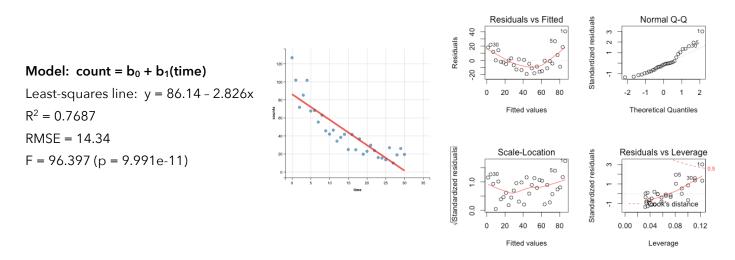
Activity #12: More regression topics: LOWESS; polynomial, nonlinear, robust, quantile; ANOVA as regression

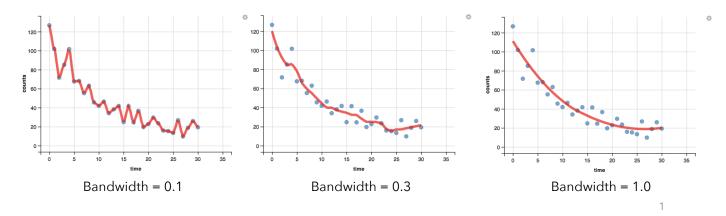
	<u>Time</u>	<u>Count</u> (above background levels)
	0	126.6
	1	101.8
	2	71.6
	•••	
	30	19.3
	=====	======
Mean =	15	43.745
SD =	9.09	29.308
N = 31		
r = -0.	877	

1. Let's model the counts as a function of time. To begin, we can fit a simple linear model. Based on the R-squared value of 0.7687, we might feel satisfied that this linear model adequately describes the data. Based on the residual plots, evaluate whether the necessary assumptions were satisfied for this linear regression analysis:



 It looks like we have a linearity issue (which would have been obvious had we plotted the data prior to fitting the linear model). To get a better idea of the "shape" of our scatterplot, we can use *locally weighted scatterplot smoothing* (LOWESS). LOWESS connects a series of models fit to small (local) subsets of the data (defined by the bandwidth or span) to describe the general relationship.

To see an animation of LOWESS in action, go to: http://bradthiessen.com/html5/stats/m301/lowess.gif



3. Based on that LOWESS curve, it's obvious that a linear function isn't the best fit for our data. So far in this course, we've only fit linear models to data. We've visualized this as a straight line (or plane) through a scatterplot.

What can we do when our data appear to have a "curved" relationship? Believe it or not, we can still use linear regression. Linear regression can include "lines" that have curved shapes.

One way to do this is to use polynomial (or curvilinear) regression to fit a curve through the data. In this Geiger counter example, we could try to fit the following models:

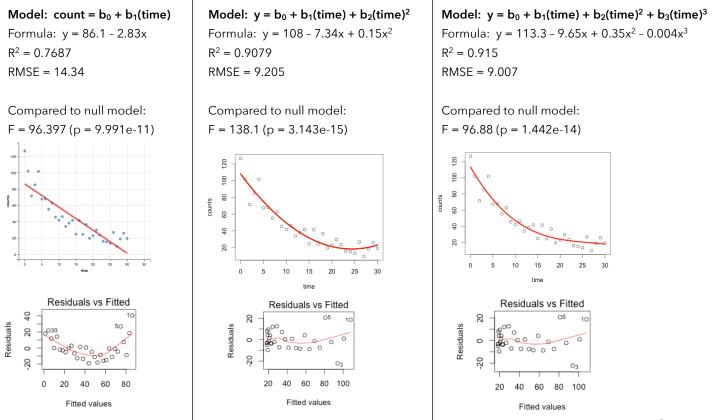
Linear model:  $\hat{y} = b_0 + b_1$  (time) Model with quadratic term:  $\hat{y} = b_0 + b_1$  (time)  $+ b_2$  (time)<sup>2</sup> Model with cubic term:  $\hat{y} = b_0 + b_1$  (time)  $+ b_2$  (time)<sup>2</sup>  $+ b_3$  (time)<sup>3</sup>

These are all considered to be linear models? Why? If you take the partial derivative of your model and the result no longer includes the unknown coefficients, then the model is considered to be linear. If, on the other hand, the partial derivative results in a function that does still include the unknown coefficients, then the model is considered to be nonlinear. Let's take a look at the partial derivative of the model with the cubic term:

$$\frac{dy}{db_0} = 1 \qquad \frac{dy}{db_1} = x \qquad \frac{dy}{db_2} = x^2 \qquad \frac{dy}{db_3} = x^3$$

Since these partial derivatives are no longer functions of the coefficients (b values), this is a linear model. It is a linear combination of predictor variables.

We can fit the models with the quadratic and cubic terms and compare them to the null model with no predictors:



4. We can compare these three models using the omnibus F-test. Verify the calculations and interpret. From this, which model would you conclude fits the data the best?

```
Analysis of Variance Table
Model 1: counts ~ 1
Model 2: counts ~ time
Model 3: counts ~ time + I(time^2)
Model 4: counts ~ time + I(time^2) + I(time^3)
              RSS Df Sum of Sq
                                      \mathbf{F}
  Res.Df
                                            Pr(>F)
1
      30 25769.0
                        19809.5 244.176 4.763e-15
2
      29
          5959.5
                   1
      28
          2372.4
                         3587.1
                                 44.215 3.897e-07
3
                   1
4
      27
          2190.5
                   1
                          182.0
                                  2.243
                                            0.1458
```

5. Look at the R-squared values for each model. What do you think would happen to the R-squared value if we fit a model with higher-powered terms (such as including all the way up to the 7th power)? Why?

6. Let's go ahead and fit the model that includes the 7th power:

```
Formula: y = 124 - 31.6x + 9.9x^2 - 1.7x^3 + 0.15x^4 - 0.007x^5 + 0.00017x^6 - 0.0000016x^7
                                                                                                     120
R^2 = 0.9314
                                                                                                     90
RMSE = 9.007
                                                                                                     80
                                                                                                  counts
                                                                                                     60
                                                                                                     40
If we compare it to the model with the quadratic term, we find:
                                                                                                     20
                                                                                                         0
                                                                                                              5
                                                                                                                  10
                                                                                                                        15
                                                                                                                             20
                                                                                                                                 25
                                                                                                                                       30
```

Analysis of Variance Table

```
Model 1: counts ~ time + I(time^2)
Model 2: counts ~ time + I(time^2) + I(time^3) + ... + I(time^6) + I(time^7)
Res.Df RSS Df Sum of Sq F Pr(>F)
28 2372.4
2 23 1767.2 5 605.22 1.5754 0.2066
```

From this, what can we conclude?

time

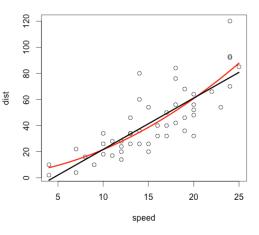
7. Just like in the last activity, we can use cross-validation to help choose the best model:

Average cross-validated mean square error:	Model
219	count = f(time)
103	$count = f(time + time^2)$
105	$count = f(time + time^2 + time^3)$
110	$count = f(time + time^2 + time^3 + time^4)$

From this, what can we conclude?

8. Let's look at another quick example. I had a dataset containing the speed and stopping distance of 50 cars. I fit models including linear, quadratic, and cubic terms and then tested each model in order:

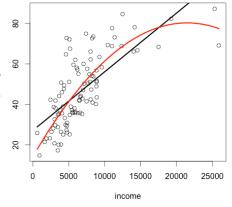
```
Analysis of Variance Table
Model 1: dist ~ 1
Model 2: dist ~ speed
Model 3: dist ~ speed + I(speed^2)
Model 4: dist ~ speed + I(speed^2) + I(speed^3)
  Res.Df
           RSS Df Sum of Sq
                                    F
                                         Pr(>F)
      49 32539
1
2
      48 11354
                 1
                     21185.5 91.6398 1.601e-12
3
      47 10825
                 1
                       528.8
                              2.2874
                                         0.1373
      46 10634
                 1
                       190.4
                             0.8234
                                         0.3689
4
```



Which model would you choose to describe this data?

9. Finally, let's go back to our "prestigious occupations" dataset. We can fit various models of prestige as a function of income. Based on this output (and the cross-validation output on the next page), which model would you choose?

```
Analysis of Variance Table
Model 1: prestige ~ 1
Model 2: prestige ~ income
Model 3: prestige ~ income + I(income^2)
Model 4: prestige ~ income + I(income^2) + I(income^3)
           RSS Df Sum of Sq
  Res.Df
                                     F
                                          Pr(>F)
1
     101 29895
2
     100 14616
                 1
                     15279.3 124.0617 < 2.2e-16 ***
3
      99 12077
                 1
                      2539.3
                              20.6179 1.597e-05 ***
4
      98 12070
                 1
                         7.4
                               0.0598
                                          0.8073
```



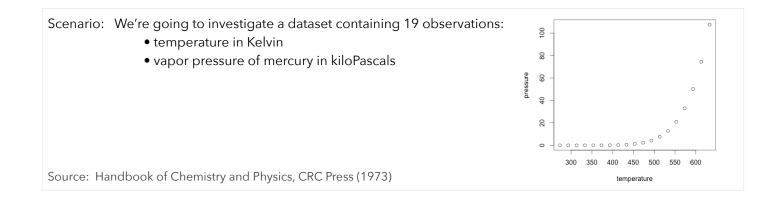
prestige

Average cross-validated mean square error:

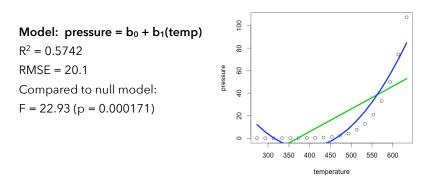
<u>Model</u>

154

- prestige = f(income)
- 130 prestige = f(income + income<sup>2</sup>)
- 131 prestige =  $f(income + income^2 + income^3)$
- 134 prestige =  $f(income + income^2 + income^3 + income^4)$

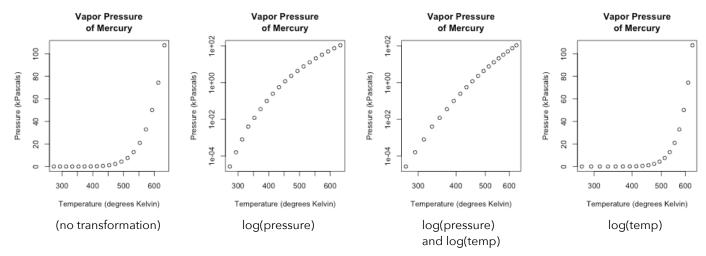


10. We can try to fit linear and quadratic models to this data. The plot shows neither model fits well, though.



Model: pressure =  $b_0 + b_1(temp) + b_2(temp)^2$   $R^2 = 0.9024$ RMSE = 9.92 Compared to null model: F = 74 (p = 8.209e-09)

We could also try to fit a nonlinear model to this data. The scatterplot indicates some kind of exponential model would fit the data. We could transform our variables to get an idea about which model might fit best.



11. Based on the graphs, it looks like a natural log transformation of both the pressure and temperature variables resulted in data that are approximately linear. This means we might want to try to fit one of these (identical) power models:

$$\hat{y} = b_0 (\text{temp})^{b_1}$$
$$\ln(\hat{y}) = b_0 + b_1 \ln(\text{temp})$$

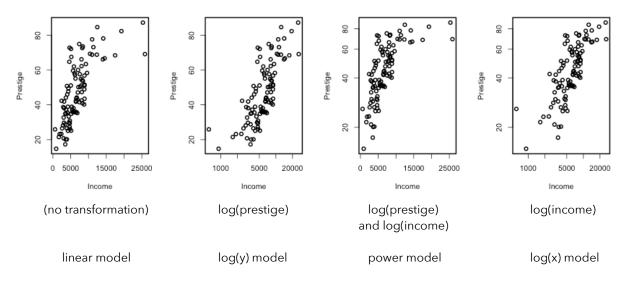
If we use the second parameterization, we can still use our ordinary least squares methods to find the line of best fit. I used R to obtain the following output:



Because this power model predicts log(pressure), we cannot use the omnibus F-test to compare it to our linear and quadratic models.

Based on this output, which model would you choose to predict pressure based on temperature?

12. We can replicate this nonlinear regression process with our prestige data. Below, I've graphed prestige as a function of income with some transformations to the variables:



Based on these plots, which transformation yielded the most "linear-looking" scatterplot?

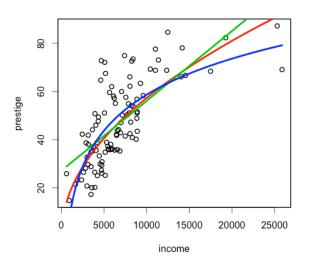
13. I then fit these models to the data an obtained the following:

```
Linear Model: prestige) = b_0 + b_1(income)
R^2 = 0.511
```

Log(y) model: log(prestige) =  $b_0 + b_1$ (income) R<sup>2</sup> = 0.452

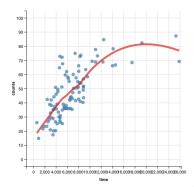
Power model: log(prestige) =  $b_0 + b_1 * log(income)$ R<sup>2</sup> = 0.566

log(x) model: prestige =  $b_0 + b_1 * log(income)$ R<sup>2</sup> = 0.549



We could then compare all these models to the LOWESS curve:

For another nonlinear regression example (including other function options), go to: <u>http://bradthiessen.com/html5/stats/m301/16e.pdf</u>



14. Let's take a step back and take a look at all the regression-related techniques we've covered thus far:

- Simple linear regression
- Diagnostic plots
- Tests for significance of coefficients (randomization-based, t-test for correlation, t-test for slope, F-test)
- Confidence intervals and prediction intervals
- Multiple linear regression
- Model comparison (using omnibus F-test)
- Adjusted R-squared
- Standardized beta coefficients
- Interaction terms
- Model selection (forward, backward, stepwise)
- Cross-validation
- Best subsets regression
- Ridge regression / Lasso
- LOWESS
- Polynomial (curvilinear) regression
- Nonlinear regression
- Robust regression
- Quantile regression
- ANOVA as regression

On the next page, we'll learn some aspects of these techniques

15. As we've discussed, the linear and nonlinear regression techniques we've covered thus far are all based on some underlying assumptions. We've investigated some techniques (visualizations and tests) to evaluate these assumptions. What can we do if we find the assumptions are violated?

If we have an issue with normality of residuals, we might choose to transform our variables. Likewise, if our linearity assumption is violated, we might turn to a curvilinear or nonlinear regression model. But what do we do if we have concerns about the homogeneity of variances assumption? Likewise, what can we do if our data have a few influential outliers?

One thing we could do is run a *robust* regression. There are two types of robust regression methods:

- Regression with robust standard errors
- Robust estimation of coefficients and standard errors

For a couple quick examples of robust regression methods, check out: <u>http://www.philender.com/courses/linearmodels/notes4/robust.html</u>

We'll briefly investigate one approach to robust regression using *bootstrap* methods. In this approach, we:

- a) Estimate regression coefficients from the data:  $\hat{y} = b_0 + b_1 x_1 + ...$
- b) Calculate predicted values  $(\hat{y})$  and residuals for each observation  $(e = \hat{y} y)$
- c) Take all *n* residuals and select a sample of *n* of them <u>with replacement</u> (the bootstrap sample).
- d) Using those sampled residuals, calculate new Y values  $(y^* = \hat{y} + e)$
- e) Now run a regression using your original x variable and the new y\* variable values
- f) Repeat steps c-e many times (say, 10,000 times)

Now that we have 10,000 estimates of our regression coefficients, we can estimate their standard errors by simply calculating the standard deviation of all our coefficient estimates. Likewise, we can find the lowest and highest 2.5% of the coefficient estimates to estimate a 95% confidence interval for each.

To read about this technique, check out either of the following:

http://socserv.mcmaster.ca/jfox/Books/Companion/appendix/Appendix-Bootstrapping.pdf http://www.sagepub.com/upm-data/21122\_Chapter\_21.pdf

Let's try this out on our prestige data. We'll model prestige as a function of income, education, and %women:

	Linear Model		Bootstrap Met	thod
	<u>Coefficient</u>	Standard Error	<u>Coefficient</u>	<u>Standard Error</u>
(intercept)	-6.794334	3.239089	-6.7918	3.24658
Income	0.001314	0.000278	0.00136	0.00028
Education	4.186637	0.388701	4.1829	0.39107
%women	-0.008905	0.030407	-0.00981	0.03072

Notice the bootstrap coefficients are slightly biased (compared to our original model). Also, notice the bootstrap standard errors are all larger. What's the consequence of having larger standard errors for the coefficients?

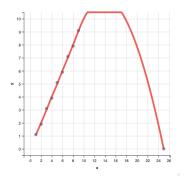
16. Let's take a different approach to bootstrapping a regression. We'll start with a fictitious dataset that has a clear outlier. When we fit a linear model to the data, we get what's pictured to the right.

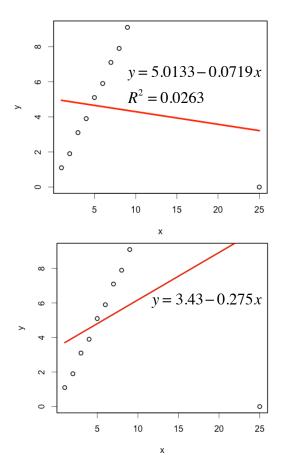
That outlier on the bottom-right obviously had a significant impact on our estimates of the regression coefficients. To mitigate the effect of that outlier, we could choose to:

- a) Take a random sample of n observations <u>with replacement</u> from our data.
- b) Estimate the regression coefficients for this bootstrap sample.
- c) Repeat this process many times to end up with lots of estimated coefficients
- d) Use the mean (or median) of those bootstrap coefficients

The bootstrap regression line is pictured to the right. While it's still not a great fit, it's markedly better than the original.

Just for comparison, a lowess curve is displayed below:

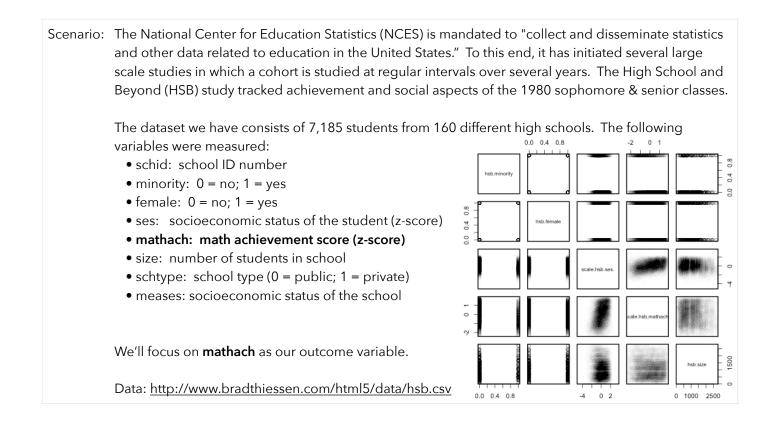




Let's see how this bootstrap method works on our prestige dataset. Below, I've pasted the coefficients using ordinary least squares and using the bootstrap method. Once again, notice that the coefficients and standard errors differ slightly.

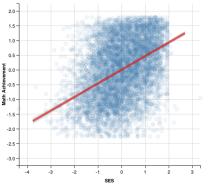
	Linear Model		Bootstrap Method		
	<u>Coefficient</u>	Standard Error	<u>Coefficient</u>	Standard Error	
(intercept)	-6.794334	3.239089	-6.71	3.1224	
Income	0.001314	0.000278	0.00142	0.0005	
Education	4.186637	0.388701	4.10	0.4673	
%women	-0.008905	0.030407	-0.00466	0.0370	

What assumptions did we make with the ordinary least squares regression? What assumptions did we make using the bootstrap method?



17. From the scatterplots, we can see math achievement is associated with socioeconomic status. We can fit the following linear model:

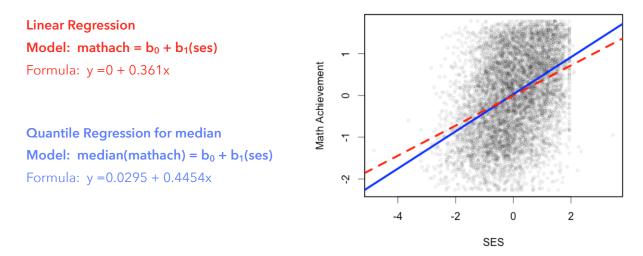
**Model:** mathach =  $b_0 + b_1$ (ses) Formula: y = 0 + 0.361x R<sup>2</sup> = 0.13 RMSE = 0.933 Comparison to null model: F = 1075 (p < 2e-16)



Take a look at the p-value and R-squared value. What can we say about the relationship between SES and math achievement? Keep in mind our variables are standardized (z-scores).

18. When we fit an ordinary least squares regression line, we're fitting a single line through the scatterplot. We can add a confidence or prediction interval, but we're assuming the relationship between our variables is virtually the same for all observations in the data. So, in this example, we're assuming a 1 standard deviation increase in SES is associated with a 0.361 standard deviation increase in math achievement for all students (regardless of just how high or low the students math achievement is).

Might we expect SES to have more or less of an impact on extremely low- or high-achieving students? Maybe. To investigate this, we can use **quantile regression**. What is a quantile?

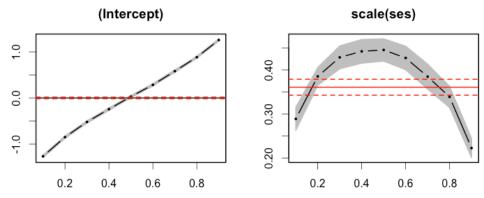


Interpret the coefficients of this quantile regression line. Remember that these coefficients only apply to the chosen quantile of interest!

20. That median regression can be useful (especially when dealing with outliers), but we're more interested in determining if the relationship between SES and math achievement differ depending on the level of math achievement.

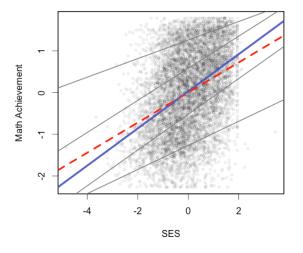
To investigate this, we can run a quantile regression for as many percentiles as we want. For example, we could run the quantile regression for the 10th, 20th, 30th, ..., 80th, and 90th percentiles. That would show us whether the relation between SES and math achievement changes across almost the entire distribution of math achievement scores.

Rather than listing out the coefficients for all 9 regression model, we can display the magnitude of the coefficients across each of the 10 deciles:



The red line shows the coefficients for our simple linear regression model (along with confidence bands). The black lines show the coefficient estimate across different percentiles of math achievement (along with grey confidence bands). From this, what can we conclude about the relationship between SES and math achievement?

21. We can also display these quantile regression lines on the scatterplot. To the right, I've plotted the regression lines for the 10th, 30th, 50th, 70th, and 90th percentiles of math achievement. Do these results match the graphs on the bottom of the previous page?



22. From these graphs, it appears as though the relationship between math achievement and SES is strongest at the median math achievement score (that's where it has the largest slope). At the median, the slope is 0.4454. At the 25th percentile (to choose another one arbitrarily), the slope is 0.4058.

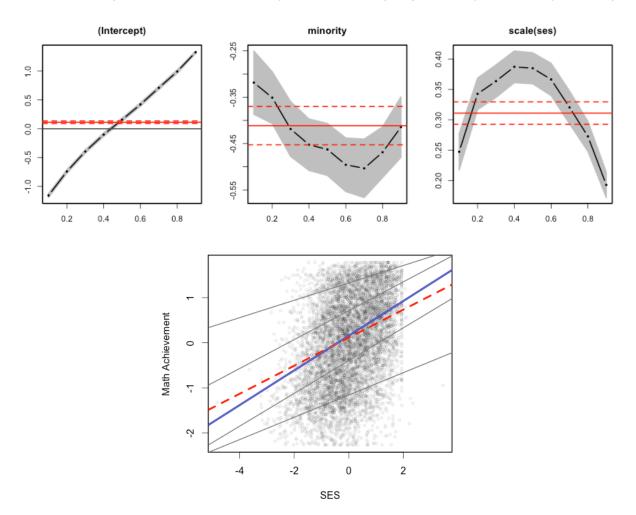
Is there a statistically significant difference between those two slopes? To check, we can compare regression models:

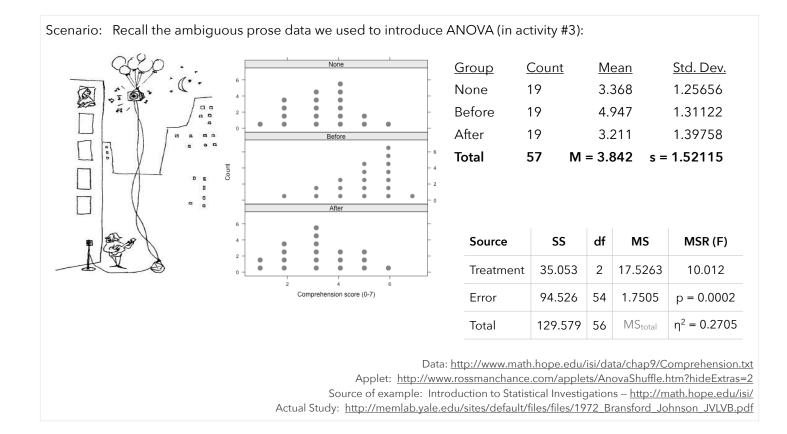
```
Quantile Regression Analysis of Deviance Table
Model: scale(mathach) ~ scale(ses)
Joint Test of Equality of Slopes: tau in { 0.25 0.5 }
Df Resid Df F value Pr(>F)
1 1 14369 7.45 0.0064 **
```

What can we conclude from this?

- (Intercept) minority -0.4 1.0 Math Achievement 0 -0.6 0.0 7 -1.0 -0.8 Ņ 0.2 0.4 0.6 0.8 0.2 0.4 0.6 0.8 0.0 0.2 0.4 0.6 0.8 1.0
- 23. We've investigated the math achievement gap associated with differences in socioeconomic status. Does the achievement gap for minority students also differ across levels of math achievement? Interpret the output.

Minority





25. The ANOVA summary table displayed above indicates at least one of the group means differs from the others. When we conducted the ANOVA, we constructed the following model:  $y_{ii} = \mu + \alpha_i + e_i$ , where  $\alpha_i = \mu_i - \mu$ .

That model is similar to many of the linear regression models we've constructed:  $y_i = b_0 + b_1 x_1 + e_i$ 

Let's take a look at the structure of our data in this example. The *original data* columns show the data that was used to generate the ANOVA summary table.

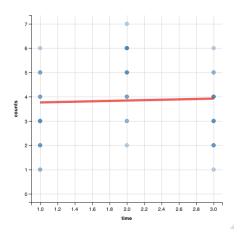
If we want to conduct a regression analysis on this data, it might make sense to convert our independent variable (condition) to numerical values. The *possible coding* column shows one way to do this. We can let 1 = after, 2 = before, and 3 = none. Since our independent variable is categorical (nominal), the actual values we use aren't meaningful (in fact, it may make more sense to code 0 = none, 1 = before, 2 = after).

Original data		Possible coding	[	Dummy codir	ig	
Subject	y = comp.score	Condition	Condition Code	After x1	Before x2	None x3
1	6	After	1	1	0	0
2	5	After	1	1	0	0
20	7	Before	2	0	1	0
21	5	Before	2	0	1	0
39	4	None	3	0	0	1
40	6	None	3	0	0	1

Using the possible coding listed in the table, I fit the model  $y_i = b_0 + b_1 (\text{condition code}) + e_i$ 

Here's the output. Interpret the slope coefficient and explain why this condition coding is a bad idea.

Model: comprehension =  $b_0 + b_1$ (condition code) Formula: y = 3.68421 + 0.07895x R<sup>2</sup> = 0.001828 RMSE = 1.534 F = 0.1007 (p = 0.7522)



26. When we want to include a categorical predictor in our regression model, we'll want to convert that categorical predictor to a series of dummy variables.

A dummy variable can take the value of 0 or 1 to indicate the absence or presence of a categorical effect. So, in this example, we could convert our condition variable into three dummy variables:

- Dummy variable #1 = 1 if the condition is **after** (and equals zero for the before and none categories)
- Dummy variable #2 = 1 if the condition is **before** (and equals zero for the after and none categories)
- Dummy variable #3 = 1 if the condition is **none** (and equals zero for the before and after categories)

These dummy variables are displayed in the table on the previous page.

Suppose we enter these dummy variables into our regression model:  $\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3$ 

I entered these variables into R and obtained the following output:

Coefficients	s: (1 not	defined be	cause of	singularities)
	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	3.3684	0.3035	11.097	1.51e-15
x1	-0.1579	0.4293	-0.368	0.714436
x2	1.5789	0.4293	3.678	0.000542
x3	NA	NA	NA	NA

Why did I get an error message?

- 27. If we include all 3 dummy variables, we have a perfect collinearity problem. All the information we need about the condition category is contained within the first two dummy variables:
  - x1 = 1 if the condition is **after** (and equals zero for the before and none categories)
  - x2 = 1 if the condition is **before** (and equals zero for the after and none categories)

To demonstrate this, identify the condition (after, before, or none) for each of the following:

<u>x1</u>	<u>x2</u>	<u>Condition</u>
1	0	
0	1	
0	0	

28. Let's run our regression again, this time using only the first two dummy variables:  $\hat{y} = b_0 + b_1 x_1 + b_2 x_2$ 

Interpret this output. What do the coefficients represent?

Coefficients:						
	Estimate	Std. Error	t value	Pr(> t )		
(Intercept)	3.3684	0.3035	11.097	1.51e-15		
x1	-0.1579	0.4293	-0.368	0.714436		
x2	1.5789	0.4293	3.678	0.000542		

Residual standard error: 1.323 on 54 degrees of freedom Multiple R-squared: 0.2705, Adjusted R-squared: 0.2435 F-statistic: 10.01 on 2 and 54 DF, p-value: 0.0002002

29. We can get an ANOVA summary table for this regression model (using the dummy variables). Compare it to the ANOVA summary table we calculated in activity #3.

Or	model					
Source	SS	df	MS	MSR (F)	x1	
Treatment	35.053	2	17.5263	10.012	x2	
Error	94.526	54	1.7505	p = 0.0002	Error	
Total	129.579	56	$MS_{total}$	$\eta^2 = 0.2705$	Total	

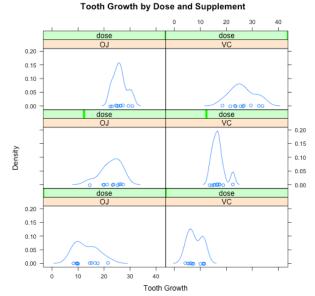
Regression Analysis							
Source	SS	df	MS	MSR (F)			
model	35.053	2	17.5263	10.012	p=0.002		
x1	11.369	1	11.369	6.494	p=0.014		
x2	23.684	1	23.684	13.530	p=0.001		
Error	94.526	54	1.7505				
Total	129.579	56	$MS_{total}$				

30. We can also conduct an AxB ANOVA as a regression analysis. To demonstrate, let's use the guinea pig tooth growth data we may have investigated back in the first unit.

This study investigated tooth growth in guinea pigs as a function of the type and dose of vitamin C. Guinea pigs were given a low, medium, or high dose of vitamin C either through orange juice (OJ) or a vitamin C supplement (VC).

Here's a quick summary of our data:

	supp	dose	n	mean	sd
1	OJ	0.5	10	13.23	4.459709
2	OJ	1	10	22.70	3.910953
3	OJ	2	10	26.06	2.655058
4	VC	0.5	10	7.98	2.746634
5	VC	1	10	16.77	2.515309
6	VC	2	10	26.14	4.797731



We can convert our dose and supplement variables into dummy variables:

Original data				Du	mmy coding	
Guinea Pig	y = tooth growth	Supplement	Dose	Supp.Code	Dose1	Dose2
1	4.2	OJ	Low	0	1	0
2	11.5	OJ	Medium	0	0	1
3	7.3	OJ	High	0	0	0
4	5.8	VC	Low	1	1	0
5	6.4	VC	Medium	1	0	1
6	10.0	VC	High	1	0	0

We can then fit a linear model, including the interaction terms.

 $\hat{y} = b_0 + b_1(\text{supp.code}) + b_2(\text{dose}_{low}) + b_3(\text{dose}_{med}) + b_4(\text{supp.code})(\text{dose}_{low}) + b_5(\text{supp.code})(\text{dose}_{med})$ 

The model results in the following coefficient estimates:

Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 13.230 1.148 11.521 3.60e-16 suppVC -5.250 1.624 -3.233 0.00209 dose1 9.470 1.624 5.831 3.18e-07 dose2 12.830 1.624 7.900 1.43e-10 suppVC:dose1 -0.680 2.297 -0.296 0.76831 suppVC:dose2 5.330 2.297 2.321 0.02411

Interpret this output.

31. Compare the AxB ANOVA summary table with the ANOVA summary table from this regression analysis.

AxB ANOVA								
Source	SS	df	MS	MSR (F)				
supplement	205.4	1	205.4	15.572	p=0.0002			
dose	2426.4	2	1213.2	92.000	p<0.00001			
interaction	108.3	2	54.2	4.107	0.02186			
Error	712.1	54	13.2					
Total	3452.2	59	$MS_{total}$					

Regression								
Source	SS	df	MS	MSR (F)				
supplement	205.4	1	205.4	15.572	p=0.0002			
dose	2426.4	2	1213.2	92.000	p<0.00001			
supp:dose	108.3	2	54.2	4.107	0.02186			
Error	712.1	54	13.2					
Total	3452.2	59	$MS_{total}$					