Assignment 1: Linear model selection

Thomas Vanpoucke, Boris Shilov

Contents

1 Variable comparison and evaluation

There are 97 data points, seven predictor variables and one response variable, Cscore. There is one binary variable, svi. Looking at the scatterplots below, there seem to be a few strong positive correlations present, such as those between Cscore and lpsa as well as lcavol and lpsa.

When looking at the first data points, we noticed that there were some recurring numbers, specifically within the lbph and lcp predictor variables.

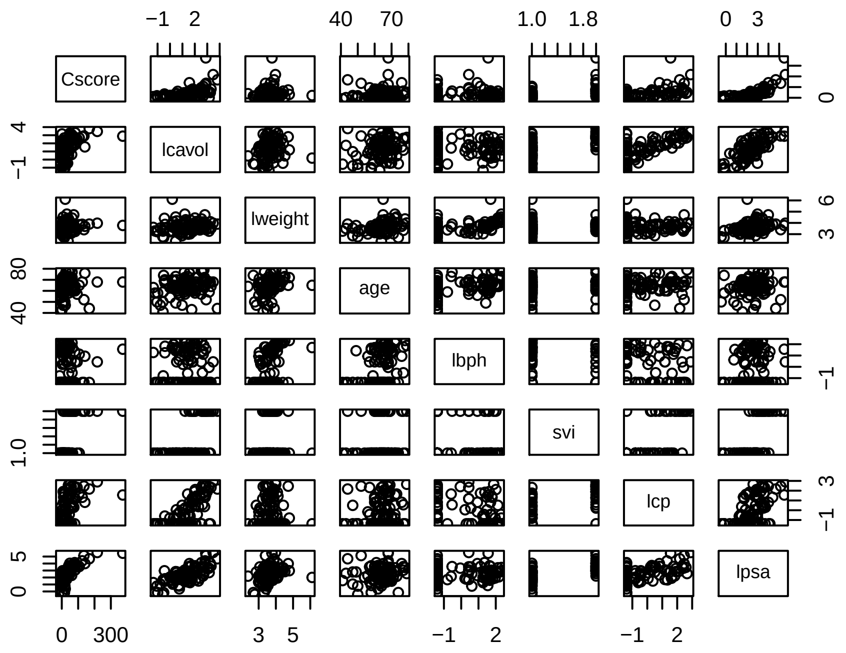
```r
head(prostate)
```

```
##   Cscore lcavol lweight age  lbph svi   lcp   lpsa
## 1  10.48 -0.580    2.77  50 -1.39   0 -1.39 -0.431
## 2   1.08 -0.994    3.32  58 -1.39   0 -1.39 -0.163
## 3  16.10 -0.511    2.69  74 -1.39   0 -1.39 -0.163
## 4 -16.39 -1.204    3.28  58 -1.39   0 -1.39 -0.163
## 5  21.08  0.751    3.43  62 -1.39   0 -1.39  0.372
## 6  18.86 -1.050    3.23  50 -1.39   0 -1.39  0.765
```

```r
summary(prostate)
```

```
##      Cscore        lcavol         lweight          age      
##  Min.   :-19   Min.   :-1.35   Min.   :2.37   Min.   :41.0  
##  1st Qu.:  9   1st Qu.: 0.51   1st Qu.:3.38   1st Qu.:60.0  
##  Median : 21   Median : 1.45   Median :3.62   Median :65.0  
##  Mean   : 36   Mean   : 1.35   Mean   :3.65   Mean   :63.9  
##  3rd Qu.: 49   3rd Qu.: 2.13   3rd Qu.:3.88   3rd Qu.:68.0  
##  Max.   :373   Max.   : 3.82   Max.   :6.11   Max.   :79.0  
##       lbph       svi          lcp              lpsa
##  Min.   :-1.39   0:76   Min.   :-1.386   Min.   :-0.43
##  1st Qu.:-1.39   1:21   1st Qu.:-1.386   1st Qu.: 1.73
##  Median : 0.30          Median :-0.799   Median : 2.59
##  Mean   : 0.10          Mean   :-0.179   Mean   : 2.48
##  3rd Qu.: 1.56          3rd Qu.: 1.179   3rd Qu.: 3.06
##  Max.   : 2.33          Max.   : 2.904   Max.   : 5.58
```

```r
plot(prostate)
```



2 Forward stepwise selection

We implemented algorithm 6.2 for forward stepwise selection. To choose which parameter to add in one round of forward stepwise selection, we used the model with the highest R^2 value, as per the algorithm. To select the single best model, we used BIC. The entire function code can be found in the source file for this document.

```
##
## Call:
## lm(formula = paste(data_vars[1], "~", paste(predictor_list, collapse = "+",
##     "+", paste(data_vars[i]))), data = data)
##
## Coefficients:
## (Intercept)         lpsa         svi1
##       -37.0         26.9         29.8

##
## Call:
## lm(formula = paste(data_vars[1], "~", paste(predictor_list, collapse = "+",
##     "+", paste(data_vars[i]))), data = data)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -60.83 -19.18  -4.72  13.51 232.87
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   -36.98       9.08   -4.07  9.7e-05 ***
## lpsa           26.90       3.80    7.08  2.6e-10 ***
## svi1           29.81      10.60    2.81    0.006 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 35.4 on 94 degrees of freedom
## Multiple R-squared:  0.558,  Adjusted R-squared:  0.549
## F-statistic: 59.3 on 2 and 94 DF,  p-value: <2e-16
```

Thus, the model returned by our algorithm as the best was one with only two predictor variables, lpsa and svi.

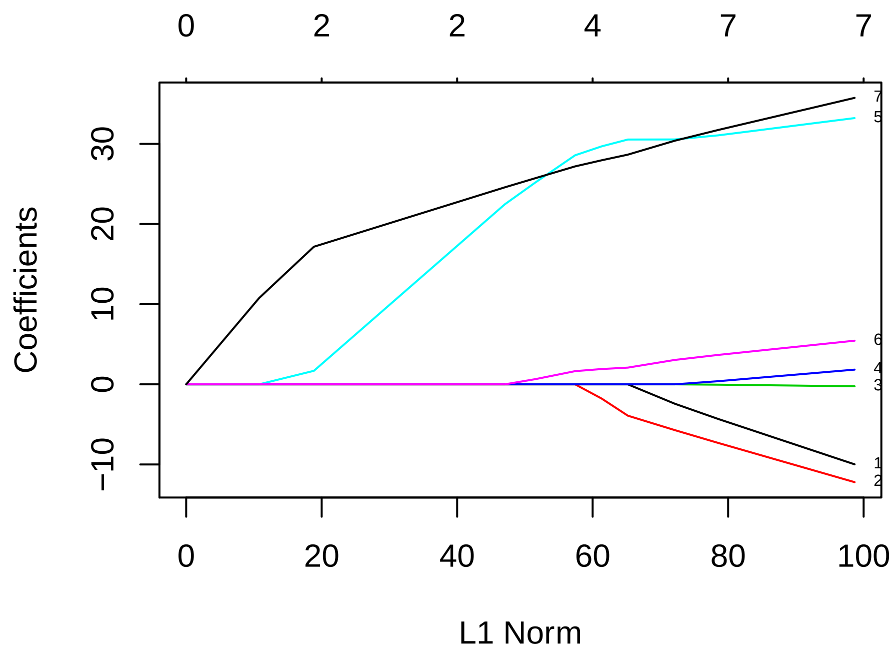
$$Cscore = -36.977 + 26.903 \times lpsa + 29.81 \times svi1$$

3 Lasso

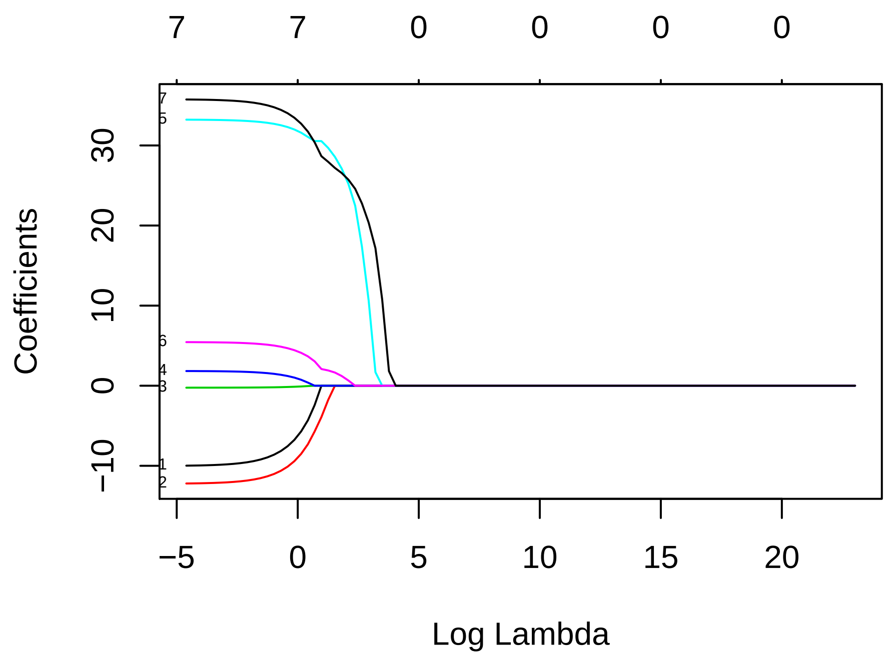
To do a cross-validated lasso and ridge, we first split up the dataset into two pieces, a training and a test dataset. We made a model, based on the training data, that was crossvalidated within this training data. The test dataset was then used to check the mean squared test error for the best lambda (which is the lowest mean squared training error). To finish off, we used the entire dataset and the best lambda value to construct our lasso model.

```r
x = model.matrix(Cscore~.,prostate)[,-1]
y = prostate$Cscore
train=sample(1:nrow(x),nrow(x)/2)
test=(-train)
y.test=y[test]

grid=10^seq(10,-2,length=100)
lasso.model=glmnet(x[train,],y[train],alpha=1,lambda=grid, thresh = 1e-12)
plot(lasso.model, label = TRUE)
```

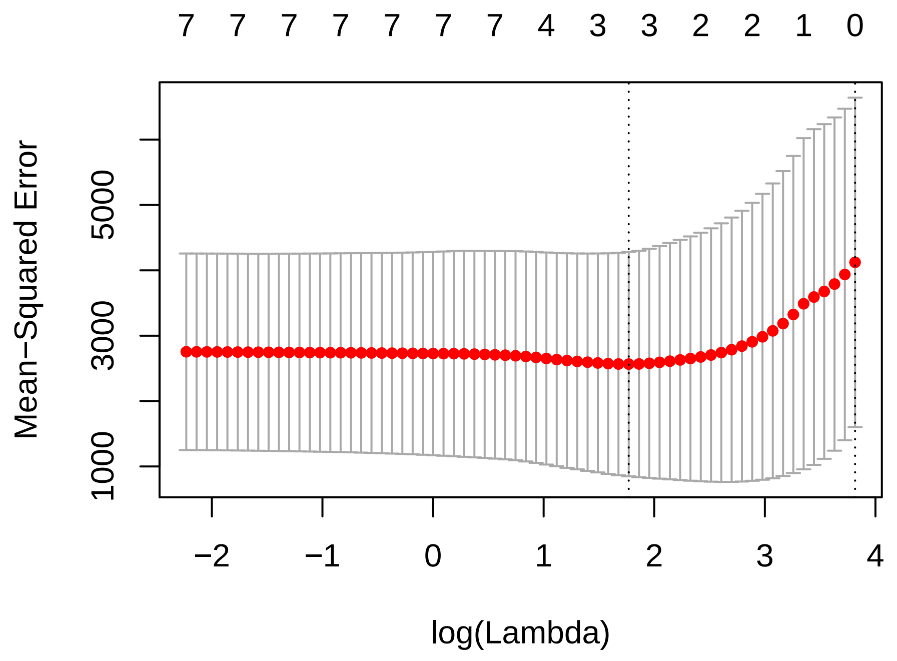


```
plot(lasso.model,xvar="lambda",label=TRUE)
```



```
lasso.model=glmnet(x[train,],y[train],alpha=1,lambda=grid, thresh = 1e-12)
OLS.model=glmnet(x[train,],y[train],alpha=1,lambda=0, thresh = 1e-12)
```

```r
cv.lasso.out=cv.glmnet(x[train,],y[train],alpha=1)
plot(cv.lasso.out)
```



```r
bestlambda.lasso=cv.lasso.out$lambda.min
out=glmnet(x,y,alpha=1,lambda=grid)

lasso.pred = predict(lasso.model,s=bestlambda.lasso,newx=x[test,])
lasso.mean = mean((lasso.pred-y.test)^2)
lasso.coef = predict(out,type="coefficients",s=bestlambda.lasso)[1:8,]

OLS.pred = predict(OLS.model, s=0, newx=x[test,])
OLS.mean = mean((OLS.pred-y.test)^2)
OLS.coef = predict(out, type="coefficients", s=0)[1:8,]

lasso.mean
```

```
## [1] 664
```

```r
OLS.mean
```

```
## [1] 736
```

```r
lasso.coef
```

```
## (Intercept)      lcavol     lweight         age        lbph        svi1
##      -23.09        0.00        0.00        0.00        0.00       15.47
##         lcp        lpsa
##        2.92       22.76
```

```r
OLS.coef
```

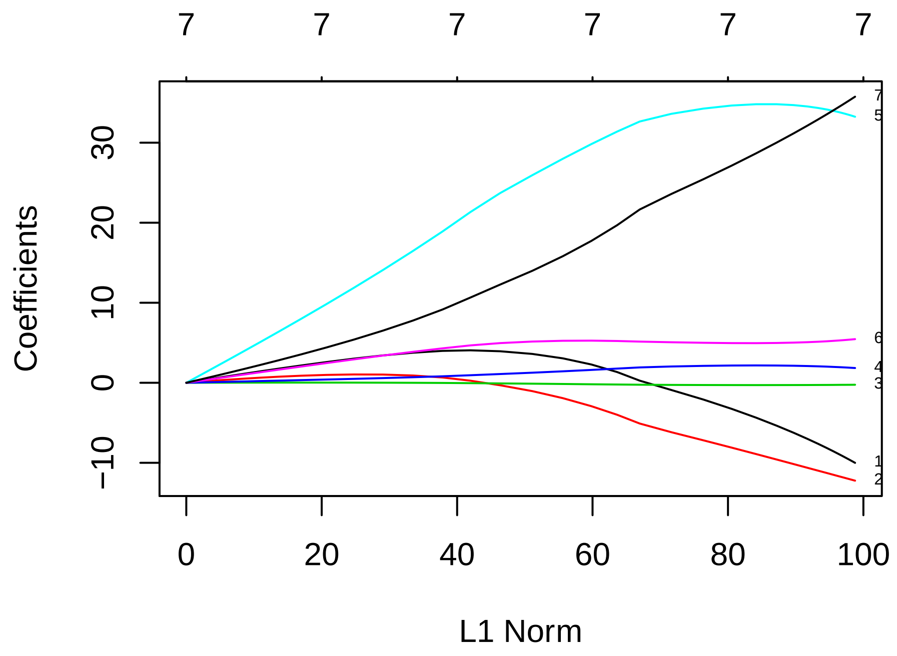
```
## (Intercept)      lcavol     lweight         age        lbph        svi1
##      -4.705     -10.071     -11.895       0.201      -0.526      18.435
##         lcp        lpsa
##       7.790      33.289
```

We can clearly see that Lasso zeroes out a large number of our variables, which is a massive reduction of complexity. Two of the variables agree with our previous best forward selection. Thus Lasso is clearly superior to ordinary least squares in this instance. The resulting Lasso model becomes:

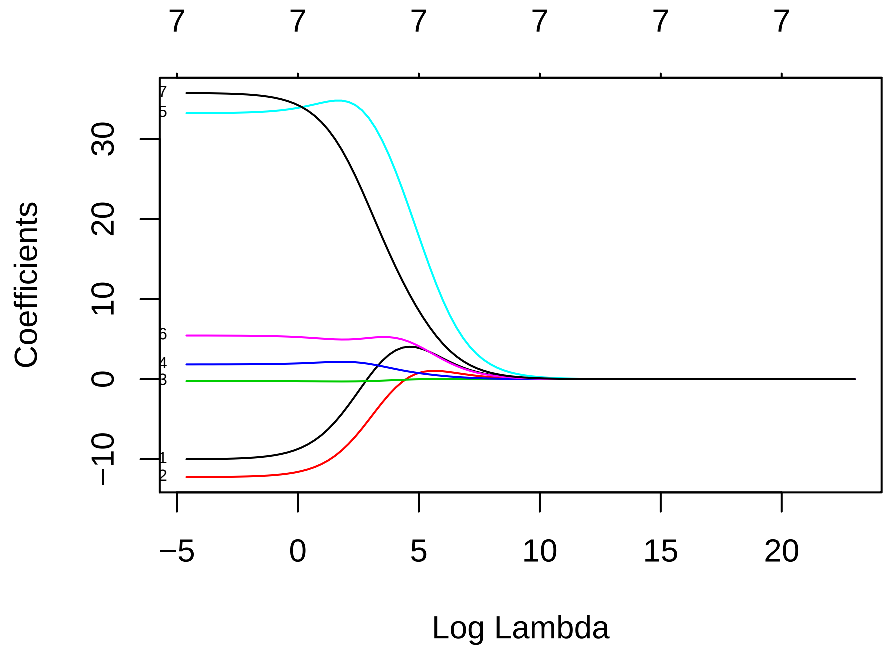
$$Cscore = -23.089 + 15.467 \times svi1 + 2.923 \times lcp + 22.763 \times lpsa$$

4 Ridge

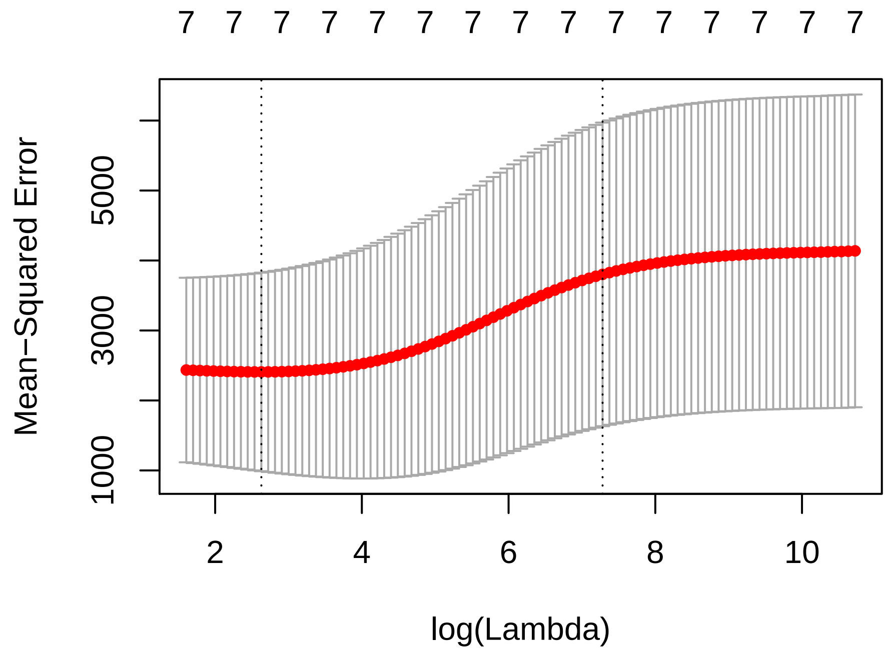
```
grid=10^seq(10,-2,length=100)
ridge.model=glmnet(x[train,],y[train],alpha=0,lambda=grid, thresh = 1e-12)
OLS.model.ridge=glmnet(x[train,],y[train],alpha=0,lambda=0, thresh = 1e-12)
plot(ridge.model, label = TRUE)
```



```
plot(ridge.model,xvar="lambda",label=TRUE)
```



```
cv.ridge.out=cv.glmnet(x[train,],y[train],alpha=0)
plot(cv.ridge.out)
```



```
bestlambda.ridge=cv.ridge.out$lambda.min
```

Lowest mean squared error here corresponds to lowest cross validation error. We can conclude that the best λ value equals 13.872.

```
bestlambda.ridge=cv.ridge.out$lambda.min
out.ridge=glmnet(x,y,alpha=1,lambda=grid)

ridge.pred = predict(ridge.model,s=bestlambda.ridge,newx=x[test,])
ridge.mean = mean((ridge.pred-y.test)^2)
ridge.coef = predict(out.ridge,type="coefficients",s=bestlambda.ridge)[1:8,]

OLS.pred.ridge = predict(OLS.model.ridge, s=0, newx=x[test,])
OLS.mean.ridge = mean((OLS.pred.ridge-y.test)^2)
OLS.coef.ridge = predict(out.ridge, type="coefficients", s=0)[1:8,]

ridge.mean
```

```
## [1] 675
```

```
OLS.mean.ridge
```

```
## [1] 736
```

```
ridge.coef
```

```
## (Intercept)      lcavol     lweight         age        lbph        svi1
##      -12.65        0.00        0.00        0.00        0.00        7.56
##         lcp        lpsa
##        0.42       19.06
```

```
OLS.coef
```

```
## (Intercept)      lcavol     lweight         age        lbph        svi1
##      -4.705     -10.071     -11.895       0.201      -0.526      18.435
##         lcp        lpsa
##       7.790      33.289
```

There is still a subsantial improvement over OLS in Ridge as most coefficients are zeroed out. The resulting Ridge model is thus:

$$Cscore = -12.651 + 7.561 \times svi1 + 0.42 \times lcp + 19.061 \times lpsa$$

5 Principal Component Regression

5.1 How many principal components would you select for yout PCR model?

We would select three principal components, because the mean squared error compared to the number of components is the lowest there. Of course, taking seven principal components is still lower, since then we practically account for all variable. Also, three components already explain approximately 78% of the variation in the data.

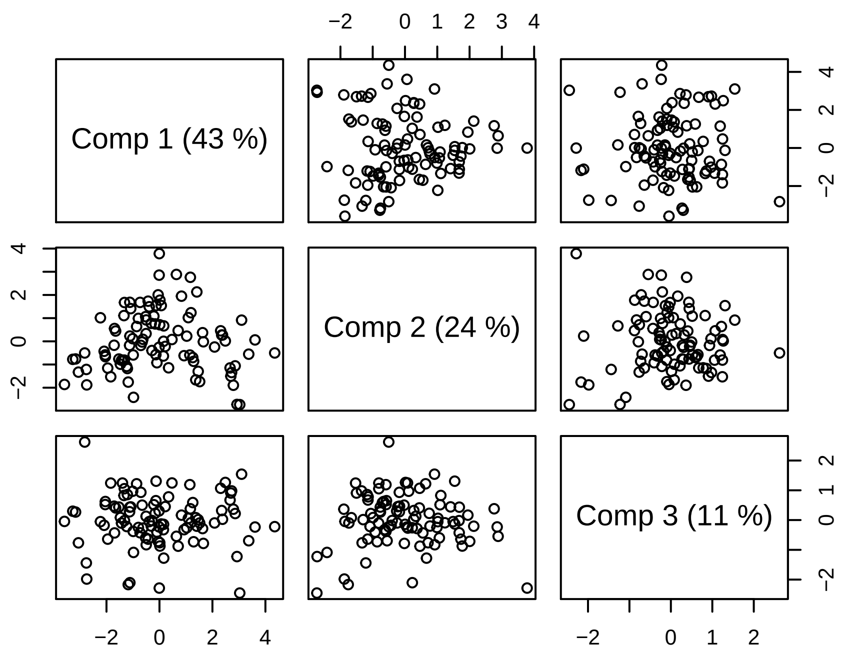
```
set.seed(10)
pcr_model=pcr(Cscore~.,data=prostate,scale=TRUE,
        validation="CV")
summary(pcr_model)
```

```
## Data:    X dimension: 97 7
##  Y dimension: 97 1
## Fit method: svdpc
## Number of components considered: 7
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##        (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## CV           52.99    40.71    40.06    39.94    39.85    40.56    39.85
## adjCV        52.99    40.61    39.95    39.83    39.71    40.43    39.66
##        7 comps
## CV       37.47
## adjCV    37.26
##
## TRAINING: % variance explained
##         1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X         43.44    66.95    77.62    85.37    92.39    97.42   100.00
## Cscore    44.91    46.93    47.77    48.25    48.28    52.84    59.22
```

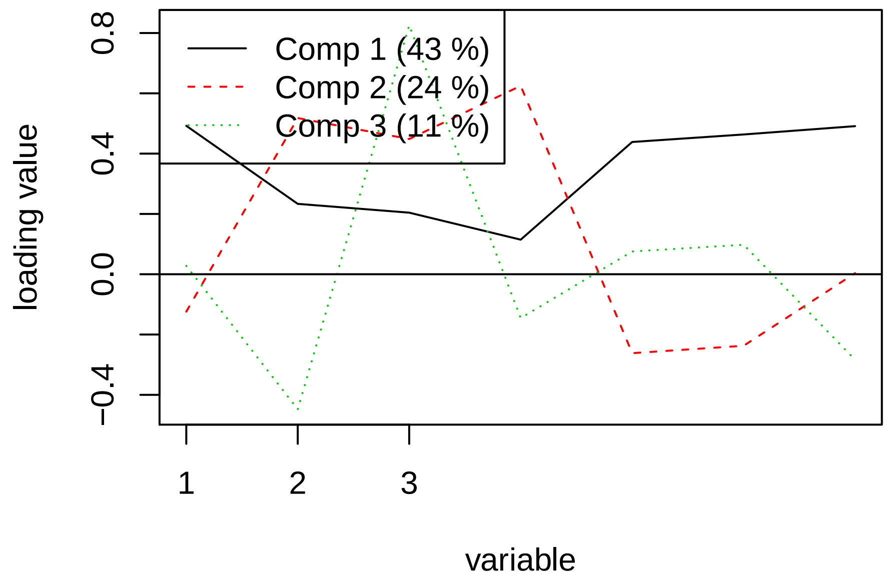
```r
explvar(pcr_model)
```

```
## Comp 1 Comp 2 Comp 3 Comp 4 Comp 5 Comp 6 Comp 7
##  43.44  23.51  10.67   7.75   7.02   5.03   2.58
```

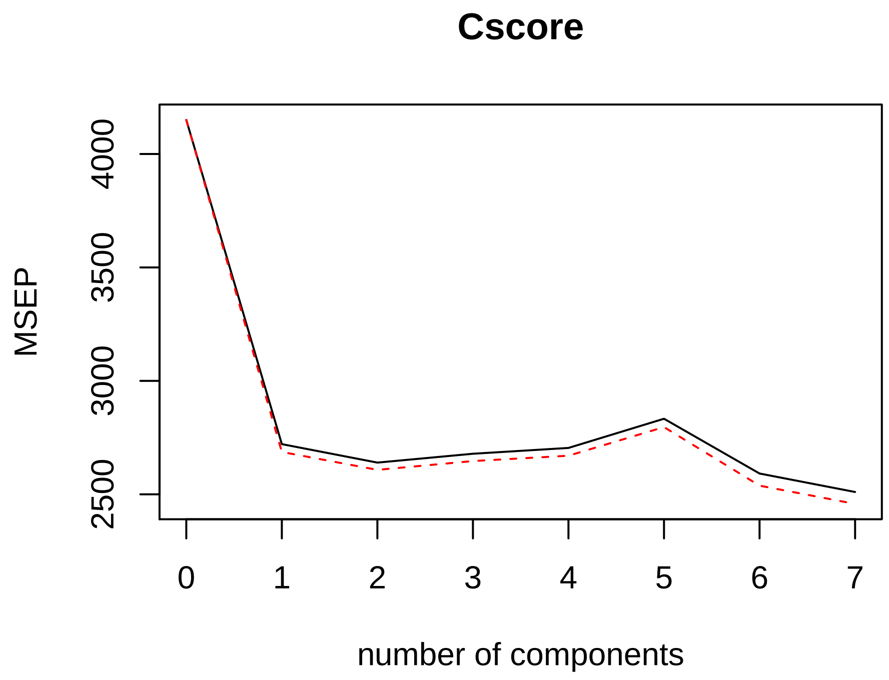
```r
plot(pcr_model, plottype = "scores", comps = 1:3)
```



```r
plot(pcr_model, "loadings", comps = 1:3, legendpos = "topleft",labels = 1:3)
abline(h = 0)
```



```r
pcr_model=pcr(Cscore~.,data=prostate,subset=train,scale=TRUE,
        validation="CV")
validationplot(pcr_model,val.type="MSEP")
```



```r
pcr_pred=predict(pcr_model,x[test,],ncomp=3)
pcr.mean = mean((pcr_pred-y.test)^2)
pcr_model=pcr(y~x,scale=TRUE,ncomp=3)
summary(pcr_model)
```

```
## Data:    X dimension: 97 7
##  Y dimension: 97 1
## Fit method: svdpc
## Number of components considered: 3
## TRAINING: % variance explained
##    1 comps  2 comps  3 comps
## X    43.44    66.95    77.62
## y    44.91    46.93    47.77
```

```r
pcr.mean
```

```
## [1] 873
```

```r
OLS.mean
```

```
## [1] 736
```

5.2 How appropriate is PCR for this dataset?

When we look at the analysis we did, we can certainly say that there is some benefit to use PCR for this dataset, since we can explain a lot of the variance with only three principal components. While the model explains most of the variance in the predictor variables, it does not predict very much variance of the response variable. So it seems that the principal components do not explain the relationship with the response very well. This means that the assumption on which PCR is based is not fulfilled.

When we use cross-validation for our 3-PC model, we can see that the test error of the PCR model is higher than the mean squared error of a normal linear regression model (see test errors above).

Based on these remarks, we conclude that PCR is not optimal for this dataset.

6 Model Comparison

6.1 How well do they perform in general?

In general, the models perform well.

6.2 Do they yield similar models?

Yes, for the most part the same variables are included. However, the coefficients differ from model to model. PCR is the only outlier, since there is no variable selection going on.

6.3 Which variables are the most important in the prediction of the progression of prostate cancer, according to each model?

The forward stepwise, Lasso and Ridge model all seem to indicate svi and lpsa are important variables. Lasso and Ridge also indicate lcp has some significant influence.

For PCR, it is a bit harder to say which variable is the most important, since every principal component has loadings of all the variables. We looked at the highest loading values of the first principal component to determine which variables are important according to PCR. In our case, those variables are approximately the 1st, 5th, 6th and 7th, which correspond to lcavol, svi, lcp and lpsa respectively (see variable loading graph in the PCR component).

6.4 Which model do you think is the most appropriate for this dataset?

We selected the best model based on the test error. For this to be valid we needed to remake the forward stepwise model with only the training data first.

```
## [1] 736

## [1] 803

## [1] 664

## [1] 675

## [1] 873
```

The values shown are the test errors for a normal OLS model, forward stepwise prediction, lasso, ridge and PCR respectively. As we can see, only the lasso and ridge test error are under the OLS test error, and lasso is still slightly lower than ridge. This leads us to conclude that our lasso model is the most appropriate model for this dataset.