Homework 05: Applied Predictive Modeling

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Exercise 6.1

(a) Start R and use these commands to load the data:

```
library (caret)
data(tecator)
```

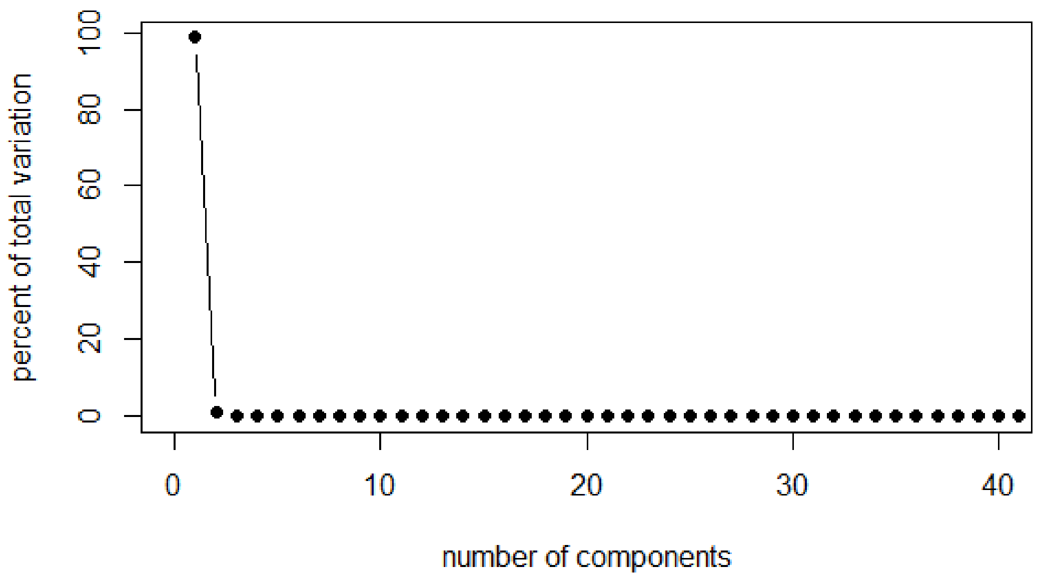
(b) In this example the predictors are the measurements at the individual frequencies. Because the frequencies lie in a systematic order (850–1,050nm), the predictors have a high degree of correlation. Hence, the data lie in a smaller dimension than the total number of predictors (215). Use PCA to determine the effective dimension of these data. What is the effective dimension?

First, apply PCA to the data

```
pc=prcomp(absorp,    scale = TRUE)
```

Then we can get the variance of each component and calculate the percentage of each variance. The first 6 percentages of variance are listed below:

```
98.626192582    0.969705229    0.279324276
 0.114429868    0.006460911    0.002624591
```



From the figure we can see that the first component account for most of the information, so there is only one effective dimension based on the linear analysis.

(c) Split the data into a training and a test set, pre-process the data, and build each variety of models described in this chapter. For those models with tuning parameters, what are the optimal values of the tuning parameter(s)?

The training and test set is built below

```
Training=createDataPartition(endpoints[, 3], p = 0.75, list= FALSE)
absorbtrain=absorp[Training,]
absorbtest=absorp[-Training,]
proteintrain =endpoints[ Training, 3]
proteintest = endpoints[-Training,3]
```

In this case we only choose the third column of endpoints----the protein as the predictor. Build the linear model

lm=train(x = absorbtrain, y = proteintrain, method = "lm", trControl = trainControl(method = "repeatedcv", repeats = 5))

The summary is printed below:

```
Linear Regression

163 samples
100 predictors

No pre-processing
Resampling: Cross-Validated (10 fold, repeated 5 times)

Summary of sample sizes: 147, 147, 146, 147, 147, 147, ...

Resampling results

  RMSE  Rsquared  RMSE SD  Rsquared SD
  1.52  0.819     0.781    0.175
```

The RMSE is 1.52

The Robust linear regression "rlm" model is built below, however, rlm does not allow the covariance matrix of the predictors to be singular to ensure that predictors are not singular, we will pre-process the predictors using PCA

rlm = train(x=absorbtrain, y=proteintrain, method="rlm",

preProcess=c("pca"),

trControl=trainControl(method="repeatedcv",repeats=5))

```
Robust Linear Model

163 samples
100 predictors

Pre-processing: principal component signal extraction, sca
led, centered
```

```
Resampling: Cross-Validated (10 fold, repeated 5 times)

Summary of sample sizes: 146, 148, 147, 146, 147, 147, ...

Resampling results

  RMSE  Rsquared  RMSE SD  Rsquared SD
  2.6   0.275     0.349    0.17
```

The PLS model:

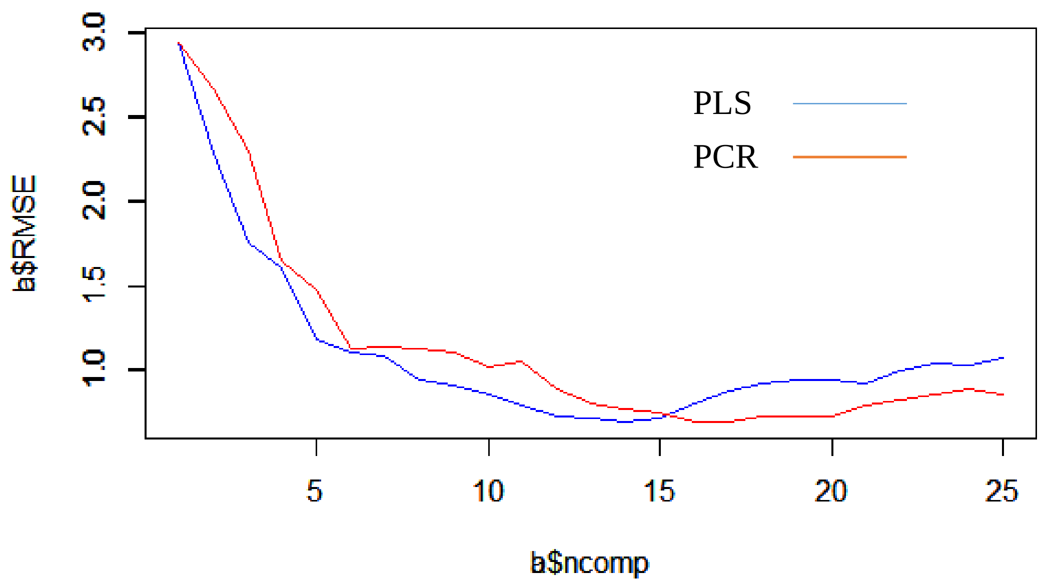
```
Partial Least Squares

163 samples
100 predictors

Pre-processing: centered, scaled
Resampling: Cross-Validated (10 fold, repeated 5 times)

Summary of sample sizes: 146, 148, 147, 146, 147, 147, ...

Resampling results across tuning parameters:

  ncomp  RMSE   Rsquared  RMSE SD  Rsquared SD
  1      2.93   0.0975    0.274    0.115
  2      2.29   0.44      0.333    0.163
  3      1.75   0.664     0.404    0.167
  4      1.61   0.712     0.401    0.159
  5      1.18   0.854     0.177    0.0467
  6      1.11   0.871     0.166    0.0437
  7      1.08   0.876     0.163    0.048
  8      0.95   0.906     0.167    0.0412
  9      0.911  0.915     0.167    0.0389
  10     0.86   0.924     0.166    0.0329
  11     0.792  0.935     0.136    0.0252
  12     0.733  0.947     0.154    0.0226
  13     0.715  0.949     0.176    0.0236
  14     0.694  0.953     0.159    0.0233
  15     0.72   0.95      0.174    0.0233
  16     0.804  0.934     0.277    0.0448
  17     0.876  0.916     0.371    0.0818
  18     0.927  0.902     0.425    0.101
  19     0.95   0.894     0.472    0.117
  20     0.941  0.894     0.483    0.121
  21     0.921  0.899     0.459    0.112
  22     1      0.877     0.566    0.161
  23     1.04   0.869     0.595    0.172
  24     1.04   0.872     0.564    0.152
  25     1.08   0.862     0.593    0.165

RMSE was used to select the optimal model using  the smalle
st value.
The final value used for the model was ncomp = 14.
```

And the PCR :

```
Principal Component Analysis

163 samples
100 predictors

No pre-processing
Resampling: Cross-Validated (10 fold, repeated 5 times)

Summary of sample sizes: 145, 147, 148, 147, 147, 147, ...

Resampling results across tuning parameters:

  ncomp  RMSE   Rsquared  RMSE SD  Rsquared SD
  1      2.94   0.106     0.274    0.113
  2      2.68   0.234     0.273    0.165
  3      2.3    0.441     0.369    0.18
  4      1.65   0.697     0.43     0.176
  5      1.47   0.766     0.286    0.102
  6      1.13   0.869     0.174    0.0413
  7      1.13   0.868     0.174    0.0408
  8      1.12   0.868     0.168    0.04
  9      1.1    0.876     0.147    0.0333
  10     1.02   0.898     0.158    0.0328
  11     1.05   0.891     0.174    0.0371
  12     0.889  0.923     0.117    0.0231
  13     0.795  0.937     0.145    0.0233
  14     0.765  0.942     0.139    0.0228
  15     0.744  0.944     0.137    0.0211
  16     0.684  0.953     0.136    0.0214
  17     0.691  0.953     0.142    0.0213
```

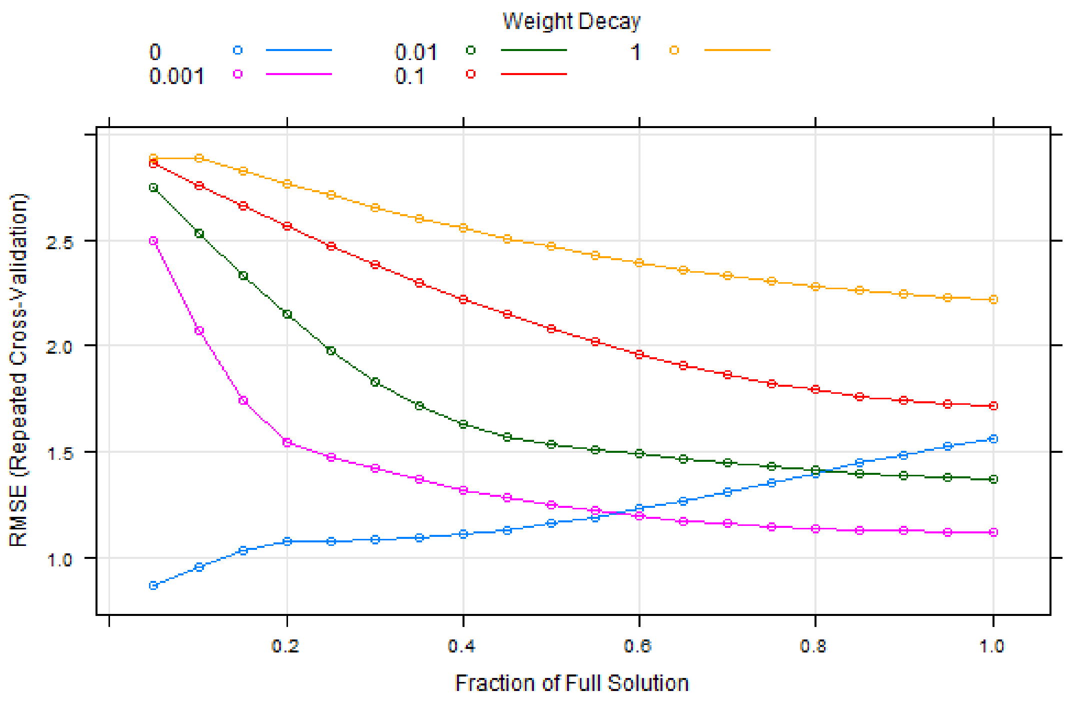
```
 18      0.721  0.951     0.159    0.0208
 19      0.718  0.951     0.18     0.0252
 20      0.722  0.95      0.19     0.0265
 21      0.782  0.94      0.247    0.0373
 22      0.819  0.932     0.296    0.0551
 23      0.853  0.925     0.324    0.0594
 24      0.882  0.918     0.362    0.0683
 25      0.853  0.922     0.341    0.07

RMSE was used to select the optimal model using  the smalle
st value.
The final value used for the model was ncomp = 16.
```

These two models have similar RMSE but the PLS requires less components.



At last we build the elastic net model:

```
ENet = train(x = absorbtrain, y = proteintrain,method = "enet",trControl = trainControl(method="repeatedcv",repeats=5), preProcess = c("center", "scale"),tuneGrid = expand.grid(lambda = c(0, .001, .01, .1, 1), fraction = seq(0.05, 1, length = 20)))
```



(d) Which model has the best predictive ability? Is any model significantly better or worse than the others?

From the RMSE result of different model, we find that PLS model has better performance since it is especially suited to handling highly correlated data. And linear model has the worst performance overall.

(e) Explain which model you would use for predicting the fat content of a sample.

PLS model can be used to predict the fat content as predicting protein in the previous problems.

Execise 6.2

(a) Start R and use these commands to load the data:

```
library (AppliedPredictiveModeling)
data (permeability)
```

(b) The fingerprint predictors indicate the presence or absence of substructures of a molecule and are often sparse meaning that relatively few of the molecules contain each substructure. Filter out the predictors that have low frequencies using the nearZeroVar function from the caret package. How many predictors are left for modeling?

```
zero = nearZeroVar( fingerprints )
fingerprints = fingerprints[,-zero]
```

There are 719 near-zero variance fingerprints, leaving 388 left for modeling
There are 165*1107=182655 elements in the previous matrix and after removing 0, there are only 165*388=64020 elements.

(c) Split the data into a training and a test set, pre-process the data, and tune a partial least squares model. How many latent variables are optimal and what is the corresponding resampled estimate of R2?

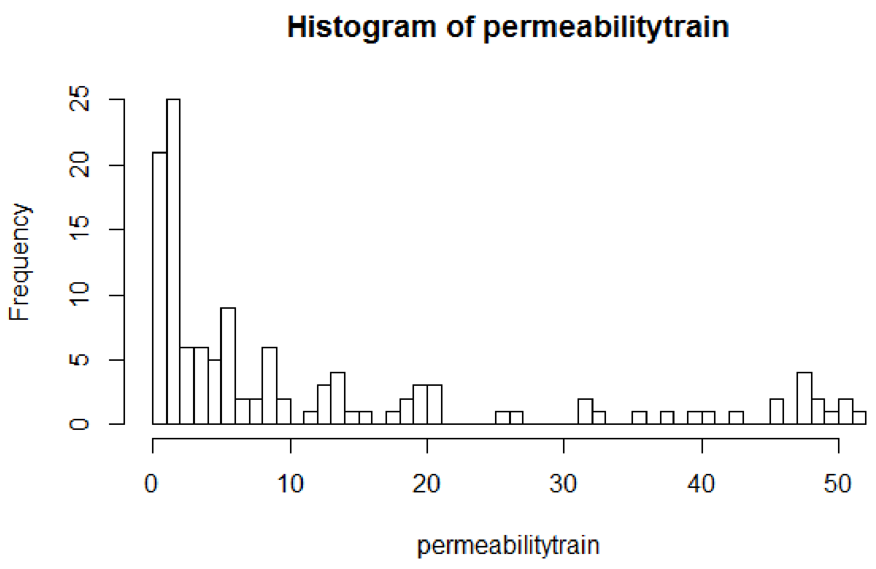
Training = createDataPartition(permeability, p=0.75)

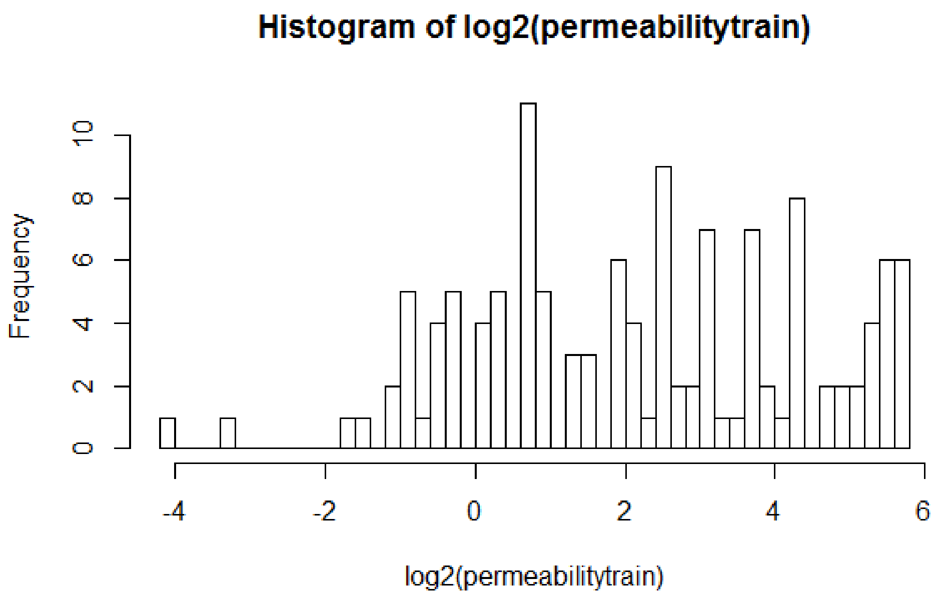
Set p=0.75 and

fingerprintstrain <- fingerprintsnonzero [Training$Resample1,]

permeabilitytrain <- permeability[Training$Resample1,]

Create the training dataset for PLS model, however, the permeability is not a symmetric distribution. We also need to pre-process the permeability before building the model





I choose log2 to modify the data and build the model.

The result of PLS model (tunelength=25) is listed below:

```
Partial Least Squares

125 samples
388 predictors

No pre-processing
Resampling: Repeated Train/Test Splits Estimated (25 reps,
 0.75%)

Summary of sample sizes: 96, 96, 96, 96, 96, 96, ...

Resampling results across tuning parameters:

  ncomp  RMSE  Rsquared  RMSE SD  Rsquared SD
  1      1.93  0.281     0.272    0.145
  2      1.71  0.436     0.302    0.142
  3      1.66  0.471     0.279    0.123
  4      1.67  0.475     0.29     0.119
  5      1.68  0.478     0.251    0.111
  6      1.69  0.485     0.272    0.114
  7      1.68  0.493     0.276    0.116
  8      1.65  0.513     0.266    0.11
  9      1.63  0.528     0.245    0.101
  10     1.64  0.537     0.233    0.0949
  11     1.69  0.523     0.239    0.0982
  12     1.72  0.513     0.237    0.0943
  13     1.75  0.503     0.246    0.104
  14     1.81  0.479     0.243    0.108
  15     1.84  0.471     0.252    0.112

RMSE was used to select the optimal model using  the smalle
st value.
The final value used for the model was ncomp = 9.
```

when n=10, the Rsquared reach the maximum value 0.537

(d) Predict the response for the test set. What is the test set estimate of R2?

ypredict = predict(plsTune, newdata=fingerprintstest)

And the R-squared is 0.56 which is not very far from the real value.

(e) Try building other models discussed in this chapter. Do any have better predictive performance?

For different models, I test lm, rlm, PCR, Enet.

LM:

lm = train(fingerprintstrain, permeabilitytrain, method="lm", preProcess=c("center","scale"), trControl=trainControl(method="repeatedcv",repeats=5))

```
Linear Regression

125 samples
388 predictors

Pre-processing: centered, scaled
Resampling: Cross-Validated (10 fold, repeated 5 times)

Summary of sample sizes: 113, 111, 112, 112, 113, 113, ...

Resampling results

  RMSE  Rsquared  RMSE SD  Rsquared SD
  32.5  0.192    11.1     0.193
```

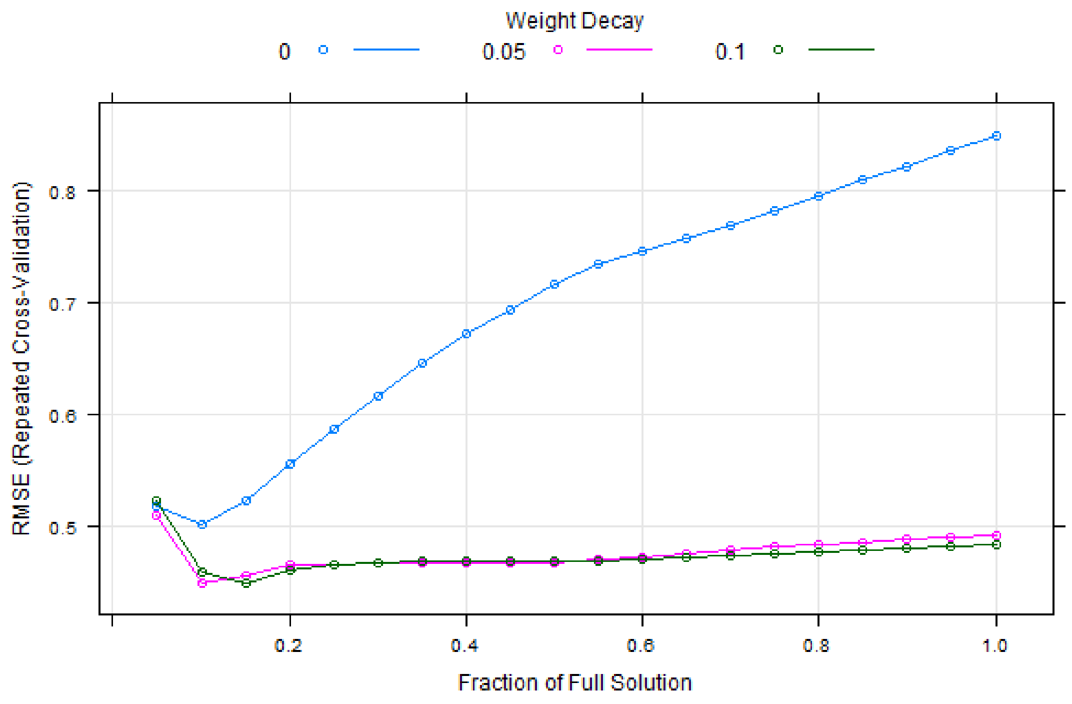
rlm

```
Robust Linear Model

125 samples
388 predictors

Pre-processing: principal component signal extraction, sca
led, centered
Resampling: Cross-Validated (10 fold, repeated 5 times)

Summary of sample sizes: 113, 111, 112, 112, 113, 113, ...

Resampling results

  RMSE  Rsquared  RMSE SD  Rsquared SD
  11.7  0.517     3.57     0.235
```

PCR

```
Principal Component Analysis

125 samples
388 predictors

Pre-processing: principal component signal extraction, sca
led, centered
Resampling: Repeated Train/Test Splits Estimated (25 reps,
 0.75%)

Summary of sample sizes: 96, 96, 96, 96, 96, 96, ...

Resampling results across tuning parameters:

  ncomp  RMSE  Rsquared  RMSE SD  Rsquared SD
  1      16    0.0599    1.47     0.0787
  2      16    0.0597    1.47     0.0785
  3      14.8  0.196     0.0232   0.229
  4      12.5  0.401     0.445    0.164
  5      11.9  0.466     0.652    0.127
  6      11.9  0.461     0.657    0.127
  7      12.3  0.416     0.538    0.125
  8       12.3  0.427      0.791     0.132
  9       12.7  0.393      0.246     0.177
  10      12.4  0.432      0.697     0.125
  11      12    0.47      0.293     0.153
  12      11.9  0.471      0.238     0.152
  13      12    0.463      0.257     0.152
  14      12.1  0.458      0.0867    0.164
  15      12    0.461      0.0297    0.168
  16      12.3  0.44       0.14      0.163
  17      12.2  0.462      0.0875    0.129
  18      11.9  0.461      0.144     0.155
  19      11.9  0.457      0.289     0.14
  20      11.9  0.461      0.127     0.146
  21      11.6  0.481      0.374     0.18
  22      11.5  0.486      0.315     0.175
  23      11.5  0.488      0.328     0.178
  24      11.6  0.493      0.326     0.143
  25      12    0.48      0.18      0.157

RMSE was used to select the optimal model using  the smalle
st value.
The final value used for the model was ncomp = 23
```

Enet



(f) Would you recommend any of your models to replace the permeability laboratory experiment?

From the result above, the elastic net solution the best penalized model choice for this problem. It has the lowest RMSE value.

Appendix

```
Q1
library(caret)
data(tecator)

#calculate the mean and variance of each column of endpoints
apply(absorp,    2,    mean)
apply(absorp,    2,    var)

pc=prcomp(absorp,    scale = TRUE)

print( pc$center )
print( pc$scale )



biplot(pc,    scale = 0)

#calculate the largest 6 eigenvalues percentage
pc_var = pc$sdev^2
pve = pc_var/sum(pc_var)*100
head(pve,10)
plot( pve, xlim=c(0,40), type='b', pch=16, xlab='number of components', 
ylab='percent of total variation' )
# 98.626192582    0.969705229    0.279324276    0.114429868    0.006460911 
0.002624591
#only the first dimension is effective
#we use the third attribute in the endpoints
set.seed(0)

Training=createDataPartition(endpoints[, 3], p = 0.75, list= FALSE)

absorbtrain=absorp[Training,]
```

```
absorbtest=absorp[-Training,]

proteintrain =endpoints[ Training, 3]
proteintest = endpoints[-Training,3]


control = trainControl(method = "repeatedcv", repeats = 5)


#linear model
set.seed(1)
lm=train(x = absorbtrain, y = proteintrain, method = "lm", trControl =
trainControl(method = "repeatedcv", repeats = 5))
mean(proteintrain)

#rlm
rlm = train( x = absorbtrain, y = proteintrain, method="rlm",
preProcess=c("pca"), trControl=trainControl(method="repeatedcv",repeats=5) )

#pcr
set.seed(1)
PCR=train(x = absorbtrain, y = proteintrain,  method = "pcr",
preProcess=c("pca"),trControl = control, tuneLength = 25)
#pls
set.seed(1)
PLS=train(x = absorbtrain, y = proteintrain, method =
"pls",trControl=trainControl(method="repeatedcv",repeats=5), preProcess =
c("center", "scale"),tuneLength = 25)
#PCR

PCR <- train(x = absorbtrain, y = proteintrain,method = "pcr", trControl =
trainControl(method="repeatedcv",repeats=5), tuneLength = 25)

comps <- rbind(PLS$results, PCR$results)
comps$Model <- rep(c("PLS", "PCR"), each = 25)
a=comps[1:25,1:6]
b=comps[26:50,1:6]

plot(a$ncomp,a$RMSE,col="blue",type="l")
par(new=TRUE)
plot(b$ncomp,b$RMSE,col="red",type="l")
legend(col=c("red","blue"))
set.seed(1)
#enet
```

```
ENet = train(x = absorbtrain, y = proteintrain,method = "enet",trControl = trainControl(method="repeatedcv",repeats=5), preProcess = c("center", "scale"),tuneGrid = expand.grid(lambda = c(0, .001, .01, .1, 1), fraction = seq(0.05, 1, length = 20)))
plot(ENet)
```

Q2

```
library(caret)
library(AppliedPredictiveModeling)
data(permeability)


zero = nearZeroVar( fingerprints )
fingerprintsnonzero = fingerprints[,-zero]

Training = createDataPartition( permeability, p=0.75 )
fingerprintstrain = fingerprintsnonzero [Training$Resample1,]
permeabilitytrain =permeability[Training$Resample1,]

fingerprintstest=fingerprintsnonzero [-Training$Resample1,]
permeabilitytest=permeability[-Training$Resample1,]

hist(permeabilitytrain,breaks=50)
hist(log2(permeabilitytrain),breaks=50)
set.seed(3)
control=trainControl(method = "LGOCV")
plsTune =train(x = fingerprintstrain, y =log10(permeabilitytrain) , method = "pls",tuneGrid = expand.grid(ncomp = 1:15),trControl = control)
plsTune

ypredict = predict( plsTune, newdata=fingerprintstest )
rsquared_pls = cor(ypredict,permeabilitytest,method="pearson")^2


set.seed(3)
lm = train( fingerprintstrain, permeabilitytrain, method="lm", preProcess=c("center","scale"),
trControl=trainControl(method="repeatedcv",repeats=5) )
ypredict_lm = predict( lm, newdata=fingerprintstest )
r2_lm = cor(ypredict_lm,permeabilitytest,method="pearson")^2
```

```
set.seed(3)
rlm = train( fingerprintstrain, permeabilitytrain, method="rlm", preProcess=c("pca"), trControl=trainControl(method="repeatedcv",repeats=5) )
ypredict_rlm = predict( rlm, newdata=fingerprintstest )
r2_rlm = cor(ypredict_rlm,permeabilitytest,method="pearson")^2



set.seed(3)
PCR=train(fingerprintstrain, permeabilitytrain, method = "pcr", preProcess=c("pca"),trControl = control, tuneLength = 25)

set.seed(3)

enet = train( fingerprintstrain, permeabilitytrain, method="enet", tuneGrid = expand.grid(lambda = c(0, .05, .1), fraction = seq(0.05, 1, length = 20)), trControl=trainControl(method="repeatedcv",repeats=5) )
plot(enet)
```