000000	3.98998747
Erythrom	4	19.0750000	1.80623919
Penicill	4	28.6000000	3.21765960
Streptom	4	7.8250000	2.38379949
Tetracyc	4	31.3750000	3.17109340

Find an estimate of our contrast $\theta = \mu_1 - \mu_2$. Find an estimate for θ_6 and θ_8 .

We now have a point estimate of the quantity in our null hypothesis, in order to conduct our test we must also know about the variability of this estimate, i.e. What is $\hat{Var}(\hat{\theta})$ or $\hat{SE}(\hat{\theta})$?

The variance of a linear combination of means in One-way ANOVA has a very nice form:

Due to the normality assumption on our errors we can use a t-test. Let θ_0 be a value of interest for our contrast (often 0). To test $H_0 : \theta = \theta_0$ vs $H_A : \theta \neq \theta_0$ we can use

$$t = \frac{\hat{\theta} - \theta_0}{\hat{SE}(\hat{\theta})} \sim t_{t(n-1)} \text{ under } H_0$$

What is the value of this test statistic for our contrast $\theta = \mu_1 - \mu_2$? Compare it to $t(0.975, 15) = 2.13$, what is your conclusion? What is your interpretation?

Likewise a confidence interval can be formed using

$$\hat{\theta} \pm t(\alpha/2, t(n-1)) \hat{SE}(\hat{\theta}) = \sum_{i=1}^t c_i \bar{y}_{i+} \pm t(\alpha/2, t(n-1)) \sqrt{MS(E) \sum_{i=1}^t \frac{c_i^2}{n_i}}$$

What is a 95% CI for $\theta = \mu_1 - \mu_2$? Does your conclusion here match the conclusion using the test statistic?

Note: A contrast that has only two nonzero c 's is called a pairwise contrast (as it looks at only two means). These can be had easily in proc glm using the code below.

A **complex** contrast is a contrast that involves more than two non-zero coefficients. For example, $\theta_{10} = \frac{\mu_1 + \mu_2}{2} - \frac{\mu_3 + \mu_4}{2}$ is a complex contrast.

```
proc glm data=binding;
class antibiotic;
model bindfrac=antibiotic/solution;
means antibiotic/ lsd cldiff lines;
lsmeans antibiotic/stderr pdiff;
run;
```

*Generally we'll want to use lsmeans not means, but ok here since no covariates involved and a balanced design was done.

The SAS System12:³**The GLM Procedure****t Tests (LSD) for BindFrac**

Note: This test controls the Type I comparisonwise error rate, not the experimentwise

Alpha	0.05
Error Degrees of Freedom	15
Error Mean Square	9.054833
Critical Value of t	2.13145
Least Significant Difference	4.5352

The SAS System

12:34 Sunday, February 16,

The GLM Procedure**t Tests (LSD) for BindFrac**

Note: This test controls the Type I comparisonwise error rate, not the experimentwise error rate.

Alpha	0.05
Error Degrees of Freedom	15
Error Mean Square	9.054833
Critical Value of t	2.13145
Least Significant Difference	4.5352

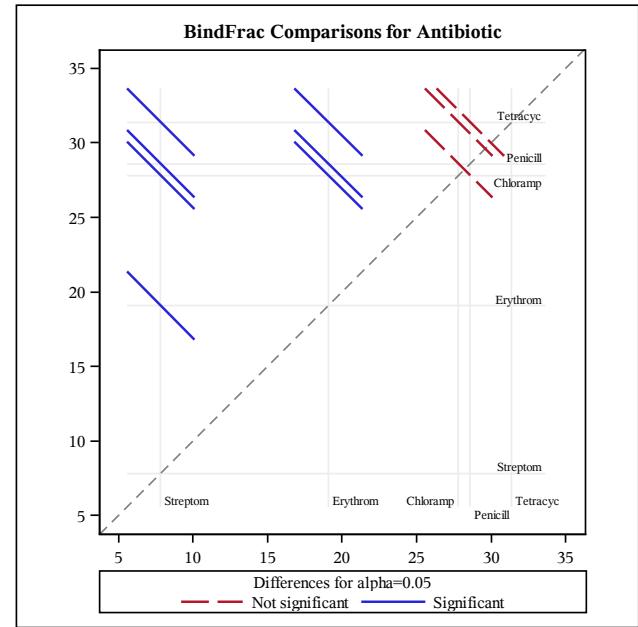
Comparisons significant at the 0.05 level are indicated by ***.				
Antibiotic Comparison	Difference Between Means	95% Confidence Limits		
Tetracyc - Penicill	2.775	-1.760	7.310	
Tetracyc - Chloramp	3.575	-0.960	8.110	
Tetracyc - Erythrom	12.300	7.765	16.835	***
Tetracyc - Streptom	23.550	19.015	28.085	***
Penicill - Tetracyc	-2.775	-7.310	1.760	
Penicill - Chloramp	0.800	-3.735	5.335	
Penicill - Erythrom	9.525	4.990	14.060	***
Penicill - Streptom	20.775	16.240	25.310	***
Chloramp - Tetracyc	-3.575	-8.110	0.960	
Chloramp - Penicill	-0.800	-5.335	3.735	
Chloramp - Erythrom	8.725	4.190	13.260	***
Chloramp - Streptom	19.975	15.440	24.510	***
Erythrom - Tetracyc	-12.300	-16.835	-7.765	***
Erythrom - Penicill	-9.525	-14.060	-4.990	***
Erythrom - Chloramp	-8.725	-13.260	-4.190	***
Erythrom - Streptom	11.250	6.715	15.785	***
Streptom - Tetracyc	-23.550	-28.085	-19.015	***
Streptom - Penicill	-20.775	-25.310	-16.240	***
Streptom - Chloramp	-19.975	-24.510	-15.440	***
Streptom - Erythrom	-11.250	-15.785	-6.715	***

Means with the same letter are not significantly different.			
t Grouping	Mean	N	Antibiotic
A	31.375	4	Tetracyc
A			
A	28.600	4	Penicill
A			
A	27.800	4	Chloramp
B	19.075	4	Erythrom
C	7.825	4	Streptom

The GLM Procedure
Least Squares Means

Antibiotic	BindFrac LSMEAN	Standard Error	Pr > t	LSMEAN Number
Chloramp	27.800000	1.5045625	<.0001	1
Erythrom	19.075000	1.5045625	<.0001	2
Penicill	28.600000	1.5045625	<.0001	3
Streptom	7.825000	1.5045625	0.0001	4
Tetracyc	31.375000	1.5045625	<.0001	5

Least Squares Means for effect Antibiotic Pr > t for H0: LSMean(i)=LSMean(j)					
Dependent Variable: BindFrac					
i/j	1	2	3	4	5
1		0.0009	0.7122	<.0001	0.1136
2	0.0009		0.0004	<.0001	<.0001
3	0.7122	0.0004		<.0001	0.2118
4	<.0001	<.0001	<.0001		<.0001
5	0.1136	<.0001	0.2118	<.0001	

The GLM Procedure
Least Squares Means


Note: To ensure overall protection level, only probabilities associated with pre-planned comparisons should be used.

Use the output to construct a 95% CI for θ_{10} .

To get the estimate for θ_{10} (and a few other linear combinations of means) in SAS we can use glm but it will be easiest to use proc mixed:

```

proc glm data=binding;
class antibiotic;
model bindfrac=antibiotic/clparm;
estimate 'lsmean for trt 2' intercept 1 antibiotic 0 1 0 0 0;
estimate 'avg of trt 2 mean and trt 3 mean' intercept 2 antibiotic 0 1 1 0 0/divisor=2;
estimate 'trt 1 vs trt 5' intercept 0 antibiotic 1 0 0 0 -1;
estimate 'avg of 1 and 2 vs avg of 3 and 4' intercept 0 antibiotic 1 1 -1 -1 0/divisor=2;
run;

proc mixed data=binding;
class antibiotic;
model bindfrac=antibiotic;
lsmeans antibiotic 'lsmean for trt 2' [1,2]/cl;
lsmeans antibiotic 'avg of trt 2 mean and trt 3 mean' [0.5,2] [0.5,3]/cl;
lsmeans antibiotic 'trt 1 vs trt 5' [1,1] [-1,5]/cl;
lsmeans antibiotic 'avg of 1 and 2 vs avg of 3 and 4' [1,1] [1,2] [-1,3] [-1,4]/divisor=2 cl;
run;

```

Least Squares Means Estimate									
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper
Antibiotic	lsmean for trt 2	19.0750	1.5046	15	12.68	<.0001	0.05	15.8681	22.2819

Least Squares Means Estimate									
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper
Antibiotic	avg of trt 2 mean and trt 3 mean	23.8375	1.0639	15	22.41	<.0001	0.05	21.5699	26.1051

Least Squares Means Estimate									
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper
Antibiotic	trt 1 vs trt 5	-3.5750	2.1278	15	-1.68	0.1136	0.05	-8.1102	0.9602

Least Squares Means Estimate									
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper
Antibiotic	avg of 1 and 2 vs avg of 3 and 4	5.2250	1.5046	15	3.47	0.0034	0.05	2.0181	8.4319

Parameter		Estimate	Standard Error	t Value	Pr > t	95% Confidence Limits		
lsmean for trt 2		19.0750000	1.50456251	12.68	<.0001	15.8681009	22.2818991	
avg of trt 2 mean and trt 3 mean		23.8375000	1.06388635	22.41	<.0001	21.5698799	26.1051201	
trt 1 vs trt 5		-3.5750000	2.12777270	-1.68	0.1136	-8.1102402	0.9602402	
avg of 1 and 2 vs avg of 3 and 4		5.2250000	1.50456251	3.47	0.0034	2.0181009	8.4318991	

Multiple Comparisons Corrections

It is not safe to go carrying out many many significance tests suggested by the data all willy-nilly. If we do, our *experiment wide* type I error rate will not be controlled.

Recall: $\alpha = P(\text{Type I Error})$

Decision	H_0 true	H_0 false
Reject H_0	Type I Error	Correct!
Fail to Reject H_0	Correct!	Type II Error

For a given test, we fix the probability of a type I error to be small (often 0.05) as it is usually considered worse than a type II error.

Consider the case with $t = 5$ (antibiotic treatments):

- the number of pairwise contrasts of the form $\theta = \mu_i - \mu_j$ is $\binom{5}{2} = 10$
- each test has type I error $\alpha = 0.05$, but overall what is our type I error rate?
i.e. $P(\text{rejecting at least one null hypothesis that is true})$
- This is called the *experimentwise* or *familywise* (fwe) type I error rate. We should really control this instead of the type I error for each test!

Example: Is a certain type of coin fair (equal probability of flipping a head and a tail)?

$$H_0 : \text{Coin fair}, p = 0.5 \quad H_A : \text{Coin biased}, p \neq 0.5$$

Experiment - flip one of these coins 10 times, if 9 or 10 heads appear or if 9 or 10 tails appear then declare coin biased.

Assuming the coin is fair,

$$\begin{aligned} \alpha &= P(\text{Concluding coin is biased}) \\ &= P(9 \text{ heads}) + P(9 \text{ tails}) + P(10 \text{ heads}) + P(10 \text{ tails}) \\ &= 2 * 10(1/2)^{10} + 2 * (1/2)^{10} = 0.021 \end{aligned}$$

This is our type I error rate for testing this particular coin (a little smaller than the usual 0.05).

Now suppose we have 100 coins of this type and we test each in the same manner. If the coins were truly fair, how many of the experiments would we expect to conclude we have a biased coin?

For a particular coin to come up heads or tails 9-10 times is very unlikely, but seeing any 1 coin of the 100 behave this way would be more likely than not.

In fact,

$$P(\text{All 100 coins identified as fair}) = 0.34$$

$$P(\text{At least 1 coin of the 100 is classified as biased}) = 0.66$$

This is why we need to control the fwe rate when we do many data-driven comparisons!

Comparisons can be categorized as *a priori* or *post-hoc*:

- *A priori*: Significance tests which will be carried out without regard to the observed outcome of the experiment.
- *Post-hoc* or data-driven: Significance tests which are suggested by the observed outcome of the experiment.

Methods for simultaneous inference for multiple comparisons include (but there are many many of these)

- Bonferroni
- Scheffé
- Tukey

Bonferroni Correction

Suppose interest lies in exactly k contrasts. **Bonferroni correction** is to replace the usual α with

$$\alpha' = \frac{\alpha}{k}$$

By doing so our fwe rate will be less than α

$$\text{fwe rate} = \alpha^* = 1 - (1 - \alpha')^k = 1 - (1 - \frac{\alpha}{k})^k \leq \alpha$$

We can now create **simultaneous** CIs. These are a group of CIs we are $(1 - \alpha)\%$ confident will all contain their true value.

Simultaneous 95% confidence intervals for the k contrasts given by

$$\begin{aligned} a_1\bar{y}_{1+} + a_2\bar{y}_{2+} + \cdots + a_t\bar{y}_{t+} &\pm t(\alpha'/2, t(n-1)) \sqrt{MS(E) \sum_{i=1}^t \frac{a_i^2}{n_i}} \\ b_1\bar{y}_{1+} + b_2\bar{y}_{2+} + \cdots + b_t\bar{y}_{t+} &\pm t(\alpha'/2, t(n-1)) \sqrt{MS(E) \sum_{i=1}^t \frac{a_i^2}{n_i}} \\ &\vdots \\ k_1\bar{y}_{1+} + k_2\bar{y}_{2+} + \cdots + k_t\bar{y}_{t+} &\pm t(\alpha'/2, t(n-1)) \sqrt{MS(E) \sum_{i=1}^t \frac{a_i^2}{n_i}} \end{aligned}$$

Note: $t(\alpha'/2, t(n-1))$ might have to be obtained using software.

For the binding fraction example, consider only pairwise comparisons with Chloramphenicol (μ_1):

$$\theta_1 = \mu_1 - \mu_2, \quad \theta_2 = \mu_1 - \mu_3, \quad \theta_3 = \mu_1 - \mu_4, \quad \theta_4 = \mu_1 - \mu_5$$

We have $k = 4$, $\alpha' = 0.05/k = 0.0125$, and $t(\alpha'/2, 15) = 2.84$.

What is the Margin of Error for one of these contrasts? Find the simultaneous 95% intervals for the four contrasts. Which of these antibiotic means differ significantly from the chloramphenicol mean?

Scheffé Correction

Scheffé correction scales the t multiplier in an interesting way.

Rather than $t(\alpha/2, t(n-1))$ we use $\sqrt{(t-1)F(\alpha, t-1, t(n-1))}$

**Doesn't depend on the number of contrasts done!

For **simultaneous** 95% confidence intervals for **any number** of contrasts, use

$$\sum_{i=1}^t c_i \bar{y}_{i+} \pm \sqrt{(t-1)F(\alpha, t-1, t(n-1))MS[E] \sum_{i=1}^t \frac{c_i^2}{n_i}}$$

For a pairwise comparisons of means, say $\mu_1 - \mu_2$, this yields

$$\bar{y}_{1+} - \bar{y}_{2+} \pm \sqrt{(t-1)F(\alpha, t-1, t(n-1))MS[E](1/n_1 + 1/n_2)}$$

For binding fraction data, what is the Margin of Error for testing one of the contrasts?
(Note: $F(\alpha, t-1, t(n-1)) = 3.06$)

Tukey-Kramer Correction (or just Tukey)

Tukey's correction is the best method when making inference on **all pairwise** comparisons in balanced designs. That is, for simple contrasts of the form

$$\theta = \mu_j - \mu_k$$

it will tend to have a lower type II error rate in these cases than Scheffé and bonferroni corrections. (It has a greater chance of detecting differences i.e. is more powerful.)

- Uses multipliers from a distribution called the ‘studentized range distribution’
- Denoted $q(\alpha, t, t(n - 1))$

For **simultaneous** 95% confidence intervals for $\theta = \mu_j - \mu_k$ use

$$\begin{aligned}\hat{\theta} &\pm \frac{q(\alpha, t, t(n - 1))}{\sqrt{2}} \hat{SE}(\hat{\theta}) \\ \bar{y}_{j+} - \bar{y}_{k+} &\pm \frac{q(\alpha, t, t(n - 1))}{\sqrt{2}} \sqrt{MS(E)\left(\frac{1}{n} + \frac{1}{n}\right)} \\ \bar{y}_{j+} - \bar{y}_{k+} &\pm q(\alpha, t, t(n - 1)) \sqrt{\frac{MS(E)}{n}}\end{aligned}$$

How to do these multiple comparison corrections in SAS?

- Bonferroni can be done by manually changing the α level SAS uses. For the example above, $\alpha' = 0.05/4 = 0.0125$:

```
proc glm data=binding;
class antibiotic;
model bindfrac=antibiotic/clparm alpha=0.0125;
*Can drop intercept since it has 0 coefficient;
estimate 'theta 1' antibiotic 1 -1;
estimate 'theta 2' antibiotic 1 0 -1;
estimate 'theta 3' antibiotic 1 0 0 -1 0;
estimate 'theta 4' antibiotic 1 0 0 0 -1;
run;

proc mixed data=binding;
class antibiotic;
model bindfrac=antibiotic;
lsmestimate antibiotic 'theta 1' [1,1] [-1,2]/cl alpha=0.0125;
lsmestimate antibiotic 'theta 2' [1,1] [-1,3]/cl alpha=0.0125;
lsmestimate antibiotic 'theta 3' [1,1] [-1,4]/cl alpha=0.0125;
lsmestimate antibiotic 'theta 4' [1,1] [-1,5]/cl alpha=0.0125;
run;
```

- Scheffe and Tukey corrections are options:

```
proc glm data=binding;
class antibiotic;
model bindfrac=antibiotic;
lsmeans antibiotic/pdiff adjust=scheffe cl;
lsmeans antibiotic/pdiff adjust=tukey cl;
run;

proc mixed data=binding;
class antibiotic;
model bindfrac=antibiotic;
lsmeans antibiotic/pdiff adjust=tukey cl;
lsmestimate antibiotic 'theta 1' [1,1] [-1,2]/cl adjust=scheffe;
lsmestimate antibiotic 'theta 2' [1,1] [-1,3]/cl adjust=scheffe;
lsmestimate antibiotic 'theta 3' [1,1] [-1,4]/cl adjust=scheffe;
lsmestimate antibiotic 'theta 4' [1,1] [-1,5]/cl adjust=scheffe;
run;
```

Bonferroni GLM output:

Parameter	Estimate	Standard Error	t Value	Pr > t	98.75% Confidence Limits		
theta 1	8.7250000	2.12777270	4.10	0.0009	2.6893015	14.7606985	
theta 2	-0.8000000	2.12777270	-0.38	0.7122	-6.8356985	5.2356985	
theta 3	19.9750000	2.12777270	9.39	<.0001	13.9393015	26.0106985	
theta 4	-3.5750000	2.12777270	-1.68	0.1136	-9.6106985	2.4606985	

Bonferroni Mixed output:

Least Squares Means Estimate Adjustment for Multiplicity: Bonferroni												
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper
Antibiotic	theta 1	8.7250	2.1278	15	4.10	0.0009	0.0009	0.05	4.1898	13.2602	4.1898	13.2602

Least Squares Means Estimate Adjustment for Multiplicity: Bonferroni												
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper
Antibiotic	theta 2	-0.8000	2.1278	15	-0.38	0.7122	0.7122	0.05	-5.3352	3.7352	-5.3352	3.7352

Least Squares Means Estimate Adjustment for Multiplicity: Bonferroni												
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper
Antibiotic	theta 3	19.9750	2.1278	15	9.39	<.0001	<.0001	0.05	15.4398	24.5102	15.4398	24.5102

Least Squares Means Estimate Adjustment for Multiplicity: Bonferroni												
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper
Antibiotic	theta 4	-3.5750	2.1278	15	-1.68	0.1136	0.1136	0.05	-8.1102	0.9602	-8.1102	0.9602

Scheffe and Tukey GLM output:

The GLM Procedure Least Squares Means Adjustment for Multiple Comparisons: Scheffe						The GLM Procedure Least Squares Means Adjustment for Multiple Comparisons: Tukey					
Antibiotic	BindFrac L SMEAN	L SMEAN Number	Antibiotic	BindFrac L SMEAN	L SMEAN Number	Antibiotic	BindFrac L SMEAN	L SMEAN Number	Antibiotic	BindFrac L SMEAN	L SMEAN Number
Chloramp	27.800000	1	Chloramp	27.800000	1	Erythrom	19.075000	2	Erythrom	19.075000	2
Erythrom	19.075000	2	Penicill	28.600000	3	Penicill	28.600000	3	Streptom	7.825000	4
Penicill	28.600000	3	Streptom	7.825000	4	Tetracyc	31.375000	5	Tetracyc	31.375000	5
Least Squares Means for effect Antibiotic Pr > t for H0: LSMean(i)=LSMean(j) Dependent Variable: BindFrac											
i/j	1	2	3	4	5	i/j	1	2	3	4	5
1	0.0177	0.9973	<.0001	0.6003		1	0.0072	0.9953	<.0001	0.4738	
2	0.0177		0.0091	0.0022	0.0009	2	0.0072		0.0035	0.0007	0.0003
3	0.9973	0.0091		<.0001	0.7881	3	0.9953	0.0035		<.0001	0.6928
4	<.0001	0.0022	<.0001		<.0001	4	<.0001	0.0007	<.0001		<.0001
5	0.6003	0.0099	0.7881	<.0001		5	0.4738	0.0003	0.6928	<.0001	
Least Squares Means for Effect Antibiotic Pr > t for H0: LSMean(i)=LSMean(j) Dependent Variable: BindFrac											
Antibiotic	BindFrac L SMEAN	95% Confidence Limits	Antibiotic	BindFrac L SMEAN	95% Confidence Limits	Antibiotic	BindFrac L SMEAN	95% Confidence Limits	Antibiotic	BindFrac L SMEAN	95% Confidence Limits
Chloramp	27.800000	24.593101 31.006899	Chloramp	27.800000	24.593101 31.006899	Erythrom	19.075000	15.868101 22.281899	Erythrom	19.075000	15.868101 22.281899
Erythrom	19.075000	15.868101 22.281899	Penicill	28.600000	25.393101 31.806899	Penicill	28.600000	25.393101 31.806899	Streptom	7.825000	4.618101 11.031899
Penicill	28.600000	25.393101 31.806899	Streptom	7.825000	4.618101 11.031899	Tetracyc	31.375000	28.168101 34.581899	Tetracyc	31.375000	28.168101 34.581899
Least Squares Means for Effect Antibiotic											
i	j	Difference Between Means	Simultaneous 95% Confidence Limits for LSMean(i)-LSMean(j)			i	j	Difference Between Means	Simultaneous 95% Confidence Limits for LSMean(i)-LSMean(j)		
1	2	8.725000	1.286228 16.163772			1	2	8.725000	2.154598 15.295402		
1	3	-0.800000	-8.238772 6.638772			1	3	-0.800000	-7.370402 5.770402		
1	4	19.975000	12.536228 27.413772			1	4	19.975000	13.404598 26.545402		
1	5	-3.575000	-11.013772 3.863772			1	5	-3.575000	-10.145402 2.995402		
2	3	-9.525000	-16.963772 -2.088228			2	3	-9.525000	-16.095402 -2.954598		
2	4	11.250000	3.811228 18.688772			2	4	11.250000	4.679598 17.820402		
2	5	-12.300000	-19.738772 -4.861228			2	5	-12.300000	-18.870402 -5.729598		
3	4	20.775000	13.336228 28.213772			3	4	20.775000	14.204598 27.345402		
3	5	-2.775000	-10.213772 4.663772			3	5	-2.775000	-9.345402 3.795402		
4	5	-23.550000	-30.988772 -16.111228			4	5	-23.550000	-30.120402 -16.979598		

Scheffe and Tukey Mixed output:

Least Squares Means Estimate Adjustment for Multiplicity: Scheffe														
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper		
Antibiotic	theta 1	8.7250	2.1278	15	4.10	0.0009	0.0009	0.05	4.1898	13.2602	4.1898	13.2602		
Least Squares Means Estimate Adjustment for Multiplicity: Scheffe														
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper		
Antibiotic	theta 2	-0.8000	2.1278	15	-0.38	0.7122	0.7122	0.05	-5.3352	3.7352	-5.3352	3.7352		
Least Squares Means Estimate Adjustment for Multiplicity: Scheffe														
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper		
Antibiotic	theta 3	19.9750	2.1278	15	9.39	<.0001	<.0001	0.05	15.4398	24.5102	15.4398	24.5102		
Least Squares Means Estimate Adjustment for Multiplicity: Scheffe														
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper		
Antibiotic	theta 4	-3.5750	2.1278	15	-1.68	0.1136	0.1136	0.05	-8.1102	0.9602	-8.1102	0.9602		
Least Squares Means														
Effect	Antibiotic	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper					
Antibiotic	Chloramp	27.8000			1.5046	15	18.48	<.0001	0.05	24.5931	31.0089			
Antibiotic	Erythrom	19.0750			1.5046	15	12.68	<.0001	0.05	15.8881	22.2819			
Antibiotic	Penicill	28.6000			1.5046	15	19.01	<.0001	0.05	25.3831	31.8089			
Antibiotic	Streptom	7.8250			1.5046	15	5.20	0.0001	0.05	4.6181	11.0319			
Antibiotic	Tetracyc	31.3750			1.5046	15	20.85	<.0001	0.05	28.1681	34.5819			
Differences of Least Squares Means														
Effect	Antibiotic	_Antibiotic	Estimate	Standard Error	DF	t Value	Pr > t	Adjustment	Adj P	Alpha	Lower	Upper	Adj Lower	Adj Upper
Antibiotic	Chloramp	Erythrom	8.7250	2.1278	15	4.10	0.0009	Tukey	0.0072	0.05	4.1898	13.2602	2.1546	15.2954
Antibiotic	Chloramp	Penicill	-0.8000	2.1278	15	-0.38	0.7122	Tukey	0.9953	0.05	-5.3352	3.7352	-7.3704	5.7704
Antibiotic	Chloramp	Streptom	19.9750	2.1278	15	9.39	<.0001	Tukey	<.0001	0.05	15.4398	24.5102	13.4046	26.5454
Antibiotic	Chloramp	Tetracyc	-3.5750	2.1278	15	-1.68	0.1136	Tukey	0.4738	0.05	-8.1102	0.9602	-10.1454	2.9954
Antibiotic	Erythrom	Penicill	-9.5250	2.1278	15	-4.48	0.0004	Tukey	0.0035	0.05	-14.0602	-4.9898	-16.0954	-2.9546
Antibiotic	Erythrom	Streptom	11.2500	2.1278	15	5.29	<.0001	Tukey	0.0007	0.05	6.7148	15.7852	4.6796	17.8204
Antibiotic	Erythrom	Tetracyc	-12.3000	2.1278	15	-5.78	<.0001	Tukey	0.0003	0.05	-16.8352	-7.7648	-18.8704	-5.7296
Antibiotic	Penicill	Streptom	20.7750	2.1278	15	9.76	<.0001	Tukey	<.0001	0.05	16.2398	25.3102	14.2046	27.3454
Antibiotic	Penicill	Tetracyc	-2.7750	2.1278	15	-1.30	0.2118	Tukey	0.6928	0.05	-7.3102	1.7602	-9.3454	3.7954
Antibiotic	Streptom	Tetracyc	-23.5500	2.1278	15	-11.07	<.0001	Tukey	<.0001	0.05	-28.0852	-19.0148	-30.1204	-16.9796

Independent Contrasts

Consider a contrast θ , then

$$\theta = c_1\mu_1 + c_2\mu_2 + \dots + c_t\mu_t$$

where $\sum_{i=1}^t c_i = 0$. The estimate of a contrast is

$$\hat{\theta} = c_1\bar{y}_{1+} + c_2\bar{y}_{2+} + \dots + c_t\bar{y}_{t+}$$

and the estimated variance is given by

$$\hat{Var}(\hat{\theta}) = MS(E) \sum_{i=1}^t \frac{c_i^2}{n_i}$$

Recall: The idea behind ANOVA is that we partition $SS(TOT)$ into independent components $SS(Trt)$ and $SS[E]$.

Similarly, we can take $SS(Trt)$ and partition it into $t - 1$ independent contrasts each with 1 df.

Orthogonal contrasts:

Let

$$\theta_1 = \sum_{i=1}^t c_i\mu_i \text{ and } \theta_2 = \sum_{i=1}^t d_i\mu_i$$

be two contrasts. θ_1 and θ_2 are **orthogonal** if

$$c_1d_1 + c_2d_2 + \dots + c_td_t = \sum_{i=1}^t c_id_i = 0$$

A set of k contrasts is mutually orthogonal if all pairs are orthogonal.

Examples:

$(-1, 1, 0, 0, 0)$ and $(0, 0, -1, 1, 0)$ orthogonal ?

$(1, -1/2, -1/2, 0, 0)$ and $(0, 0, 0, -1, 1)$ orthogonal ?

$(-1, 1, 0, 0, 0)$ and $(0, -1, 1, 0, 0)$ orthogonal ?

Due to the joint normality, **orthogonality implies independence!**

Sums of squares for contrasts

Recall we are going to partition $SS(Trt)$ into $t - 1$ independent contrasts. The sums of squares for a contrast are

$$SS(\hat{\theta}) = \frac{\hat{\theta}^2}{\left(\frac{c_1^2}{n_1} + \dots + \frac{c_t^2}{n_t}\right)} = \frac{\hat{\theta}^2}{\left(\sum_{i=1}^t \frac{c_i^2}{n_i}\right)}$$

This contrast has 1 df associated with it.

We can define $MS(\hat{\theta}) = SS(\hat{\theta})/1 = SS(\hat{\theta})$ and can then test

$$H_0 : \theta = 0 \quad vs \quad H_A : \theta \neq 0$$

using the F-statistic

$$F = \frac{MS(\hat{\theta})}{MS(E)} \sim F_{1,t(n-1)}$$

Compare this to the t -test done earlier for testing a contrast

$$t = \frac{\hat{\theta} - \theta_0}{\hat{SE}(\hat{\theta})} \sim t_{t(n-1)}$$

(Remember if we square a t stat we get an F stat!)

We can also test multiple contrasts all equal to 0 at once

$$H_0 : \theta_1 = \theta_2 = \dots = \theta_k = 0 \quad vs \quad H_A : \text{At least 1 } \theta \neq 0$$

using the F-statistic

$$F = \frac{\frac{SS(\hat{\theta}_1) + SS(\hat{\theta}_2) + \dots + SS(\hat{\theta}_k)}{k}}{MS(E)} \sim F_{k,t(n-1)}$$

How to relate this to $SS(Trt)$? Generally, if $\theta_1, \theta_2, \dots, \theta_{t-1}$ are $t - 1$ mutually orthogonal contrasts then

$$SS(Trt) = SS(\hat{\theta}_1) + SS(\hat{\theta}_2) + \dots + SS(\hat{\theta}_{t-1})$$

and $df_{Trt} = df_{\hat{\theta}_1} + \dots + df_{\hat{\theta}_{t-1}} = 1 + \dots + 1 = t - 1$

Notice, testing all $t - 1$ contrasts equal to 0 is equivalent to testing our global F -test!

Again consider the Binding Fraction data. In this case we have $5 - 1 = 4$ df for treatment. Consider the following set of 4 mutually orthogonal contrasts:

$$\begin{aligned}\theta_1 &= (-2 \quad -1 \quad 0 \quad 1 \quad 2) \\ \theta_2 &= (2 \quad -1 \quad -2 \quad -1 \quad 2) \\ \theta_3 &= (-1 \quad 2 \quad 0 \quad -2 \quad 1) \\ \theta_4 &= (1 \quad -4 \quad 6 \quad -4 \quad 1)\end{aligned}$$

Since these are mutually orthogonal, they are all independent.

Let's use SAS to get estimates. Test for $\theta_4 = 0$ using both the t and F tests. Then show that $SS(Trt) = SS(\theta_1) + SS(\theta_2) + SS(\theta_3) + SS(\theta_4)$ and conduct the global F test.

```
proc glm data=binding; class antibiotic; model bindfrac=antibiotic;
contrast 'theta 1' antibiotic -2 -1 0 1 2;
contrast 'theta 2' antibiotic 2 -1 -2 -1 2;
contrast 'theta 3' antibiotic -1 2 0 -2 1;
contrast 'theta 4' antibiotic 1 -4 6 -4 1; run;

proc mixed data=binding; class antibiotic; model bindfrac=antibiotic;
lsmeans antibiotic 'theta 1' [-2,1] [-1,2] [0,3] [1,4] [2,5];
lsmeans antibiotic 'theta 2' [2,1] [-1,2] [-2,3] [-1,4] [2,5];
lsmeans antibiotic 'theta 3' [-1,1] [2,2] [0,3] [-2,4] [1,5];
lsmeans antibiotic 'theta 4' [1,1] [-4,2] [6,3] [-4,4] [1,5]; run;
```

Least Squares Means Estimate						
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t
Antibiotic	theta 1	-4.1000	4.7578	15	-0.86	0.4024
Least Squares Means Estimate						
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t
Antibiotic	theta 2	34.2500	5.6296	15	6.08	<.0001
Least Squares Means Estimate						
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t
Antibiotic	theta 3	26.0750	4.7578	15	5.48	<.0001
Least Squares Means Estimate						
Effect	Label	Estimate	Standard Error	DF	t Value	Pr > t
Antibiotic	theta 4	123.18	12.5881	15	9.79	<.0001

Consider a new dataset: Data consists of the number of contaminants in IV fluids made by $t = 3$ pharmaceutical companies

	Cutter	Abbott	McGaw
	255	105	577
	264	288	515
	342	98	214
	331	275	413
	234	221	401
	217	240	260
\bar{y}_{i+}	273.8	204.5	396.7

Source	d.f.	Sum of squares	Mean Square	F
Treatments (or pharmacies)	2	113646	56823	5.81
Error	15	146753	9784	
Total	17	260400		

Consider the following 2 contrasts:

$$\theta_1 = \mu_M - \mu_A \quad \text{and} \quad \theta_2 = \mu_C - \frac{\mu_M + \mu_A}{2}$$

Which levels of the factor will each of these be in SAS? Rewrite these contrasts in terms of μ_1 , μ_2 , and μ_3 .

Are these contrasts orthogonal?

Are the estimated contrasts $\hat{\theta}_1$ and $\hat{\theta}_2$ independent?

Use the output to compute $SS(\hat{\theta}_1)$ and $SS(\hat{\theta}_2)$. What should these add up to and why?

```

proc glm data=pharm; class company; model contam=company;
contrast 'McGaw vs Abbot' company -1 0 1;
estimate 'McGaw vs Abbot' company -1 0 1;
contrast 'Cutter vs avg of McGaw and Abbot' company -1 2 -1;
estimate 'Cutter vs avg of McGaw and Abbot' company -1 2 -1/divisor=2; run;

```

Note: We should really do a multiple comparison correction for our two contrasts. Bonferroni is easiest, compare our p-values to $0.05/2 = 0.025$.

The GLM Procedure

Class Level Information		
Class	Levels	Values
Company	3	Abbott Cutter McGaw

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	113646.3333	56823.1667	5.81	0.0136
Error	15	146753.6667	9783.5778		
Corrected Total	17	260400.0000			

R-Square	Coeff Var	Root MSE	contam Mean
0.436430	33.91268	98.91197	291.6667

Source	DF	Type I SS	Mean Square	F Value	Pr > F
Company	2	113646.3333	56823.1667	5.81	0.0136

Source	DF	Type III SS	Mean Square	F Value	Pr > F
Company	2	113646.3333	56823.1667	5.81	0.0136

Contrast	DF	Contrast SS	Mean Square	F Value	Pr > F
McGaw vs Abbot	1	110784.0833	110784.0833	11.32	0.0043
Cutter vs avg of McGaw and Abbot	1	2862.2500	2862.2500	0.29	0.5965

Parameter	Estimate	Standard Error	t Value	Pr > t
McGaw vs Abbot	192.166667	57.1068524	3.37	0.0043
Cutter vs avg of McGaw and Abbot	-26.750000	49.4559849	-0.54	0.5965

Company	contam LSMEAN
Abbott	204.500000
Cutter	273.833333
McGaw	396.666667

Polynomial contrasts

For one-way ANOVA, if the factor is actually on the interval scale but observed at only a few levels we can test for polynomial relationships.

With t levels, we can fit any polynomial of degree $t - 1$ or less. (Polynomial of degree $t - 1$ is equivalent to fitting ANOVA model.) That is, every polynomial model of degree $t - 2$ or less is nested in the full ANOVA model!

Example: A poultry science experiment measures bodyweights of chickens from $t = 4$ diet groups. Diets are characterized by protein concentration in diet.

- Response $Y = 21$
- A balanced CRD was done with diet and $N = 72$ total chickens. (Implying $n = 18$).

Experiment Summary:

diet group	x : level of protein	diet mean \bar{y}_i
1	21.8	994.9
2	23.5	1000.6
3	25.2	1025.8
4	26.9	1056.0

Here we can see that our factor is actually on an interval scale but measured at only 4 levels.

Consider the One-way ANOVA model using diet and the Linear Regression model cubic in protein:

```
proc glm data=chickens; class diet;
model gain=diet; run;

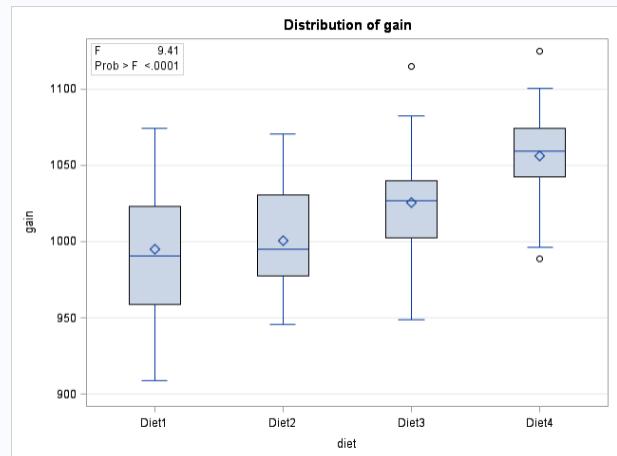
proc glm data=chickens;
model gain=protein protein*protein protein*protein*protein; run;
```

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	42020.4921	14006.8307	9.41	<.0001
Error	68	101214.9702	1488.4554		
Corrected Total	71	143235.4623			

R-Square	Coeff Var	Root MSE	gain Mean
0.293367	3.785046	38.58051	1019.288

Source	DF	Type I SS	Mean Square	F Value	Pr > F
diet	3	42020.49206	14006.83069	9.41	<.0001

Source	DF	Type III SS	Mean Square	F Value	Pr > F
diet	3	42020.49206	14006.83069	9.41	<.0001



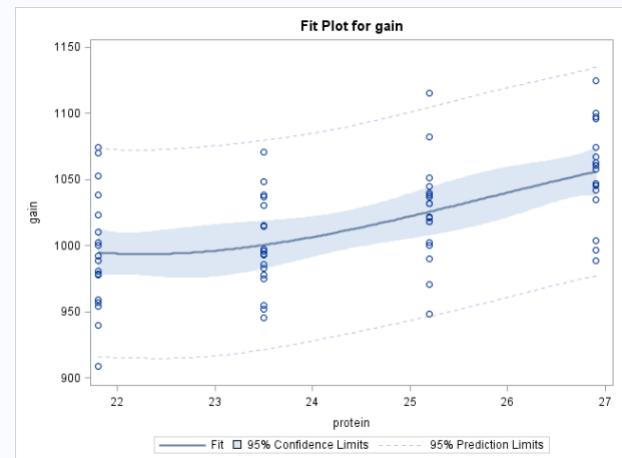
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	42020.4921	14006.8307	9.41	<.0001
Error	68	101214.9702	1488.4554		
Corrected Total	71	143235.4623			

R-Square	Coeff Var	Root MSE	gain Mean
0.293367	3.785046	38.58051	1019.288

Source	DF	Type I SS	Mean Square	F Value	Pr > F
protein	1	39129.40362	39129.40362	26.29	<.0001
protein*protein	1	2700.51253	2700.51253	1.81	0.1825
protein*protein*protein	1	190.57591	190.57591	0.13	0.7216

Source	DF	Type III SS	Mean Square	F Value	Pr > F
protein	1	232.0108148	232.0108148	0.16	0.6942
protein*protein	1	213.5806599	213.5806599	0.14	0.7060
protein*protein*protein	1	190.5759142	190.5759142	0.13	0.7216

Parameter	Estimate	Standard Error	t Value	Pr > t
Intercept	9025.320090	19740.84174	0.46	0.6490
protein	-966.091671	2446.98971	-0.39	0.6942
protein*protein	38.179905	100.79101	0.38	0.7060
protein*protein*protein	-0.493645	1.37959	-0.36	0.7216



Investigate the two ANOVA tables. Also inspect the Type I Sums of Squares for the MLR model, these would be useful in model building! We can test for the adequacy of a model linear or quadratic in protein rather than the full ANOVA (equivalent to the cubic model).

If we have equally spaced levels (differences between levels all the same), we can actually write down the different polynomial parts in terms of contrasts. Below gives the contrasts you would use for equally spaced levels for 3, 4, or 5 levels.

Factor levels	Poly. Degree	Contrast	Coefficients for					$SS(\hat{\theta}_i)$
			\bar{y}_{1+}	\bar{y}_{2+}	\bar{y}_{3+}	\bar{y}_{4+}	\bar{y}_{5+}	
3	1	$\hat{\theta}_1$	-1	0	1			$R(\beta_1 \beta_0)$
	2	$\hat{\theta}_2$	1	-2	1			$R(\beta_2 \beta_0, \beta_1)$
4	1	$\hat{\theta}_1$	-3	-1	1	3		$R(\beta_1 \beta_0)$
	2	$\hat{\theta}_2$	1	-1	-1	1		$R(\beta_2 \beta_0, \beta_1)$
	3	$\hat{\theta}_3$	-1	3	-3	1		$R(\beta_3 \beta_0, \beta_1, \beta_2)$
5	1	$\hat{\theta}_1$	-2	-1	0	1	2	$R(\beta_1 \beta_0)$
	2	$\hat{\theta}_2$	2	-1	-2	-1	2	$R(\beta_2 \beta_0, \beta_1)$
	3	$\hat{\theta}_3$	-1	2	0	-2	1	$R(\beta_3 \beta_0, \beta_1, \beta_2)$
	4	$\hat{\theta}_4$	1	-4	6	-4	1	$R(\beta_4 \beta_0, \beta_1, \beta_2, \beta_3)$

Rightmost column indicates extra SS in MLR of the form

$$\mu(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots$$

The contrast corresponding to a polynomial of degree p can be used to test for a p^{th} degree association:

- large $|\hat{\theta}_1|$ indicates linear association between y and x .
- large $|\hat{\theta}_2|$ indicates quadratic association between y and x .
- large $|\hat{\theta}_3|$ indicates cubic association between y and x .

```
proc glm data=chickens; class diet; model gain=diet;
contrast 'linear' diet -3 -1 1 3;
contrast 'quadratic' diet 1 -1 -1 1;
contrast 'cubic' diet -1 3 -3 1; run;
```

Contrast	DF	Contrast SS	Mean Square	F Value	Pr > F
linear	1	39129.40362	39129.40362	26.29	<.0001
quadratic	1	2700.51253	2700.51253	1.81	0.1825
cubic	1	190.57590	190.57590	0.13	0.7216

Note the equivalence between this output and the linear regression model cubic in protein. Conclusion? Go ahead and use the linear model rather than the full ANOVA. No need to look at pairwise comparisons etc.

F-ratio for lack-of-fit:

To test for lack-of-fit of a polynomial (*reduced*) model of degree p , use extra sum-of-squares F-ratio on $t - 1 - p$ and $N - t$ df:

$$F = \frac{SS(\text{lack of fit})/(t - 1 - p)}{MS(E)_{\text{full}}}$$

where

$$\begin{aligned} SS(\text{lack-of-fit}) &= SS(Trt) - SS(R)_{\text{poly}} \\ &= SS(E)_{\text{poly}} - SS(E)_{\text{full}} \end{aligned}$$

For illustration purposes (i.e. this isn't necessary), let's test if the quadratic model is sufficient or if the full ANOVA model is necessary.