1. Statistical assumptions

The standard regression model assumes that the residuals, or $\epsilon$’s, are independently, identically distributed (usually called “iid” for short) as normal with $\mu = 0$ and variance $\sigma^2$.

(a) Independence

A residual should not be related to another residual. Situations where independence could be violated include repeated measures and time series because two or more residuals come from the same subject and hence may be correlated. Another violation of independence comes from nested designs where subjects are clustered (such as in the same school, same family, same neighborhood). There are regression techniques that relax the independence assumption, as we saw in the repeated measures section of the course.

(b) Identically distributed

As stated above, we assume that the residuals are distributed $N(0, \sigma^2)$. That is, we assume that each residual is sampled from the same normal distribution with a mean of zero and the same variance throughout. This is identical to the normality and equality of variance assumptions we had in the ANOVA. The terminology applies to regression in a slightly different manner, i.e., defined as constant variance along the entire range of the predictor variable, but the idea is the same.

The MSE from the regression source table provides an estimate of the variance $\sigma^2$ for the $\epsilon$’s.

Usually, we don’t have enough data at any given level of X to check whether the Y’s are normally distributed with constant variance, so how should this assumption be checked?
One may plot the residuals against the predicted scores (or instead the predictor variable). There should be no apparent pattern in the residual plot. However, if there is fanning in (or fanning out), then the equality of variance part of this assumption may be violated.

To check the normality part of the assumption, look at the histogram of the residuals to see whether it resembles a symmetric bell-shaped curve. Better still, look at the normal probability plot of the residuals (recall the discussion of this plot from the ANOVA lectures).

2. Below I list six problems and discuss how to deal with each of them (see Ch. 3 of KNNL for more detail)

(a) The association is not linear. You check this by looking at the scatter plot of X and Y. If you see anything that doesn’t look like a straight line, then you shouldn’t run a linear regression. You can either transform or use a model that allows curvature such as polynomial regression or nonlinear regression, which we will discuss later. Plotting residuals against the predicted scores will also help detect nonlinearity.

(b) Error terms do not have constant variance. This can be observed in the residual plots. You can detect this by plotting the residuals against the predictor variable. The residual plot should have near constant variance along the levels of the predictor; there should be no systematic pattern. The plot should look like a horizontal band of points.

(c) The error terms are not independent. We can infer the appropriateness of this assumption from the details of study design, such as if there are repeated measures variables. You can perform a scatter plot of residuals against time to see if there is a pattern (there shouldn’t be a correlation). Other sources of independence violations are due to grouping such as data from multiple family members or multiple students from the same classroom; there may be correlations between individuals in the same family or individuals in the same classroom.

(d) Outliers. There are many ways to check for outliers (scatter plot of Y and X, examining the numerical value of the residuals, plotting residuals against the predictor). We’ll also cover a more quantitative method of determining the degree to which an outlier influences the regression line.

(e) Residuals are not normally distributed. This is checked by either looking at the histogram of the residuals or the normal-normal plot of the residuals.
(f) You have the wrong structural model (aka a mispecified model). You can also use residuals to check whether an additional variable should be added to a regression equation. For example, if you run a regression with two predictors, you can take the residuals from that regression and plot them against other variables that are available. If you see any systematic pattern other than a horizontal band, then that is a signal that there may be useful information in that new variable (i.e., information not already accounted for by the linear combination of the two predictors already in the regression equation that produced those residuals).

3. Nonlinearity

What do you do if the scatterplot of the raw data, or the scatterplot of the residuals against the predicted scores, suggests that the association between the criterion variable Y and the predictor variable X is nonlinear? One possibility is that you can re-specify the model. Rather than having a simple linear model of the form $Y = \beta_0 + \beta_1 X$, you could add more predictors. Perhaps a polynomial of the form $Y = \beta_0 + \beta_1 X + \beta_2 X^2$ would be a better fit. Along similar lines, you may be able to transform one of the variables to convert the model into a linear model. Either way (adding predictors or transforming existing predictors) we have an exciting challenge in regression because you are trying to find a model that fits the data. Through the process of finding such a model, you might learn something about theory or the psychological processes underlying your phenomenon. There could be useful information in the nature of the curvature (processes that speed up or slow down at particular critical points).

There are sensible ways of diagnosing how models are going wrong and how to improve a model. You could examine residuals. If a linear relation holds, then there won’t be much pattern in the residuals. To the degree there is a relation in the residuals when plotted against a predictor variable, then that is a clue that the model is misspecified.

4. The “Rule of the Bulge” to decide on transformations.

Here is a heuristic for finding power transformations to linearize data. It’s basically a mnemonic for remembering which transformation applies in which situation, much like the mnemonics that help you remember the order of the planets (e.g., My Very Educated Mother Just Saved Us Nine Pies; though recent debate now questions whether the last of those pies should be saved...). A more statistics-related mnemonic can help you remember the three key statistical assumptions. INCA: independent normal constant-variance assumptions (Hunt, 2010, *Teaching Statistics*, 32, 73-74).

The rule operates within the power family of transformations $x^p$ that we discussed in an earlier lecture notes (see syntax there for implementing power transformations in R and SPSS). Recall that within the power family, the identity transformation (i.e., no transformation) corresponds to $p = 1$. Taking $p = 1$ as the reference point, we can talk about either increasing $p$...
(say, making it 2 or 3) or decreasing $p$ (say, making it 0, which leads to the log, or -1, which is the reciprocal).

With two variables $Y$ and $X$ it is possible to transform either variable. That is, either of these are possible: $Y^p = \beta_0 + \beta_1 X$ or $Y = \beta_0 + \beta_1 X^p$. Of course, the two exponents in these equations will usually not be identical.

The rule of the bulge is a heuristic for determining what exponent to use on either the dependent variable ($Y$) or the predictor variable ($X$) to help linearize the relation between two variables. First, identify the shape of the “one-bend” curve you observe in the scatter plot with variable $Y$ on the vertical axis and variable $X$ on the horizontal axis (all that matters is the shape, not the quadrant that your data appear in). Use the figure below to identify one of the four possible one-bend shapes. The slope is irrelevant, just look at the shape (i.e., is it “J” shaped, “L” shaped, etc.).

Once you identify a shape (for instance, a J-shape pattern in the far right of the previous figure), then go to the “rule of the bulge” graph below and identify whether to increase or decrease the exponent. The graph is a gimmick to help you remember what transformation to use given a pattern you are trying to deal with. For example, a J-shape data pattern is in the south-east portion of the plot below. The “rule of the bulge” suggests you can either increase the exponent on $X$ so you could try squaring or cubing the $X$ variable, or instead you could decrease the exponent on $Y$ such as with a log or a reciprocal. The action to “increase” or “decrease” is determined by whether you are in the positive or negative part of the “rule of the bulge” figure, and which variable to transform ($X$ or $Y$) is determined by the axis (horizontal or vertical, respectively).
If you decide to perform a transformation to eliminate nonlinearity, it makes sense to transform the predictor variable $X$ rather than the criterion variable $Y$. The reason is that you may want to eventually test more complicated regressions with multiple predictors. If you tinker with $Y$ you might inadvertently mess up a linear relation with some other predictor variable.

An aside with a little calculus. Sometimes transformations follow from theory. For example, if a theory presupposes that changes in a dependent variable are inversely related to another variable, as in the differential equation

$$\frac{dY(X)}{dX} = \frac{\alpha}{X}$$  \hspace{1cm} (7-1)

then this differential equation has the solution

$$Y(X) = \alpha \ln X + \beta$$  \hspace{1cm} (7-2)

The $Y(X)$ notation denotes that $Y$ is a function of $X$. The point here is that the theoretical statement about how change works in a particular situation, implies a nonlinear transformation on $X$. In the current example, the theory (from its statement about the nature of change over time) leads naturally to the log transformation. For many more examples of this kind of approach, see Coleman’s *Introduction to Mathematical Sociology*. 
When working with nonlinear data one needs to be careful about extrapolating to data points outside the range of observation. Figure 7-1 presents an interesting clip from the *Economist*.

5. Constant Variance Assumption

Dealing with the equality of variance assumption is tricky. In a few cases it may be possible to transform a variable to eliminate the equality of variance (as was the case in ANOVA), but you have to be careful that the transformation does not mess up other assumptions (in particular, linearity). Conversely, if you perform a transformation to “clean up” a nonlinearity problem, you need to be careful that the transformation did not inadvertently mess up the equality of variance assumption.
Another possible remedial measure in this case is to perform a weighted regression. If your subjects are clustered and the variances depend on the cluster, then you could weight each data point by the inverse of the variance. See KNNL ch 11 for details on weighted regression.

6. Outliers

By outlier we mean a data point that has the potential to exert a “disproportionate” degree of influence on the regression line. A simple index of an outlier is the residual (i.e., the observed score - predicted score). If a residual for a particular subject is large, then that data point is suspect as a possible outlier.

With more than one predictor, spotting an outlier is difficult because we need to think about all the variables (dimensions) concurrently. For instance, with three predictors, an outlier means that the point “sticks out” in comparison to all the other points within the four dimensional plot (one dependent variable and three predictors). So simple pairwise scatterplots won’t always be an option.

Chapter 10 of KNNL discusses various normalizations on the residuals that can be performed. For instance, is a residual of 3 large or small? In order to tell we can normalize the residuals into a common scale. Obviously, the magnitude of the residual depends, in part, on the scale of the dependent variable. There is one normalization that is analogous to a Z score (dividing the residual by the square root of the MSE). Another set of normalizations involve deleted residuals (if interested, see chapter 10 KNNL).

One of the best ways to detect an outlier, and whether it is an influential outlier, is through the use of Cook’s D. This is a measure of the influence on the overall regression of the single data point in question. Each data point has a Cook’s D. To develop intuition on Cook’s D, I’ll present an example involving midterm exams. We first look at the scatter plot (Figure 7-2) and the correlation.

data list free/ test1 test2.
bEGIN DATA
{data go here} 
END DATA.

plot format=regression
/plot test2 with test1.
correlation test2 test1
/print= twotail
/statistics=all.
Figure 7-2: SPSS scatter plot
Next, we’ll run a regression analysis. The syntax also shows you how to produce scatter plots within the regression command (redundant with the plots we did above). Also, the last line of the command creates two new columns of data (labelled resid and fits), which contain residuals and predicted Y values, respectively. You may need to use a “set width=132.” command before running the regression command to get all the columns next to the “casewise” plot (and if using a windowing system, you may need to scroll horizontally as well to view the columns on your monitor).

Figure [7-3] displays the residuals plotted against the predictor variable. This plot was generated by the plot command below.

```
regression variables= test1 test2
/statistics = r anov coeff ci
/dependent=test2
/method=enter test1
/residuals outliers(cook)
/casewise=all sepred cook zpred sresid
/scatterplot (test2, test1)
/save resid(resid) pred(fits).
```

GRAPH
/SCATTERPLOT(BIVAR)= test1 WITH resid.

Comment: you can double click on the resulting residual plot to add a horizontal reference line at Y=0 to provide a visual cue for the horizontal band.

Multiple R .67211
R Square .45174
Adjusted R Square .43065
Standard Error 4.55742
### Analysis of Variance

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\[ F = 21.42235 \quad \text{Signif} \ F = .0001 \]

### Variables in the Equation

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### Casewise Plot of Standardized Residual

* : Selected  M: Missing

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### Residuals Statistics:
It appears that subject 23 is an outlier because the residual (-12.71) is much larger in magnitude than any other residual. We'll omit that subject for now and redo the analysis. That
particular subject was the only one to have a test2 score of 21 so we can conveniently select that subject out by asking SPSS to not use subjects whose test2 score equals 21. Had the data file included a subject ID index (e.g., a subject number), then it would have been more efficient to select directly on subject number.

`select if (test2 ne 21).`  
`execute.`

[abbreviated output]

```
Multiple R .66568 Analysis of Variance
R Square .44313 DF Sum of Squares Mean Square
Adjusted R Square .42085 Regression 1 286.98276 286.98276
Standard Error 3.79814 Residual 25 360.64687 14.42587
F = 19.89361 Signif F = .0002

Variable B SE B 95% Confidnce Interval B Beta T Sig T
TEST1 .794477 .178125 .427622 1.161332 .665679 4.460 .0002
(Constant) .950880 .871922 -17.006703 18.908463 .109 .9140

Caseewise Plot of Standardized Residual
*: Selected  M: Missing
```

Case TEST2 *PRED *RESID *ZPRED *SRESID *COOK D *SEPRED
Residuals Statistics:  

```
Min  Max  Mean  Std Dev  N
```
Lecture Notes #7: Residual Analysis and Multiple Regression

In the two regressions the slopes are comparable but the intercepts differ in absolute terms. Further, the $R^2$'s are not very different across the two regressions suggesting that the two regressions are comparable. Perhaps that point we suspected to be an outlier is not very influential because its presence or absence has relatively little impact on the regression.

The main things to note in this example are the effects of the outlier on the parameter estimates and how the residuals, and associated printouts, were used to decipher where the assumptions were being violated. The way we detected whether this suspected point was an outlier was to remove it and re-run the regression. We compared the effects of the model with the suspected outlier included and the model without the suspected outlier. For this example, both cases yielded comparable results. So, for this example including the outlier will not do too much damage.

**I am not advocating that outliers be dropped in data analysis.** Rather, I simply compared two different regressions (one with the outlier and one without) to see whether the results differed. The comparison of these two regressions lets me assess how much “influence” the particular data point has on the overall regression. This time the two regressions were similar so I feel pretty confident in reporting results with all subjects. In this example the outlier appears to have little impact on the final result.

This idea of comparing the model with the outlier and the model without the outlier can be extended. Why not do this for every data point? First, perform one regression with all the data included. Then perform N different regressions; for each regression a single data point is removed. This would tell us how “influential” each data point is on the regression line. Luckily, there is a quick way of doing this computation (if you had 200 subjects, the technique I just outlined would require 201 separate regressions). The quick way is Cook’s D (D stands for distance). The formula for Cook’s D involves quite a bit of matrix algebra so I won’t present it here (see KNNL for a derivation). Cook’s D is basically a measure of the difference between the regression one gets by including subject i and the regression one gets by omitting subject i. So, each subject gets his or her own Cook’s D. A subject’s individual

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<td>-1.5482</td>
<td>1.9286</td>
<td>.0000</td>
<td>.9806</td>
<td>27</td>
</tr>
<tr>
<td>Standardized Residual</td>
<td>-.7320</td>
<td>2.0542</td>
<td>.9787</td>
<td>.3390</td>
<td>27</td>
</tr>
<tr>
<td>Differential Residual</td>
<td>-6.1071</td>
<td>7.6331</td>
<td>.0777</td>
<td>3.9971</td>
<td>27</td>
</tr>
<tr>
<td>Mahalanobis</td>
<td>.0028</td>
<td>6.6426</td>
<td>.9630</td>
<td>1.5666</td>
<td>27</td>
</tr>
<tr>
<td>Cook’s D</td>
<td>.0000</td>
<td>.2073</td>
<td>.0370</td>
<td>.0499</td>
<td>27</td>
</tr>
<tr>
<td>Leverage</td>
<td>.0001</td>
<td>.2555</td>
<td>.0603</td>
<td>27</td>
<td></td>
</tr>
</tbody>
</table>

Total Cases = 27
D is an index of how influential that subject’s data are on the regression line. Large values of Cook’s D indicate that the particular data point (subject) has a big effect on the regression equation. Cook’s D is influenced both by the residual and the leverage of the predictors.

Determining what constitutes a large value of Cook’s D involves calculating the sampling distribution for F, so we’ll just have to make good guesses as to constitutes high values of Cook’s D. A rule of thumb is to look for Cook’s D values that are relatively greater than the majority of the D’s in the sample. Some people use a different rule of thumb, such as any Cook’s D greater than 4/N is a potential influential outlier. In this example with 27 observations 4/27 = .148 so two points are potential influential outliers since they have Cook D values greater than .148. I’ve seen variants of this rule such as 2p/N where p is the number of predictors.

Another strategy for determining key values of Cook’s D is to use the F table to set up critical values. Use α = 0.50 (not 0.05), the numerator degrees of freedom are the number of parameters in the structural model (including the intercept), and the denominator degrees of freedom are N minus the number of parameters (the same df associated with MSE). For example, with two predictors (so a total of 3 parameters including the intercept), 24 df in the error, and α = .50, we find a tabled value of 0.812. Cook’s original 1977 paper in Technometrics proposed using α = 0.50 with an argument that if the removal of a point makes the estimate of the slope (here slope can be a vector of multiple slopes corresponding to multiple predictors as we will see later in these notes and in LN8 and LN9) move outside the 50% confidence band, then it should be considered an influential point and treated as a potential outlier.

In the present example, there was one predictor so there were 2 parameters including the intercept, there were 26 residual degrees of freedom. The F value corresponding to .50 with 2,26 degrees of freedom is .712. This gives a numerical benchmark for Cook’s D in this particular example: any observed Cook’s D greater than 0.712 is suspect because it might be an influential outlier.

One could use the built in F function in SPSS (or Excel) to find the necessary value of F. In SPSS, for example, with the menu system under TRANSFORM-COMPUTE you will find a list of functions. Select IDF.F. For this example you would type IDF.F(.50,2,26), define the new variable you want the output to go into, and click on OK. Or, in the syntax window type this command and you will get a new column of identical numbers that give the F cutoff (“Fcrit” is an arbitrary name for the new column this command creates).

For a definition of leverage see KNNL. It turns out that SPSS has its own definition of leverage. SPSS uses a centered leverage, i.e., $\hat{h}_i - \frac{1}{n}$ where n is the number of subjects. Most people just use $\hat{h}_i$. SPSS prints out the leverage values as part of the casewise plot (labeled LEVER; in most versions of SPSS you have to write “lever” on the casewise line to get this to print out).
compute Fcrit = idf.f(.50, 2, 26).
execute.

An alternative but identical approach to finding the critical Cook’s D value would be to use the inverse $F$ function on the column of Cook D scores to find the cumulative area under the $F$. That is, if you save Cook’s D scores in a new column called cook (or any other arbitrary variable name you like), then you can run this command on that column of saved Cook D scores:

compute pval = cdf.f(cook, 2, 26).
execute.

This syntax will produce a new column of “pvals”. Look for any “pval” greater than .50 and those are potential influential outliers. Both the cdf.f and idf.f approaches will lead to identical conclusions based on the $F$ test.

This logic of comparing regressions with and without a data point can also be extended to examine the effect on individual regression parameters like intercept and slopes. Cook’s D focuses on the effect of the entire regression rather than individual $\beta$s. There is an analogous measure DFBETA that examines the effect of each single data point on each regression parameter. SPSS computes the change for each $\beta$ in standardized units of removing each data point. To get this within SPSS just add a

\SAVE SDBETA(name)

... to your regression syntax. If you have two predictors, this command will create three new columns in your data file labeled name1, name2 and name3 for the standardized difference in beta of that point on each of the intercept and the two predictors. A value of say -.1 means that particular beta drops .1 standard error units when that data point is added as compared to when it is omitted. Some people treat a standardized DFBETA greater than one a potential influential outlier, others use the rule 2/sqrt(N), so any standardized DFBETA greater than 2/sqrt(N) becomes a suspicious influential outlier.

7. What to do if you have influential outliers?

As I said before, don’t automatically drop the outliers. Check whether there was a data entry error or if something was different about that particular data collection session (e.g., a new RA’s first subject and the RA messed up the protocol).
If there is a small cluster of outliers, you may want to check whether there is something informative about this small group. It could be error, but it could be a signal about a relatively small class of participants. For example, in a dataset with 250 families there may be 6 kids who act out aggressively, and these may be the kids who are at high risk.

You can run nonparametric or robust regression, which are not as sensitive to outliers as the typical regressions we run though can exhibit lower power.

8. Relation between the two sample t test and regression with one predictor.

Now I’ll show the connection between ANOVA and regression.

Let’s begin with a simple example with two experimental groups. Here are the data. Note the three extra columns. These columns represent three different ways to code the predictor variable. All are fine as long as you keep track of the values you used (much like interpreting a contrast value that depends on the particular coefficients). The means for the two groups are 8.56 and 5.06, the grand mean is 6.81, and the treatment effect \( \alpha \) is 1.75. Think about what each of the three scatterplots (the first column on the y-axis and each of the three remaining columns on separate x-axes) will look like.

```
5.4 1 1 1
6.2 1 1 1
3.1 1 1 1
3.8 1 1 1
6.5 1 1 1
5.8 1 1 1
6.4 1 1 1
4.5 1 1 1
4.9 1 1 1
4.0 1 1 1
8.8 0 -1 2
9.5 0 -1 2
10.6 0 -1 2
9.6 0 -1 2
7.5 0 -1 2
6.9 0 -1 2
7.4 0 -1 2
6.5 0 -1 2
10.5 0 -1 2
8.3 0 -1 2
```

data list free / dv dummy contrast group.

REGRESSION USING 0 AND 1 TO CODE FOR GROUPS

```
regrssion variables = dv dummy
/statistics = r anova coeff ci
/dependent = dv
/method=enter dummy.
```

Multiple R .80955 Analysis of Variance
Lecture Notes #7: Residual Analysis and Multiple Regression

R Square .65537
Adjusted R Square .63623
Standard Error 1.33766

DF Sum of Squares Mean Square

Regression 1 61.25000 61.25000
Residual 18 32.20800 1.78933

F = 34.23063 Signif F = .0000

Variable B SE B 95% Confidence Interval B Beta T Sig T
DUMMY -3.50000 .598220 -4.756813 -2.243187 -.809552 -5.851 .0000
(Constant) 8.560000 .423005 7.671299 9.448701 20.236 .0000

A SECOND REGRESSION USING 1 AND -1 TO CODE FOR GROUPS

regression variables = dv contrast
/statistics = r anova coeff ci
(dependent = dv
/method-enter contrast.

Multiple R .80955
R Square .65537
Adjusted R Square .63623
Standard Error 1.33766

DF Sum of Squares Mean Square

Regression 1 61.25000 61.25000
Residual 18 32.20800 1.78933

F = 34.23063 Signif F = .0000

Variable B SE B 95% Confidence Interval B Beta T Sig T
CONTRAST -1.750000 .299110 -2.378406 -1.121594 -.809552 -5.851 .0000
(Constant) 6.8100000 .299110 6.181594 7.438701 22.768 .0000

The test of significance for these two regressions are identical. The slope is reduced by 1/2 as compared to the first regression. This is because the coding on the predictor variable is two units apart (1 and -1) rather than one unit (1 and 0). The intercept also changes because of two reasons: the line has shifted over to the left and the slope has changed.

Below is yet another predictor variable (using codes 1 and 2) as well as the usual two-sample t test and the output from a one-way ANOVA so that you can compare regression and ANOVA.

t-test groups= group
/variables dv.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Number of Cases</th>
<th>Mean</th>
<th>SD</th>
<th>SE of Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>DV</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GROUP 1</td>
<td>10</td>
<td>5.0600</td>
<td>1.189</td>
<td>.376</td>
</tr>
<tr>
<td>GROUP 2</td>
<td>10</td>
<td>8.5600</td>
<td>1.471</td>
<td>.465</td>
</tr>
</tbody>
</table>
Mean Difference = -3.5000

t-test for Equality of Means

<table>
<thead>
<tr>
<th>Variance</th>
<th>t-value</th>
<th>df</th>
<th>2-Tail Sig</th>
<th>SE of Diff</th>
<th>95% CI for Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equal</td>
<td>-5.85</td>
<td>18</td>
<td>.000</td>
<td>.598</td>
<td>(-4.757, -2.243)</td>
</tr>
<tr>
<td>Unequal</td>
<td>-5.85</td>
<td>17.24</td>
<td>.000</td>
<td>.598</td>
<td>(-4.761, -2.239)</td>
</tr>
</tbody>
</table>

oneway dv by group(1,2)

A THIRD REGRESSION USING A CODE OF 1 AND 2 FOR THE TWO GROUPS

regression variables = dv group
/statistics = r anova coeff ci
/dependent = dv
/method=enter group.

Multiple R: .80955
R Square: .65537
Adjusted R Square: .63623
Standard Error: 1.33766

Analysis of Variance

<table>
<thead>
<tr>
<th>SOURCE</th>
<th>D.F.</th>
<th>SUM OF SQUARES</th>
<th>MEAN SQUARES</th>
<th>F</th>
<th>F Ratio</th>
<th>F Prob.</th>
</tr>
</thead>
<tbody>
<tr>
<td>BETWEEN GROUPS</td>
<td>1</td>
<td>61.2500</td>
<td>61.2500</td>
<td>34.2306</td>
<td>.0000</td>
<td></td>
</tr>
<tr>
<td>WITHIN GROUPS</td>
<td>18</td>
<td>32.2080</td>
<td>1.7893</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>TOTAL</td>
<td>19</td>
<td>93.4580</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

F = 34.23063 Signif F = .0000

Variable:

<table>
<thead>
<tr>
<th>GROUP</th>
<th>B</th>
<th>SE B</th>
<th>95% Confidence Interval</th>
<th>Beta</th>
<th>T</th>
<th>Sig T</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Constant)</td>
<td>1.560000</td>
<td>.945868</td>
<td>-.427195 to 3.547195</td>
<td>1.649</td>
<td>.1164</td>
<td></td>
</tr>
</tbody>
</table>

In this last regression I reversed the group codes so the sign of the slope changed. That is, in the first two regressions the subjects listed in the first group had a greater group code than subjects listed in the second group (e.g., 1 and 0, respectively). But in the third regression I switched so that the first group had the lesser value than the second group (i.e., 1 and 2). I did this to show you that except for sign, the $t$ test is identical across all three regressions; hence all that matters is that the two groups have unique group codes. The regression equation does rest.

I have shown by example that one can reproduce the classic two sample $t$-test through regression. You can anticipate that the correct predictor variables in regression can give you the same results as any ANOVA. Later, I will show the general connection between regression and ANOVA, but first we need to generalize our conception of regression to include more than one predictor.
9. Multiple regression

Multiple regression is a simple and natural extension of what we have been talking about with one predictor variable. Multiple regression permits any number of (additive) predictor variables. Multiple regression simply means “multiple predictors.”

The model is similar to the case with one predictor; it just has more X’s and β’s.

\[ Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 \ldots + \beta_p X_p + \epsilon \]  

(7-3)

where p is the number of predictor variables. The assumptions are the same as for linear regression with one predictor. Each \( \beta_i \) corresponds to the slope on the ith variable holding all other predictor variables constant (i.e., the “unique” slope, or the partial slope). This idea corresponds to the partial derivative in calculus. Ideally, the predictors should not be correlated with the other predictors because this creates multicollinearity problems—the standard error of the slope will be larger than it should be. More on this “multicollinearity problem” later.

With two predictors there is a three dimensional scatterplot that corresponds to the regression problem. Figure 7-4 shows a scatterplot in three dimensions. The three dimensions refer to the predictors and the two dependent variable, with the points in the plot representing subjects.

For two predictors, the regression is finding the plane that minimizes the residuals. Figure 7-5 shows the same scatter plot but with a plane of best fit. The analog with the pegboard demonstration should be obvious—rather than fitting a line there is now a plane.

Three or more predictor variables are difficult to display in a plot because we need more than three dimensions but the idea and intuition scales to any number of dimensions.

Variance decomposition is also extended to the case of multiple regression. The degrees of freedom in the numerator take into account the number of predictors. The \( F \) ratio from the source table is interpreted as whether all the variables as a set account for a significant proportion of the variability in the dependent variable. That is, the \( F \) ratio is comparing “the model” as a whole (MS regression) to “what’s left over” (MS residuals). This corresponds to the simple ANOVA design that decomposed sums of squares into between and within components. The form of the multiple regression source table is

<table>
<thead>
<tr>
<th>SS</th>
<th>df</th>
<th>MS</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSR= ( \sum (Y_i - \bar{Y})^2 )</td>
<td>number of parameters - 1</td>
<td>SSR/df</td>
<td>MSR/MSE</td>
</tr>
<tr>
<td>SSE= ( \sum (Y_i - \hat{Y}_i)^2 )</td>
<td>N - number of parameters</td>
<td>SSE/df</td>
<td></td>
</tr>
</tbody>
</table>
Figure 7-4: Scatterplot with two predictor variables
Figure 7-5: Linear fit with residuals plotted.
variance in Y that can be accounted for by the set of X variables. Recall the pie chart we played with earlier in the term with ANOVA. The square root of $R^2$, sometimes denoted $r_{\hat{y},y}$, is the correlation between the observed data and the fitted values. Both are indices of how well a linear model fits the data.

The $F$ given by MSR/MSE is an omnibus test that shows how well the model as a whole (all predictors as an aggregate) fit the data. This $F$ tests whether $R^2$ is significantly different from zero. As with all omnibus tests, this particular $F$ is not very useful. We usually care more about how specific predictors are performing, especially in relation to other predictors. Thus, we are usually interested in each slope. This is analogous to the “I hats” from contrasts in ANOVA.

Each slope is an index representing each predictor’s unique contribution to the overall regression. In a two predictor regression there will, of course, be two slopes. The interpretation of these two slopes is as follows. The slope $\beta_1$ is attached to predictor $X_1$ and the slope $\beta_2$ is attached to predictor $X_2$. The slope $\beta_1$ can be interpreted as follows: if predictor $X_2$ is held constant and predictor $X_1$ increases by one unit, then a change of $\beta_1$ will result in the criterion variable $Y$. Similarly, the slope $\beta_2$ means that if predictor $X_1$ is held constant and predictor $X_2$ increases by one unit, then a change of $\beta_2$ will result in the criterion variable $Y$. Thus, each slope is an index of the unique contribution of each predictor variable to the criterion variable $Y$. This logic extends to any number of predictors such that the slope $\beta_i$ refers to the unique contribution of variable $i$ holding all other variables constant.

We can test each individual slope $\hat{\beta}_i$ against the null hypothesis that the population $\beta_i = 0$ as well as build confidence intervals around the estimates of the slopes. The test for each slope is a test of whether the predictor variable accounts for a significant unique portion of the variance in the criterion variable $Y$. SPSS output conveniently provides both the estimates of the $\beta$ parameters as well as their standard errors. The $t$ test is the ratio of the slope estimate over its standard error and the confidence interval is the usual estimate plus or minus the margin of error.

We need to be careful when interpreting the $t$ test for each $\hat{\beta}_i$ because those tests depend on the intercorrelations among the predictor variables. If the predictors are correlated, then there is no single way to assess the unique contribution of each predictor separately. That is, when a correlation between predictors is present, there is no sensible way to “hold all other predictors constant”. Thus, the presence of correlations between the predictor variables introduces redundancy. This problem is similar to what we encountered with unequal sample sizes in the factorial ANOVA.

As we saw with simple linear regression, the multiple regression function (Equation 7-3) can be used to make predictions, both mean $E(\hat{Y})$ and individual $\hat{Y}$. There is also a standard error prediction (SEPRED) corresponding to each subject.
Those interested in a full explanation of the relevant formulae should consult KNNL who develop the matrix algebra approach to multiple regression. The value of matrix notation becomes clear when dealing with multiple regression. I will not emphasize the details of definitional and computational formulae for multiple regression in this class because they are generalizations of the simple linear regression case using matrix algebra concepts. If you understand the case for simple linear regression, then you understand multiple regression too. In this class I will emphasize the ability to interpret the results from a regression rather than how to compute a regression.

10. Testing “sets of variables”

Sometimes one wants to test whether a subset of predictor variables increases predictability. For example, I may have a regression with five variables. I want to test whether the last three variables increase the fit to the data (i.e., minimize the residuals, or equivalently, increase $R^2$) significantly over and above whatever the first two variables are already doing. An example of this is with the use of blocking variables. Suppose I have two variables that I want to use as blocking factors to soak up error variance and three other variables of interest. I am mainly interested in whether these latter three variables can predict the dependent variable over and above the two blocking factors.

The way to do this is through the “increment in $R^2$ test.” You do two separate regression equations. One is the full model with five variables included; the other is the reduced model with the particular subset under consideration omitted from the regression. You then test the difference in $R^2$; that is, how much did $R^2$ increase from the reduced to the full regression. The formula is

$$F = \frac{\text{SSE}(R) - \text{SSE}(F)}{\text{SSE}(F)} \left( \frac{\text{df}_{\text{full}}}{\text{df}_{\text{reduced}} - \text{df}_{\text{full}}} \right)$$

where $\text{SSE}(R)$ and $\text{SSE}(F)$ are the sum of squares error for the reduced and full models, respectively, and $\text{df}_{\text{reduced}}$ and $\text{df}_{\text{full}}$ are the degrees of freedom (for the denominator) in the reduced regression and the full regression, respectively. In Lecture Notes #8, I'll present a version of this same equation in terms of $R^2$ rather than SSE. In the example with the blocking variables, the full regression would include all five predictors and the reduced regression would include only the two predictors that are being used as blocking factors (i.e., the reduced regression omits the three variables of interest). This $F$ test is comparing the difference in error between the two models. This is the approach the Maxwell and Delaney used throughout their book for explaining ANOVA.

The observed $F$ in Equation (7-4) is compared to the tabled $F$, where $\text{df}_{\text{red}} - \text{df}_{\text{full}}$ the degrees of
freedom for the numerator and df full is the degrees of freedom for the denominator.

The \( F \) test in Equation 7-4 provides an omnibus test for whether the omitted variables (the ones that appear in the full model but not the reduced model) account for a significant portion of the variance in the criterion variable \( Y \). Thus, in my example with the two blocking factors and three variables of interest, the \( F \) test in Equation 7-4 tells me whether the three predictor variables of interest as a set account for a significant portion of the variance in \( Y \), over and above that previously accounted for by the two blocking factors. As such, this \( F \) test is an omnibus test because it gives information about the set of three variables rather than information about the separate usefulness of each predictor.

If you think about it, one could perform an increment in \( R^2 \) for each independent variable separately (i.e., looking at each predictor variable’s “independent” contribution to \( R^2 \))? In other words, the full regression includes all \( p \) predictors and one performs a sequence of reduced regressions each with \( p - 1 \) predictors, where for each of the reduced regressions one of the predictor variables is omitted. It turns out that this is a sensible idea because it gives the significance test for the unique contribution of each predictor variable. Earlier I noted that the t-test associated with the slope provides a test for the unique contribution of the variable associated with that slope. As you would expect, the two tests (t-test on the individual slope or the F-test using Equation 7-4 where only one variable is omitted in the reduced regression) are identical; both are testing the unique contribute of that particular predictor variable.

11. Fun with residuals

I have focused on residuals because they carry a lot of useful information that helps diagnose the fit of a model. Much of the material in these lecture notes illustrates this point. I want to convince you that residuals carry much information by illustrating how one can embed hidden messages that plots of residuals can uncover

A simple example first. I’ll read in some data that has one predictor and one dependent variable. I present a scatterplot of the data with the regression line superimposed on the scatterplot and show the normal probability plot of the residuals. Something clearly looks off with the normal probability plot. The scatterplot show some structure beyond following a relatively straight line; the dark points are merely several points near each other.
qqnorm(resid(fit1))
qqline(resid(fit1))
Let’s plot the residuals from the regression I just ran against the predictor variable. The plot does not look like any plot we have seen before: it reveals a hidden message. That message was not evident in the original scatterplot but was uncovered by running the regression and plotting the residuals.

```r
plot(data$X, resid(fit1), pch = 19)
```
Here is another data set that looks quite typical of most data sets. I print out the first few rows of the 5 columns (one column is the dependent variable and the remaining columns are predictors). I present a set of scatterplots of all possible pairs of variables along with density plots illustrating the distributions of each variable. Then I run a regression and plot the residuals. With over 8000 observations, the normal probability plot points to a violation of normality given that the points do not follow a straight line. Having looked at the data one doesn’t see much structure.

```r
data <- read.table("/Users/gonzo/rich/teach/Gradst`1/Lect7/simpson.txt")
names(data) <- c("dv", "X1", "X2", "X3", "X4")
head(data)
```
<table>
<thead>
<tr>
<th>dv</th>
<th>X1</th>
<th>X2</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2.2334</td>
<td>-0.123090</td>
<td>0.1166100</td>
</tr>
<tr>
<td>-2.2075</td>
<td>0.313110</td>
<td>-0.0808860</td>
</tr>
<tr>
<td>-2.1816</td>
<td>0.016508</td>
<td>0.0352500</td>
</tr>
<tr>
<td>-2.3055</td>
<td>-0.024318</td>
<td>0.0339400</td>
</tr>
<tr>
<td>-2.2796</td>
<td>-0.018672</td>
<td>-0.0023774</td>
</tr>
<tr>
<td>-2.2666</td>
<td>-0.356240</td>
<td>0.1129400</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>X3</th>
<th>X4</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.2748900</td>
<td>-0.18969</td>
</tr>
<tr>
<td>0.3515900</td>
<td>-0.96198</td>
</tr>
<tr>
<td>0.2542200</td>
<td>-0.71549</td>
</tr>
<tr>
<td>-0.0025414</td>
<td>-0.43821</td>
</tr>
<tr>
<td>-0.0797500</td>
<td>-0.33685</td>
</tr>
<tr>
<td>0.0578740</td>
<td>-0.26380</td>
</tr>
</tbody>
</table>

# librarys for fancy multiple scatterplots on same page
library(ggplot2)
library(GGally)
ggpairs(data)
# run a regression with all 5 predicts; the .
# means all other variables besides the column dv
out.lm <- lm(dv ~ ., data = data)

summary(out.lm)
```
## Coefficients:
##            Estimate Std. Error t value     Pr(>|t|)
## (Intercept)  -0.002008   0.010928 -0.184 0.854000
## X1             0.910275   0.063618 14.308 <2e-16 ***
## X2             0.991121   0.067346 14.717 <2e-16 ***
## X3             0.883462   0.064311 13.737 <2e-16 ***
## X4             0.977337   0.046513 21.012 <2e-16 ***
##
## Residual standard error: 1 on 8401 degrees of freedom
## Multiple R-squared:  0.05004, Adjusted R-squared:  0.04955
## F-statistic: 110.5 on 4 and 8401 DF,  p-value: < 2.2e-16
```

```r
par(mfcol = c(1, 2))
hist(resid(out.lm))
qqnorm(resid(out.lm))
qqline(resid(out.lm))
```
But, let’s plot the residuals from that multiple regression against the predicted values \( \hat{Y} \) and we see the residuals do contain additional information in the form of an interesting image.

```r
par(mfcol = c(1, 1))
plot(predict(out.lm), resid(out.lm), pch = ".")
```
For more examples of hiding information in residuals, and to learn how to do this, see Stefaniski’s (2007) article in the *American Statistician*. 
Appendix 1: Relevant R syntax

Cook’s distance

If you save the `lm()` output, then you can run the `cooks.distance()` command on the output.

data <- read.table("data.outlier")
colnames(data) <- c("x", "y")

lm.out <- lm(y ~ x, data)

summary(lm.out)

## Call:
## lm(formula = y ~ x, data = data)
## ## Residuals:
## Min 1Q Median 3Q
## -12.7095 -3.2694 0.4445 3.2685
## Max
## 7.5986

## Coefficients:
## Estimate Std. Error t value
## (Intercept) -7.3979 10.0692 -0.735
## x 0.9560 0.2065 4.628
## Pr(>|t|)
## (Intercept) 0.469
## x 8.96e-05 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05
## '. ' 0.1 ' ' 1

## Residual standard error: 4.557 on 26 degrees of freedom
## Multiple R-squared: 0.4517, Adjusted R-squared: 0.4306
## F-statistic: 21.42 on 1 and 26 DF, p-value: 8.964e-05

c.d <- cooks.distance(lm.out)
round(c.d, 3)

## 1 2 3 4 5 6
## 0.022 0.065 0.002 0.045 0.060 0.000
Now you can treat c.d like a variable that you can plot or perform other computations.

To find the critical F for Cook’s at .50 you can use this command (following the example given earlier in the lecture notes)

```r
qf(0.5, 3, 24)
```

```
# [1] 0.8115318
```

R has an entire suite of additional diagnostics such as the dfbetas(), rstandard(), rstudent(), etc. The R command dfbetas() is the standardized version, whereas, dfbeta() is the unstandardized version.

### Multiple Regression

It is easy to perform multiple regression in R. Just list all predictors in the lm command. If you want a full factorial design you can use the asterisk instead of the plus sign; if you want specific interactions you can use the colon (see Lecture Notes 4 for a similar description in the case of the aov() command). We will talk about interactions in regression in more detail in a later lecture notes.

```r
lm.out <- lm(y ~ x1 + x2 + x3 + x4)
summary(lm.out)
cooks.distance(lm.out)
```

### Two sample t-test example

Here is the example I did earlier in the lecture notes showing that a regression can reproduce the results of a two sample t test. For easy reference, here are the key summary statistics: the cell means are 5.06 and 8.56; the mean difference is -3.5; the grand mean is 6.81 and the $\alpha$s of the structural model are $5.06 - 6.81 = -1.75$ and $8.56 - 6.81 = 1.75$. 

```r
##  7  8  9 10 11 12
## 0.030 0.074 0.009 0.002 0.023 0.002
## 13 14 15 16 17 18
## 0.112 0.021 0.000 0.006 0.003 0.023
## 19 20 21 22 23 24
## 0.000 0.036 0.258 0.019 0.477 0.000
## 25 26 27 28
## 0.028 0.018 0.000 0.006
```
data <- read.table("data.ttest")
colnames(data) <- c("dv", "dummy", "contrast", "group")
data

## dv dummy contrast group
## 1  5.4  1  1  1
## 2  6.2  1  1  1
## 3  3.1  1  1  1
## 4  3.8  1  1  1
## 5  6.5  1  1  1
## 6  5.8  1  1  1
## 7  6.4  1  1  1
## 8  4.5  1  1  1
## 9  4.9  1  1  1
##10 4.0  1  1  1
##11 8.8  0 -1  2
##12 9.5  0 -1  2
##13 10.6 0 -1  2
##14 9.6  0 -1  2
##15 7.5  0 -1  2
##16 6.9  0 -1  2
##17 7.4  0 -1  2
##18 6.5  0 -1  2
##19 10.5 0 -1  2
##20 8.3  0 -1  2

# report typical two sample t test for
# comparison; assume equal var t test for
# consistency with regression

t.test(dv ~ group, data, var.equal = T)

##
## Two Sample t-test
##
## data:  dv by group
## t = -5.8507, df = 18, p-value =
## 1.532e-05
## alternative hypothesis: true difference in means between group 1 and group 2
## 95 percent confidence interval:
## -4.756813 -2.243187
## sample estimates:
## mean in group 1 mean in group 2
## 5.06   8.56
# dummy code (1 and 0) regression

```r
summary(lm(dv ~ dummy, data))
```

## Call:
## lm(formula = dv ~ dummy, data = data)

## Residuals:
##    Min   1Q Median   3Q   Max
## -2.060 -1.085   0.040  1.065  2.040

## Coefficients:
##             Estimate Std. Error t value
## (Intercept)   8.5600     0.4230  20.236
## dummy        -3.5000     0.5982  -5.851
## Pr(>|t|)
## (Intercept) 7.86e-14 ***
## dummy       1.53e-05 ***

## Signif. codes:
##  0 '***' 0.001 '**' 0.01 '*' 0.05
## '.' 0.1 ' ' 1

## Residual standard error: 1.338 on 18 degrees of freedom
## Multiple R-squared: 0.6554, Adjusted R-squared: 0.6362
## F-statistic: 34.23 on 1 and 18 DF,  p-value: 1.532e-05

# contrast code (1 and -1) regression

```r
summary(lm(dv ~ contrast, data))
```

## Call:
## lm(formula = dv ~ contrast, data = data)

## Residuals:
##    Min   1Q Median   3Q   Max
## -2.060 -1.085   0.040  1.065  2.040

## Coefficients:
##             Estimate Std. Error t value
## (Intercept)   6.8100     0.2991  22.768
## contrast     -1.7500     0.2991  -5.851
## Pr(>|t|)
## (Intercept) 7.86e-14 ***
## contrast     1.53e-05 ***

## Signif. codes:
##  0 '***' 0.001 '**' 0.01 '*' 0.05
## '.' 0.1 ' ' 1

## Residual standard error: 1.338 on 18 degrees of freedom
## Multiple R-squared: 0.6554, Adjusted R-squared: 0.6362
## F-statistic: 34.23 on 1 and 18 DF,  p-value: 1.532e-05
## (Intercept) 1.02e-14 ***
## contrast 1.53e-05 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05
## '.' 0.1 ' ' 1
##
## Residual standard error: 1.338 on 18 degrees of freedom
## Multiple R-squared: 0.6554, Adjusted R-squared: 0.6362
## F-statistic: 34.23 on 1 and 18 DF, p-value: 1.532e-05

# group code (1 and 2) regression
summary(lm(dv ~ contrast, data))

##
## Call:
## lm(formula = dv ~ contrast, data = data)
##
## Residuals:
## Min 1Q Median 3Q Max
## -2.060 -1.085 0.040 1.065 2.040
##
## Coefficients:
## Estimate Std. Error t value
## (Intercept) 6.8100 0.2991 22.768
## contrast -1.7500 0.2991 -5.851
##
## Pr(>|t|)
## (Intercept) 1.02e-14 ***
## contrast 1.53e-05 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05
## '.' 0.1 ' ' 1
##
## Residual standard error: 1.338 on 18 degrees of freedom
## Multiple R-squared: 0.6554, Adjusted R-squared: 0.6362
## F-statistic: 34.23 on 1 and 18 DF, p-value: 1.532e-05