Module 5 Lab Examples

Introduction

This lab covers the following topics.

- 1. Confidence and prediction intervals
- 2. Manually performing a Sum of Squares F-test
- 3. Using anova() to perform a Sum of Squares F-test
- 4. Using model selection criteria functions AIC() and BIC() to compare models
- 5. Exploring the usefulness of \mathbb{R}^2 for model comparison

You'll explore these concepts in the context of a study looking at the energy costs of echo-location in bats. The data is available in the Sleuth3 package, in the object case1002.

case1002

```
##
       Mass
                              Type Energy
## 1
     779.0 non-echolocating bats
                                     43.70
     628.0 non-echolocating bats
      258.0 non-echolocating bats
                                     23.30
## 4
     315.0 non-echolocating bats
                                     22.40
## 5
       24.3 non-echolocating birds
                                      2.46
       35.0 non-echolocating birds
                                      3.93
## 7
       72.8 non-echolocating birds
                                      9.15
     120.0 non-echolocating birds
                                     13.80
     213.0 non-echolocating birds
                                     14.60
## 10 275.0 non-echolocating birds
                                     22.80
## 11 370.0 non-echolocating birds
                                     26.20
## 12 384.0 non-echolocating birds
                                     25.90
## 13 442.0 non-echolocating birds
                                     29.50
## 14 412.0 non-echolocating birds
                                     43.70
## 15 330.0 non-echolocating birds
                                     34.00
## 16 480.0 non-echolocating birds
                                     27.80
       93.0
                 echolocating bats
                                      8.83
                 echolocating bats
                                      1.35
## 18
        8.0
## 19
        6.7
                 echolocating bats
                                      1.12
## 20
                 echolocating bats
        7.7
                                      1.02
```

?case1002

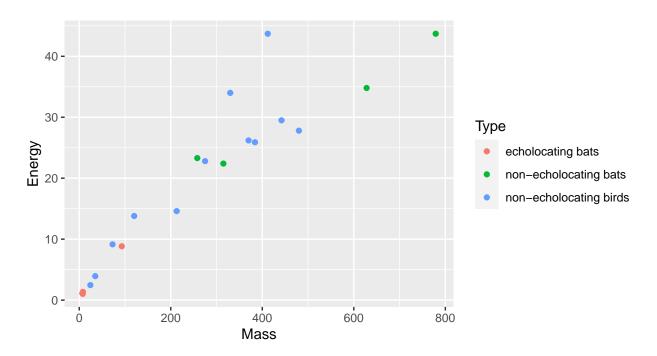
Here's the context: Some bats use echolocation to orient themselves. Zoologists have hypothesized the energy costs of echolocation during flight are the sum of the energy cost of flight plus the energy cost of echolocation. If they can show bats that echolocate use about the same energy as non-echolocating bats, they have evidence these bats have evolved to echo-locate efficiently. But there is a complication, the energy costs of flight depend on how heavy you are.

The data are on in–flight energy expenditure and body mass from 20 energy studies on three types of flying vertebrates: echolocating bats, non–echolocating bats and non–echolocating birds.

Exploratory Analysis

Let's take a quick look at what we have:

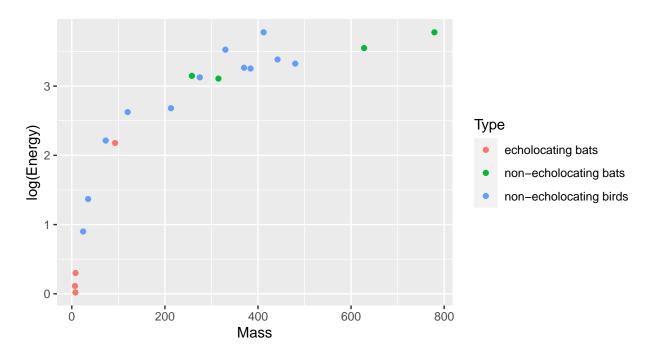
```
qplot(Mass, Energy, data = case1002, color = Type)
```



Notice the general relationship, that increasing mass is associated with increasing energy costs. It's a little hard to see any substantial difference between the three types. You might notice there seems to be a lot more variation in energy with higher mass, this is often a sign a transformation might result in a cleaner relationship. Let's try looking at log(Energy) instead.

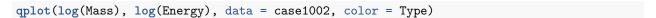
Plot Mass vs. log(Energy).

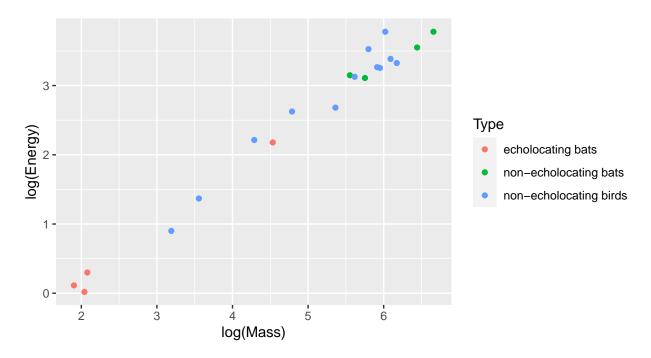
```
qplot(Mass, log(Energy), data = case1002, color = Type)
```



The variation looks a little more constant, but the relationship between energy and mass looks rather non-linear. Let's try log(Mass) as well:

Plot log(Mass) vs. log(Energy).





Much better: nice linear relationship, and constant variance.

Multiple Linear Regression

We are going to be interested in three models.

Model 1: Both birds and non-echolocating bats have possibly different energy costs in flight to echolocating bats, after accounting for a linear relationship between log energy and log mass,

$$\log(Energy_i) = \beta_0 + \beta_1 \log(Mass_i) + \beta_2 non-ebat_i + \beta_3 bird_i + \epsilon_i$$

Model 2: The energy costs for non-echolocating bats and echolocating bats is the same, but possibly different to birds, after accounting for a linear relationship between log energy and log mass,

$$\log(Energy_i) = \beta_0 + \beta_1 \log(Mass_i) + \beta_3 bird_i + \epsilon_i$$

Model 3: All types have the same energy costs in flight, after accounting for a linear relationship between log energy and log mass,

$$\log(Energy_i) = \beta_0 + \beta_1 \log(Mass_i) + \epsilon_i$$

where $non\text{-}ebat_i$ is an indicator variable that the Type of the i^{th} observation is a non-echo-locating bat, and $bird_i$ is an indicator variable that the Type of the i^{th} observation is a bird.

Fit all three of the models specified above using lm() and store them in the variables mod1, mod2, and mod3, respectively.

Note: Model 2 is a little tricky, we need to create a new indicator that is TRUE only for "non-echolocating birds".

```
mod1 <- lm(log(Energy) ~ log(Mass) + Type, data = case1002)
mod2 <- lm(log(Energy) ~ log(Mass) +
        I(Type == "non-echolocating birds"), data = case1002)
mod3 <- lm(log(Energy) ~ log(Mass), data = case1002)</pre>
```

We don't actually have to fit model 2 to answer our question of interest. Since Model 2 only differs from Model 1 by dropping the β_2 term, we can ask if $\beta_2 = 0$ in Model 1, to decide if Model 2 is more appropriate.

We fit it here to demonstrate the difference between the fit of the two models, which we'll do by examining their predictions.

Prediction and Confidence Intervals

If you want prediction and/or confidence intervals for the mean response variable value at new explanatory variable values, the procedure is similar to the one we used for SLR. You need to specify a new data frame containing the values of the variables of interest, then use predict(). Let's compare the predictions between Model 1 and Model 2, for echo-locating and non-echo-locating bats of the same weight:

First we will make a new data frame to use as new data.

```
same_weight_bats <- data.frame(
   Type = rep(c("echolocating bats", "non-echolocating bats"), 3),
   Mass = rep(c(100, 400, 700), each = 2)
)
same_weight_bats</pre>
```

```
## Type Mass
## 1 echolocating bats 100
## 2 non-echolocating bats 100
```

```
## 3 echolocating bats 400
## 4 non-echolocating bats 400
## 5 echolocating bats 700
## 6 non-echolocating bats 700
```

You must be careful to keep the column names exactly the same as those in the input data to lm() and any categorical variables must use the same values. OK, let's take a look at the predictions for mod1:

```
cbind(same_weight_bats, pred_log_energy = predict(mod1, newdata = same_weight_bats))
```

```
##
                      Type Mass pred_log_energy
## 1
         echolocating bats
                            100
                                        2.255321
## 2 non-echolocating bats
                                        2.176658
## 3
         echolocating bats
                             400
                                        3.385092
## 4 non-echolocating bats
                             400
                                        3.306429
## 5
         echolocating bats
                             700
                                        3.841155
## 6 non-echolocating bats
                                        3.762492
```

In the first model, notice first that the predictions for echo and non-echo locating bats of the same weight are different, and second they always differ by the same amount (i.e. 2.255321-2.176658 = 3.385092-3.306429 = 0.078663). This amount is our estimate of β_2 , which you can confirm by examining coef (mod1).

Do the same as above for mod2: make predictions for the log-energy-usage using mod2.

```
cbind(same_weight_bats, pred_log_energy = predict(mod2, newdata = same_weight_bats))
```

```
##
                       Type Mass pred_log_energy
## 1
                                        2.212898
         echolocating bats
                            100
## 2 non-echolocating bats
                             100
                                        2.212898
         echolocating bats
                             400
                                        3.324432
## 4 non-echolocating bats
                             400
                                        3.324432
## 5
         echolocating bats
                             700
                                        3.773134
                                        3.773134
## 6 non-echolocating bats
                            700
```

In the second model, β_2 has been forced to zero and the predictions for echo and non-echo locating bats of the same weight are always the same.

These predictions are on the transformed response scale. To go back to energy (rather than log energy) you can backtransform the predictions (and confidence interval endpoints if needed):

```
cbind(same_weight_bats, pred_energy = exp(predict(mod1, newdata = same_weight_bats)))
```

```
##
                      Type Mass pred_energy
## 1
                             100
         echolocating bats
                                    9.538359
## 2 non-echolocating bats
                             100
                                    8.816789
         echolocating bats
                             400
                                   29.520721
## 4 non-echolocating bats
                             400
                                   27.287500
## 5
         echolocating bats
                             700
                                   46.579266
## 6 non-echolocating bats
                            700
                                   43.055579
```

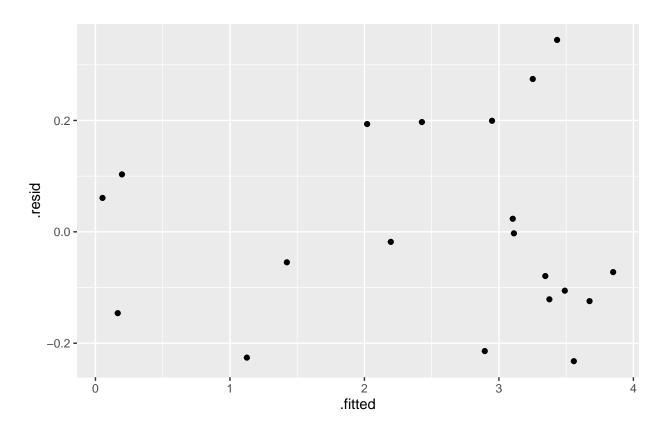
If you need a confidence interval or prediction interval, you can add the interval argument as usual.

Diagnostics

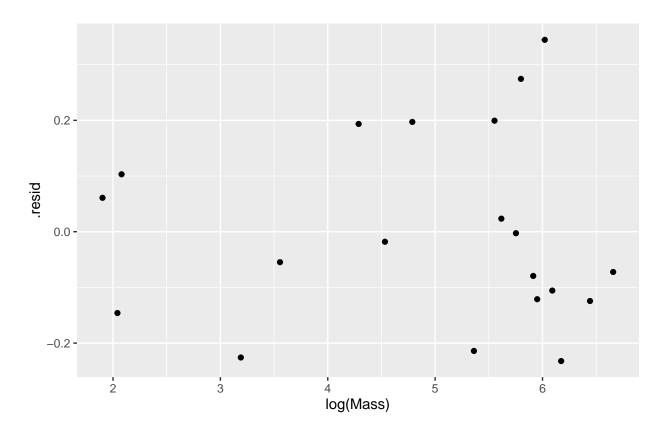
Hopefully you are convinced that we can answer the scientific question of interest with inference on β_2 in Model 1. Before we do, we should take a look at the fit of the models. You should generally do these checks on the most complicated model you are considering.

**Use augment() on mod1 to create a data frame with diagnostics. Save it to the variable case1002_diags. Then plot each .fitted, 'log(Mass), and Type against .resid.

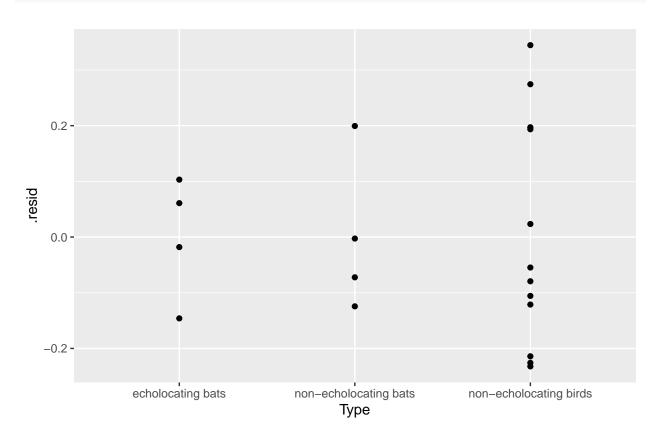
```
case1002_diag <- augment(mod1, case1002)
qplot(.fitted, .resid, data = case1002_diag)</pre>
```



```
qplot(log(Mass), .resid, data = case1002_diag)
```



qplot(Type, .resid, data = case1002_diag)



To review, we are looking for signs that our model assumptions—linearity, normality, independence, constant variance—may have been violated. If they have, it could show up as systematic patterns in the residual plots.

The one plot that may raise eyebrows in this example is the residuals versus Type. It looks like the residuals for non-echolocating birds are much more spread out. However, there is not too much cause for concern: since there are many more birds than either kind of bats, you are more likely to see extremes just because you have more observations for that group.

Inference on single parameters

Take a look at the summary of Model 1

```
summary(mod1)
```

```
##
## Call:
## lm(formula = log(Energy) ~ log(Mass) + Type, data = case1002)
## Residuals:
##
        Min
                  1Q
                       Median
                                    3Q
                                            Max
## -0.23224 -0.12199 -0.03637 0.12574
                                        0.34457
##
## Coefficients:
##
                              Estimate Std. Error t value Pr(>|t|)
                                                   -9.993 2.77e-08 ***
## (Intercept)
                              -1.49770
                                          0.14987
## log(Mass)
                               0.81496
                                          0.04454
                                                   18.297 3.76e-12 ***
## Typenon-echolocating bats -0.07866
                                          0.20268
                                                   -0.388
                                                              0.703
## Typenon-echolocating birds 0.02360
                                          0.15760
                                                    0.150
                                                              0.883
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.186 on 16 degrees of freedom
## Multiple R-squared: 0.9815, Adjusted R-squared: 0.9781
## F-statistic: 283.6 on 3 and 16 DF, p-value: 4.464e-14
```

The output includes the t-tests for the null hypothesis that each parameter is zero. This isn't always the hypothesis of interest, but in this case, the scientific question can be answered by examining the row for β_2 , the parameter associated with the non-echolocating bat indicator variable.

There is no evidence that non-echolocating bats have a different energy cost in flight to echo-locating bats, after accounting for body mass (p-value = 0.70 from t-test echo-locating indicator variable in a regression of log energy on log mass and type).

Confidence intervals for model parameters can be obtained with the confint() function. Use it on mod1.

confint(mod1)

With 95% confidence, the mean log energy cost for non-echolocating bats is between 0.51 units lower and 0.35 units higher than echolocating bats.

Inference on more than one parameter

You might be interested in comparing Model 1 to Model 3. Since these two models differ by two parameters the appropriate comparison uses and Extra Sum of Squares F-test.

A Sum of Squares F-test allows us to compare any two nested models, (which we typically call the "reduced model" and a more complex "full model"), where the reduced model is "nested" in the full model. Nested means that the full model has all predictors the reduced model has, plus additional predictors. Put another way, the predictors in the reduced model are a subset of the predictors in the full model. Note that this is the only setting where we can use an F-test.

Sum of Squares F-test

Basically, we want to compare the proportion of total variability explained by each model, and ask if the increase in explained variability is sufficient to justify adding the additional term/s into the model. Equivalently, is the *decrease* in *unexplained* variability sufficient to justify the more complex model? The F-statistic contains the information we need, and its distribution has an answer.

$$F = \frac{(RSS_{red} - RSS_{full})/(df_{red} - df_{full})}{RSS_{full}/df_{full}} \sim F_{(df_{red} - df_{full}, df_{full})}$$

"RSS" stands for Residual Sum of Squares, "df" stands for degrees of freedom, and the subscripts denote the full and reduced model. The following code calculates the necessary pieces, and then performs a Sum of Squares F-test.

```
rss1 <- deviance(mod1) # Model 1 RSS
rss3 <- deviance(mod3) # Model 3 RSS
df1 <- df.residual(mod1) # Model 1 Residual Degrees of Freedom
df3 <- df.residual(mod3) # Model 3 Residual Degrees of Freedom
fstat <- ((rss3 - rss1)/(df3 - df1))/(rss1/df1) # F-statistic
1 - pf(fstat, df3 - df1, df3) # p-value</pre>
```

```
## [1] 0.6585362
```

The first two lines extract the residuals sum of squares from each model fit. The next two lines extract the residual degrees of freedom from each model. The next line calculates the F-statistic, and the final line calculates the p-value. To review, the p-value is the probability of seeing an F-statistic this unlikely, or more unlikely, if the null hypothesis (simple model) is true. What do we conclude?

There is no evidence for the more complicated model. The extra terms aren't worth it. You can probably guess, there is an easier way to perform the same test.

```
anova(mod3, mod1) # Sum of Squares F-test
```

```
## Analysis of Variance Table
##
## Model 1: log(Energy) ~ log(Mass)
## Model 2: log(Energy) ~ log(Mass) + Type
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 18 0.58289
## 2 16 0.55332 2 0.029574 0.4276 0.6593
```

The analysis of variance table contains all the information we just calculated. Conveniently, the two models being compared are provided in the output (note that Model 1 is just the first model object you provided—in this case, mod3; likewise, Model 2 is the second model object you provided—in this case, mod1). After the summary of the models being compared, the output displays the ANOVA table. The columns give the residual degrees of freedom, residual sum of squares, difference in degrees of freedom (numerator degrees of freedom), difference in sum of squares between the two models, F-statistic, and p-value.

Perform the Sum of Squares F-test on mod2 and mod1.

```
## Analysis of Variance Table
##
## Model 1: log(Energy) ~ log(Mass) + I(Type == "non-echolocating birds")
## Model 2: log(Energy) ~ log(Mass) + Type
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 17 0.55853
## 2 16 0.55332 1 0.0052094 0.1506 0.703
```

What other ways can we compare two or more models?

Model Comparison Criteria

An analyst may want additional model comparison criteria. Two commonly used tools are the Akaike information criterion (AIC), and the Bayesian information criterion (BIC). The details of these measures are beyond the scope of this lab, but suffice it to say that the lower the score for each of these two criteria, the better the fit (**discussion of "better" below). A strength of AIC and BIC, in contrast to the F-test, is that not only can we compare more than two models simultaneously, but we can compare models that are not nested.

```
AIC(mod1, mod2, mod3)
##
        df
                  AIC
## mod1
         5 -4.993569
## mod2
         4 -6.806154
## mod3
        3 -7.952201
BIC(mod1, mod2, mod3)
##
        df
                    BIC
## mod1
         5 -0.01490754
## mod2
         4 -2.82322519
## mod3
         3 -4.96500445
```

Both criteria agree with the F-test: the simplest of the three models is sufficient. We know this because mod3 has the lowest AIC and BIC scores.

**What does "better" mean to AIC and BIC? There is not a simple answer, but there are a few ideas worth mentioning. AIC and BIC place value on model "parsimony," in the Occam's Razor sense of the word. If two models explain variation in the response equally well, then AIC and BIC tend to prefer the simpler model (with fewer terms). AIC and BIC implement this preference by penalizing a model (that is, giving it a higher, less "desirable" score) for extra predictors. This preference aids interpretation; the greater the

number of terms in a model, typically the more difficult it is to understand and interpret the meaning of those terms. For example, imagine interpreting a marginally useful squared three-way interaction term! However, this preference for simpler, more interpretable models makes AIC and BIC somewhat ill-suited to model selection for prediction. If prediction is your ultimate goal, and that squared three-way interaction term improves prediction, then so be it!

R^2 - Coefficient of Determination

What about R^2 as a model comparison metric? R^2 is sometimes called the "Coefficient of Determination," and described as the proportion of total variation in the response explained by the model.

Revisiting the models we fit, R^2 did increase with the addition of Type:

```
summary(mod1) # Multiple R-squared: 0.9815
```

```
##
## Call:
## lm(formula = log(Energy) ~ log(Mass) + Type, data = case1002)
##
  Residuals:
##
        Min
                  1Q
                       Median
                                    30
                                            Max
   -0.23224 -0.12199 -0.03637
                              0.12574
                                        0.34457
##
## Coefficients:
##
                              Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                              -1.49770
                                          0.14987
                                                   -9.993 2.77e-08 ***
## log(Mass)
                               0.81496
                                                   18.297 3.76e-12 ***
                                          0.04454
## Typenon-echolocating bats -0.07866
                                                   -0.388
                                                              0.703
                                          0.20268
## Typenon-echolocating birds 0.02360
                                          0.15760
                                                    0.150
                                                              0.883
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.186 on 16 degrees of freedom
## Multiple R-squared: 0.9815, Adjusted R-squared: 0.9781
## F-statistic: 283.6 on 3 and 16 DF, p-value: 4.464e-14
```

summary(mod3) # Multiple R-squared: 0.9806

```
##
## lm(formula = log(Energy) ~ log(Mass), data = case1002)
##
## Residuals:
##
                       Median
                                             Max
        Min
                  1Q
                                    3Q
## -0.21143 -0.14422 -0.04284 0.09681
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -1.46826
                           0.13716
                                    -10.71 3.1e-09 ***
## log(Mass)
                0.80861
                           0.02684
                                     30.13 < 2e-16 ***
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
```

```
##
## Residual standard error: 0.18 on 18 degrees of freedom
## Multiple R-squared: 0.9806, Adjusted R-squared: 0.9795
## F-statistic: 907.6 on 1 and 18 DF, p-value: < 2.2e-16</pre>
```

Does this mean mod1 is superior to mod3? To explore this answer, consider adding another explanatory variable, but this time a completely meaningless one. We will generate Normal random variables with the same mean as the response variable log(Energy), and a standard deviation of one. What will happen to R^2 if we include this predictor in the model?

```
set.seed(12345)
noise <- rnorm(nrow(case1002), mean(log(case1002$Energy)), 1)
mod4 <- lm(log(Energy) ~ log(Mass) + Type + noise, data = case1002)
summary(mod4) # Multiple R-squared: 0.9823</pre>
```

```
##
## Call:
## lm(formula = log(Energy) ~ log(Mass) + Type + noise, data = case1002)
##
## Residuals:
                      Median
##
       Min
                 1Q
                                    3Q
## -0.22849 -0.10940 -0.05392 0.12741 0.36124
## Coefficients:
                              Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                              -1.40198
                                         0.19327 -7.254 2.81e-06 ***
## log(Mass)
                                          0.04529 18.076 1.36e-11 ***
                              0.81863
## Typenon-echolocating bats -0.08586
                                          0.20521
                                                  -0.418
                                                             0.682
## Typenon-echolocating birds 0.01406
                                          0.15986
                                                   0.088
                                                             0.931
## noise
                              -0.04162
                                          0.05213
                                                  -0.798
                                                             0.437
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.1881 on 15 degrees of freedom
## Multiple R-squared: 0.9823, Adjusted R-squared: 0.9776
## F-statistic: 208 on 4 and 15 DF, p-value: 6.077e-13
```

 R^2 increased! Did we really *explain* more of the variation in our data? Of course not. In fact, R^2 will never decrease when you add more terms; it can only increase. AIC and BIC, on the other hand, take into consideration the number of terms included in a model.

Check AIC and BIC for mod1 and mod4.

```
## df AIC

## mod1 5 -4.993569

## mod4 6 -3.825931

BIC(mod1, mod4)

## df BIC

## mod1 5 -0.01490754

## mod4 6 2.14846307
```

Note that AIC and BIC are both smaller for mod1 than for mod4, so mod1 would be the preferred model according to both of these criteria. The AIC and BIC do a better (but of course not perfect) job of identifying models that contain useful variables vs. models that contain "noise" (useless) variables.