Prediction with Linear Modelling

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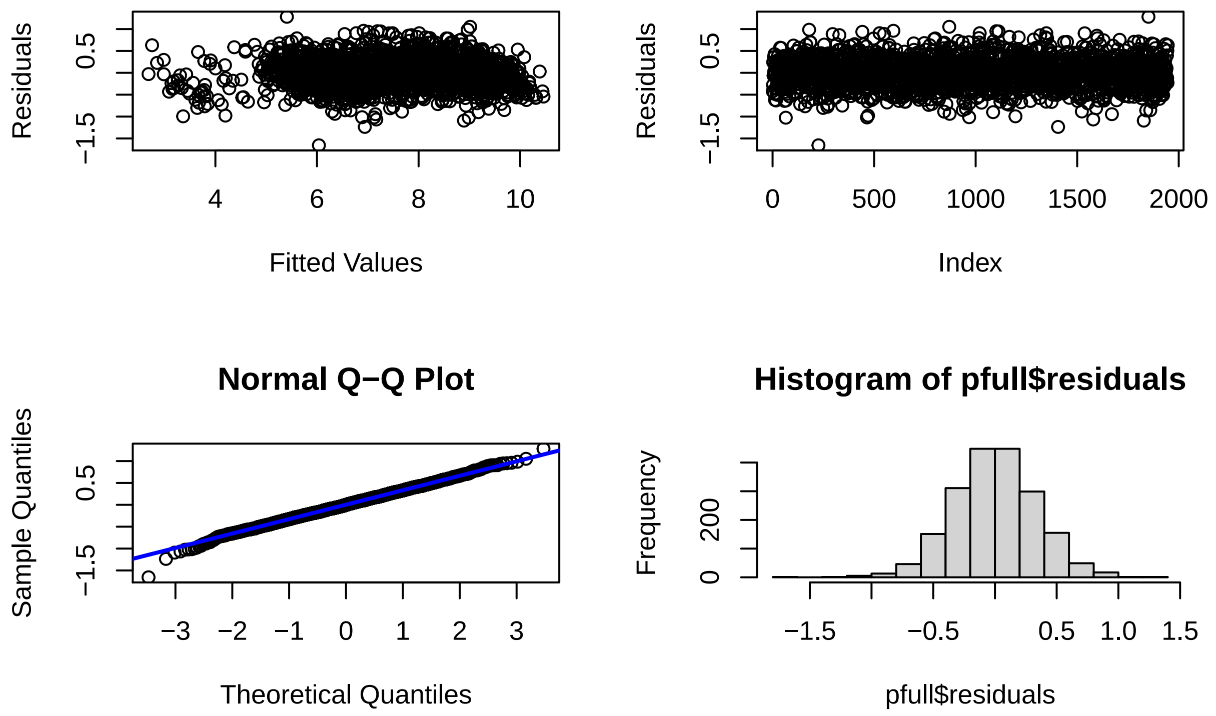
Summary

Ever since computers were invented, scientists have tried to predict the 3-D structures of proteins based on their amino acid sequences coded by the underlying DNA: this is often referred to as the famous "protein folding problem". Proteins carry out vital functions in our bodies, from blood transport (hemoglobin) to digestion (pepsin). On the other hand, proteins also play a key role allowing disease-causing viruses to be infectious. I will look at a subset of data from a specific spike protein associated with COVID-19, that enables the virus to attack human cells. Much research around the world has been devoted to better understanding this protein in the past 10 months. The file protein-train.csv contains 1946 samples of computer-generated structures for the COVID-19 spike protein. The response variable of interest is accuracy, which is a measure of how close that computer-generated structure is to a known benchmark structure. There are 685 explanatory variables.

The objective of my analysis is to construct the best possible fitted model to predict accuracy from these variables based on the 1946 observations of computer-generated structures for the Covid-19 protein. I decided to start off by constructing the full multiple linear regression model with all the predictors. I then decided to remove multicollinearity from the 685 predictors in protein-train.csv. I assessed regression model assumptions, and addressed outliers, then tested different model selection methods on a single train/validation set. Looking back, I should have utilized regularization methods like LASSO or ridge regression that can deal with multicollinearity and variable selection. I considered forwards selection, backwards selection, and forwards/backwards selection, with both Akaike information criterion (AIC) and Bayesian information criterion (BIC). I also considered Iterative conditional minimization (ICM) as a selection method, with AIC and BIC, and a harsher penalty than BIC. I then chose the best candidates and cross validated them, and found the best model selection method, which I then applied on the full data set in order to get the final model. I then assessed multiple linear regression assumptions for my final model. Finally, I used my final model to predict the values of the response variables of protein-test.csv. I found in my main results that forward selection with AIC as criteria had the lowest average root mean squared error (RMSPE), after cross validation, and so the model constructed with forward selection with AIC criteria would be my final model.

Exploratory analysis of dataset



In the data, there are 1946 observations and 685 predictors with 1 response. I observed that in the data, there are no categorical predictors, and that there are cases of perfect multicollinearity, indicating I should remove those predictors. In order to take a closer look at the data, I decided to construct a full multiple linear regression model based on all the observations and predictors given, and plot the residuals. In the residuals vs fitted values, we see that the data is randomly scattered around y=0, indicating the independence assumption is satisfied. We see that since the data was generated in temporal order, we also look at the residuals vs index plot, which also satisfies model assumptions. From the histogram and QQ plot of the residuals, we see that the normality assumption is also satisfied. The R squared value of the model is 0.9482963, which is very large and either indicates the full model is very accurate at predicting or overfitting. So we have an idea on reducing predictors to get a better model for prediction.

Methods

In order to remove multicollinearity from the data, I used the vif function from the "faraway" package in order to determine the variance inflation factor (VIF) of each predictor and I then used the method of removing the predictor with the largest VIF in a while loop until the largest VIF was less than 10.

In order to determine whether or not I should use a model transformation, I examined residual plots (residuals vs fitted values, residuals vs index, as well as the QQ plot and histogram of residuals). I did not look at residuals vs predictors since there are too many. Since the residual plots did not reveal any problems with assumptions, I decided not to use any transformations with my multiple linear regression model.

I also considered the effects of individual observations on my fitted multiple linear regression model. I recorded the studentized residuals, leverages and Cook's distances for my model (after removing multicollinearity). I then plotted studentized residuals vs fitted values, and noted the observations that lay outside of 3 standard deviations. I also plotted the leverages and noted the leverages greater than twice the average. Then, to put it together, I looked at a plot of the Cook's distances. Cook's distances of > 0.5 are generally considered outliers. Thus, I found no outliers in the data. However, I would like to note that I used 0.5 as a cutoff point since it is the one used in the lectures, but some other general rule of thumb cutoff points are 4/(number of observations), or 4/(number of observations - number of predictors - 1). When testing the latter cutoff point, I got around 200 outliers. Due to time constraints, I decided not to test its impact on prediction in a train/validation split, but I would have if time was not an issue.

Now that I removed multicollinearity and considered the effects of individual observations, I began to consider different model selection strategies.

I noted that since there were more than 500 predictors even after removing multicollinearity, it was too difficult to do an all possible regressions search. Thus I started off with a single train/validation split (80/20) and tested out each of forward/backward/forward-backward selections with both AIC and BIC as criteria. I then also tested ICM with BIC and AIC as criteria. Additionally, I tested out ICM with a harsher penalty of 2 * BIC's. I narrowed down to a few model selection methods by comparing the root mean squared error for train and validation from each model selection method. I noticed that backward selection took much longer than forward selection or forward/backward selection and ICM was the fastest. AIC was also generally slower than BIC.

I cross validated the final candidates with $K = 5$ folds. I compared the average of each model's root mean square error (RMSE) to find the lowest in order to determine the best procedure/selection method. To get my final model, I applied this method on the full dataset. Using this final model, I predicted the response values of protein-test.csv.

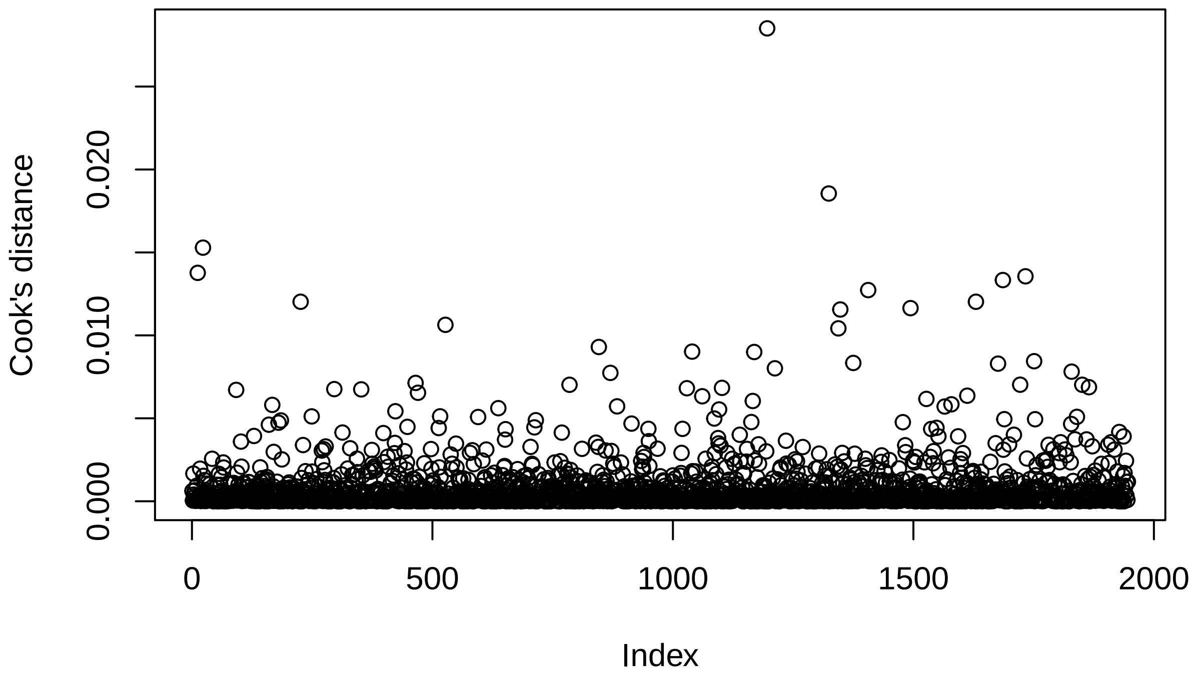
Results and discussion

Results of removing multicollinearity

After removing multicollinearity, I ended up with 551 predictors, so a total of 134 predictors were removed to get rid of multicollinearity.

Results of assessing the effects of individual observations

Using a Cook's distance cutoff point of 0.5, I observed 0 outliers in the data.



As seen in the plot, there are no points higher than y = 0.5.

Results of model selection

During my single train/validation split, I tested a total of 9 selection methods. Forward/backward/forward-backward, each with both AIC and BIC criteria, and ICM with AIC, BIC and a 2*BIC penalty. I recorded the train RMSE and validation RMSE for each model constructed with each of the 9 methods.

Selection method	Train RSME	Validation RMSE	AIC/BIC
Forward with AIC	0.4101569	0.6022125	2151.3292283
Backward with AIC	0.3987215	0.6339674	2109.2762061
Forward-backward with AIC	0.4115107	0.6168919	2123.5912774
Forward with BIC	0.5195751	0.6122045	2982.4444807
Backward with BIC	0.4872484	0.6298803	2988.2240144
Forward-backward BIC	0.5158826	0.6404971	2967.5852432
ICM with AIC	0.4030746	0.4512895	2103.0893615
ICM with BIC	0.5132434	0.5708434	2929.5618959
ICM with 2*BIC penalty	0.5943295	0.5708434	
Full model	0.380513	0.6227402	

Firstly, I see that both BIC and AIC values are lowest when I used ICM, with AIC/BIC when compared to the stepwise methods.

Since train RMSE can be made arbitrarily small by adding linearly independent predictors, we mainly care about the lowest validation RMSE, as long as they are approximately equal.

Since this is only a single train/validation split, I use this data to help me narrow down a few candidates for K fold cross validation.

I will note here that I tested out the ICM methods multiple times, and I got varying RMSE's for both train and validation. Sometimes they were better than the stepwise methods and sometimes they were worse, indicating a level of variability that I tested further with cross validation.

We can see that the validation RMSE is lower in forward with AIC(253 predictors) than the full model, which means the full model(551 predictors) is overfitting, so my exploratory analysis was correct in predicting we should get rid of some predictors. The stepwise methods with BIC as criteria yielded models with around 80 predictors, and had higher RMSE than forward with AIC, so I concluded they were underfitting.

With these results, I conclude that I should cross validate forward with AIC, forward with BIC, ICM with AIC and ICM with BIC to further evaluate selection strategies.

I decided on cross validation with 5 folds. If I had more time, I would have liked to use more folds.

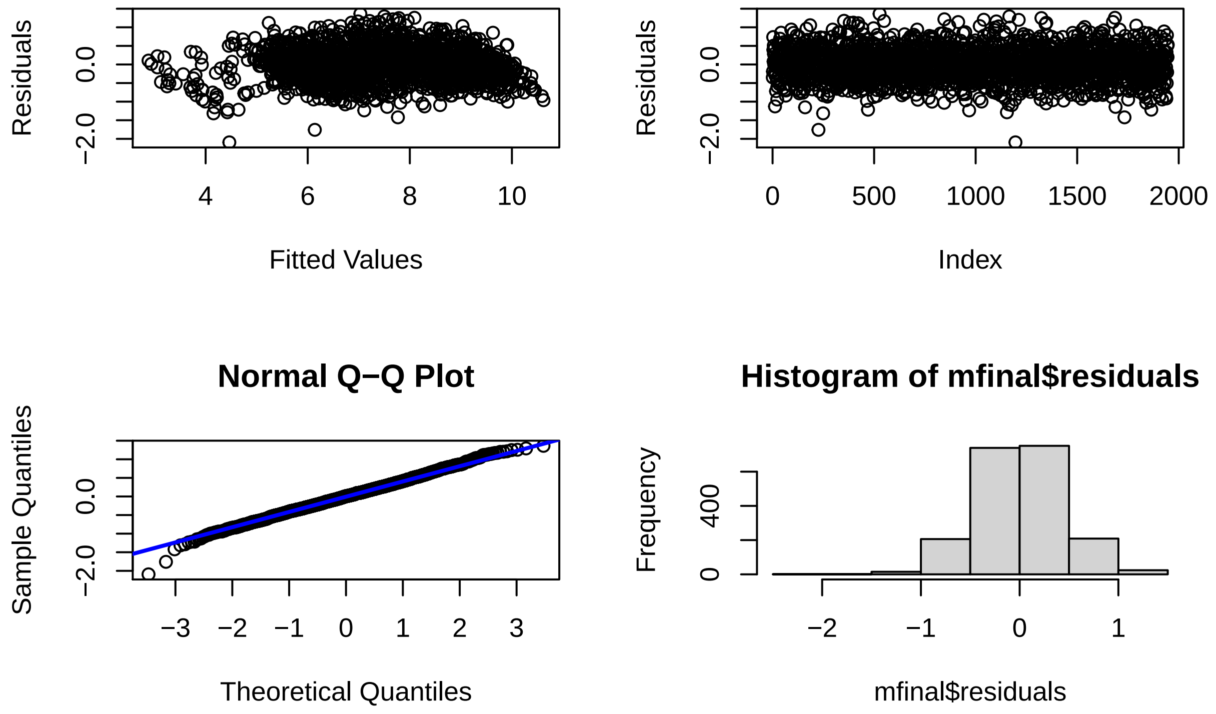
The results of cross validation are

Selection method	Average RMSE (RMSPE)
Forward AIC	0.6054771
ICM AIC	0.6093815
Forward BIC	0.6409394
ICM BIC	0.6251201

Thus I can conclude that the model constructed with forward with AIC has the lowest

RMSPE and so I can conclude that it is the best model selection method for prediction. I then apply this selection method to the entire data set to get my final model.

My final model selection method evaluated 112158 models before finishing. The R squared value for my final model is 0.9159083, and my final model has 267 predictors and 1 response. A full list of these predictors can be found in the appendix. The regression coefficient for the first 3 predictors are 0.033416, -0.097572 , and -0.052900. They are all statistically significant since the corresponding p-values are much less than 0.005. (< 1.51e-05)



Overall my final model fits the data very well. All the regression assumptions are reasonably satisfied by my final model. In the residuals vs fitted values and residuals vs index plot,the points are randomly scattered around y=0. In the QQplot and histogram, normality seems to be satisfied.

I would predict the MSPE to be 0.3666026, if I applied the fitted model on new data. I am fairly confident my model should generalize well to doing prediction on new data since my model selection strategy yielded the lowest MSPE with cross validation, but since I only cross validated with 5 folds, I know I'm not as confident as I could be. If I had more time I would try 10 or even more folds.

Some interesting findings are that I noticed ICM with AIC sometimes yielded lower RMSE's than forward selection with AIC, but there was more variability, so the average RMSE was still lower. In addition, my final model did not include angles, a predictor that represents a score based on the configuration of angles in the computer generated structure of each

Covid-19 spike protein.

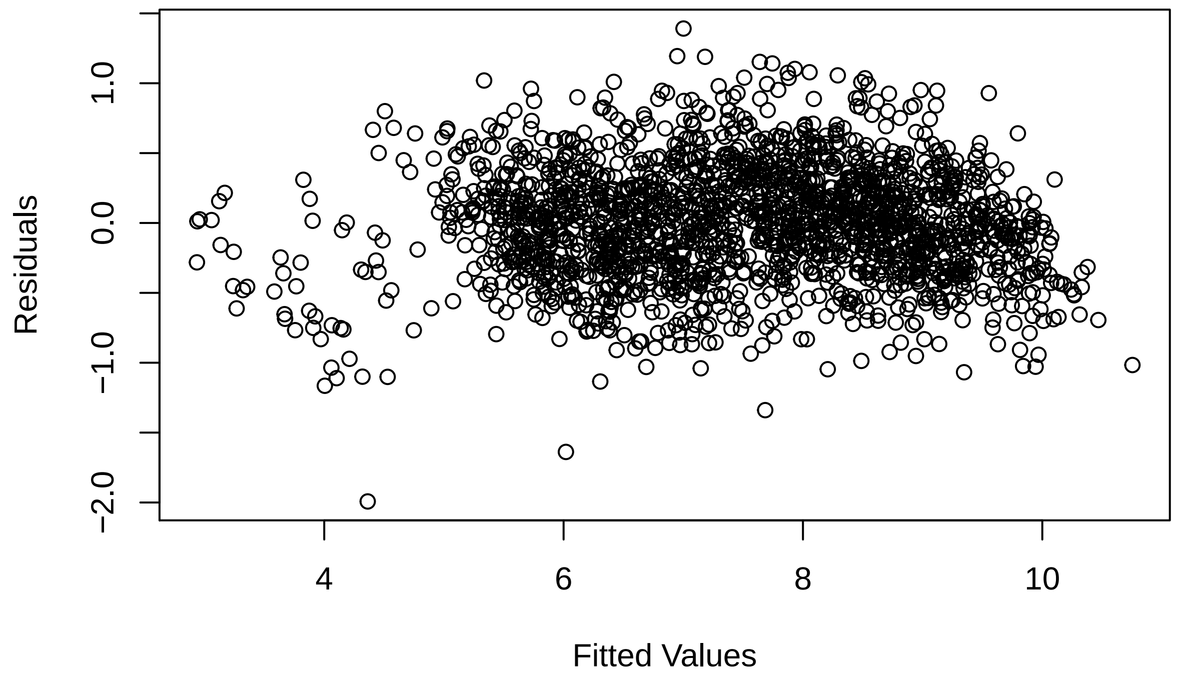
Appendix

```r
# Detect and remove multicollinearity / commented since I saved after running

library("faraway")
```

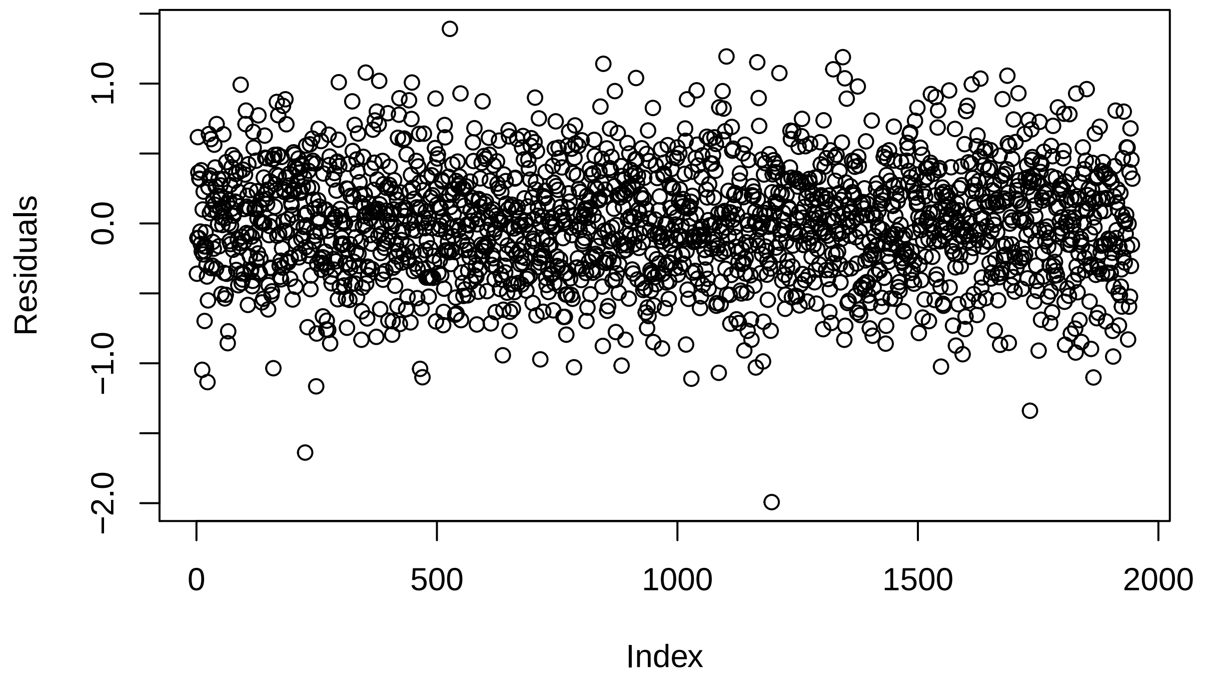
```
## Warning: package 'faraway' was built under R version 4.0.3
```

```r
ptrain <- read.csv ("protein-train.csv")

i <- 0
pred <- c()

# full model
pfull <- lm(accuracy ~ .,data = ptrain)

# vector of VIF's of predictors
# npred <- vif(pfull)
# vifpred <- unname(npred)

# copy of full model
ctrain <- ptrain[]

load("ptrain")

# # while the largest VIF >= 10
# while(max(vifpred) >= 10)
# {
#
#   # find the index of the max VIF
#   j <- which.max(vifpred) + 1
#   ptrain <- ptrain[,-j]
#   # vifpred only includes the predictors (685) while ptrain has the
#   # response as well (686), so we add 1 to j
#
#
#   premov <- lm(accuracy ~ .,data = ptrain) # fit new model without predictor
#   # with largest VIF
#
#   npred <- vif(premov)
#   vifpred <- unname(npred) # find new vector of VIF's and loop until
#   # every VIF is less than 10
#
#
#   i <- i + 1 # count of how many predictors removed
#
# }
load("premov")
```

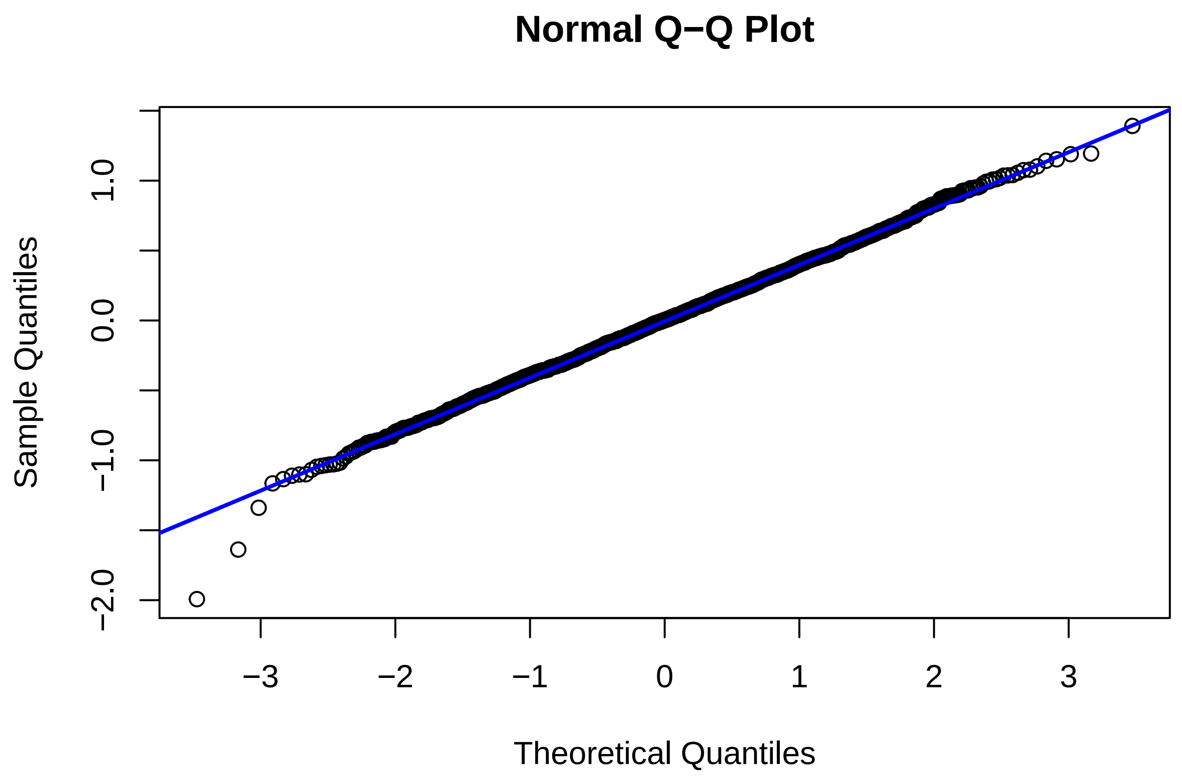
```
# after removing multicollinearity, we assess model linear regression
# assumptions

#summary(premov)
plot(premov$fitted.values, premov$residuals, xlab = "Fitted Values",
     ylab = "Residuals")
```



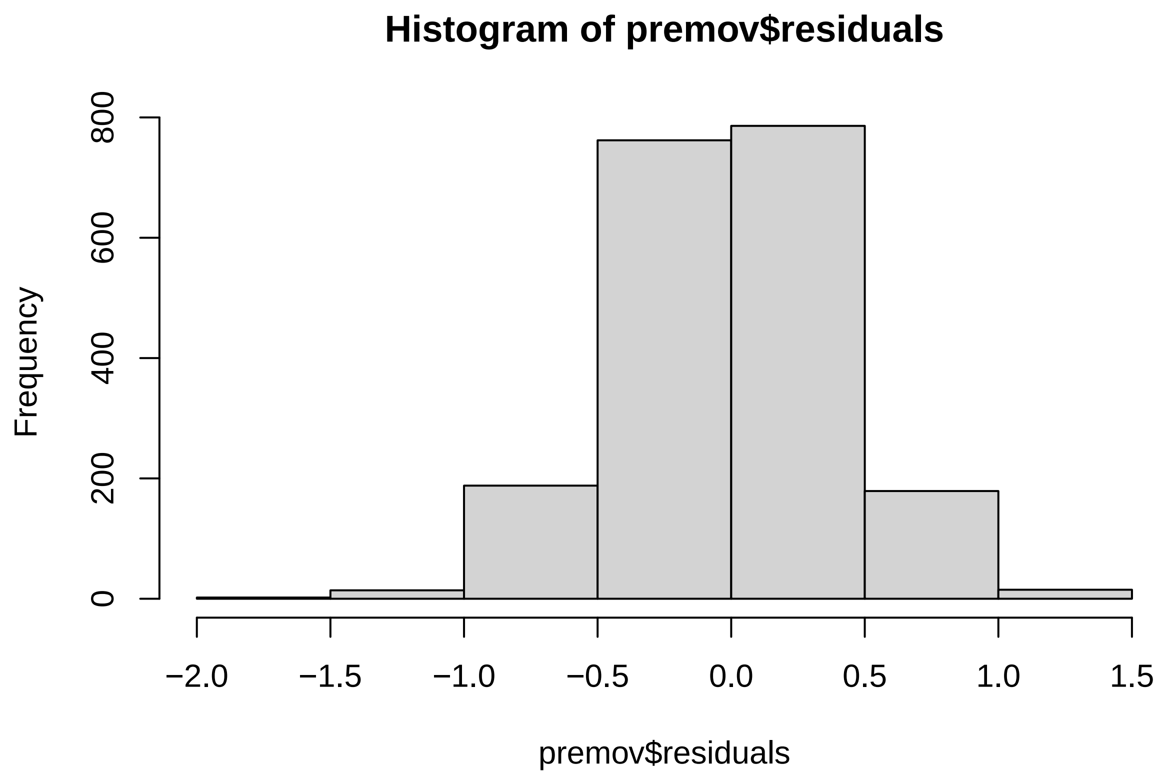
```
plot (1: nrow (ptrain), premov$residuals , xlab = " Index ", ylab =
        " Residuals ")
```



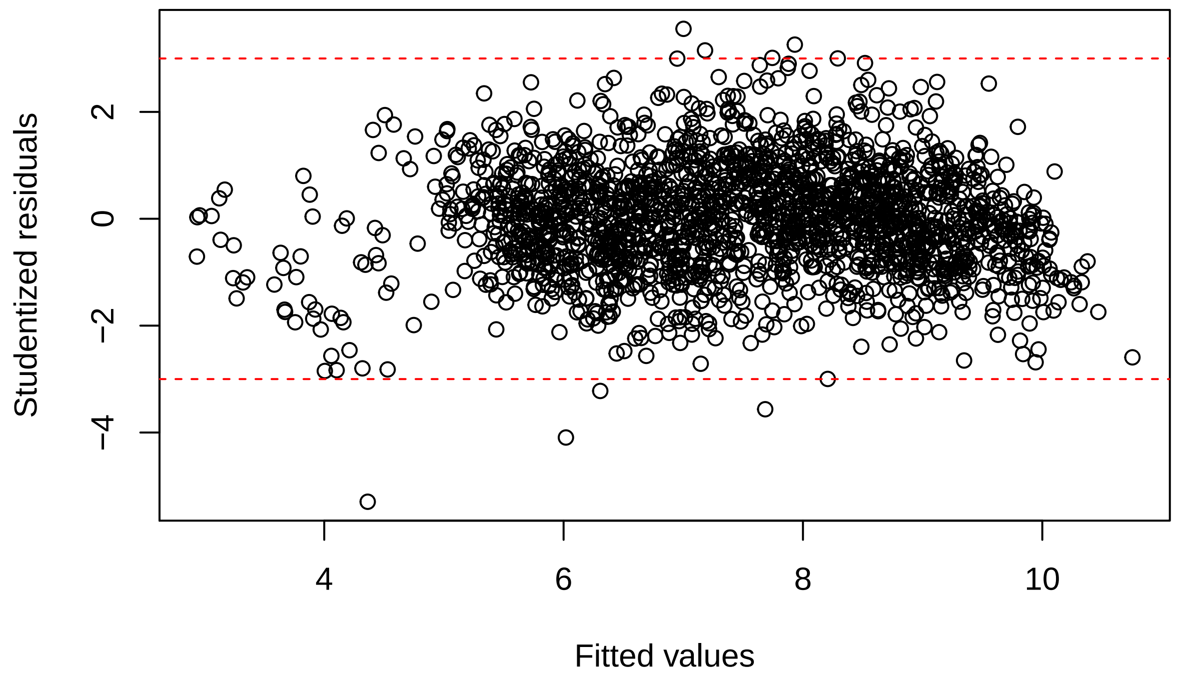
```r
qqnorm(premov$residuals)
qqline(premov$residuals, col="blue", lwd = 2)
```



```r
hist(premov$residuals)
```



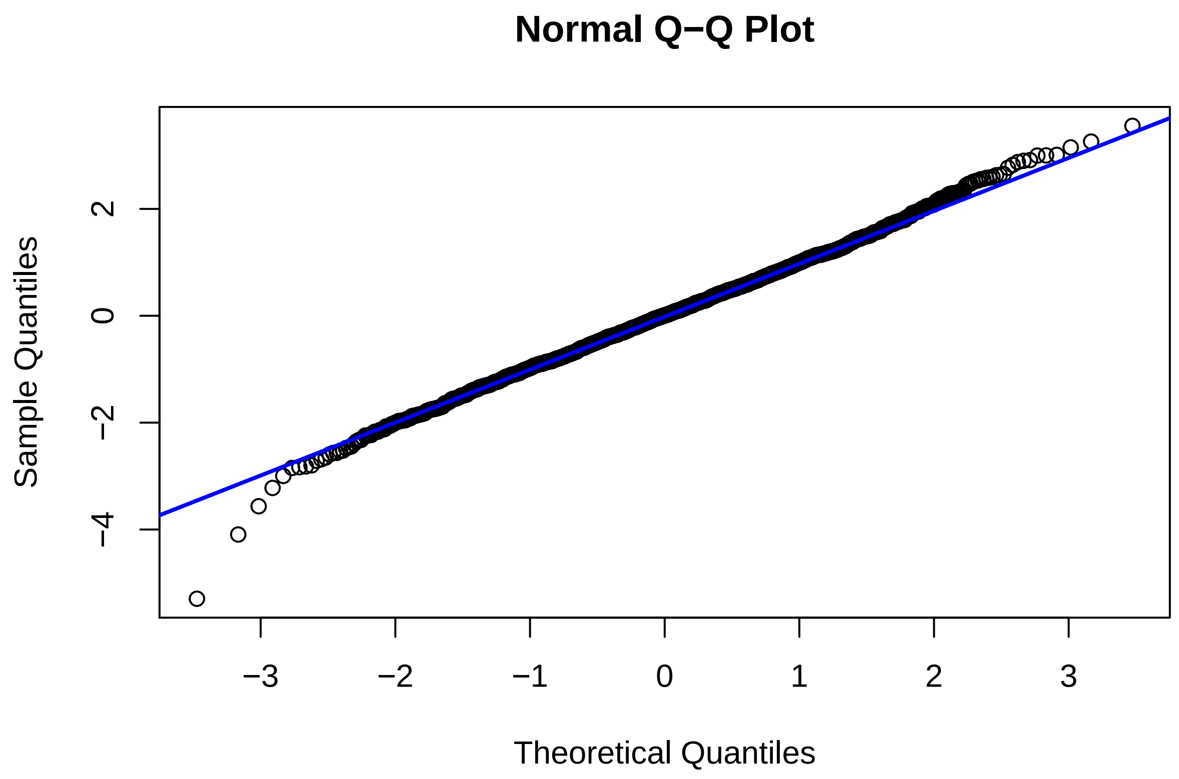
```
library(MASS)

# quantities for individual observations
sres <- studres(premov) # studentized residuals
lev <- hatvalues(premov) # leverage
cd <- cooks.distance(premov) # Cook's distance


# plot of studentized residuals vs fitted values
plot(premov$fitted.values, sres, xlab = "Fitted values",
     ylab = "Studentized residuals")
# plots look the same
abline(h = c(3,-3), col = "red", lty=2) # lie within 3 standard deviations
```



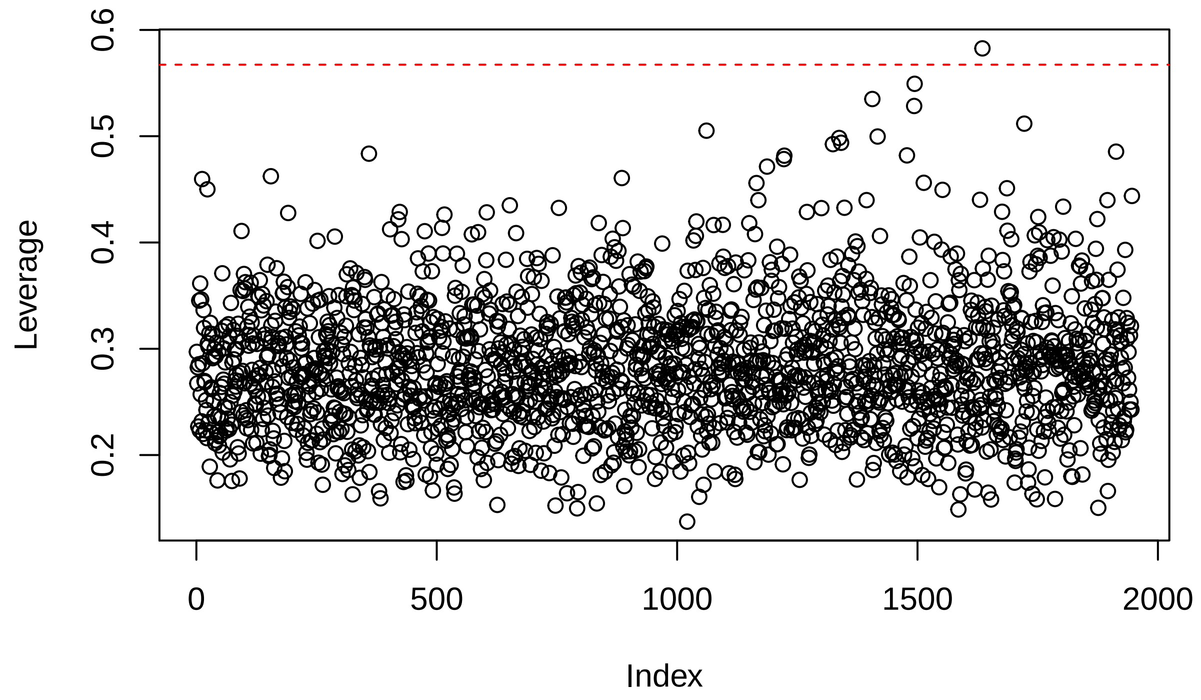
```r
# of 0
which(abs(sres) > 3) # find the observations that don't lie within 3
```

```
##   23  226  527  846 1196 1324 1344 1686 1733
##   23  226  527  846 1196 1324 1344 1686 1733
```

```r
# standard deviations
#   23  226  527  846 1196 1324 1344 1686 1733
qqnorm(sres)
qqline(sres, col = "blue", lwd = 2)
```



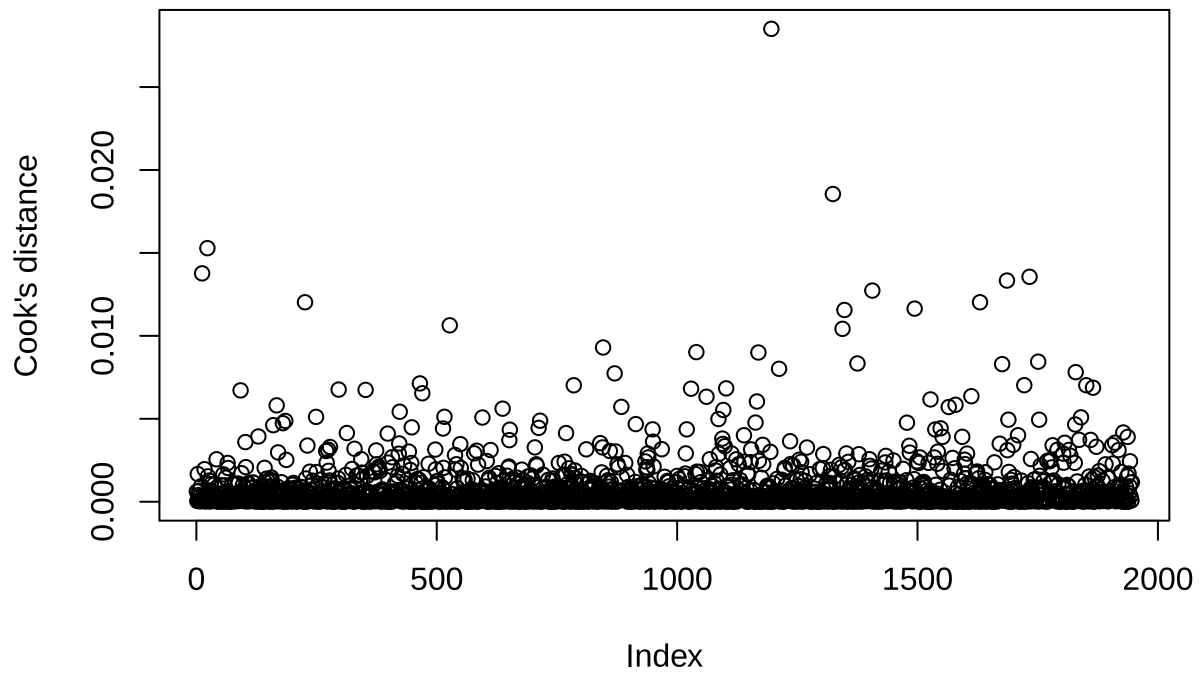
```r
#leverage

plot(lev, ylab = "Leverage")
abline(h = 2 * mean(lev), col = "red", lty = 2) # leverages twice than average
```



```
# leverage are considered high
which(lev > 2 * mean(lev)) # 1635
```

```
## 1635
## 1635
```

```
# Cook's distance

plot(cd, ylab = "Cook's distance")
abline(h = 0.5, col = "red", lty = 2)
```



```
 h <- unname(which(cd > 0.5))
# Cook's distance greater than 0.5 is generally considered large
# Thus, there are no outliers
# Other rules of thumb are 4/n, and 4/n-k-1

 otrain <- ptrain[-h,]
 new <- lm(accuracy ~ .,data = ptrain)
# summary(new)
```

```
# Check model regression assumptions after outliers removed

# plot(new$fitted.values, new$residuals, xlab = "Fitted Values",
#      ylab = "Residuals")
# qqnorm(new$residuals)
# qqline(new$residuals, col="blue", lwd = 2)
# hist(new$residuals)
```

```
# First we test out different model selection methods with a single
# train/validation split.

library(MASS)
```

```
N <- nrow(ptrain)
set.seed(20688307)

trainInd <- sample(1: N ,round(N*0.8) ,replace = F)
# 80/20 train/validation split
trainSet <- ptrain[trainInd ,]
validSet <- ptrain[-trainInd ,]

full <- lm(accuracy ~ ., data = trainSet)
empty <- lm(accuracy ~ 1, data = trainSet)

# stepwise forward with aic

load("m_aicf")

#m_aicf <- stepAIC(object = empty, scope = list(upper = full, lower = empty), directio



# stepwise backward with aic

load("m_aicb")

#m_aicb <- stepAIC(object = full, scope = list(upper = full, lower = empty), direction



# stepwise forward/backward with aic

load("m_aich")

#m_aich <- stepAIC(object = empty, scope = list(upper = full, lower = empty), directio
#= "both")



# stepwise forward with bic

load("m_bicf")

#m_bicf <- stepAIC(object = empty, scope = list(upper = full, lower = empty), directio
```

```r
# stepwise backward with bic

load("m_bicb")

#m_bicb <- stepAIC(object = full, scope = list(upper = full, lower = empty), direction



#stepwise forward-backward with bic

load("m_bich")

#m_bich <- stepAIC(object = empty, scope = list(upper = full, lower = empty), directio
```

```r
# We calculate the RMSE on train and validation for each model


# Full model (after removing multicollinearity)

 predfull <- predict(full, newdata = validSet)
 fullv <- sqrt(mean((validSet$accuracy - predfull)^2)) #RMSE for validation
 fullt <- sqrt(mean(full$residuals^2)) # RMSE for train




# AIC-forward selection

 predaf <- predict(m_aicf, newdata = validSet)
 aicfv <- sqrt(mean((validSet$accuracy - predaf)^2))
 aicft <- sqrt(mean(m_aicf$residuals ^2))

 faic <- AIC(m_aicf)

# AIC-backward selection

 predab <- predict(m_aicb, newdata = validSet)
 aicbv <- sqrt(mean((validSet$accuracy - predab)^2))
 aicbt <- sqrt(mean(m_aicb$residuals^2))

 baic <- AIC(m_aicb)

# AIC-forward/backward selection

 predah <- predict(m_aich, newdata = validSet)
 aichv <- sqrt(mean((validSet$accuracy - predah )^2))
 aicht <- sqrt(mean(m_aich$residuals ^2))

 haic <- AIC(m_aich)

# BIC-forward selection

 predbf <- predict (m_bicf , newdata = validSet)
 bicfv <- sqrt(mean((validSet$accuracy - predbf )^2))
 bicft <- sqrt(mean(m_bicf$residuals^2))

 fbic <- BIC(m_bicf)

# BIC-backward selection

 predbb <- predict(m_bicb, newdata = validSet)
 bicbv <- sqrt(mean((validSet$accuracy - predbb)^2))
 bicbt <- sqrt(mean(m_bicb$residuals^2))

 bbic <- BIC(m_bicb)


# BIC-forward/backward selection

 predbh <- predict(m_bich, newdata = validSet)
 bichv <- sqrt(mean((validSet$accuracy - predbh)^2))
 bicht <- sqrt(mean(m_bich$residuals ^2))

 hbic <- BIC(m_bich)
```

```
#ICM with no penalty (AIC)
library(MASS)

N <- nrow(ptrain)

load("m_bestA")

#set.seed(20688307)

# trainInd <- sample(1: N ,round(N*0.8) ,replace = F)
# # 80/20 train/validation split
# trainSet <- ptrain[trainInd ,]
# validSet <- ptrain[-trainInd ,]
#
```

```
# full <- lm(accuracy ~ ., data = trainSet)
# empty <- lm(accuracy ~ 1, data = trainSet)
#
# varlist = c()
# varnames = names(trainSet)
# n = nrow(trainSet)
# varoder <- sample(1:ncol(trainSet)) #random order of variables
# minCrit = Inf
# noChange = F
#
# while(!noChange) {
#   noChange = T
#   for (i in varoder) {
#     if (i == 1)
#       next
#
#     if (i %in% varlist & length(varlist) > 1) {
#       index = c(1, varlist[varlist != i])
#     trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit) < minCrit) {
#           minCrit = AIC (fit)
#           varlist = varlist[varlist != i]
#           #print(paste0(" Criterion : ", round(minCrit, 1) , ", variables : ",
#             #           paste0 (varnames[varlist], collapse = " ")))
#           bestA_model = fit
#           noChange = F
#       }
#
#     }  else if  (!i %in% varlist) {
#       index = c(1, varlist, i)
#       trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit) < minCrit) {
#           minCrit = AIC(fit)
#           varlist = c(varlist, i)
#          # print(paste0(" Criterion : ", round(minCrit, 1), ", variables : ",
#                     #  paste0(varnames[varlist], collapse = " ")))
#
#           bestA_model = fit
#            noChange = F
#         }
#      }
#   }
# }
```

```
# ICM with BIC penalty
library(MASS)

N <- nrow(ptrain)
#set.seed(20688307) different AIC each time without seed

load("m_bestB")

# trainInd <- sample(1: N ,round(N*0.8) ,replace = F)
# # 80/20 train/validation split
# trainSet <- ptrain[trainInd ,]
# validSet <- ptrain[-trainInd ,]
#
# full <- lm(accuracy ~ ., data = trainSet)
# empty <- lm(accuracy ~ 1, data = trainSet)
#
# pen <- log (nrow (trainSet))
# varlist = c()
# varnames = names(trainSet)
# n = nrow(trainSet)
# varoder <- sample(1:ncol(trainSet)) #random order of variables
# minCrit = Inf
# noChange = F
#
# while(!noChange) {
#   noChange = T
#   for (i in varoder) {
#     if (i == 1)
#       next
#
#     if (i %in% varlist & length(varlist) > 1) {
#       index = c(1, varlist[varlist != i])
#     trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit, k=pen) < minCrit) {
#           minCrit = AIC (fit, k = pen)
#             varlist = varlist[varlist!= i]
#           #  print(paste0(" Criterion : ", round(minCrit, 1) , ", variables : ",
#           #                paste0 (varnames[varlist], collapse = " ")))
#             bestB_model = fit
#             noChange = F
#         }
#
#     }  else if  (!i %in% varlist) {
#         index = c(1, varlist, i)
#         trainVars = trainSet[, index]
#
#         fit = lm(accuracy ~ ., data = trainVars)
#
#         if (AIC(fit, k = pen) < minCrit) {
#             minCrit = AIC(fit, k = pen)
#             varlist = c(varlist, i)
#           #  print(paste0(" Criterion : ", round(minCrit, 1), ", variables : ",
#                   #     paste0(varnames[varlist], collapse = " ")))
#
#             bestB_model = fit
#             noChange = F
#          }
#     }
#   }
# }
```

```
# ICM with 2*BIC penalty
library(MASS)

N <- nrow(ptrain)
#set.seed(20688307) different AIC each time without seed

load("m_bestC")

# trainInd <- sample(1: N ,round(N*0.8) ,replace = F)
# # 80/20 train/validation split
# trainSet <- ptrain[trainInd ,]
# validSet <- ptrain[-trainInd ,]
#
# full <- lm(accuracy ~ ., data = trainSet)
# empty <- lm(accuracy ~ 1, data = trainSet)
#
# pen <- 2 * log (nrow (trainSet))
# varlist = c()
# varnames = names(trainSet)
# n = nrow(trainSet)
# varoder <- sample(1:ncol(trainSet)) #random order of variables
# minCrit = Inf
# noChange = F
#
# while(!noChange) {
#   noChange = T
#   for (i in varoder) {
#     if (i == 1)
#       next
#
#     if (i %in% varlist & length(varlist) > 1) {
#       index = c(1, varlist[varlist != i])
#     trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit, k=pen) < minCrit) {
#           minCrit = AIC (fit, k = pen)
#           varlist = varlist[varlist!= i]
#         #  print(paste0(" Criterion : ", round(minCrit, 1) , ", variables : ",
#         #               paste0 (varnames[varlist], collapse = " ")))
#           bestC_model = fit
#           noChange = F
#       }
#
#     }  else if  (!i %in% varlist) {
#       index = c(1, varlist, i)
#       trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit, k = pen) < minCrit) {
#           minCrit = AIC(fit, k = pen)
#           varlist = c(varlist, i)
#         #  print(paste0(" Criterion : ", round(minCrit, 1), ", variables : ",
#                 #     paste0(varnames[varlist], collapse = " ")))
#
#           bestC_model = fit
#           noChange = F
#        }
#     }
#   }
# }
```

```
# ICM RMSE - we get varying RMSE's since different orderings for ICM
# Sometimes we get a higher RMSE, sometimes lower. So we can cross validate to
# check further.

# ICM - no penalty

 bestA <- predict(bestA_model, newdata = validSet)
 bestAv <- sqrt(mean((validSet$accuracy - bestA)^2))
 bestAt <- sqrt(mean(bestA_model$residuals ^2))

 bestaic <- AIC(bestA_model)


# ICM -BIC penalty

 bestB <- predict(bestB_model, newdata = validSet)
 bestBv <- sqrt(mean((validSet$accuracy - bestB)^2))
 bestBt <- sqrt(mean(bestB_model$residuals ^2))

 bestbic <- BIC(bestB_model)

 # ICM -2 * BIC penalty

 bestC <- predict(bestC_model, newdata = validSet)
 bestCv <- sqrt(mean((validSet$accuracy - bestC)^2))
 bestCt <- sqrt(mean(bestC_model$residuals ^2))
```

```
load("RMSE1")
load("RMSE2")
load("RMSE3")
load("RMSE4")

RMSPE1 <- mean(RMSE1)
RMSPE2 <- mean(RMSE2)
RMSPE3 <- mean(RMSE3)
RMSPE4 <- mean(RMSE4)


# Cross Validation to determine the best selection method
# library (MASS)
# N <- nrow(ptrain)
# set.seed(20688307)
```

```
#
# K<-5
#
# validSetSplits <- sample((1:N)%%K + 1)
# RMSE1 <- c()
# RMSE2 <- c()
# RMSE3 <- c()
# RMSE4 <- c()
#
# for (p in 1:K) {
#   validSet <- ptrain[validSetSplits == p ,]
#   trainSet <- ptrain[validSetSplits != p ,]
#
#   full <- lm (accuracy ~ . , data = trainSet)
#   empty <- lm (accuracy ~ 1 , data = trainSet)
#
#
# m1 <- stepAIC(object = empty, scope = list(upper = full, lower = empty), direction =
#
# pred1 <- predict( m1, newdata = validSet)
# RMSE1[p] <- sqrt(mean((validSet$accuracy - pred1)^2))
#
#
#
# varlist = c()
# varnames = names(trainSet)
# n = nrow(trainSet)
# varoder <- sample(1:ncol(trainSet)) #random order of variables
# minCrit = Inf
# noChange = F
#
# while(!noChange) {
#   noChange = T
#   for (i in varoder) {
#     if (i == 1)
#       next
#
#     if (i %in% varlist & length(varlist) > 1) {
#       index = c(1, varlist[varlist != i])
#     trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit) < minCrit) {
```

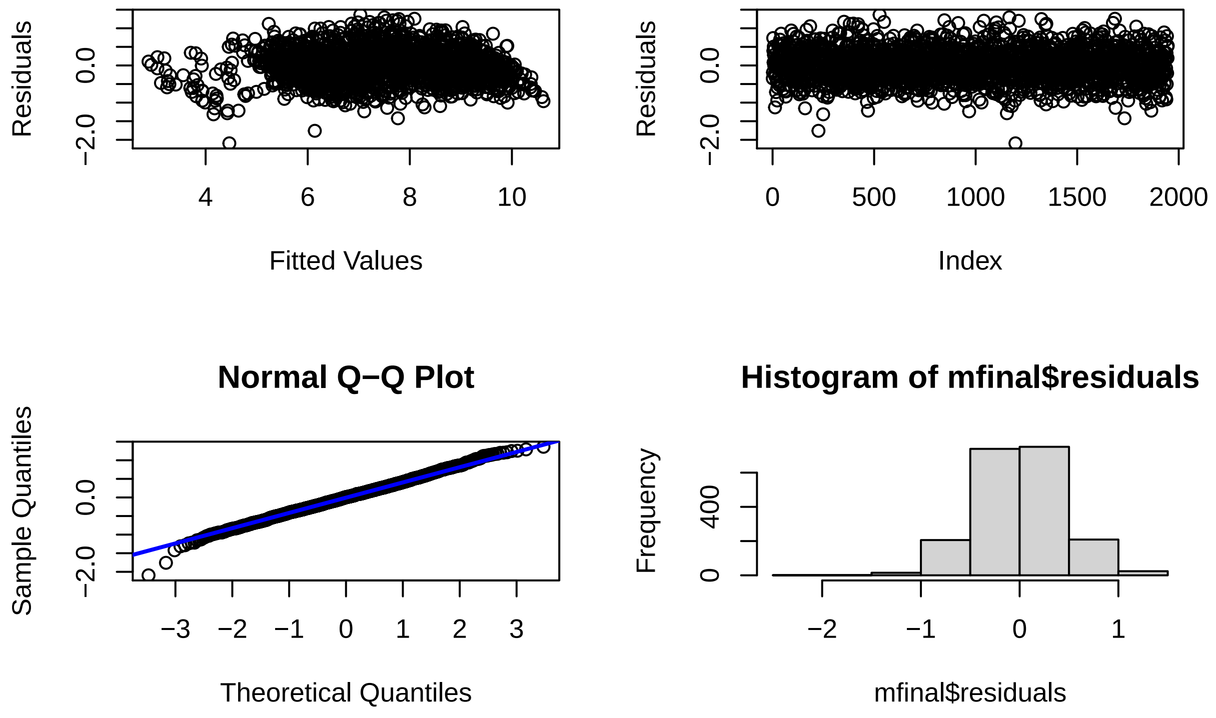
```
#            minCrit = AIC (fit)
#            varlist = varlist[varlist != i]
#            #print(paste0(" Criterion : ", round(minCrit, 1) , ", variables : ",
#                         #paste0 (varnames[varlist], collapse = " ")))
#            m2 = fit
#            noChange = F
#        }
#
#     }  else if  (!i %in% varlist) {
#        index = c(1, varlist, i)
#        trainVars = trainSet[, index]
#
#        fit = lm(accuracy ~ ., data = trainVars)
#
#        if (AIC(fit) < minCrit) {
#            minCrit = AIC(fit)
#            varlist = c(varlist, i)
#           # print(paste0(" Criterion : ", round(minCrit, 1), ", variables : ",
#                    #   paste0(varnames[varlist], collapse = " ")))
#
#             m2 = fit
#             noChange = F
#          }
#       }
#     }
# }
#
#  pred2 <- predict(m2 ,newdata = validSet)
#  RMSE2[p] <- sqrt(mean((validSet$accuracy - pred2)^2))
#
#
#
#
#  m3 <- stepAIC(object = empty, scope = list(upper = full, lower = empty), direction
#  pred3 <- predict(m3 , newdata = validSet )
#  RMSE3[p] <- sqrt(mean(( validSet$accuracy - pred3)^2))
#
#
#
#
# pen <- log (nrow (trainSet))
# varlist = c()
# varnames = names(trainSet)
# n = nrow(trainSet)
# varoder <- sample(1:ncol(trainSet)) #random order of variables
# minCrit = Inf
# noChange = F
#
# while(!noChange) {
#   noChange = T
#   for (z in varoder) {
#     if (z == 1)
#       next
#
#     if (z %in% varlist & length(varlist) > 1) {
#       index = c(1, varlist[varlist != z])
#     trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit, k=pen) < minCrit) {
#           minCrit = AIC (fit, k = pen)
#           varlist = varlist[varlist!= z]
#           #print(paste0(" Criterion : ", round(minCrit, 1) , ", variables : ",
#                         #paste0 (varnames[varlist], collapse = " ")))
#           m4 = fit
#           noChange = F
#       }
#
#     }  else if  (!z %in% varlist) {
#       index = c(1, varlist, z)
#       trainVars = trainSet[, index]
#
#       fit = lm(accuracy ~ ., data = trainVars)
#
#       if (AIC(fit, k = pen) < minCrit) {
#           minCrit = AIC(fit, k = pen)
#           varlist = c(varlist, z)
#          # print(paste0(" Criterion : ", round(minCrit, 1), ", variables : ",
#                       #paste0(varnames[varlist], collapse = " ")))
#
#           m4 = fit
#           noChange = F
#        }
#     }
#   }
# }
#
```

```
# pred4 <- predict(m4, newdata = validSet)
# RMSE4[p] <- sqrt(mean((validSet$accuracy - pred4)^2))
#
#
# }
#
#
```

```
# We apply selected procedure to the full dataset

load("mfinal")

# full <- lm(accuracy ~ ., data = ptrain)
# empty <- lm(accuracy ~ 1, data = ptrain)
#
# mfinal <- stepAIC(object = empty, scope = list(upper = full, lower = empty), directi

mfinal$coefficients
```

```
##                 (Intercept)       aliph1HC_aliph2HC_long
##                 3.085736324                  0.033415822
##              scLysN_bbC_vlong        aliph2HC_bbN_medshort
##                -0.097572193                 -0.052900348
##  aliph1HC_aromaticC_medshort  aromaticC_hydroxylO_medlong
##                 0.110722520                 -0.039630202
##    carbonylC_aromaticC_short     aliph1HC_aromaticC_vlong
##                 0.110159934                  0.080347635
##                bbC_bbO_short       aliph1HC_aliph1HC_vlong
##                -0.027907824                  0.149503560
##        carboxylC_scLysN_vlong             sulfur_bbC_vlong
##                 0.041247792                 -0.017002155
##      aliph1HC_aromaticC_long     aromaticC_hydroxylO_long
##                 0.082598536                 -0.030726393
##         aliph2HC_scLysN_vlong           aliph3HC_bbC_vlong
##                 0.037928555                  0.010450667
##            aliph1HC_bbN_vlong                 bbN_bbO_long
##                -0.013684296                 -0.011956478
##            aliph2HC_bbN_vlong           sulfur_bbC_medlong
##                 0.001059020                 -0.063075774
##           carboxylO_bbC_vlong        aromaticC_sulfur_long
##                 0.024634615                  0.037697347
##   aliph1HC_aromaticC_medlong         aromaticC_scAGN_short
##                 0.070662023                  0.012264308
##             aliph1HC_bbO_long        aliph1HC_bbC_medshort
##              -0.080248036                  0.076676022
##     aliph2HC_aromaticC_vlong             scLysN_bbN_vlong
##               0.012469819                 -0.074743867
##           bbN_bbC_medshort                 bbO_bbO_short
##              -0.023752349                 -0.022324954
##        aliph1HC_sulfur_short           aliph3HC_bbN_short
##               0.198692224                  0.100834275
##         aliph1HC_bbO_medlong     aliph2HC_carboxylO_vlong
##              -0.126807275                 -0.009171958
##      aliph3HC_aliph3HC_short               scAGN_bbN_long
##               0.038660284                  0.034621603
##      aliph3HC_aromaticC_long         aliph2HC_scArgN_vlong
##              -0.016014025                  0.113686020
##      aliph2HC_aliph3HC_short       aliph1HC_aliph3HC_short
##               0.035877308                  0.145722316
##          scArgN_bbO_medlong           aliph1HC_bbCA_vlong
##               0.465020986                  0.006617271
##          carboxylC_bbN_long    carboxylO_carboxylO_vlong
##               0.074742456                 -0.010173256
##           scAGN_bbN_medlong       aliph1HC_bbProN_medlong
##               0.014973172                  0.283258729
##            bbCA_bbO_vshort          aliph1HC_scArgN_long
##              -0.362888385                  0.362998718
##           sulfur_bbCA_short         scLysN_carboxylO_long
##              -0.126617592                  0.132046893
##    carbonylC_hydroxylO_vlong       aliph2HC_aliph3HC_vlong
##              -0.055209272                  0.013393611
##      aliph2HC_hydroxylO_long      carbonylC_bbProN_medlong
##               0.011610725                 -0.154285898
##           bbN_bbN_medshort         aliph3HC_scArgN_vlong
##              -0.051056941                  0.268086387
##        aliph1HC_bbProN_vlong            aromaticC_bbO_vlong
##               0.048928470                  0.013720180
##      aliph2HC_aliph2HC_short           scLysN_bbN_medlong
##               0.044249959                 -0.026692625
##    aliph1HC_aliph3HC_medlong         aliph1HC_bbN_medshort
##              -0.044883584                 -0.099658805
##       aliph1HC_aliph1HC_long       carboxylC_aromaticC_long
##               0.139026676                  0.009206965
##        carbonylC_bbProN_long               sulfur_bbO_vlong
##              -0.097289640                 -0.031887005
##            bbN_bbC_medlong        aliph2HC_aromaticC_long
##              -0.016180792                  0.004385553
##     scAGN_carbonylO_medshort       bbProN_carboxylO_vlong
##              -0.080649720                  0.091184664
##              bbO_bbO_vshort              bbProN_bbO_long 
##                 0.146228095                  0.035606456 
##          bbCA_bbO_medshort     aliph1HC_hydroxylO_vlong 
##                -0.028972857                  0.077876330 
##     aliph3HC_aromaticC_vlong    carboxylC_carboxylC_vlong 
##                -0.018148494                 -0.230068159 
##    carboxylC_hydroxylO_short       carboxylO_bbCA_medlong 
##                -0.247938453                  0.059548280 
##   aliph2HC_hydroxylO_medlong   aliph3HC_aromaticC_medlong 
##                 0.010365249                 -0.014508451 
##       aromaticC_bbO_medlong          aromaticC_bbO_vshort 
##                 0.016919610                 -0.189646813 
##         aromaticC_bbC_short    aromaticC_aromaticC_vlong 
##                 0.098443505                 -0.008677942 
##        aromaticC_bbProN_vlong     aliph3HC_hydroxylO_short 
##                -0.043302601                 -0.080619545 
##               bbC_bbC_long         aliph1HC_bbO_medshort 
##                -0.001633968                 -0.083598662 
##      aliph3HC_hydroxylO_long       carbonylC_bbProN_vlong 
##                 0.002522520                 -0.084920281 
##   carbonylC_aliph3HC_medlong        carbonylC_sulfur_vlong 
##                 0.016342590                 -0.051448147 
##       aromaticC_scLysN_vlong          carboxylO_bbCA_long 
##                -0.059700876                  0.037532441 
##  aromaticC_carbonylO_medlong       carbonylC_sulfur_short 
##                 0.015775515                 -0.160344227 
##     aliph2HC_scLysN_medshort         scAGN_hydroxylO_long 
##                -0.112110634                 -0.044511253 
##       hydroxylO_sulfur_short    hydroxylO_sulfur_medshort 
##                 0.169724232                  0.141965152 
##        hydroxylO_sulfur_long        hydroxylO_sulfur_vlong 
##                 0.055146213                  0.037033233 
##         sulfur_bbCA_medshort        carbonylC_scLysN_vlong 
##                -0.033038837                  0.017447277 
##          carbonylC_bbN_vlong   aliph3HC_hydroxylO_medlong 
##                -0.026666517                  0.001390584 
##     aliph2HC_aliph3HC_vshort          carbonylC_bbC_medlong 
##                 0.093825630                 -0.031946936 
##           scAGN_bbO_medlong            aliph1HC_bbO_short 
##                 0.034180334                 -0.104519186 
##         aliph2HC_scLysN_long               sulfur_bbO_long 
##                 0.012691939                 -0.028302323 
##         bbProN_bbCA_medshort               scAGN_bbO_short 
##                 0.053310119                  0.077763462 
##     aromaticC_sulfur_medlong   aromaticC_hydroxylO_vshort 
##                0.036376737                -0.139132948
##      aliph1HC_hydroxylO_long         aliph3HC_bbN_medlong
##                0.094946454                 0.010331282
##            aliph3HC_bbN_long               bbN_bbO_medlong
##                0.009687819                -0.006754636
##              bbProN_bbN_long        hydroxylO_bbC_medlong
##                0.059957710                 0.019037832
##     aromaticC_bbProN_medlong              bbN_bbO_medshort
##               -0.062357352                -0.015189454
## carbonylC_hydroxylO_medshort  aliph2HC_aromaticC_medshort
##               -0.030684302                 0.020226009
##  aliph1HC_hydroxylO_medshort   aliph1HC_hydroxylO_medlong
##                0.133336205                 0.143327723
##  aliph3HC_hydroxylO_medshort        carboxylO_bbC_medshort
##               -0.052614362                -0.003362942
##           aliph2HC_bbC_vlong        aliph3HC_bbO_medshort
##                0.005501942                 0.024198115
##          aliph2HC_bbO_vshort      aliph1HC_aliph3HC_vlong
##                0.078716145                -0.045279213
##     hydroxylO_sulfur_medlong              sulfur_bbO_short
##                0.057980490                -0.045000808
##      aliph2HC_bbProN_medlong              scLysN_bbCA_long
##               -0.036046483                -0.061679233
##      carboxylC_aliph2HC_long        scLysN_hydroxylO_long
##               -0.033814766                 0.034865570
##           scLysN_bbC_medlong      aliph3HC_aliph3HC_vlong
##               -0.038809919                 0.042269473
##      aliph3HC_bbProN_medlong          aromaticC_scAGN_long
##               -0.046140394                 0.016416593
##        aliph1HC_bbN_medlong            bbProN_bbN_medlong
##               -0.033305850                 0.049402040
##       scAGN_carboxylO_vshort        scAGN_carbonylO_vshort
##               -0.103702815                -0.181275377
##              bbN_bbC_vshort   aliph2HC_aliph3HC_medshort
##               -0.034485953                 0.013959357
##              scAGN_bbO_long     carbonylC_aliph3HC_short
##                0.020451777                -0.054674429
##  aliph1HC_carbonylO_medshort          aliph3HC_scArgN_long
##                0.049188422                 0.147521127
##             scArgN_bbO_long      aliph3HC_scAGN_medshort
##               -0.167596507                 0.037133114
##             scAGN_bbC_vlong          aliph3HC_bbCA_short
##               -0.011720693                 0.032853035
##       aromaticC_sulfur_vlong          carbonylC_bbO_short
##                0.006866154                -0.053511772
##        aliph1HC_bbCA_medshort            sulfur_sulfur_vlong
##                   0.089850472                    0.101705497
##         carbonylC_scLysN_long    carbonylC_carbonylO_vlong
##                  -0.063068273                    0.053671218
##            aromaticC_bbN_vlong aromaticC_hydroxylO_medshort
##                   0.005685735                   -0.034600715
##     hydroxylO_carboxylO_long    hydroxylO_carboxylO_vshort
##                  -0.040825251                    0.128573027
##     aliph3HC_sulfur_medshort     aliph1HC_sulfur_medshort
##                   0.091243632                   -0.065549264
##      aliph3HC_sulfur_medlong     aliph3HC_carboxylO_vlong
##                   0.070642595                   -0.039253563
##    carbonylC_carbonylO_short       aromaticC_sulfur_short
##                   0.125956082                   -0.049771200
##         aliph3HC_sulfur_vlong         carbonylO_bbN_medlong
##                   0.035178195                   -0.022447784
##         hydroxylO_bbN_medlong     carboxylO_sulfur_medlong
##                   0.018727370                    0.064175413
##       carboxylO_sulfur_vlong         aliph2HC_bbC_medshort
##                   0.049402755                    0.015149426
##              bbCA_bbO_short           bbProN_sulfur_vlong
##                  -0.037120901                   -0.077863378
##    carboxylO_sulfur_medshort          aliph3HC_sulfur_long
##                   0.055188545                    0.035887993
##     carbonylC_sulfur_medlong        scLysN_carbonylO_vlong
##                  -0.080799206                   -0.045165791
##         aliph1HC_scAGN_short    carboxylC_aliph2HC_medlong
##                  -0.035500366                   -0.023592740
##           carboxylC_bbN_vlong            bbProN_bbN_medshort
##                   0.033677823                    0.036127352
##    carbonylO_carboxylO_vlong   aliph3HC_carbonylO_medshort
##                  -0.050357059                    0.057780707
##           scAGN_bbO_medshort         scAGN_carbonylO_short
##                   0.033740243                   -0.092842141
## carbonylC_carbonylO_medshort      aliph2HC_carbonylO_long
##                   0.070085778                    0.012806071
##        aliph3HC_bbProN_vlong        scArgN_hydroxylO_short
##                   0.034847864                   -0.104232851
##             bbProN_bbO_vlong     aromaticC_scAGN_medshort
##                   0.028829040                   -0.020626043
##           aliph1HC_bbN_short     carbonylC_aliph2HC_short
##                  -0.066846762                    0.015064798
##    hydroxylO_carboxylO_short         carbonylC_sulfur_long
##                   0.052280040                   -0.067967872
##     aliph2HC_carbonylO_vlong     carbonylC_carbonylC_vlong
##                    0.013665337                  -0.053412695
##          scAGN_bbProN_medshort               scAGN_bbO_vshort
##                   -0.110165410                   0.058690082
##              carboxylC_bbC_vlong     aromaticC_scLysN_medlong
##                   -0.023729055                  -0.074723138
##            carboxylO_bbC_medlong         aliph3HC_sulfur_short
##                   -0.046276599                   0.059825467
##          aliph1HC_aliph2HC_short          aromaticC_bbCA_vlong
##                   -0.099632709                   0.006726620
##       aliph1HC_aliph2HC_medshort           aromaticC_bbC_vlong
##                   -0.032012144                  -0.007449817
##           aliph2HC_aliph3HC_long                 bbCA_bbO_long
##                   -0.013490532                  -0.005993055
##         aliph2HC_sulfur_medshort            scLysN_bbO_medlong
##                   -0.021344664                   0.051987113
##        aliph2HC_carbonylO_vshort     carboxylC_aliph2HC_vlong
##                    0.065010336                   0.029854412
##            scArgN_carboxylO_long           aromaticC_bbN_long
##                   -0.062484734                   0.005016098
##         carboxylC_aliph3HC_vlong           carbonylO_bbO_short
##                   -0.029941360                   0.026266941
##     aliph2HC_carboxylO_medshort       aliph2HC_scLysN_medlong
##                   -0.032709942                  -0.042976497
##             aliph3HC_bbO_medlong     aliph1HC_carbonylO_vlong
##                    0.014514297                   0.019793344
##           aliph2HC_aliph2HC_vlong          carboxylC_bbC_medlong
##                    0.005725962                   0.037538066
##     aliph3HC_aromaticC_medshort            carboxylO_bbN_vshort
##                    0.010878726                   0.101576622
##          carboxylO_bbCA_medshort            carboxylC_bbO_vlong
##                    0.052583382                  -0.024579277
##             aliph1HC_scAGN_vlong     aliph1HC_carboxylO_vlong
##                    0.019577410                  -0.052434293
##               carbonylC_bbN_long          aliph3HC_aliph3HC_long
##                   -0.008464008                   0.041788129
##        aliph3HC_aliph3HC_medlong              hydroxylO_bbN_long
##                    0.032817099                   0.010621954
##      aliph3HC_carbonylO_medlong  carbonylC_aliph1HC_medshort
##                    0.019437489                  -0.051558885
##   hydroxylO_hydroxylO_medlong     bbProN_carbonylO_medlong
##                    0.029409867                   0.044446613
##            scAGN_scLysN_medlong     aliph3HC_carbonylO_short
##                   -0.071215490                   0.027438451
##              carboxylO_bbO_vlong                scLysN_bbN_long
##                    0.009993058                  -0.058036401
##          carbonylO_bbCA_long                   bbN_bbN_long
##                 -0.010172362                   -0.011761693
##                 bbN_bbN_vlong     aliph2HC_hydroxylO_vlong
##                 -0.011307629                    0.005828448
##          aliph3HC_scLysN_vlong                sulfur_bbN_long
##                  0.054436693                    0.015240198
##         aliph3HC_bbCA_medshort            sulfur_bbN_medshort
##                 -0.016090571                    0.031679472
##              sulfur_bbN_short    carboxylC_carboxylO_vlong
##                  0.053296717                    0.026011662
## hydroxylO_carboxylO_medshort     carboxylO_carboxylO_long
##                 -0.073726235                    0.056920368
##            aromaticC_bbO_long    aromaticC_aromaticC_short
##                  0.006316804                   -0.009064569
##         aromaticC_bbN_medshort    carbonylO_sulfur_medshort
##                 -0.009741127                    0.033785599
##              aliph2HC_bbC_long  aliph3HC_carboxylO_medshort
##                  0.004397429                    0.049722809
```

```
# We check the model for linear regression assumptions again


 #summary(premov)
par ( mfrow = c (2 ,2) )

 plot(mfinal$fitted.values, mfinal$residuals, xlab = "Fitted Values",
      ylab = "Residuals")
 plot (1: nrow (ptrain), mfinal$residuals , xlab = " Index ", ylab =
         " Residuals ")

 qqnorm(mfinal$residuals)
 qqline(mfinal$residuals, col="blue", lwd = 2)
 hist(mfinal$residuals)
```



```r
# use final model to predict response for protein-test.csv

ptest <- read.csv ("protein-test.csv")


predfinal <- predict(mfinal, newdata = ptest)

writeLines(as.character(predfinal), "mypreds1.txt.txt")
```