TDDE01 – Machine Learning
Individual Laboration Report 2

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1 Assignment 1

In this assignment we were tasked with implementing *feature selection* using the *k-fold cross validation* and *linear regression* algorithms. The result of this can be found in appendix: A - Code assignment 1.

The feature selection algorithm iterates through all possible combinations of *features* from the predictor variables and apply the *k-fold* cross validation on all of them. The feature combination with the lowest *sum of squared error* gets picked as the best combination.

First all the combinations of features a iterated through.

$$\mathbf{A} = \{c_1, c_2, ..., c_n\}, 1 \leq n \leq ncol(X) \tag{1}$$

A in the equation above represents all the permutations of column index for the response variable. Each of theses combinations are sent to the *k-fold cross validation* where the data is split into K parts of equal size. The K are then iterated through and each data subset is used as testing data with the other $K-1$ sets as training data. The *k-fold cross validation* uses the *linear regression* with *ordinary least squares* estimator. The produced predictions are then error checked with the *sum of squared error*

$$\sum_{i=1}^{n} (\hat{y}_i - y_i)^2, n = nrow(y) \tag{2}$$

for fold K. After all the K folds for a given combination of features are calculated, the mean of all fold errors are calculated and returned as the final error value for the feature combination.

$$s \in \{1, ..., n\} \tag{3}$$

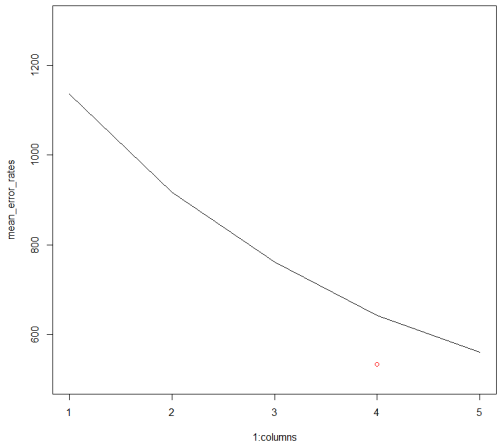
where s symbolizes a set of indexes. We then create all combinations of indexes from 1 to $2^n 1 - 1$ (because we don't need the empty feature set).

$$\mathbf{A} = \{s_1, s_2, ..., s_{2^n-1}\} \tag{4}$$

$$\bigcap_{i=1}^{|\mathbf{A}|} (s_i) = \emptyset \tag{5}$$

where $K = |folds|$ and $n = |y|$.

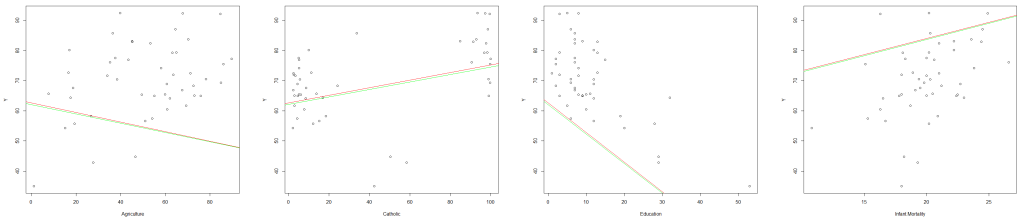
In the figure below the mean error for a given number of selected features can be shown.



Figur 1: The mean error rate for different number of feature combinations.

The red dot indicates the best feature combination, i.e. the one with the lowest error score. For this data set it's $\{Agriculture, Education, Catholic, Infant.Mortality\}$. In general terms we can observe that the more features that are selected, the lower the error rate becomes.

The following graphs show the linear regression result for each of the different features that was returned by the best feature subset function described above.



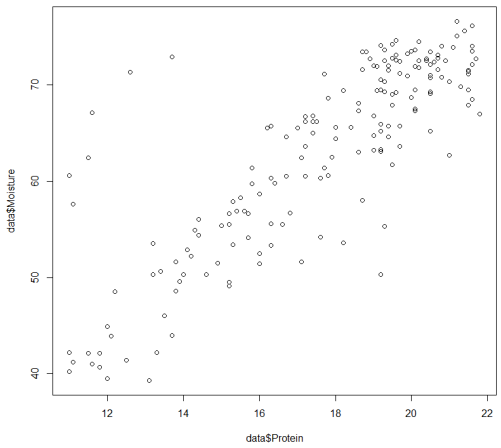
The models manges to hit fairly close to what humans would recognize as the best linear function for each data set.

2 Assignment 2

In this assignment we are tasked with analyzing the data set found in the file **tecator.xlsx**. The data is grouped into the columns:

$$\{Sample, Channel1, ..., Channel100, Moisutre, Fat, Protein\} \tag{6}$$

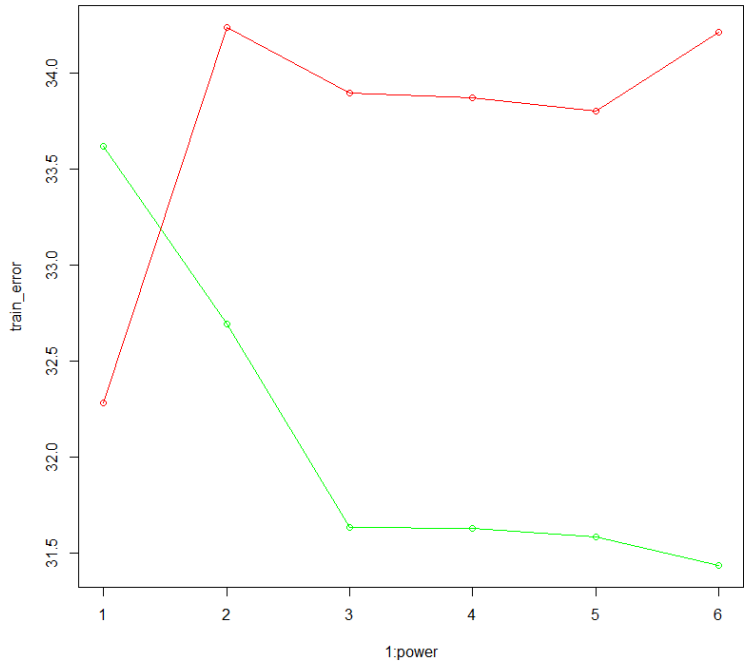
The first task is to plot the *Moisture* and *Protein* and determine if a linear model would be a good approximation for the data. The plot can be seen in the figure below.



Figur 2: The *Moisture* plotted by *Protein*.

A linear approximation seems to be a good fit for the data.

Next we examine if a polynomial approximation of the data up to the nth power is a suitable estimation. We also use the *mean squared error* (MSE) to examine the fitness of the polynomial model. The data set is split into two sets of equal size where one of the sets are the training set and the other the validation set.



Figur 3: The training and validation error rate for the polynomial estimation given the MSE.

The **green line** is the error rate for the training data and the **red line** is the error rate for the validation set over the different power-levels. We can observe in the graph that the fitting of the training data decreases when the power-level increases but the error rate for the validation data increases with about the same magnitude. This can be explained with the fact that, as observed in the plot of the full data set above, the data would follow a linear model and the polynomial approximation leads to over fitting of the training set.

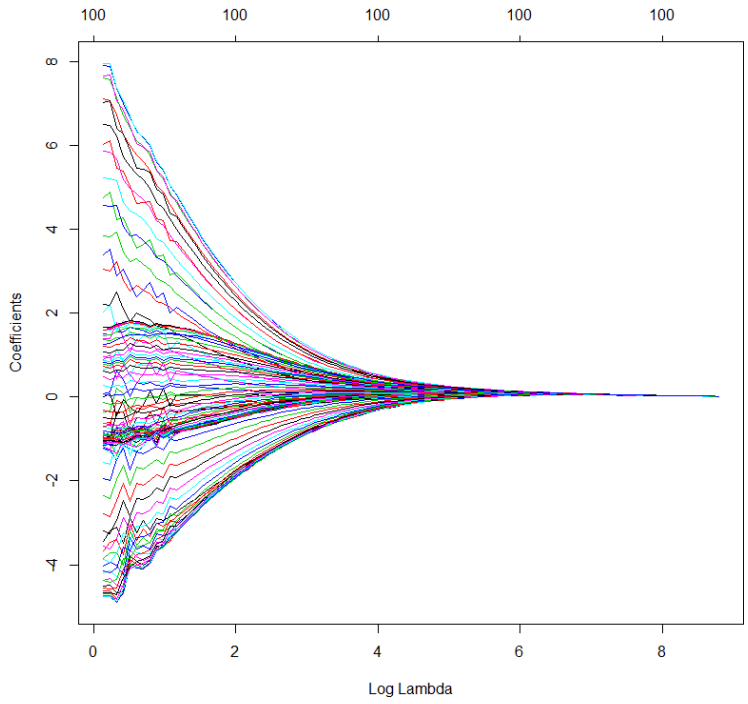
We perform best features selection using the full data set with the *step* cross validation function. We get 64 coefficients from the step function.

The next part involves fitting a *ridge regression model* to the data set.

$$min \sum_{i=1}^{n} V(\hat{x_i} \cdot w, \hat{y_i}) + \lambda \|w\|_2^2 \tag{7}$$

The equations results in the ridge estimation to intersect the linear regression estimation in an edge point. This property will result in none to few coefficients being zeroed although many will be very small.

The result can be observed in the following plot. We can see as the lambda increases, the coefficients converges to zero.



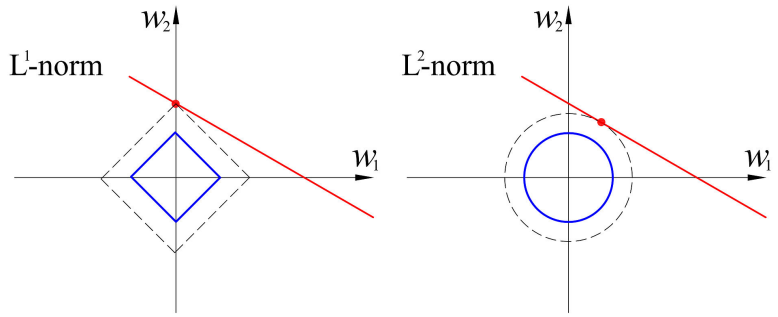
Figur 4: Size of the coefficients over the log of the penalty factor lambda.

We can observe that the number of coefficients stay high over all the lambdas but the penalty factor causes the size of the coefficients to decrease.

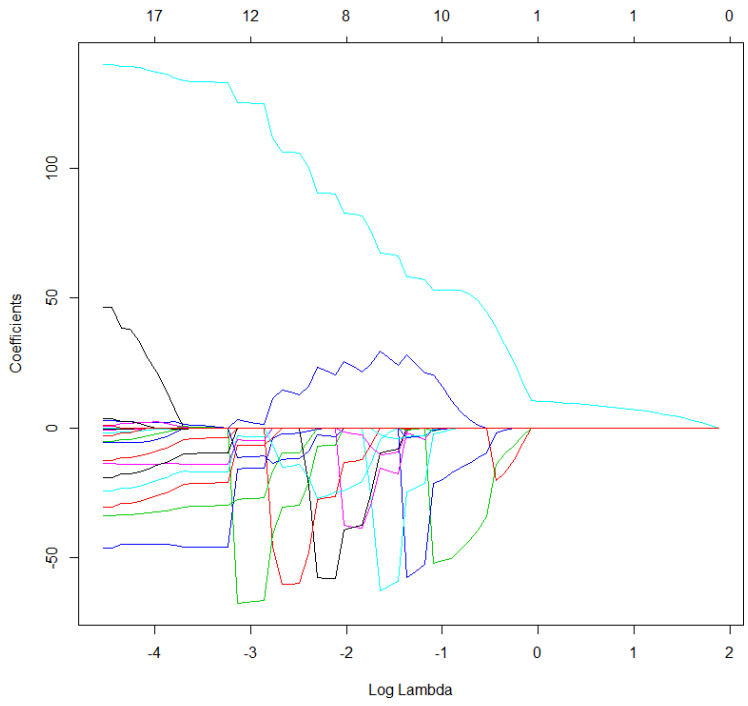
$$min \sum_{i=1}^{n} V(\hat{x_i} \cdot w, \hat{y_i}) + \lambda \|w\| \tag{8}$$

The equation is similar to the ridge estimation with the big difference being

that the estimation bound has a different shape where coefficients can be zeroed. This can be observed in the figure below.



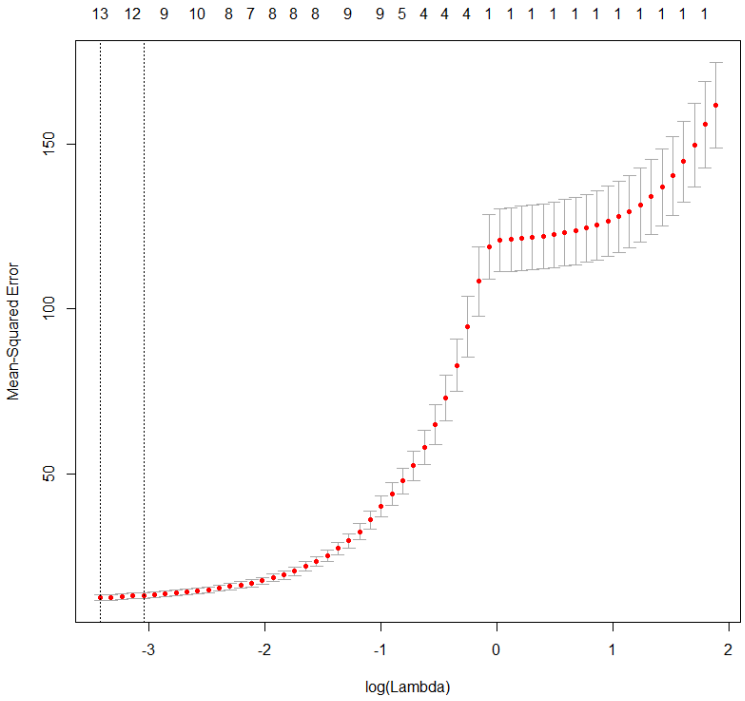
Figur 5: Shape of the Ridge and LASSO estimation bounds respectively, credit to Rezamohammadighazi for original image.



Figur 6: Size of the coefficients over the log of the penalty factor lambda.

As observed with the ridge regression the coefficients decrease over log lambda but the number of coefficients is drastically decreased, resulting in 13 coefficients.

The final part involves plotting to cross validation score using the lasso model, the result can be observed in the graph below. The variance increase with the lambda and the validation score.



Figur 7: Mean squared error over the log lambdas with variance included.

From the graph above we can observe how the MSE increases exponentially up to log lambda of 0. After this the error rate increases exponentially again. We can also observe how the variance increases with lambda.

In comparison with the step aic model the cross validation using lasso and k-fold resulted in much less coefficients.

3 Appendix: A - Code assignment 1

Listing 1: Code for assignment 1

```
library(readxl)

# folding indexes, returns start indexes for each
   fold
indexes <- function(n,k){
  s = floor(n/k)
  indexes = matrix(1,k,2)
  for(i in 1:k){
    indexes[i,1] = (i-1) * s
    indexes[i,2] = i * s -1
  }
  indexes = indexes +1
  indexes[k,2] = n
  return(indexes)
}

# Deprecated because of reasons
binary_permutations <- function(n){
  indexes = matrix(0,2^n-1,n)
  for(i in 1:2^n-1){
    indexes[i,] = as.numeric(intToBits(i))[1:n]
  }
  return(indexes)
}

k_fold <- function(X,Y,K){
  n = nrow(X)
  fold_errors = matrix(0,K,1)
  fold_weights = matrix(0,K,(ncol(X)+1))
  indexes = indexes(n,K)
  for( i in 1:K){
    test_fold_indexes = indexes[i,1]:indexes[i,2]
    train_fold_indexes = (1:n)[-test_fold_indexes]

    test_y = Y[test_fold_indexes]
    test_x = X[test_fold_indexes,]
    train_x = X[train_fold_indexes,]
    train_y = Y[train_fold_indexes]
    result = linear_regression(as.matrix(train_x),
```

```
      train_y,as.matrix(test_x),test_y)
    fold_errors[i,] = result$err
    fold_weights[i,] = result$param
  }

  return (list(weights=colMeans(fold_weights), err=
     fold_errors))
}
best_subset <- function(X,Y,K){
  n = nrow(X)
  columns = ncol(X)
  print(columns)

  errors = matrix(0,columns,2^columns)
  mean_error_rates = matrix(0,columns,1)
  best_error = Inf
  best_indexes = c()
  best_weights = c()
  for(n_features in 1:columns){
    binary_permutations = binary_permutations(ncol(X
       ))
    binary_permutations = t(combn(1:columns,n_
       features))
    n_combinations = nrow(binary_permutations)

    combination_errors = matrix(Inf,n_combinations
       ,1)

    for(combination in 1:n_combinations){
      current_features = binary_permutations[
         combination,]
      filtered_x = as.matrix(X[current_features])
      k_fold = k_fold(filtered_x,Y,K)
      combination_errors[combination,] = mean(k_fold
         $err)
      best_combination_index = which.min(combination
         _errors)

      if(combination_errors[best_combination_index,]
          < best_error){
        best_weights = k_fold$weights
```

```
        best_indexes = binary_permutations[
           combination,]
        best_error = combination_errors[best_
           combination_index,]
      }

    }
    mean_error_rates[n_features,] = mean(combination
       _errors)

  }
  plot(1:columns,mean_error_rates, type = "l", ylim
     = c(500,1300))
  points(length(best_indexes),best_error, col="Red")
  print(best_error)
  return(list(indexes=best_indexes, weights=best_
     weights, err=best_error))
}

 # Linear regression between two samples, one as x-
    values and one as y-values
 linear_regression <- function(x_train,y_train,x_
    test,y_test){
    x_train = cbind(matrix(1,nrow(x_train),1),x_
       train)
    x_test = cbind(matrix(1,nrow(x_test),1),x_test)
    w = solve(t(x_train) %*% x_train) %*% t(x_train)
        %*% y_train
    w = as.vector(w)
    pY = x_test %*% w
    errors = sum((y_test - pY)^2)
   return(list(param=w, pred=pY, err=errors))
 }


data = swiss
set.seed(12345)
s = sample(1:nrow(data),nrow(data))
data = data[s,]
# ============
#fold_indexes(nrow(data),5)
```

```
X = data[,2:ncol(data)]
Y = as.matrix(data$Fertility)
best_features = best_subset(X,Y,5)
print(best_features)
X = X[,best_features$indexes]
print(X)
model = linear_regression(x_train = as.matrix(X),y_
   train = Y,x_test = as.matrix(X),y_test = Y)
for(i in 1:ncol(X)){
  plot(X[,i],Y, xlab = colnames(X)[i])
  # From best_features
  abline(best_features$weights[1],best_features$
     weights[i+1],col="Red")
  # From new regression
  abline(model$param[1],model$param[i+1],col="Green"
     )

}
```

4 Appendix: B - Code assignment 2

Listing 2: Code for assignment2

```
library(MASS)
library(readxl)
library(Matrix)
library(glmnet)

data = read_excel("tecator.xlsx")
plot(data$Protein,data$Moisture)
# answer: yes

# task 2
# Find a probailist model explaining Mi. where M is
   a polynomial model of the protein up to power i
# Why is it important to use mean squared error whne
    fitting model?

# We approximate the model as w0 + w1x^1 + w2x^2 ...
# Use MSE instead of SSE because MSE is normalized
```

```
set.seed(12345)
n = nrow(data)
train_indexes = sample(1:n,floor(n*0.5))
train_data = data[train_indexes,]
test_data = data[-train_indexes,]
poly = 6
train_error = matrix(0,poly,1)
test_error = matrix(0,poly,1)

for(i in 1:poly) {
  model = lm(Moisture ~ poly(Protein,i), data=train_
     data)
  train_predictions = predict(model,train_data)
  test_predictions = predict(model,test_data)

  train_error[i,] = mean((train_data$Moisture -
     train_predictions)^2)
  test_error[i,] = mean((test_data$Moisture - test_
     predictions)^2)
}

ylim = c(min(rbind(train_error,test_error)),max(
   rbind(train_error,test_error)))
plot(1:poly,train_error, col="Green", ylim=ylim)
lines(1:poly,train_error, col="Green")
points(1:poly,test_error,col="Red")
lines(1:poly,test_error, col="Red")

# Observation of the plot indicates that as we
   increase the polynomial level the functiuon
   becomes more fitted for the training data and
   results in increasingly worse fit for the test
   data

model = lm(Fat ~ . - Protein - Moisture - Sample,
   data=data)
steps = stepAIC(model,direction="both", trace=FALSE)
coeff_aics = steps$coefficients
n_coeff_aics = length(coeff_aics)
```

```
print(n_coeff_aics)
# 64 columns were selected

data_y = data$Fat

data = data[,-which(colnames(data) == "Sample")]
data = data[,-which(colnames(data) == "Fat")]
data = data[,-which(colnames(data) == "Protein")]
data = as.matrix(data[,-which(colnames(data) == "
   Moisture")])

ridge = glmnet(x=data, y=data_y, alpha=0)
plot(ridge, xvar="lambda")

# task 6
# Do the same stuff but with LASSO, compare with
   ridge
lasso = glmnet(x=data, y=data_y, alpha=1)
plot(lasso, xvar="lambda")

# task 7
#   CV to find the optimal LASSO, report the optimal
    lambda and how many variables were chosen by the
    model '
#   make conculsions
#   show a plot of CV scores in comparasion to
   lambda

lasso_cv = cv.glmnet(data,data_y, alpha=1)
lasso_cv_lambda = min(lasso_cv$lambda)
n_lass_cv = sum(coef(lasso_cv) != 0)
print(lasso_cv_lambda)
print(n_lass_cv)
plot(lasso_cv)
# task 8
# compare result from 4 and 7
```