Section 1: Multiple Regression

Section 2: Model Selection

Section 3: Stepwise Regression

Section 4: Non-Linear Models

Section 5: Practical Exercises

Multiple Regression with R

Code **▼**

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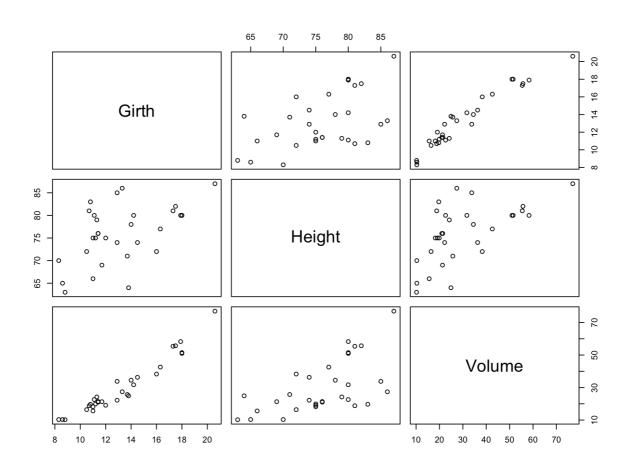
Last modified: 04 Mar 2019

Section 1: Multiple Regression

The in-built dataset trees contains data pertaining to the Volume, Girth and Height of 31 felled black cherry trees. In the Simple Regression session, we constructed a simple linear model for Volume using Girth as the independent variable. Now we will expand this by considering Height as another predictor.

Start by plotting the dataset:

plot(trees)



This plots all variables against each other, enabling visual information about correlations within the dataset.

Re-create the original model of Volume against Girth:

```
Hide
```

```
m1 = lm(Volume~Girth, data=trees)
summary(m1)
##
## Call:
```

```
## lm(formula = Volume ~ Girth, data = trees)
## Residuals:
     Min
##
             10 Median
                           3Q
                                 Max
## -8.065 -3.107 0.152 3.495 9.587
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -36.9435
                          3.3651 -10.98 7.62e-12 ***
## Girth
               5.0659
                           0.2474
                                   20.48 < 2e-16 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.252 on 29 degrees of freedom
## Multiple R-squared: 0.9353, Adjusted R-squared: 0.9331
## F-statistic: 419.4 on 1 and 29 DF, p-value: < 2.2e-16
```

Now include Height as an additional variable:

```
Hide
```

```
m2 = lm(Volume~Girth+Height,data=trees)
summary(m2)
```

```
## Call:
## lm(formula = Volume ~ Girth + Height, data = trees)
##
## Residuals:
##
      Min
               1Q Median
                              3Q
## -6.4065 -2.6493 -0.2876 2.2003 8.4847
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -57.9877
                          8.6382 -6.713 2.75e-07 ***
## Girth
               4.7082
                           0.2643 17.816 < 2e-16 ***
                0.3393
                          0.1302 2.607 0.0145 *
## Height
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 3.882 on 28 degrees of freedom
## Multiple R-squared: 0.948, Adjusted R-squared: 0.9442
## F-statistic: 255 on 2 and 28 DF, p-value: < 2.2e-16
```

Note that the R^2 has improved, yet the Height term is less significant than the other two parameters.

Try including the interaction term between Girth and Height:

```
m3 = lm(Volume~Girth*Height,data=trees)
summary(m3)
```

```
##
## Call:
## lm(formula = Volume ~ Girth * Height, data = trees)
##
## Residuals:
      Min
##
              1Q Median
                            3Q
## -6.5821 -1.0673 0.3026 1.5641 4.6649
##
## Coefficients:
##
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 69.39632 23.83575
                                 2.911 0.00713 **
## Girth
            -5.85585 1.92134 -3.048 0.00511 **
              ## Height
## Girth:Height 0.13465
                        0.02438 5.524 7.48e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.709 on 27 degrees of freedom
## Multiple R-squared: 0.9756, Adjusted R-squared: 0.9728
## F-statistic: 359.3 on 3 and 27 DF, p-value: < 2.2e-16
```

All terms are highly significant. Note that the Height is more significant than in the previous model, despite the introduction of an additional parameter.

We'll now try a different functional form - rather than looking for an additive model, we can explore a multiplicative model by applying a log-log transformation (leaving out the interaction term for now).

```
m4 = lm(log(Volume)~log(Girth)+log(Height),data=trees)
summary(m4)
```

```
##
## Call:
## lm(formula = log(Volume) ~ log(Girth) + log(Height), data = trees)
## Residuals:
##
        Min
                   1Q
                         Median
                                       3Q
                                                Max
## -0.168561 -0.048488 0.002431 0.063637 0.129223
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -6.63162
                         0.79979 -8.292 5.06e-09 ***
                          0.07501 26.432 < 2e-16 ***
## log(Girth)
               1.98265
## log(Height) 1.11712
                          0.20444
                                    5.464 7.81e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 0.08139 on 28 degrees of freedom
## Multiple R-squared: 0.9777, Adjusted R-squared: 0.9761
## F-statistic: 613.2 on 2 and 28 DF, p-value: < 2.2e-16
```

All terms are significant. Note that the residual standard error is much lower than for the previous models. However, this value cannot be compared with the previous models due to transforming the response variable. The R^2 value has increased further, despite reducing the number of parameters from four to three.

```
## 2.5 % 97.5 %

## (Intercept) -8.269912 -4.993322

## log(Girth) 1.828998 2.136302

## log(Height) 0.698353 1.535894
```

Looking at the confidence intervals for the parameters reveals that the estimated power of Girth is around 2, and Height around 1. This makes a lot of sense, given the well-known dimensional relationship between Volume, Girth and Height!

For completeness, we'll now add the interaction term.

```
m5 = lm(log(Volume)~log(Girth)*log(Height),data=trees)
summary(m5)
```

```
##
## Call:
## lm(formula = log(Volume) ~ log(Girth) * log(Height), data = trees)
## Residuals:
##
         Min
                    1Q
                          Median
                                        3Q
                                                 Max
## -0.165941 -0.048613 0.006384 0.062204 0.132295
##
## Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                           -3.6869
                                       7.6996 -0.479
                                                         0.636
                                                         0.799
## log(Girth)
                            0.7942
                                       3.0910
                                                0.257
## log(Height)
                            0.4377
                                       1.7788
                                                0.246
                                                         0.808
## log(Girth):log(Height)
                            0.2740
                                       0.7124
                                                0.385
                                                         0.704
##
## Residual standard error: 0.08265 on 27 degrees of freedom
## Multiple R-squared: 0.9778, Adjusted R-squared: 0.9753
## F-statistic: 396.4 on 3 and 27 DF, p-value: < 2.2e-16
```

The R^2 value has increased (of course, as all we've done is add an additional parameter), but interestingly none of the four terms are significant. This means that none of the individual terms alone are vital for the model - there is duplication of information between the variables. So we will revert back to the previous model.

Given that it would be reasonable to expect the power of Girth to be 2, and Height to be 1, we will now fix those parameters, and instead just estimate the one remaining parameter.

```
m6 = lm(log(Volume)-log((Girth^2)*Height)~1,data=trees)
summary(m6)
```

```
##
## Call:
## lm(formula = log(Volume) - log((Girth^2) * Height) ~ 1, data = trees)
##
## Residuals:
##
                   1Q
                         Median
                                        3Q
  -0.168446 -0.047355 -0.003518  0.066308  0.136467
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -6.16917
                          0.01421 -434.3
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0791 on 30 degrees of freedom
```

Note that there is no R² (as only the intercept was included in the model), and that the Residual Standard Error is incomparable with previous models due to changing the response variable.

We can alternatively construct a model with the response being y, and the error term additive rather than multiplicative.

```
m7 = lm(Volume~0+I(Girth^2):Height,data=trees)
summary(m7)
```

```
##
## Call:
## lm(formula = Volume ~ 0 + I(Girth^2):Height, data = trees)
##
## Residuals:
      Min
               10 Median
##
                               3Q
                                      Max
## -4.6696 -1.0832 -0.3341 1.6045 4.2944
##
## Coefficients:
##
                     Estimate Std. Error t value Pr(>|t|)
                                                  <2e-16 ***
## I(Girth^2):Height 2.108e-03 2.722e-05
                                           77.44
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 2.455 on 30 degrees of freedom
## Multiple R-squared: 0.995, Adjusted R-squared: 0.9949
## F-statistic: 5996 on 1 and 30 DF, p-value: < 2.2e-16
```

Note that the parameter estimates for the last two models are slightly different... this is due to differences in the error model.

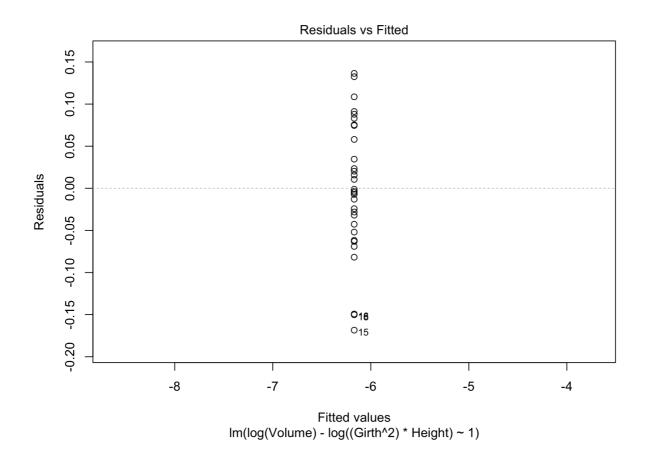
Section 2: Model Selection

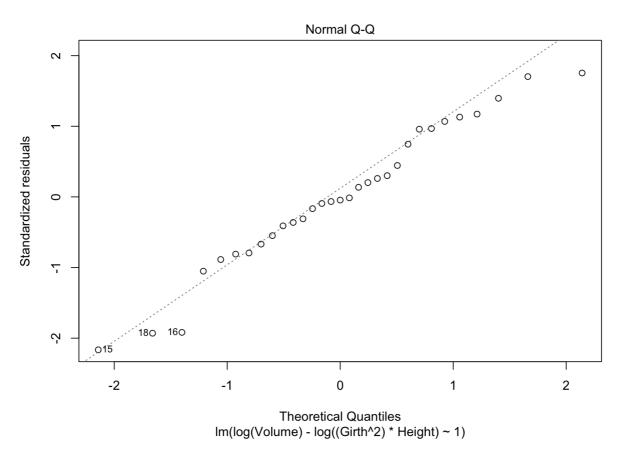
Of the last two models, the one with the log-Normal error model would seem to have the more Normal residuals. This can be inspected by looking at diagnostic plots, by and using the shapiro.test():

Hide

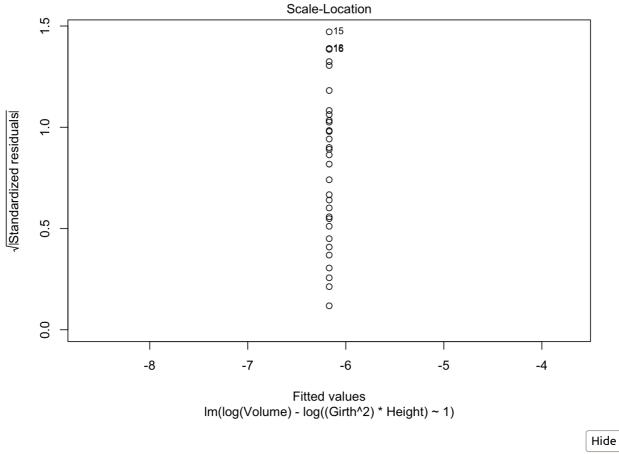
https://bioinformatics-core-shared-training.github.io/linear-models-r/multiple regression.html

plot(m6)

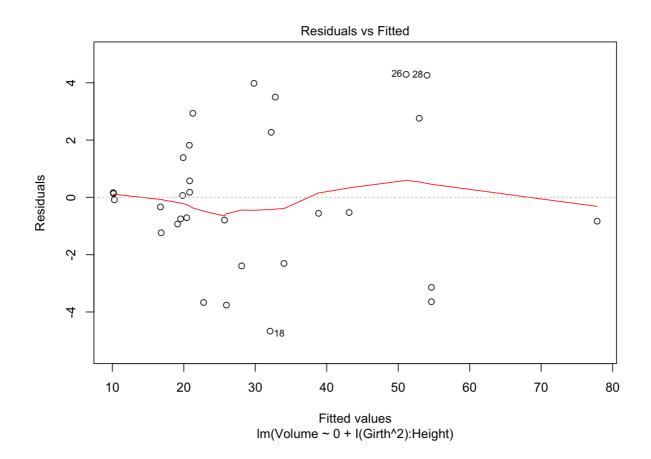


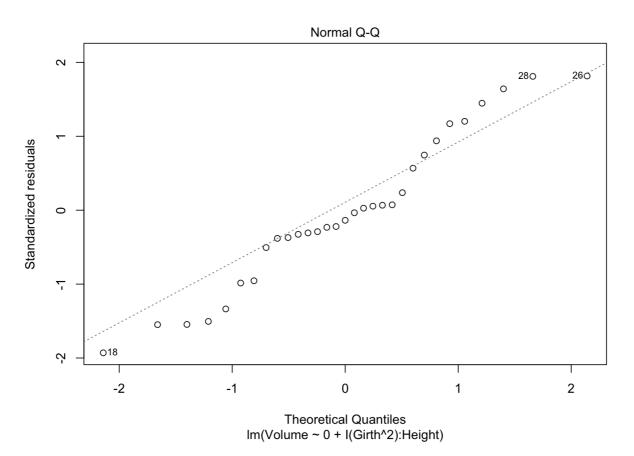


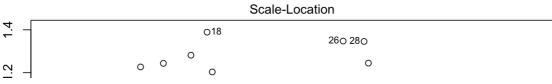
hat values (leverages) are all = 0.03225806
and there are no factor predictors; no plot no. 5

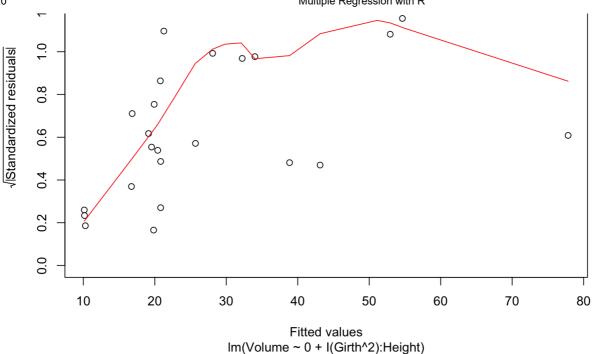


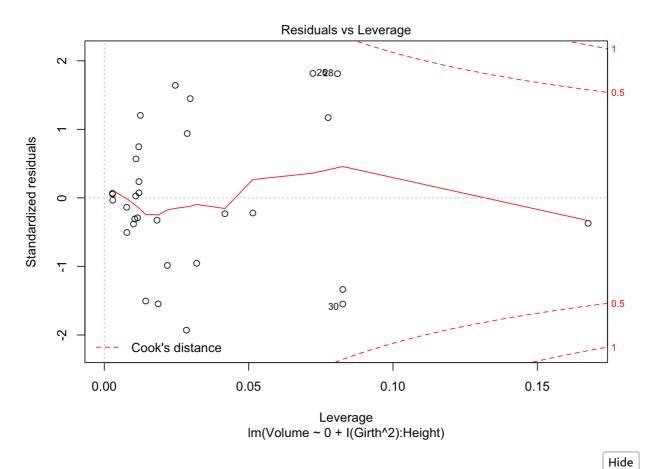
plot(m7)











```
shapiro.test(residuals(m6))
```

```
##
## Shapiro-Wilk normality test
##
## data: residuals(m6)
## W = 0.97013, p-value = 0.5225
```

```
shapiro.test(residuals(m7))
```

```
##
## Shapiro-Wilk normality test
##
## data: residuals(m7)
## W = 0.95846, p-value = 0.2655
```

The Akaike Information Criterion (AIC) can help to make decisions regarding which model is the most appropriate. Now calculate the AIC for each of the above models:

Hide

```
summary(m1)
##
## Call:
## lm(formula = Volume ~ Girth, data = trees)
## Residuals:
     Min
##
             1Q Median
                           3Q
                                 Max
## -8.065 -3.107 0.152 3.495 9.587
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -36.9435
                           3.3651 -10.98 7.62e-12 ***
## Girth
                5.0659
                           0.2474
                                    20.48 < 2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 4.252 on 29 degrees of freedom
## Multiple R-squared: 0.9353, Adjusted R-squared: 0.9331
## F-statistic: 419.4 on 1 and 29 DF, p-value: < 2.2e-16
```

Hide

```
AIC(m1)
```

```
## [1] 181.6447
```

```
summary(m2)
```

```
##
## Call:
## lm(formula = Volume ~ Girth + Height, data = trees)
## Residuals:
##
      Min
               1Q Median
                               3Q
                                      Max
## -6.4065 -2.6493 -0.2876 2.2003 8.4847
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
                          8.6382 -6.713 2.75e-07 ***
## (Intercept) -57.9877
## Girth
                4.7082
                           0.2643 17.816 < 2e-16 ***
## Height
                0.3393
                           0.1302 2.607 0.0145 *
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 3.882 on 28 degrees of freedom
## Multiple R-squared: 0.948, Adjusted R-squared: 0.9442
## F-statistic: 255 on 2 and 28 DF, p-value: < 2.2e-16
```

```
AIC(m2)
```

```
## [1] 176.91
```

Hide

summary(m3)

```
##
## Call:
## lm(formula = Volume ~ Girth * Height, data = trees)
##
## Residuals:
      Min
               1Q Median
                              3Q
                                      Max
## -6.5821 -1.0673 0.3026 1.5641 4.6649
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) 69.39632 23.83575 2.911 0.00713 **
                        1.92134 -3.048 0.00511 **
## Girth
               -5.85585
## Height
               -1.29708
                           0.30984 -4.186 0.00027 ***
## Girth:Height 0.13465
                        0.02438 5.524 7.48e-06 ***
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.709 on 27 degrees of freedom
## Multiple R-squared: 0.9756, Adjusted R-squared: 0.9728
## F-statistic: 359.3 on 3 and 27 DF, p-value: < 2.2e-16
```

```
AIC(m3)
```

```
## [1] 155.4692
```

```
summary(m4)
```

```
##
## Call:
## lm(formula = log(Volume) ~ log(Girth) + log(Height), data = trees)
## Residuals:
##
        Min
                   10
                         Median
                                       3Q
                                               Max
## -0.168561 -0.048488 0.002431 0.063637 0.129223
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -6.63162   0.79979   -8.292   5.06e-09 ***
                          0.07501 26.432 < 2e-16 ***
## log(Girth)
               1.98265
## log(Height) 1.11712
                          0.20444 5.464 7.81e-06 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 0.08139 on 28 degrees of freedom
## Multiple R-squared: 0.9777, Adjusted R-squared: 0.9761
## F-statistic: 613.2 on 2 and 28 DF, p-value: < 2.2e-16
```

Hide

AIC(m4)

```
## [1] -62.71125
```

Hide

summary(m5)

```
##
## lm(formula = log(Volume) ~ log(Girth) * log(Height), data = trees)
##
## Residuals:
##
        Min
                    1Q
                          Median
                                        3Q
## -0.165941 -0.048613 0.006384 0.062204 0.132295
##
## Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                           -3.6869
                                       7.6996 -0.479
                                                         0.636
## log(Girth)
                                       3.0910
                                                0.257
                                                         0.799
                            0.7942
                            0.4377
                                       1.7788
                                                0.246
## log(Height)
                                                         0.808
## log(Girth):log(Height)
                            0.2740
                                       0.7124
                                                0.385
                                                         0.704
## Residual standard error: 0.08265 on 27 degrees of freedom
## Multiple R-squared: 0.9778, Adjusted R-squared: 0.9753
## F-statistic: 396.4 on 3 and 27 DF, p-value: < 2.2e-16
```

```
AIC(m5)
## [1] -60.88061
                                                                            Hide
summary(m6)
##
## Call:
## lm(formula = log(Volume) - log((Girth^2) * Height) ~ 1, data = trees)
## Residuals:
##
        Min
                  10
                        Median
                                     3Q
## -0.168446 -0.047355 -0.003518 0.066308 0.136467
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0791 on 30 degrees of freedom
                                                                            Hide
AIC(m6)
## [1] -66.34198
                                                                            Hide
summary(m7)
##
## lm(formula = Volume ~ 0 + I(Girth^2):Height, data = trees)
##
## Residuals:
##
      Min
               1Q Median
                              3Q
                                    Max
## -4.6696 -1.0832 -0.3341 1.6045 4.2944
##
## Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
## I(Girth^2):Height 2.108e-03 2.722e-05 77.44 <2e-16 ***
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 2.455 on 30 degrees of freedom
## Multiple R-squared: 0.995, Adjusted R-squared: 0.9949
## F-statistic: 5996 on 1 and 30 DF, p-value: < 2.2e-16
```

AIC(m7)

```
Hide
```

```
## [1] 146.6447
```

Whilst the AIC can help differentiate between similar models, it cannot help deciding between models that have different responses. Which model would you select as the most appropriate?

Section 3: Stepwise Regression

The in-built dataset swiss contains data pertaining to fertility, along with a variety of socioeconomic indicators. We want to select a sensible model using stepwise regression. First regress Fertility agains all available indicators:

```
m8 = lm(Fertility~.,data=swiss)
summary(m8)
```

```
##
## Call:
## lm(formula = Fertility ~ ., data = swiss)
##
## Residuals:
      Min
                1Q
                    Median
                                3Q
                                       Max
## -15.2743 -5.2617
                    0.5032
                            4.1198 15.3213
##
## Coefficients:
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                 66.91518 10.70604 6.250 1.91e-07 ***
                 -0.17211
                            0.07030 -2.448 0.01873 *
## Agriculture
## Examination
                 -0.25801 0.25388 -1.016 0.31546
## Education
                 ## Catholic
                  0.10412
                            0.03526 2.953 0.00519 **
## Infant.Mortality 1.07705
                            0.38172 2.822 0.00734 **
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 7.165 on 41 degrees of freedom
## Multiple R-squared: 0.7067, Adjusted R-squared: 0.671
## F-statistic: 19.76 on 5 and 41 DF, p-value: 5.594e-10
```

Are all terms significant?

Now use stepwise regression, performing backward elimination in order to automatically remove inappropriate terms:

```
library(MASS)
summary(stepAIC(m8))
```

```
## Start: AIC=190.69
## Fertility ~ Agriculture + Examination + Education + Catholic +
##
      Infant.Mortality
##
##
                     Df Sum of Sq
                                    RSS
                                           AIC
## - Examination
                     1
                          53.03 2158.1 189.86
## <none>
                                 2105.0 190.69
## - Agriculture 1 307.72 2412.8 195.10
## - Infant.Mortality 1
                          408.75 2513.8 197.03
## - Catholic
                          447.71 2552.8 197.75
                      1
                      1 1162.56 3267.6 209.36
## - Education
##
## Step: AIC=189.86
## Fertility ~ Agriculture + Education + Catholic + Infant.Mortality
##
##
                     Df Sum of Sq
                                    RSS
                                           AIC
## <none>
                                 2158.1 189.86
## - Agriculture
                          264.18 2422.2 193.29
                     1
## - Infant.Mortality 1
                          409.81 2567.9 196.03
## - Catholic
                    1
                          956.57 3114.6 205.10
                      1 2249.97 4408.0 221.43
## - Education
```

```
##
## Call:
## lm(formula = Fertility ~ Agriculture + Education + Catholic +
     Infant.Mortality, data = swiss)
##
##
## Residuals:
##
      Min
              1Q Median
                             3Q
                                    Max
## -14.6765 -6.0522 0.7514 3.1664 16.1422
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                62.10131 9.60489 6.466 8.49e-08 ***
## Agriculture
                ## Education
## Catholic
                 ## Infant.Mortality 1.07844 0.38187 2.824 0.00722 **
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 7.168 on 42 degrees of freedom
## Multiple R-squared: 0.6993, Adjusted R-squared: 0.6707
## F-statistic: 24.42 on 4 and 42 DF, p-value: 1.717e-10
```

Are all terms significant? Is this model suitable? What are the pro's and con's of this approach?

Section 4: Non-Linear Models

The in-built dataset trees contains data pertaining to the Volume, Girth and Height of 31 felled black cherry trees.

In the Simple Regression session, we constructed a simple linear model for Volume using Girth as the independent variable. Using Multiple Regression we trialled various models, including some that had multiple predictor variables and/or involved log-log transformations to explore

power relationships.

However, due to limitations of the method, we were not able to explore other options such as a parameterised power relationship with an additive error model. We will now attempt to fit this model:

[Math Processing Error]

Parameters for non-linear models may be estimated using the nls package in R.

```
Hide
```

```
volume = trees$Volume
height = trees$Height
girth = trees$Girth
m9 = nls(volume~beta0*girth^beta1*height^beta2,start=list(beta0=1,beta1=2,beta2=1))
summary(m9)
```

```
##
## Formula: volume ~ beta0 * girth^beta1 * height^beta2
##
## Parameters:
## Estimate Std. Error t value Pr(>|t|)
## beta0 0.001449    0.001367    1.060 0.298264
## beta1 1.996921    0.082077    24.330    < 2e-16 ***
## beta2 1.087647    0.242159    4.491 0.000111 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.533 on 28 degrees of freedom
##
## Number of iterations to convergence: 5
## Achieved convergence tolerance: 8.255e-07</pre>
```

Note that the parameters beta0, beta1 and beta2 weren't defined prior to the function callnls knew what to do with them. Also note that we had to provide starting points for the parameters. What happens if you change them?

Are all terms significant? Is this model appropriate? What else could be tried to achieve a better model?

Section 5: Practical Exercises

Puromycin

The in-built R dataset Puromycin contains data regarding the reaction velocity versus substrate concentration in an enzymatic reaction involving untreated cells or cells treated with Puromycin.

- Plot conc (concentration) against rate. What is the nature of the relationship between conc and rate?
- Find a transformation that linearises the data and stabilises the variance, making it
 possible to use linear regression. Create the corresponding linear regression model. Are all
 terms significant?
- Add the state term to the model. What type of variable is this? Is the inclusion of this term appropriate?

- Now add a term representing the interaction between rate and state. Are all terms significant? What can you conclude?
- Given this information, create the regression model you believe to be the most appropriate
 for modelling conc. Regenerate the plot of conc against rate. Draw curves
 corresponding to the fitted values of the final model onto this plot (note that two separate
 curves should be drawn, corresponding to the two levels of state).

Attitude

The in-built R dataset attitude contains data from a survey of clerical employees.

- Create a linear model regressing rating on complaints, and store the model in a variable.
- Use the step function to perform forward selection stepwise regression, in order to
 automatically add appropriate terms, using a command similar to:
 new_model = step(original_model,.~.+privileges+learning+raises+critical+advance)
- Which term(s) were added? What is Akaike's Information Criterion (AIC) corresponding to the final model? Are all terms in the resulting model significant? Check diagnostic plots. Do you think this is a suitable model?