Simple template for R Markdown

for Advanced Methods for Regression and Classification

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```
knitr::opts_chunk$set(echo = TRUE,warning=FALSE,message=FALSE)
data(College,package="ISLR")
str(College)
```

```
## 'data.frame':    777 obs. of  18 variables:
##  $ Private    : Factor w/ 2 levels "No","Yes": 2 2 2 2 2 2 2 2 2 2 ...
##  $ Apps       : num  1660 2186 1428 417 193 ...
##  $ Accept     : num  1232 1924 1097 349 146 ...
##  $ Enroll     : num  721 512 336 137 55 158 103 489 227 172 ...
##  $ Top10perc  : num  23 16 22 60 16 38 17 37 30 21 ...
##  $ Top25perc  : num  52 29 50 89 44 62 45 68 63 44 ...
##  $ F.Undergrad: num  2885 2683 1036 510 249 ...
##  $ P.Undergrad: num  537 1227 99 63 869 ...
##  $ Outstate   : num  7440 12280 11250 12960 7560 ...
##  $ Room.Board : num  3300 6450 3750 5450 4120 ...
##  $ Books      : num  450 750 400 450 800 500 500 450 300 660 ...
##  $ Personal   : num  2200 1500 1165 875 1500 ...
##  $ PhD        : num  70 29 53 92 76 67 90 89 79 40 ...
##  $ Terminal   : num  78 30 66 97 72 73 93 100 84 41 ...
##  $ S.F.Ratio  : num  18.1 12.2 12.9 7.7 11.9 9.4 11.5 13.7 11.3 11.5 ...
##  $ perc.alumni: num  12 16 30 37 2 11 26 37 23 15 ...
##  $ Expend     : num  7041 10527 8735 19016 10922 ...
##  $ Grad.Rate  : num  60 56 54 59 15 55 63 73 80 52 ...
```

```
summary(College)
```

For some Codeblocks, we hide the results as they were exploding the PDF File.

Our goal is to find a linear regression model which allows to predict the variable Apps, i.e. the number of applications received, using the remaining variables except of the variables Accept and Enroll.

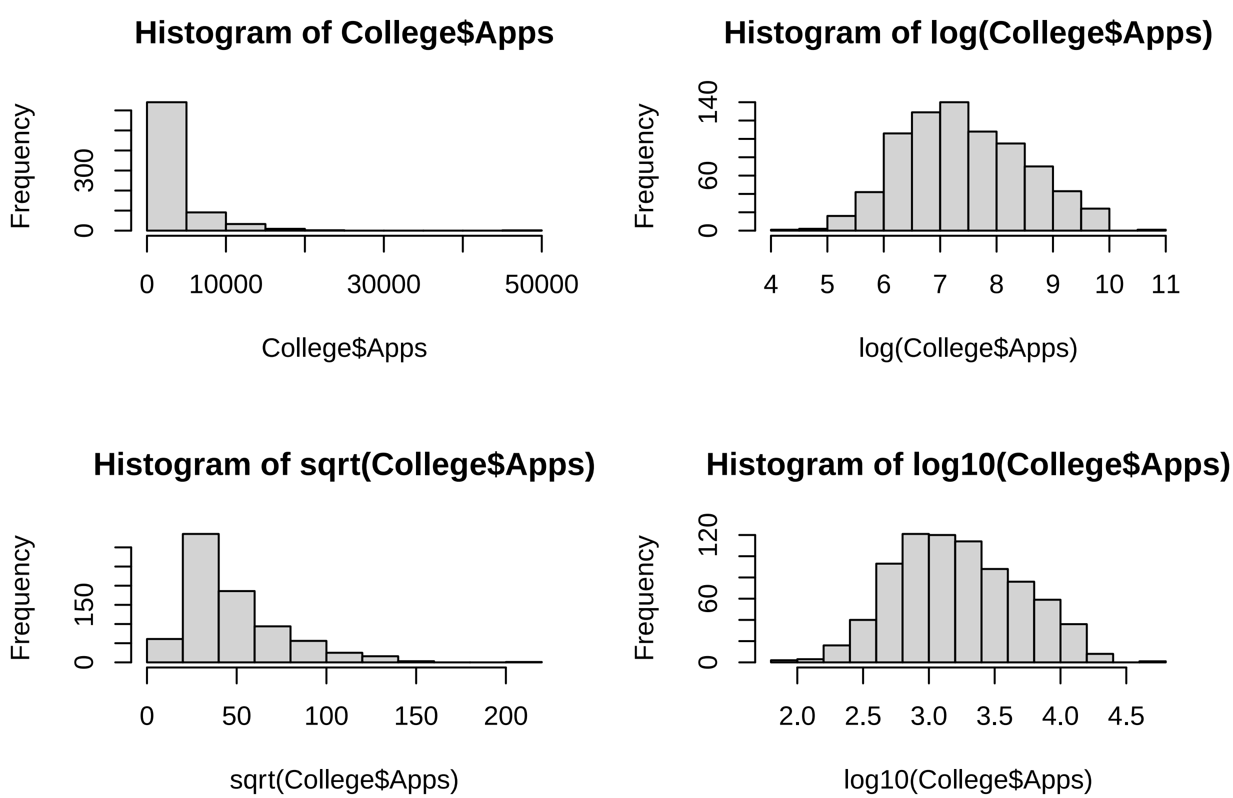
For the following tasks, split the data randomly into training and test data (about 2/3 and 1/3), build the model with the training data, and evaluate the model using the RMSE as a criterion.

split the data into training and test data:

```
n <- nrow(College)
set.seed(11835945)
train <- sample(1:n, 2*n/3)
test <- -train
```

1. Look first at your data. Is any preprocessing necessary or useful? Argue why a log-transformation of the response variable can be useful. Continue with log(Apps) as the response.

```r
par(mfrow=c(2,2))
hist(College$Apps)
hist(log(College$Apps))
hist(sqrt(College$Apps))
hist(log10(College$Apps))
```



Logarithmic values are normal distributed.

```r
College$logApps <- log(College$Apps)
College<-College[-c(2,3,4)]
train.data <- College[train,]
test.data <- College[test,]
#intersect(train.data,test.data)
```

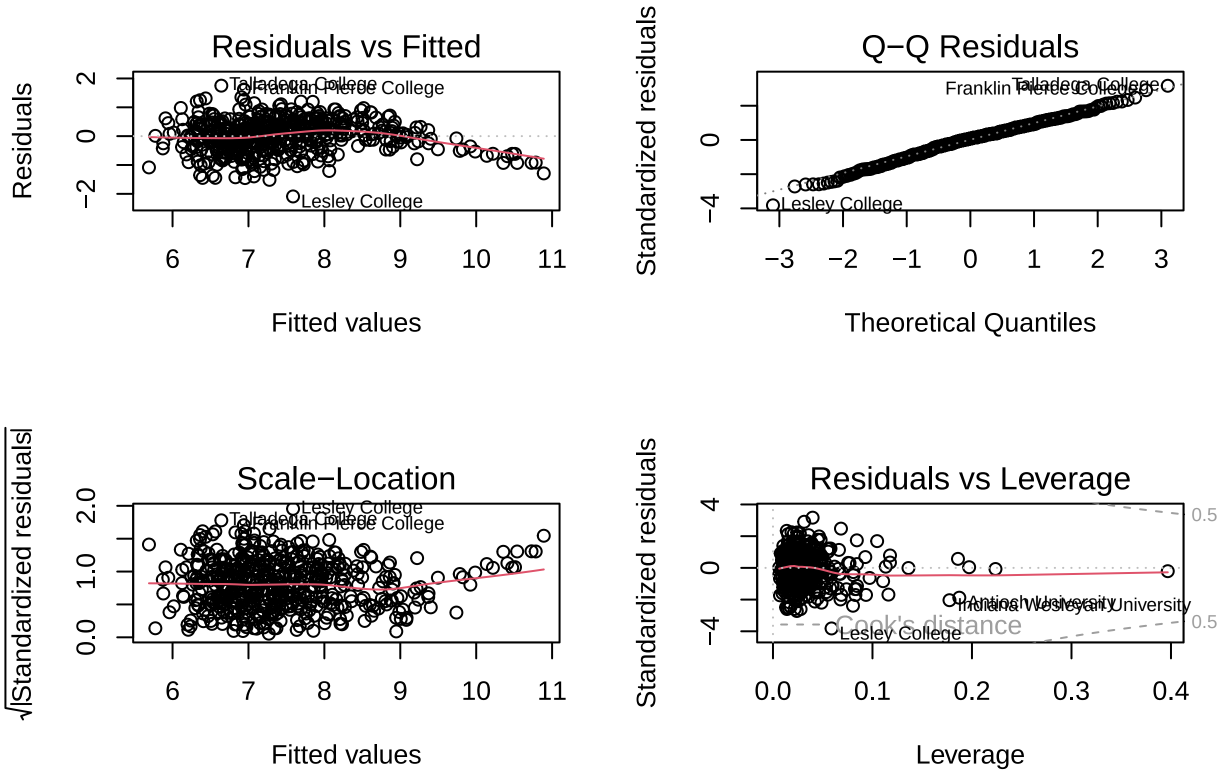
2. Full model: Estimate the full regression model and interpret the results.

(a) For that purpose, apply the function lm() to compute the estimator – for details see course notes. Interpret the outcome of summary(res), where res is the output from the lm() function. Which variables contribute to explaining the response variable? Look at diagnostics plots with plot(res). Are the model assumptions fulfilled?

```r
par(mfrow=c(2,2))
res <- lm(logApps ~ ., data=train.data)
summary(res)
```

```
##
## Call:
## lm(formula = logApps ~ ., data = train.data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.09017 -0.35901  0.04444  0.36923  1.75008
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  4.505e+00  2.627e-01  17.149  < 2e-16 ***
## PrivateYes  -5.458e-01  9.592e-02  -5.690 2.16e-08 ***
## Top10perc    8.395e-04  3.548e-03   0.237 0.813042
## Top25perc    1.784e-03  2.875e-03   0.621 0.535165
## F.Undergrad  1.096e-04  8.115e-06  13.500  < 2e-16 ***
## P.Undergrad  1.675e-05  1.908e-05   0.878 0.380440
## Outstate     4.363e-05  1.263e-05   3.456 0.000596 ***
## Room.Board   9.068e-05  3.146e-05   2.883 0.004111 **
## Books        4.742e-04  1.714e-04   2.767 0.005866 **
## Personal    -6.124e-05  4.438e-05  -1.380 0.168265
## PhD          8.776e-03  3.060e-03   2.868 0.004309 **
## Terminal     1.362e-04  3.341e-03   0.041 0.967492
## S.F.Ratio    3.887e-02  8.608e-03   4.516 7.86e-06 ***
## perc.alumni -8.729e-03  2.656e-03  -3.287 0.001085 **
## Expend       2.758e-05  7.582e-06   3.638 0.000303 ***
## Grad.Rate    7.389e-03  1.931e-03   3.827 0.000146 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.564 on 502 degrees of freedom
## Multiple R-squared:  0.7225, Adjusted R-squared:  0.7143
## F-statistic: 87.15 on 15 and 502 DF,  p-value: < 2.2e-16
```

```r
plot(res)
```



predict the number of applications for the test data:

```
pred <- predict(res, newdata=test.data)
```

calculate the RMSE:

```
rmse <- sqrt(mean((test.data$logApps - pred)^2))
rmse
```

```
## [1] 0.5939058
```

Now we check what variables are important for the prediction:

```
library(caret)
varImp(res)
```

```
##                 Overall
## PrivateYes   5.68976620
## Top10perc    0.23662776
## Top25perc    0.62056807
## F.Undergrad 13.49986698
## P.Undergrad  0.87785930
## Outstate     3.45559629
## Room.Board   2.88280220
## Books        2.76699251
## Personal     1.37979118
## PhD          2.86766202
## Terminal     0.04077427
## S.F.Ratio    4.51608349
```

```
## perc.alumni  3.28655720
## Expend       3.63796291
## Grad.Rate    3.82657917
```

(b) Now we try to manually compute the LS coefficients, in the same way as lm(). Thus, replace from the above command lm() by model.matrix(). This gives you the matrix X as it is used to estimate the regression coefficients. Now apply the formula to compute the LS estimator. You can do matrix multiplication in R by %*%, and the inverse of a matrix is computed with solve(). How is R handling binary variables (Private), and how can you interpret the corresponding regression coefficient? Compare the resulting coefficients with those obtained from lm(). Do you get the same result?

```r
X <- model.matrix(logApps ~ . , data=train.data)
y <- train.data$logApps
beta <- solve(t(X) %*% X) %*% t(X) %*% y
beta
```

```
##                      [,1]
## (Intercept)  4.504733e+00
## PrivateYes  -5.457882e-01
## Top10perc    8.395119e-04
## Top25perc    1.783999e-03
## F.Undergrad  1.095526e-04
## P.Undergrad  1.675083e-05
## Outstate     4.363130e-05
## Room.Board   9.068202e-05
## Books        4.742280e-04
## Personal    -6.123653e-05
## PhD          8.775718e-03
## Terminal     1.362216e-04
## S.F.Ratio    3.887223e-02
## perc.alumni -8.729084e-03
## Expend       2.758132e-05
## Grad.Rate    7.389273e-03
```

first 5 rows of the matrix X:

```r
head(X)
```

```
##                                 (Intercept) PrivateYes Top10perc Top25perc
## Roger Williams University                 1          1        10        20
## North Park College                        1          1        19        39
## University of Wisconsin-Stout             1          0         9        32
## Lewis University                          1          1        12        31
## Rocky Mountain College                    1          1        11        31
## Montana State University                  1          0        15        42
##                                 F.Undergrad P.Undergrad Outstate Room.Board Books
## Roger Williams University              2111        1489    12520       6050   500
## North Park College                      879         156    12580       4345   400
## University of Wisconsin-Stout          6038         579     6704       2592   376
## Lewis University                       2192        1423    10560       4520   500
## Rocky Mountain College                  743         118     8734       3362   600
## Montana State University               8730         993     5552       3710   550
##                                 Personal PhD Terminal S.F.Ratio perc.alumni
## Roger Williams University            730  44       54      16.4           8
## North Park College                   970  76       79      13.1          24
```

```
## University of Wisconsin-Stout     1750  78       78      21.0           17
## Lewis University                  1200  36       48      14.3           10
## Rocky Mountain College             625  56       78      11.3           27
## Montana State University          2300  75       83      17.6            8
##                               Expend Grad.Rate
## Roger Williams University       7957        61
## North Park College             10889        74
## University of Wisconsin-Stout   6254        65
## Lewis University                7701        61
## Rocky Mountain College          6422        68
## Montana State University        6324        37
```

As we can see the binary variable is encoded as 0 and 1. We actually get the same results as with the lm() function. In the Matrix Methods, we have get

```r
beta[,1]["PrivateYes"]
```

```
## PrivateYes
## -0.5457882
```

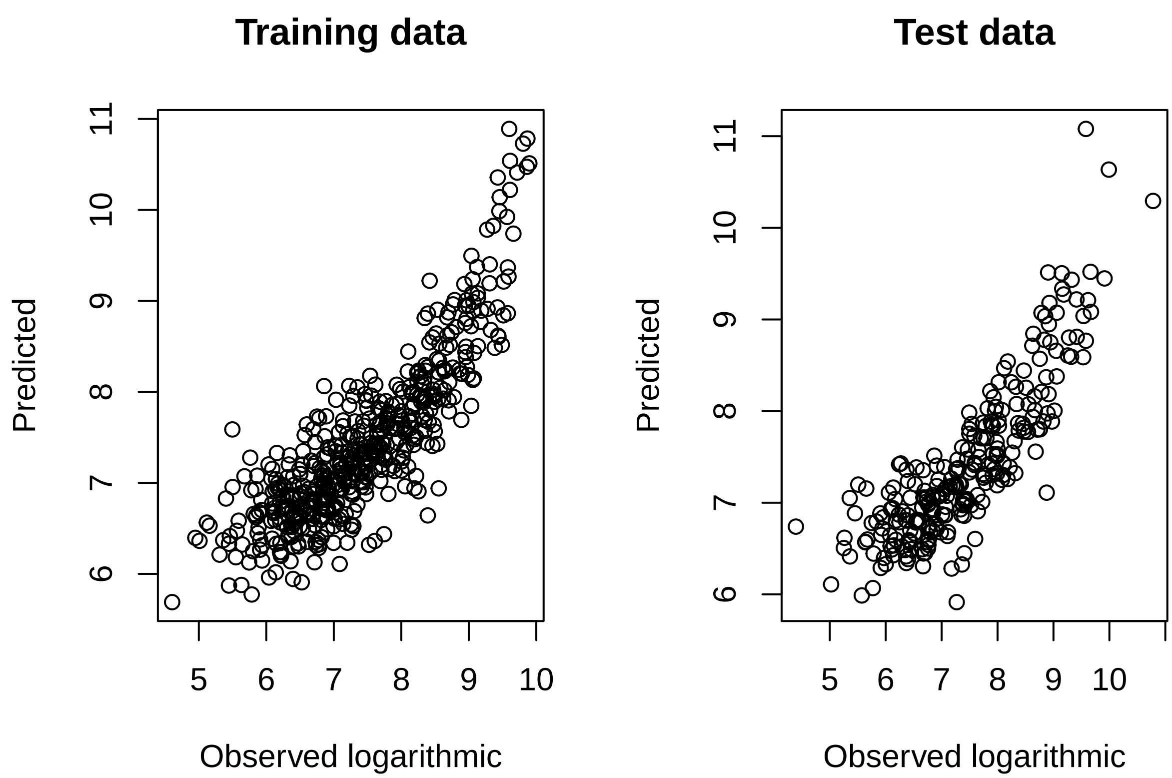
And with the lm() function we get

```r
coef(res)["PrivateYes"]
```

```
## PrivateYes
## -0.5457882
```

(c) Compare graphically the observed and the predicted values of the response variable – once only for the training data, and once for the test data. What do you think about the prediction performance of your model?

```r
par(mfrow=c(1,2))
plot(train.data$logApps, predict(res), xlab="Observed logarithmic", ylab="Predicted", main="Training da
plot(test.data$logApps, pred, xlab="Observed logarithmic", ylab="Predicted", main="Test data")
```



In both graphs, we can see a clear linear relationship between the observed and predicted values. Since the training data has more data points, the graph is more dense but one can still see that both graphs are very similar.

(d) Compute the RMSE separately for training and test data, and compare the values. What do you conclude?

```
pred.train <- predict(res, newdata=train.data)
rmse.train <- sqrt(mean((train.data$logApps - pred.train)^2))
rmse.train
```

```
## [1] 0.5552257
```

```
rmse
```

```
## [1] 0.5939058
```

Since the model was fitted to the training data, i expect the RMSE of the test data set to be bigger. This is the also the case.

3. Reduced model: Exclude all input variables from the model which were not significant in 2(a), and compute the LS-estimator.

```
reduced.model<- lm(logApps ~ .  -Top25perc -Top10perc -P.Undergrad -Personal
                                -PhD -Terminal -perc.alumni, data=train.data)
summary(reduced.model)
```

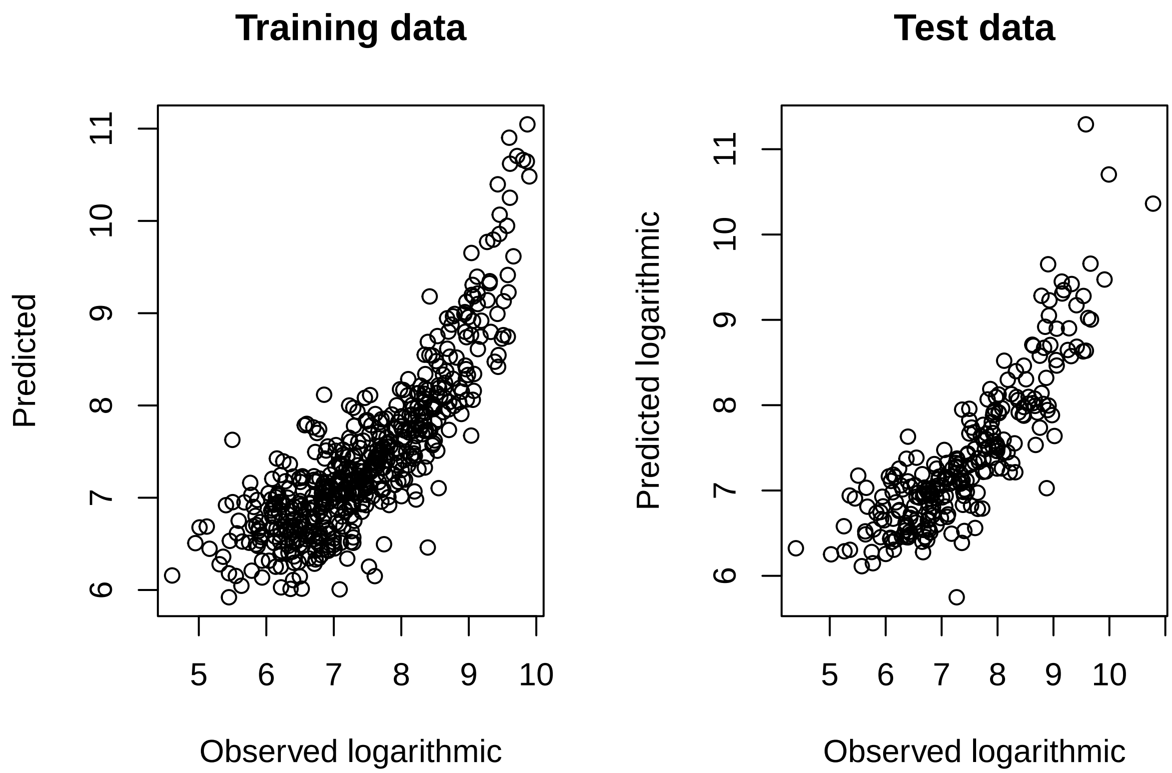
```
##
```

```
## Call:
## lm(formula = logApps ~ . - Top25perc - Top10perc - P.Undergrad -
##     Personal - PhD - Terminal - perc.alumni, data = train.data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.12992 -0.32849  0.05935  0.38432  1.93196
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  4.663e+00  2.217e-01  21.037  < 2e-16 ***
## PrivateYes  -6.938e-01  9.363e-02  -7.410 5.29e-13 ***
## F.Undergrad  1.199e-04  7.108e-06  16.867  < 2e-16 ***
## Outstate     5.309e-05  1.196e-05   4.438 1.12e-05 ***
## Room.Board   1.240e-04  3.122e-05   3.972 8.16e-05 ***
## Books        4.548e-04  1.695e-04   2.684  0.00752 **
## S.F.Ratio    4.444e-02  8.754e-03   5.076 5.41e-07 ***
## Expend       3.316e-05  7.063e-06   4.694 3.44e-06 ***
## Grad.Rate    8.100e-03  1.811e-03   4.471 9.59e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5796 on 509 degrees of freedom
## Multiple R-squared:  0.7029, Adjusted R-squared:  0.6983
## F-statistic: 150.6 on 8 and 509 DF,  p-value: < 2.2e-16
```

(a) Are now all input variables significant in the model? Why is this not to be expected in general?

Yes. Various Reasons such as Overfitting, colinearity, sample size limitations, noise and bias, etc. ### (b) Visualize the fit and the prediction from the new model, see 2(c).

```r
par(mfrow=c(1,2))
pred <- predict(reduced.model, newdata=test.data)
plot(train.data$logApps, predict(reduced.model), xlab="Observed logarithmic",
                             ylab="Predicted", main="Training data")
plot(test.data$logApps, pred, xlab="Observed logarithmic",
                             ylab="Predicted logarithmic", main="Test data")
```



(c) Compute the RMSE for the new model, see 2(d). What would we expect?

```
pred.train <- predict(reduced.model, newdata=train.data)
rmse.train <- sqrt(mean((train.data$logApps - pred.train)^2))
cat("RMSE of native model",rmse.train)
```

```
## RMSE of native model 0.5745158
```

```
rmse <- sqrt(mean((test.data$logApps - pred)^2))
cat("RMSE of reduced model",rmse)
```

```
## RMSE of reduced model 0.5908559
```

I expect the new model to have a higher RMSE, even though we only removed insignificant variables. However, the error is smaller since with all variables we did fit the model to the noise of the model (Overfitting)

(d) Compare the two models with anova(). What can you conclude?

```
anova(res,reduced.model)
```

```
## Analysis of Variance Table
##
## Model 1: logApps ~ Private + Top10perc + Top25perc + F.Undergrad + P.Undergrad +
##     Outstate + Room.Board + Books + Personal + PhD + Terminal +
##     S.F.Ratio + perc.alumni + Expend + Grad.Rate
## Model 2: logApps ~ (Private + Top10perc + Top25perc + F.Undergrad + P.Undergrad +
##     Outstate + Room.Board + Books + Personal + PhD + Terminal +
```

```
##     S.F.Ratio + perc.alumni + Expend + Grad.Rate) - Top25perc -
##     Top10perc - P.Undergrad - Personal - PhD - Terminal - perc.alumni
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    502 159.69
## 2    509 170.97 -7   -11.289 5.0697 1.413e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

4. Perform variable selection based on stepwise regression, using the function step(), see help file and course notes. Perform both, forward selection (start from the empty model) and backward selection (start from the full model). Compare the resulting models with the RMSE, and with plots of response versus predicted values.

```r
full_model <- lm(logApps~ .,data=train.data)
empty_model <- lm(logApps ~ 1, data = train.data)
forward_model <- step(empty_model,direction = "forward",scope=formula(full_model))
backward_model <-step(full_model,direction = "backward")
anova(forward_model,backward_model)
```

```r
anova(forward_model,backward_model)
```

```
## Analysis of Variance Table
##
## Model 1: logApps ~ F.Undergrad + PhD + Room.Board + Private + Outstate +
##     Grad.Rate + S.F.Ratio + Expend + perc.alumni + Books
## Model 2: logApps ~ Private + F.Undergrad + Outstate + Room.Board + Books +
##     PhD + S.F.Ratio + perc.alumni + Expend + Grad.Rate
##   Res.Df    RSS Df Sum of Sq F Pr(>F)
## 1    507 160.96
## 2    507 160.96  0         0
```

```r
# Function to calculate RMSE
rmse <- function(model){
  predictions <- predict(model, train.data)
  sqrt(mean((test.data$logApps - predictions)^2))
  }
rmse_forward <- rmse(forward_model)
rmse_backward <- rmse(backward_model)

cat("RMSE of Forward Model:", rmse_forward)
```

```
## RMSE of Forward Model: 1.447649
```

```r
cat("RMSE of Backward Model:", rmse_backward)
```

```
## RMSE of Backward Model: 1.447649
```

```r
require(gridExtra)
plot_model <- function(model, title) {
  predictions <- predict(model, newdata = test.data)
  ggplot(test.data, aes(x = predictions, y = logApps)) +
    geom_point() +
    geom_smooth(method = "lm", color = "blue") +
    labs(title = title, x = "Predicted Values", y = "Actual Values") +
    theme_minimal() } # Plotting both models
plot1 <- plot_model(forward_model, "Forward Selection Model")
```

```
plot2 <- plot_model(backward_model, "Backward Selection Model")
grid.arrange(plot1, plot2, ncol=2)
```