TMA4268 Statistical Learning V2020

Module 6: Recommended exercises - Solutions

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Spring 2020

You might need to install the following packages to run this code:

```
install.packages("pls")
install.packages("GGAlly")
install.packages("ISLR")
install.packages("leaps")
install.packages("glmnet")
```

Recommended exercise 1

1) Least square estimator

For the least square estimator, the solution can be found in the first session here.

We find the least square by minimizing the RSS with respect to the coefficients.

$$RSS = ||\mathbf{y} - \mathbf{X}\beta||^2 = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta) = \mathbf{y}^T\mathbf{y} - \beta^T\mathbf{X}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\beta + \beta^T\mathbf{X}^T\mathbf{X}\beta$$

Here, all the terms have dimension 1×1, so $\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} = \mathbf{y}^T\mathbf{X}\boldsymbol{\beta}$ and the expression becomes

$$RSS = \mathbf{y}^T\mathbf{y} - 2\beta^T\mathbf{X}^T\mathbf{y} + \beta^T\mathbf{X}^T\mathbf{X}\beta$$

We find the least square estimates by derivating this expression wrt. $\boldsymbol{\beta}$, setting the expression equal to 0 and solving for $\boldsymbol{\beta}$

$$\frac{RSS}{d\boldsymbol{\beta}} = \frac{\mathbf{y}^T\mathbf{y}}{d\boldsymbol{\beta}} - \frac{2\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y}}{d\boldsymbol{\beta}} + \frac{\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}}{d\boldsymbol{\beta}} = 0$$

$$-2\mathbf{X}^T\mathbf{y} + 2(\mathbf{X}^T\mathbf{X})\boldsymbol{\beta} = 0$$
$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

2) Maximum likelihood estimator

For the maximum likelihood estimator, the solution can be found here.

To find the maximum likelihood estimator, we minimize the likelihood wrt. the coefficients. For a linear model, we assume a normal distribution for the response where the expected value is $\mathbf{X}\boldsymbol{\beta}$, i.e. $\mathbf{y} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 I)$

$$L(\boldsymbol{\beta}|\mathbf{y}) = \prod_{i=1}^{n} f(y_i, \boldsymbol{\beta}) = \prod_{i=1}^{n}\Big(\frac{1}{\sqrt{2\pi\sigma^2}}\exp\{-\frac{1}{2\sigma^2}(y_i - X\beta)^2\}\Big) = \frac{1}{(2\pi\sigma^2)^{n/2}}\exp\{-\frac{1}{2}(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})^T(\sigma^2 I)^{-1}(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})\}$$

Minimizing the log-likelihood by taking the log of the above function and derivating with respect to $\boldsymbol{\beta}$,

$$\frac{d\log(L)}{d\boldsymbol{\beta}} = -\frac{d}{d\beta}(\frac{n}{2}\log(2\pi\sigma^2)) - \frac{d}{d\beta}(\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})^T(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})) = 0$$

The first term have no $\boldsymbol{\beta}$ and will cancel. The variance in the second term can be placed outside of the derivation, and can hance be removed. Then, we end up with the same expression as for the RSS-minimization, and we find the same $\hat{\boldsymbol{\beta}}$ as above.

$$\frac{d\log(L)}{d\boldsymbol{\beta}} = \frac{\mathbf{y}^T\mathbf{y}}{d\boldsymbol{\beta}} - \frac{2\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y}}{d\boldsymbol{\beta}} + \frac{\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}}{d\boldsymbol{\beta}} = 0$$
$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Recommended exercise 2

```r
library(ISLR) # Package with data for an Introduction to Statistical
              # Learning with Applications in R
```

```r
# Load Credit dataset
data(Credit)

# Check column names
names(Credit)
```

```
##  [1] "ID"        "Income"    "Limit"     "Rating"    "Cards"
##  [6] "Age"       "Education" "Gender"    "Student"   "Married"
## [11] "Ethnicity" "Balance"
```

```r
# Check dataset shape
dim(Credit)
```

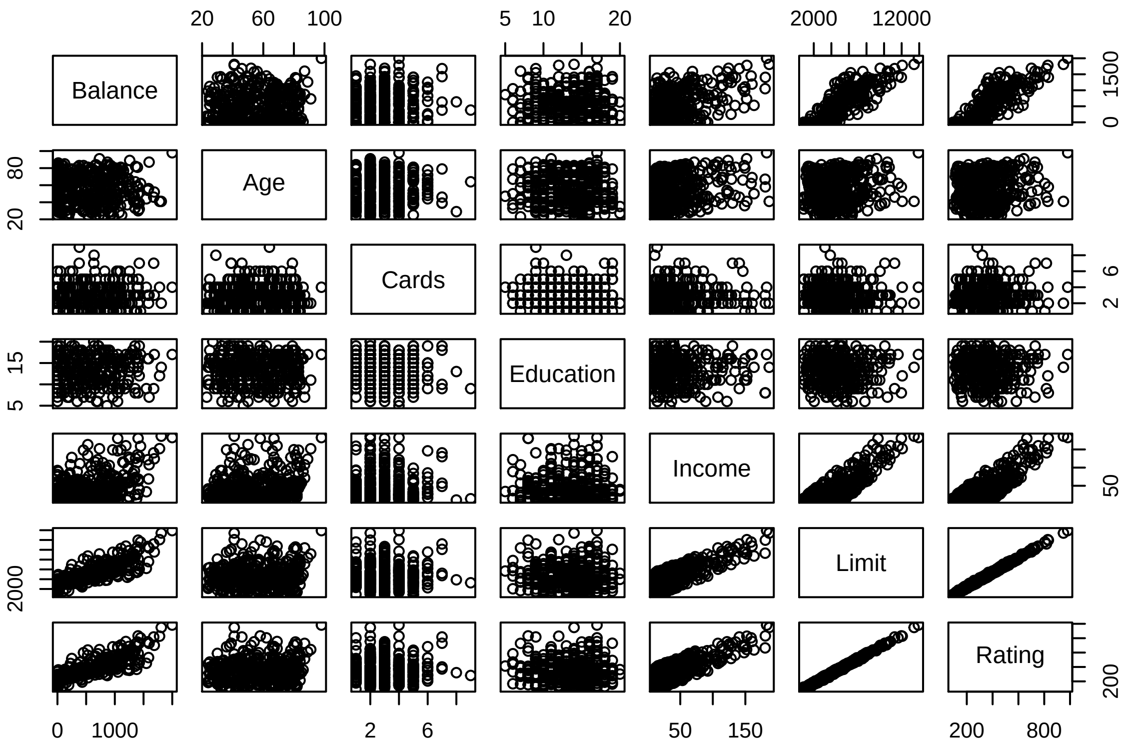
```
## [1] 400  12
```

```r
head(Credit)
```

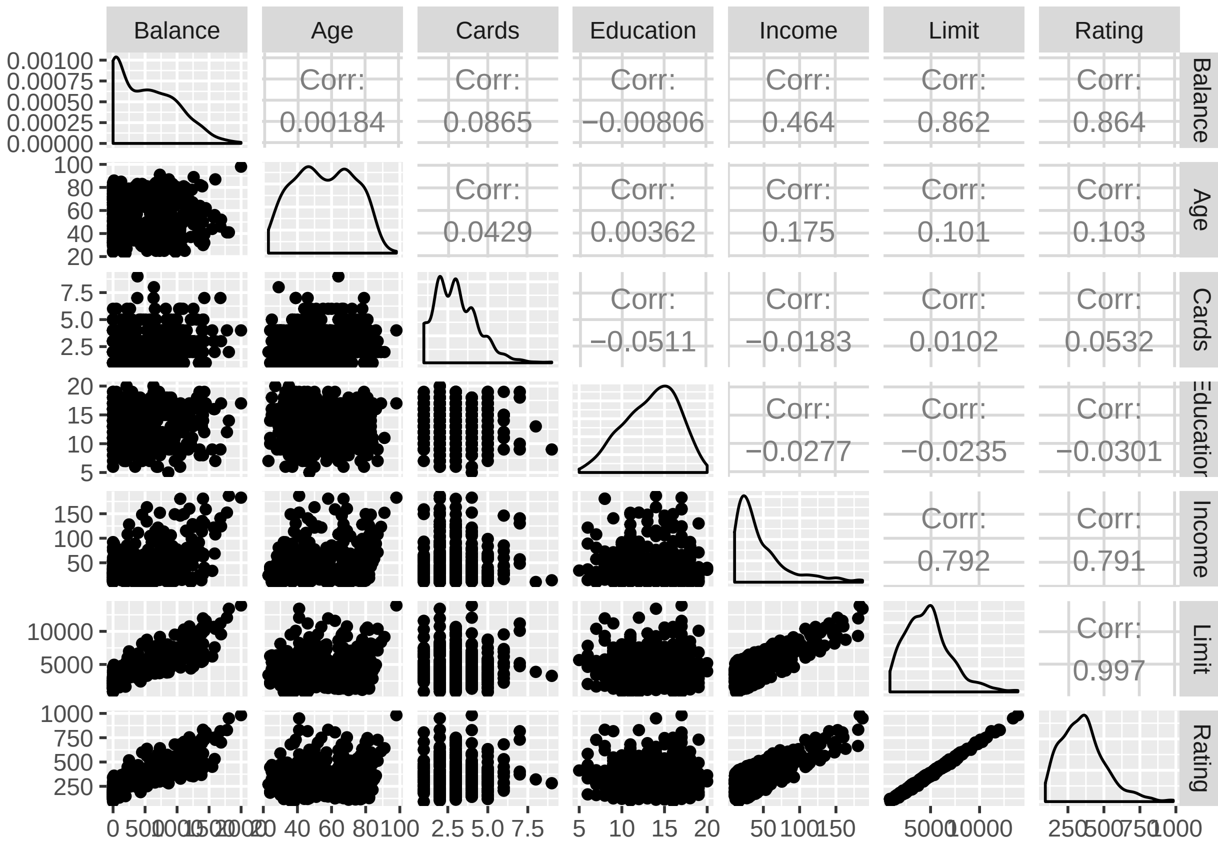
```
##   ID  Income Limit Rating Cards Age Education Gender Student Married
## 1  1  14.891  3606    283     2  34        11   Male      No     Yes
## 2  2 106.025  6645    483     3  82        15 Female     Yes     Yes
## 3  3 104.593  7075    514     4  71        11   Male      No      No
## 4  4 148.924  9504    681     3  36        11 Female      No      No
## 5  5  55.882  4897    357     2  68        16   Male      No     Yes
## 6  6  80.180  8047    569     4  77        10   Male      No      No
##   Ethnicity Balance
## 1 Caucasian     333
## 2     Asian     903
## 3     Asian     580
## 4     Asian     964
## 5 Caucasian     331
## 6 Caucasian    1151
```

```r
# Select variable to plot
pairwise_scatter_data <- Credit[,c("Balance", "Age", "Cards", "Education",
                                   "Income", "Limit", "Rating")]
```

```r
# Simplest possible pairwise scatter plot
pairs(pairwise_scatter_data)
```




```r
# More interesting but slower pairwise plot from package GGally
library(GGally)
ggpairs(data=pairwise_scatter_data)
```



Check here for quick get started to ggpairs

Recommended exercise 3

```
# Exclude 'ID' column
credit_data <- subset(Credit, select=-c(ID))

# Counting the dummy variables as well
credit_data_number_predictors <- 11

# Take a look at the data
head(credit_data)
```

```
##    Income Limit Rating Cards Age Education Gender Student Married
## 1  14.891  3606    283     2  34        11   Male      No     Yes
## 2 106.025  6645    483     3  82        15 Female     Yes     Yes
## 3 104.593  7075    514     4  71        11   Male      No      No
## 4 148.924  9504    681     3  36        11 Female      No      No
## 5  55.882  4897    357     2  68        16   Male      No     Yes
## 6  80.180  8047    569     4  77        10   Male      No      No
##   Ethnicity Balance
## 1 Caucasian     333
## 2     Asian     903
## 3     Asian     580
## 4     Asian     964
```

```
## 5 Caucasian     331
## 6 Caucasian    1151
```

```r
# Summary statistics
summary(credit_data)
```

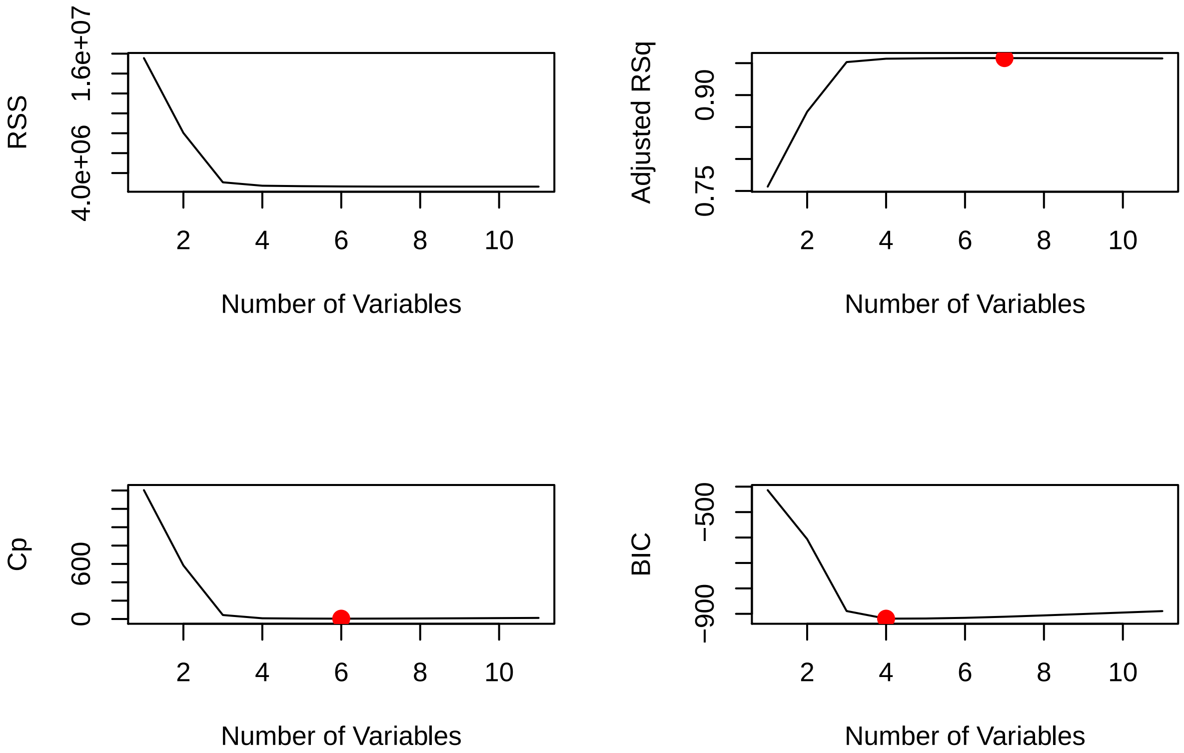
```
##      Income           Limit           Rating          Cards      
##  Min.   : 10.35   Min.   :  855   Min.   : 93.0   Min.   :1.000  
##  1st Qu.: 21.01   1st Qu.: 3088   1st Qu.:247.2   1st Qu.:2.000  
##  Median : 33.12   Median : 4622   Median :344.0   Median :3.000  
##  Mean   : 45.22   Mean   : 4736   Mean   :354.9   Mean   :2.958  
##  3rd Qu.: 57.47   3rd Qu.: 5873   3rd Qu.:437.2   3rd Qu.:4.000  
##  Max.   :186.63   Max.   :13913   Max.   :982.0   Max.   :9.000  
##       Age          Education        Gender    Student   Married  
##  Min.   :23.00   Min.   : 5.00    Male :193   No :360   No :155  
##  1st Qu.:41.75   1st Qu.:11.00   Female:207   Yes: 40   Yes:245  
##  Median :56.00   Median :14.00                                   
##  Mean   :55.67   Mean   :13.45                                   
##  3rd Qu.:70.00   3rd Qu.:16.00                                   
##  Max.   :98.00   Max.   :20.00                                   
##             Ethnicity      Balance       
##  African American: 99   Min.   :   0.00  
##  Asian           :102   1st Qu.:  68.75  
##  Caucasian       :199   Median : 459.50  
##                         Mean   : 520.01  
##                         3rd Qu.: 863.00  
##                         Max.   :1999.00  
```

```r
# Create train and test set indexes
set.seed(1)
train_perc <- 0.75
credit_data_train_index <- sample(1:nrow(credit_data), nrow(credit_data)*train_perc)
credit_data_test_index <- (-credit_data_train_index)

# Create train and test set
credit_data_training <- credit_data[credit_data_train_index, ]
credit_data_testing <- credit_data[credit_data_test_index, ]
```

```r
library(leaps)

# Perform best subset selection using all the predictors and the training data
best_subset_method=regsubsets(Balance~.,credit_data_training,nvmax=credit_data_number_predictors)

# Save summary obj
best_subset_method_summary=summary(best_subset_method)
```

```r
# Plot RSS, Adjusted R^2, C_p and BIC

par(mfrow=c(2,2))
plot(best_subset_method_summary$rss,xlab="Number of Variables",ylab="RSS",type="l")
plot(best_subset_method_summary$adjr2,xlab="Number of Variables",ylab="Adjusted RSq",type="l")
bsm_best_adjr2 = which.max(best_subset_method_summary$adjr2)

points(bsm_best_adjr2,best_subset_method_summary$adjr2[bsm_best_adjr2], col="red",cex=2,pch=20)
plot(best_subset_method_summary$cp,xlab="Number of Variables",ylab="Cp",type='l')
bsm_best_cp=which.min(best_subset_method_summary$cp)
```

```r
points(bsm_best_cp,best_subset_method_summary$cp[bsm_best_cp],col="red",cex=2,pch=20)
bsm_best_bic=which.min(best_subset_method_summary$bic)

plot(best_subset_method_summary$bic,xlab="Number of Variables",ylab="BIC",type='l')
points(bsm_best_bic,best_subset_method_summary$bic[bsm_best_bic],col="red",cex=2,pch=20)
```

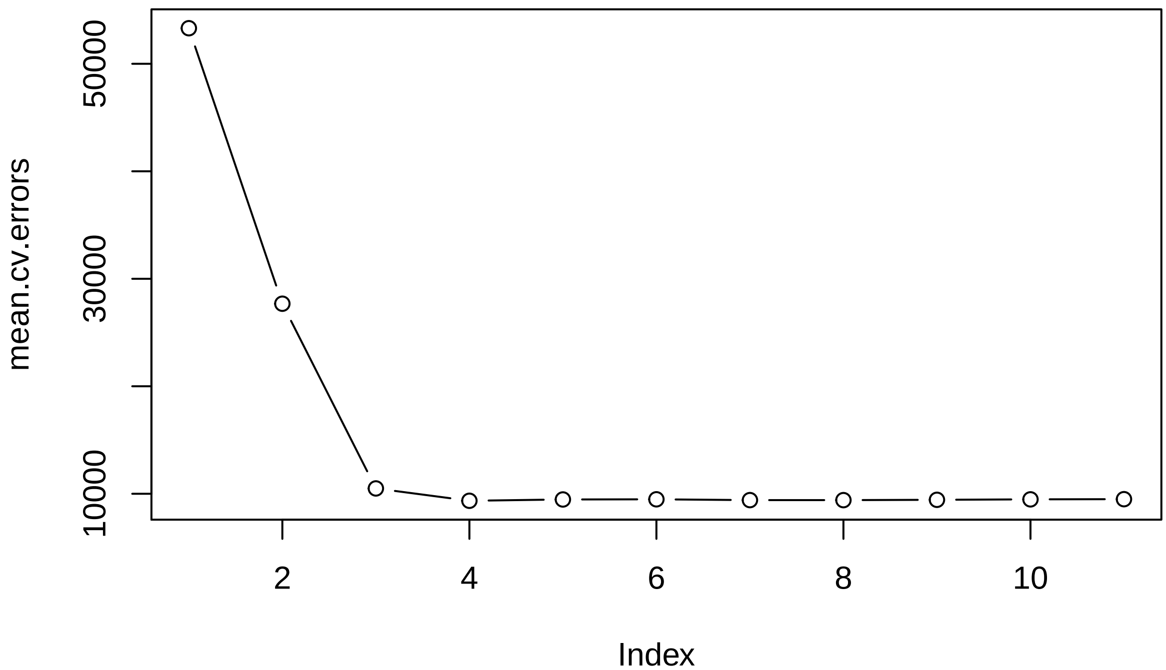



```r
# Create a prediction function to make predictions
# for regsubsets with id predictors included
predict.regsubsets=function(object,newdata,id,...){
  form=as.formula(object$call[[2]])
  mat=model.matrix(form,newdata)
  coefi=coef(object,id=id)
  xvars=names(coefi)
  mat[,xvars]%*%coefi
}

# Create indexes to divide the data between folds
k=10
set.seed(1)
folds=sample(1:k,nrow(credit_data_training),replace=TRUE)
cv.errors=matrix(NA,k,credit_data_number_predictors, dimnames=list(NULL, paste(1:credit_data_number_pre

# Perform CV
for(j in 1:k){
  best_subset_method=regsubsets(Balance~.,data=credit_data_training[folds!=j,],nvmax=credit_data_number_
  for(i in 1:credit_data_number_predictors){
    pred=predict(best_subset_method,credit_data_training[folds==j,],id=i)
    cv.errors[j,i]=mean( (credit_data_training$Balance[folds==j]-pred)^2)
    }
```

```
}

# Compute mean cv errors for each model size
mean.cv.errors=apply(cv.errors,2,mean)
mean.cv.errors
```

```
##         1         2         3         4         5         6         7 
## 53308.978 27681.063 10497.276  9349.190  9468.743  9484.566  9410.272 
##         8         9        10        11 
##  9409.024  9437.443  9480.517  9496.783
```

```
# Plot the mean cv errors
par(mfrow=c(1,1))
plot(mean.cv.errors,type='b')
```




```
# Fit the selected model using the whole training data
# and compute test error

# models selected
number_predictors_selected <- 4

# Create info for lm call
variables <- names(coef(best_subset_method,id=number_predictors_selected))
variables <- variables[!variables %in% "(Intercept)"]
bsm_formula <- as.formula(best_subset_method$call[[2]])
bsm_design_matrix <- model.matrix(bsm_formula,credit_data_training)[, variables]
bsm_data_train <- data.frame(Balance = credit_data_training$Balance, bsm_design_matrix)

# Fit a standard linear model using only the selected
# predictors on the training data
model_best_subset_method <- lm(formula = bsm_formula, bsm_data_train)
summary(model_best_subset_method)
```

```
##
```

```
## Call:
## lm(formula = bsm_formula, data = bsm_data_train)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -160.26  -76.81  -11.21   48.15  350.49
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -5.216e+02  1.758e+01 -29.670  < 2e-16 ***
## Income      -7.856e+00  2.651e-01 -29.627  < 2e-16 ***
## Limit        2.706e-01  4.001e-03  67.622  < 2e-16 ***
## Cards        2.426e+01  3.981e+00   6.094 3.43e-09 ***
## StudentYes   4.196e+02  1.782e+01  23.542  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 96.14 on 295 degrees of freedom
## Multiple R-squared:  0.9575, Adjusted R-squared:  0.9569
## F-statistic:  1661 on 4 and 295 DF,  p-value: < 2.2e-16
```

```
# Make predictions on the test set
bsm_design_matrix_test <- model.matrix(bsm_formula,credit_data_testing)[, variables]
bsm_predictions <- predict(object = model_best_subset_method, newdata = as.data.frame(bsm_design_matrix_

# Compute test squared errors
bsm_squared_errors <- (credit_data_testing$Balance-bsm_predictions)^2
squared_errors <- data.frame(bsm_squared_errors=bsm_squared_errors)


# test MSE
mean(bsm_squared_errors)
```

```
## [1] 12243.75
```

Recommended exercise 4

Similar analysis as previous exercise, simply replace Best Subset Selection

(`best_subset_method=regsubsets(Balance~.,credit_data,nvmax=credit_data_number_predictors)`)

by Forward Stepwise Selection

(`regfit.fwd=regsubsets(Balance~.,credit_data,nvmax=credit_data_number_predictors,method="forward")`)

, Backward Stepwise Selection

(`regfit.fwd=regsubsets(Balance~.,credit_data,nvmax=credit_data_number_predictors,method="backward")`)

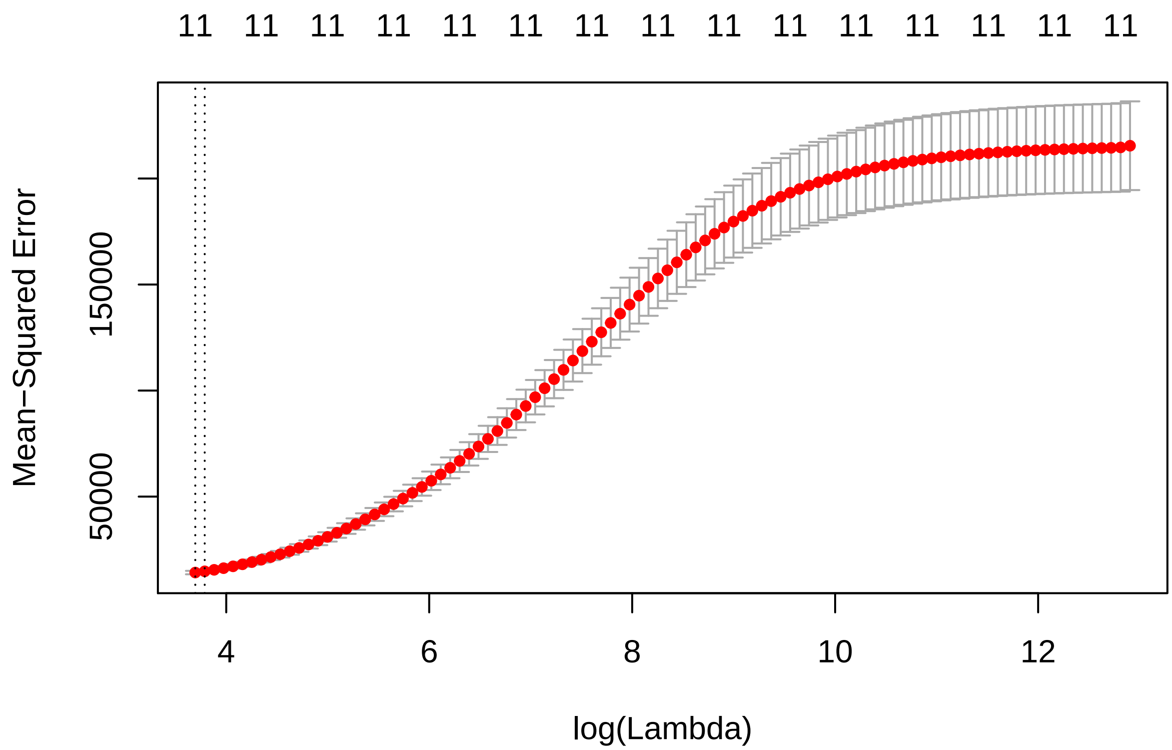
and Hybrid Stepwise Selection

(`regfit.fwd=regsubsets(Balance~.,credit_data,nvmax=credit_data_number_predictors,method="seqrep")`)

Recommended exercise 5

```r
library(glmnet) # Package Lasso and Elastic-Net Regularized
                # Generalized Linear Models
```

```r
x_train <- model.matrix(Balance~.,credit_data_training)[,-1]
y_train <- credit_data_training$Balance

x_test <- model.matrix(Balance~.,credit_data_testing)[,-1]
y_test <- credit_data_testing$Balance

ridge_mod <- glmnet(x_train,y_train,alpha=0)

set.seed(1)
cv.out=cv.glmnet(x_train, y_train,alpha=0)
plot(cv.out)
```



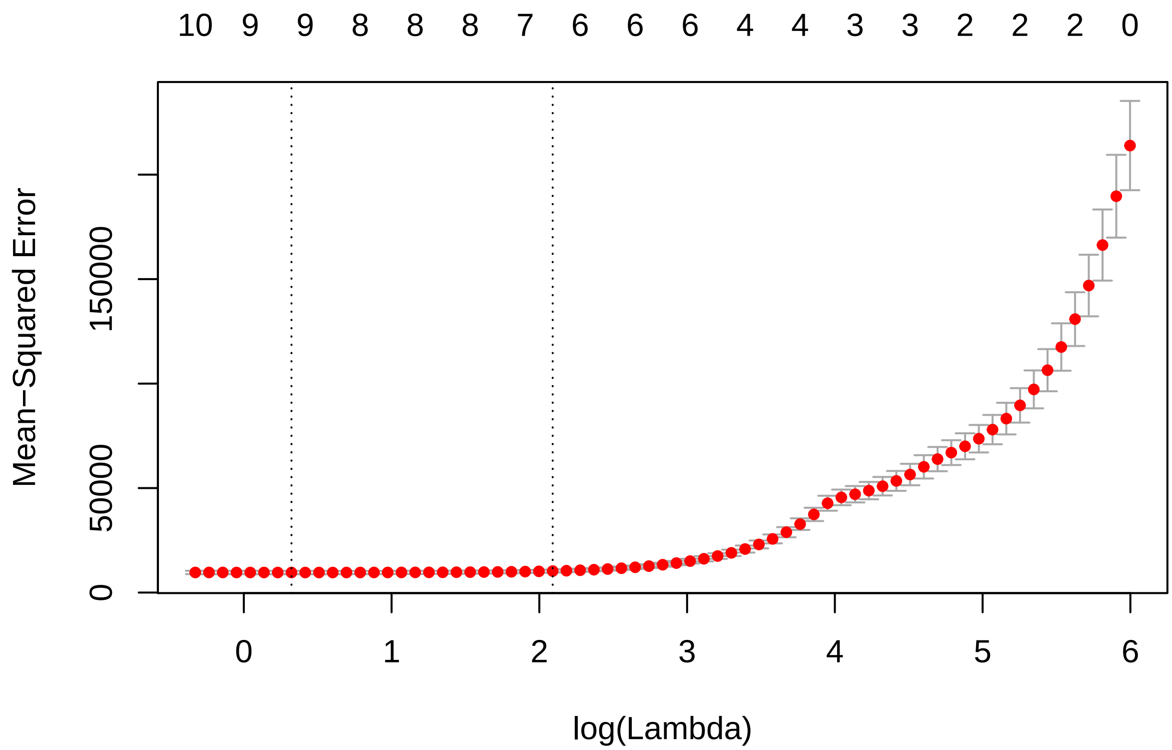

```r
best_lambda_ridge <- cv.out$lambda.min
best_lambda_ridge
```

```
## [1] 40.24862
```

```r
ridge_predictions = predict(ridge_mod,s=best_lambda_ridge,newx=x_test)
ridge_square_errors <- as.numeric((ridge_predictions-y_test)^2)
squared_errors <- data.frame(ridge_square_errors = ridge_square_errors, squared_errors)
```

Recommended exercise 6

```r
lasso_mod <- glmnet(x_train,y_train,alpha=1)

set.seed(1)
cv.out=cv.glmnet(x_train, y_train,alpha=1)
plot(cv.out)
```




```r
best_lambda_lasso <- cv.out$lambda.min
best_lambda_lasso
```

```
## [1] 1.380717
```

```r
lasso_predictions = predict(lasso_mod,s=best_lambda_lasso,newx=x_test)
lasso_square_errors <- as.numeric((lasso_predictions-y_test)^2)
squared_errors <- data.frame(lasso_square_errors = lasso_square_errors, squared_errors)
```

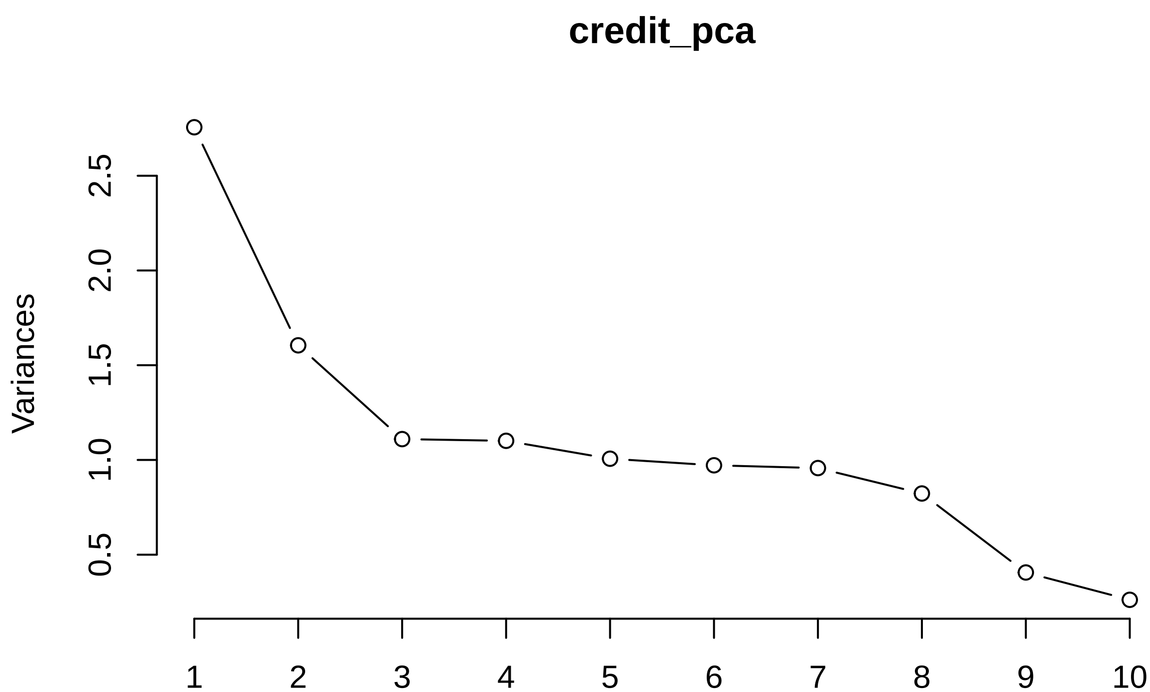
Recommended exercise 7

```r
x <- model.matrix(Balance~.,credit_data)[,-1]

credit_pca <- prcomp(x, center = TRUE, scale. = TRUE)

print(credit_pca)
```

```
## Standard deviations (1, .., p=11):
##  [1] 1.66007642 1.26685832 1.05356810 1.04926273 1.00322222 0.98576693
##  [7] 0.97830708 0.90714714 0.63722533 0.51174012 0.04617646
```

```
##
## Rotation (n x k) = (11 x 11):
##                              PC1          PC2          PC3           PC4
## Income             -0.542206953  0.029036783 -0.033270648 -6.564051e-05
## Limit              -0.586332930  0.017502630 -0.024351723  4.678929e-02
## Rating             -0.586751867  0.014971105 -0.004630758  3.687909e-02
## Cards              -0.019086978 -0.008549632  0.479005750 -2.720228e-01
## Age                -0.122783390 -0.071116603  0.107188498 -4.787335e-01
## Education           0.026797471  0.096557225 -0.475418336  1.990653e-01
## GenderFemale       -0.002519860  0.052811098 -0.334014058 -4.207748e-02
## StudentYes          0.002276904  0.125422970 -0.618650527 -2.963169e-01
## MarriedYes         -0.026218561  0.094278214  0.125718135  7.389864e-01
## EthnicityAsian      0.032769895  0.696759512  0.105703127  6.686132e-03
## EthnicityCaucasian -0.004070799 -0.686505857 -0.100240068  1.338718e-01
##                            PC5         PC6         PC7         PC8
## Income             -0.02816858  0.02297156 -0.04086888  0.03502243
## Limit               0.02393728  0.06109959  0.02753603 -0.07998103
## Rating              0.03044748  0.04901285  0.06298342 -0.07474080
## Cards               0.07450235 -0.28313105  0.77070237 -0.10917776
## Age                -0.29468570 -0.58353604 -0.35860755  0.41270188
## Education          -0.58335540 -0.40244676  0.21601791 -0.41794930
## GenderFemale        0.74620452 -0.51375214 -0.10203846 -0.22746095
## StudentYes          0.05874438  0.20236658  0.42777847  0.53366278
## MarriedYes          0.04850438 -0.32419986  0.13571418  0.53676497
## EthnicityAsian      0.02125450  0.01284830 -0.04334986  0.01824866
## EthnicityCaucasian  0.04400214 -0.02306227  0.10322555  0.06987098
##                              PC9         PC10          PC11
## Income             -0.016018928  0.836411394  0.0017092799
## Limit              -0.010697575 -0.379489022  0.7053633132
## Rating             -0.005366527 -0.373834509 -0.7081335719
## Cards               0.005357720  0.059511066  0.0305564113
## Age                -0.048994454 -0.102540342  0.0005901693
## Education          -0.021973159  0.014172918 -0.0036133922
## GenderFemale        0.014513597  0.027300122  0.0001327203
## StudentYes          0.022068488 -0.032119354  0.0044219212
## MarriedYes          0.119017609 -0.018248384  0.0051766487
## EthnicityAsian     -0.706522468 -0.014783578 -0.0035849536
## EthnicityCaucasian -0.694731116  0.008145839 -0.0004464620
```

```r
plot(credit_pca, type = "l")
```



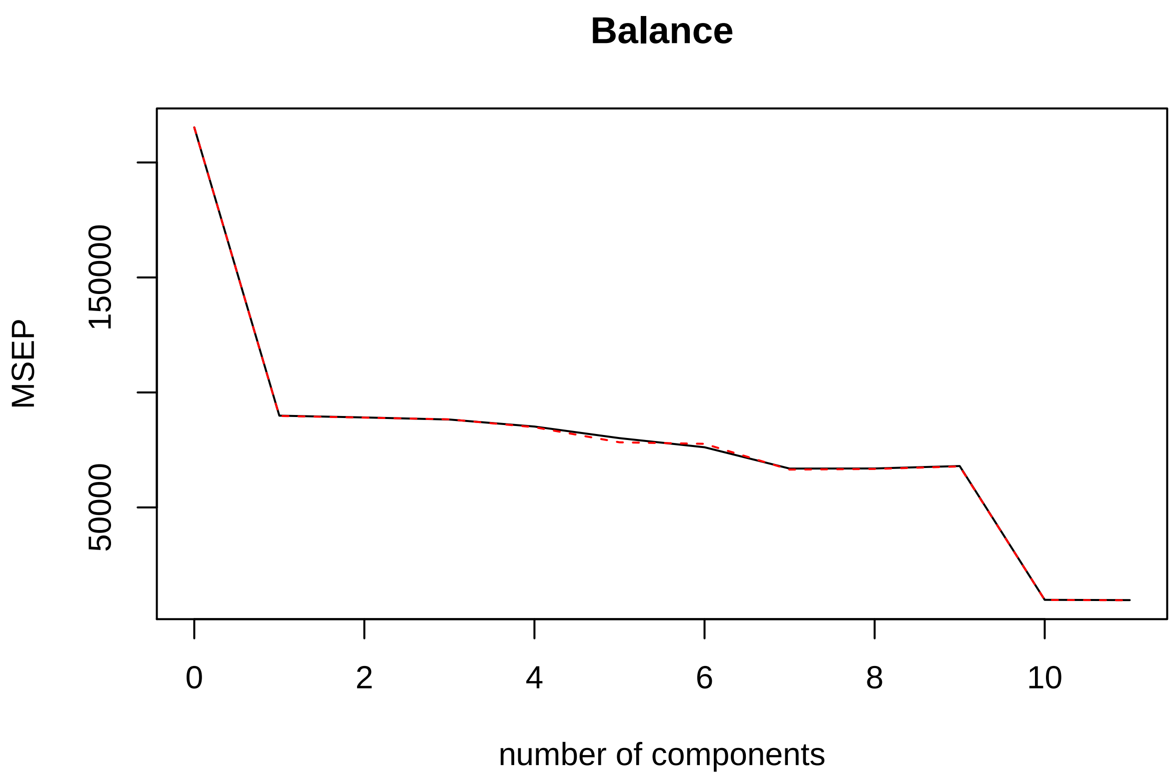

```r
summary(credit_pca)
```

```
## Importance of components:
##                           PC1    PC2    PC3    PC4    PC5     PC6     PC7
## Standard deviation     1.6601 1.2669 1.0536 1.0493 1.0032 0.98577 0.97831
## Proportion of Variance 0.2505 0.1459 0.1009 0.1001 0.0915 0.08834 0.08701
## Cumulative Proportion  0.2505 0.3964 0.4973 0.5974 0.6889 0.77727 0.86427
##                            PC8     PC9    PC10    PC11
## Standard deviation     0.90715 0.63723 0.51174 0.04618
## Proportion of Variance 0.07481 0.03691 0.02381 0.00019
## Cumulative Proportion  0.93908 0.97600 0.99981 1.00000
```

The first PC explain along 25% of the variability in the data. Then the second PC explain an extra 15% of the variability in the data. From the third PC until 8th PC the extra variability explained per PC varies between 7.5% to 10%, dropping to 3.6% on the 9th PCA. So I would likely use 8 PCs for the Credit dataset.

Recommended exercise 8

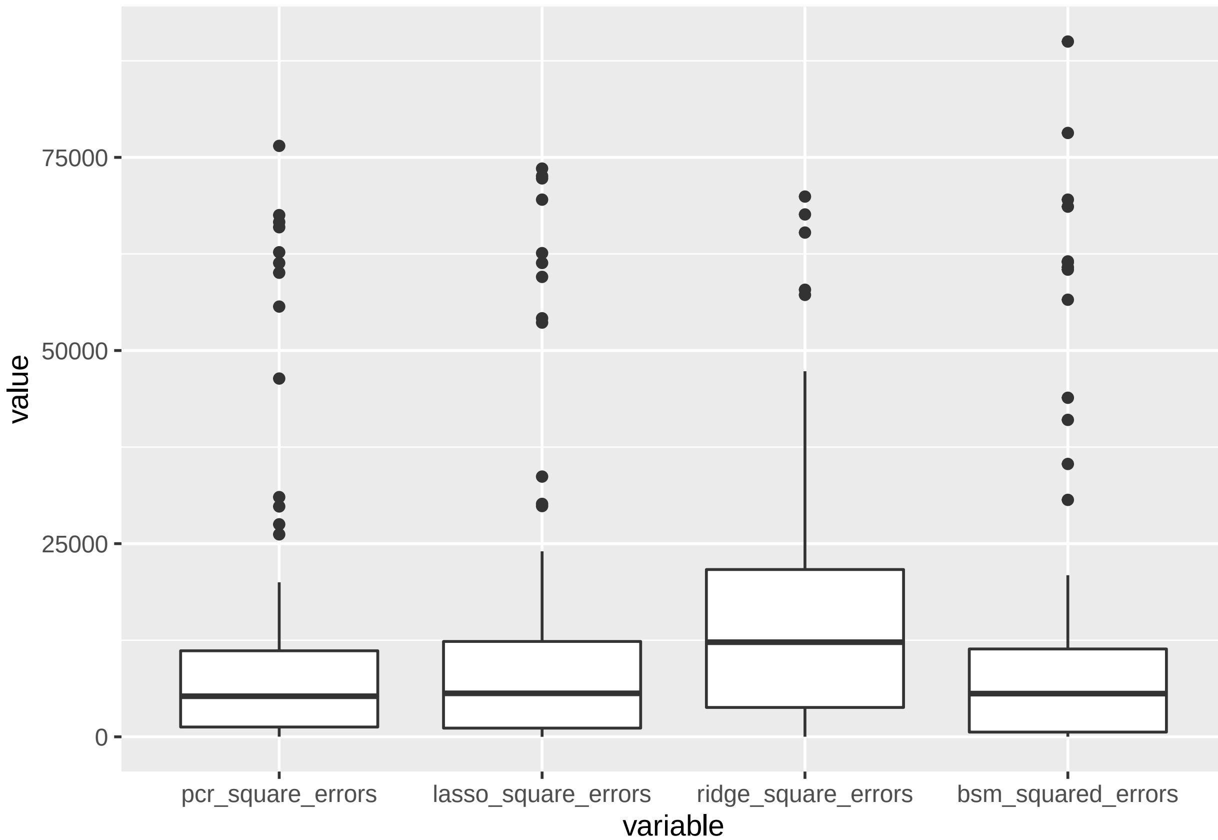
```r
library(pls)

set.seed(1)

pcr_model <- pcr(Balance~., data=credit_data_training,scale=TRUE, validation="CV")
validationplot(pcr_model,val.type="MSEP")
```




```r
pcr_predictions = predict(pcr_model,credit_data_testing,ncomp=10)
pcr_square_errors <- as.numeric((pcr_predictions-credit_data_testing$Balance)^2)
squared_errors <- data.frame(pcr_square_errors = pcr_square_errors, squared_errors)
mean(pcr_square_errors)
```

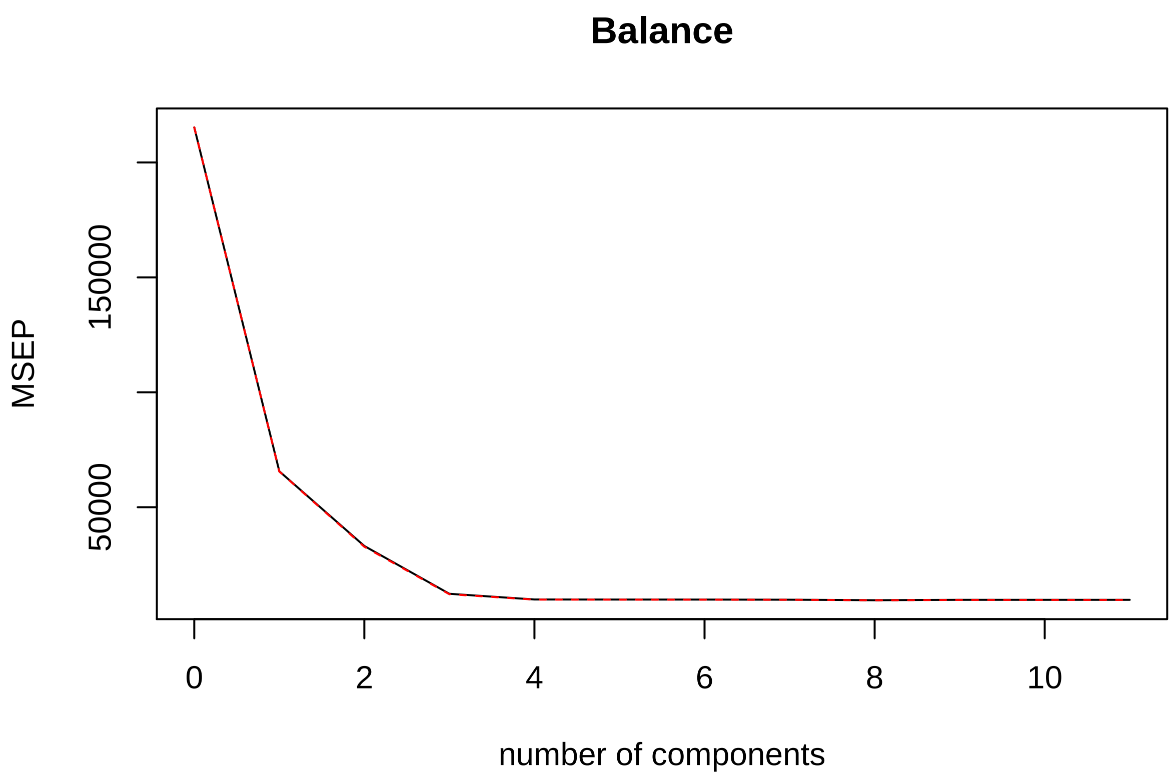
```
## [1] 11578.1
```

```r
library(ggplot2)
library(reshape2)
ggplot(melt(squared_errors)) + geom_boxplot(aes(variable, value))
```



Recommended exercise 9

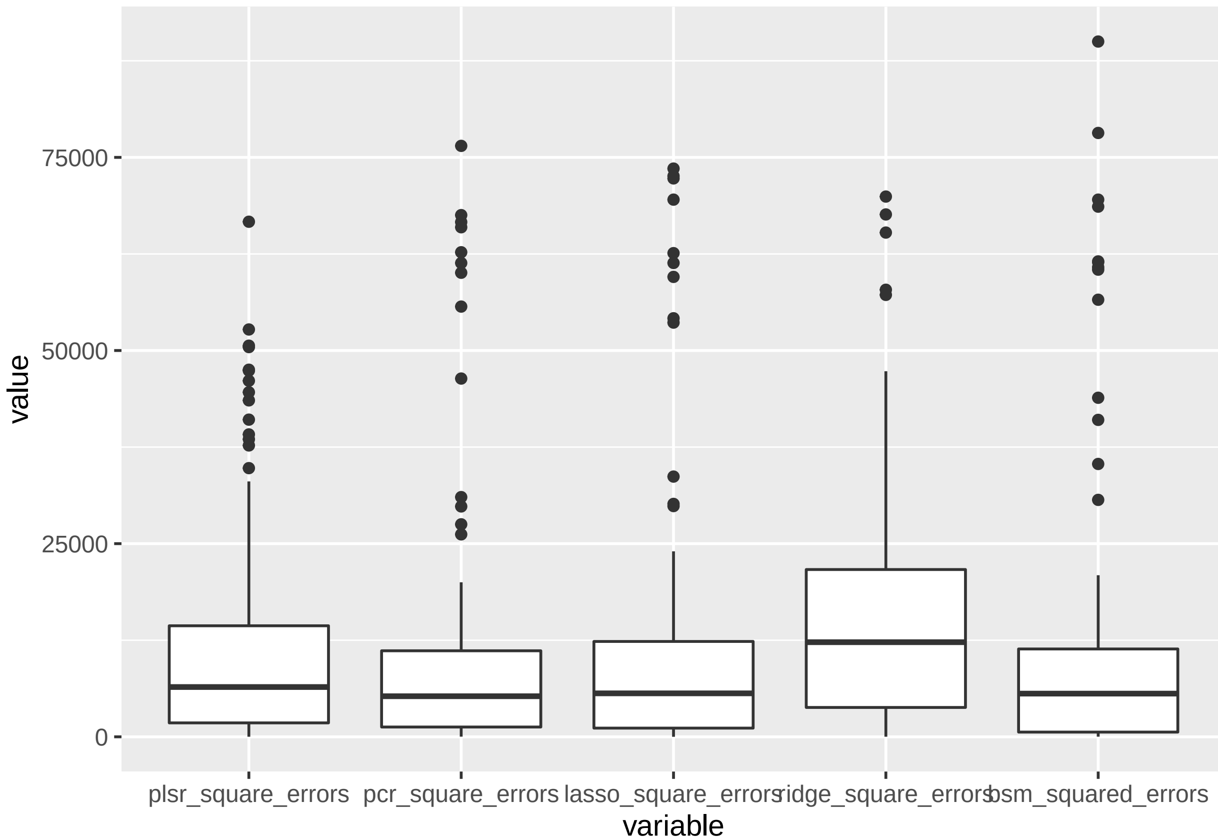
```
library(pls)

set.seed(1)

plsr_model <- plsr(Balance~., data=credit_data_training,scale=TRUE, validation="CV")
validationplot(plsr_model,val.type="MSEP")
```




```
plsr_predictions = predict(plsr_model,credit_data_testing,ncomp=3)
plsr_square_errors <- as.numeric((plsr_predictions-credit_data_testing$Balance)^2)
squared_errors <- data.frame(plsr_square_errors = plsr_square_errors, squared_errors)
mean(plsr_square_errors)
```

```
## [1] 12476.32
```

```
ggplot(melt(squared_errors)) + geom_boxplot(aes(variable, value))
```




```r
colMeans(squared_errors)
```

```
##  plsr_square_errors   pcr_square_errors lasso_square_errors
##            12476.32            11578.10            12077.15
## ridge_square_errors  bsm_squared_errors
##            15742.83            12243.75
```