Computer lab 2 block 1

Vasileia Kampouraki & Laura Julià Melis & Mengxin Liu

12/08/2019

Assignment 2. Analysis of credit scoring.

The data file creditscoring.xls contains data retrieved from a database in a private enterprise. Each row contains information about one customer. The variable good/bad indicates how the customers have managed their loans. The other features are potential predictors. Your task is to derive a prediction model that can be used to predict whether or not a new customer is likely to pay back the loan.

1. Import the data to R and divide into training/validation/test as 50/25/25: use data partitioning code specified in Lecture 1e.

See Appendix

2. Fit a decision tree to the training data by using the following measures of impurity (a. Deviance, b. Gini index) and report the misclassification rates for the training and test data. Choose the measure providing the better results for the following steps.

We have fitted two decision trees using the function `tree()` from the package **tree**, choosing `split = "deviance"` and `split = "gini"` in each one.

- Missclassification rates for the fitted tree using the deviance:

```
##   Test.data Training.data
## 1     0.268         0.212
```

- Missclassification rates for the fitted tree using the Gini index:

```
##   Test.data Training.data
## 1     0.368          0.24
```

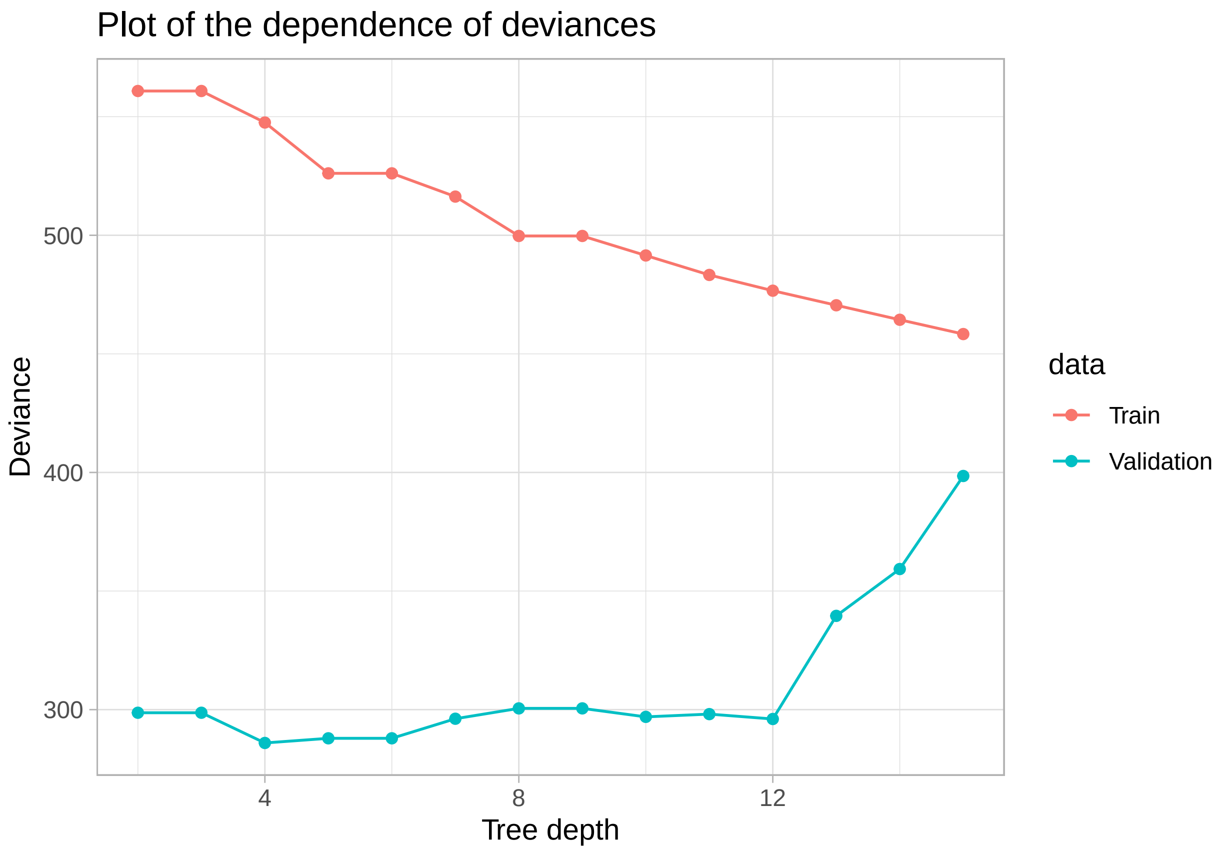
Given the missclassification rates, the best performance is the one obtained by the tree fitted with the deviance as measure of impurity. For both trees the rate for the training data is quite similar but the error rate for the test data is smaller in the deviance case.

For this reason, from now on we will use the tree with `deviance`.

3. Use training and validation sets to choose the optimal tree depth. Present the graphs of the dependence of deviances for the training and the validation data on the number of leaves. Report the optimal tree, report it's depth and the variables used by the tree. Interpret the information provided by the tree structure. Estimate the misclassification rate for the test data.

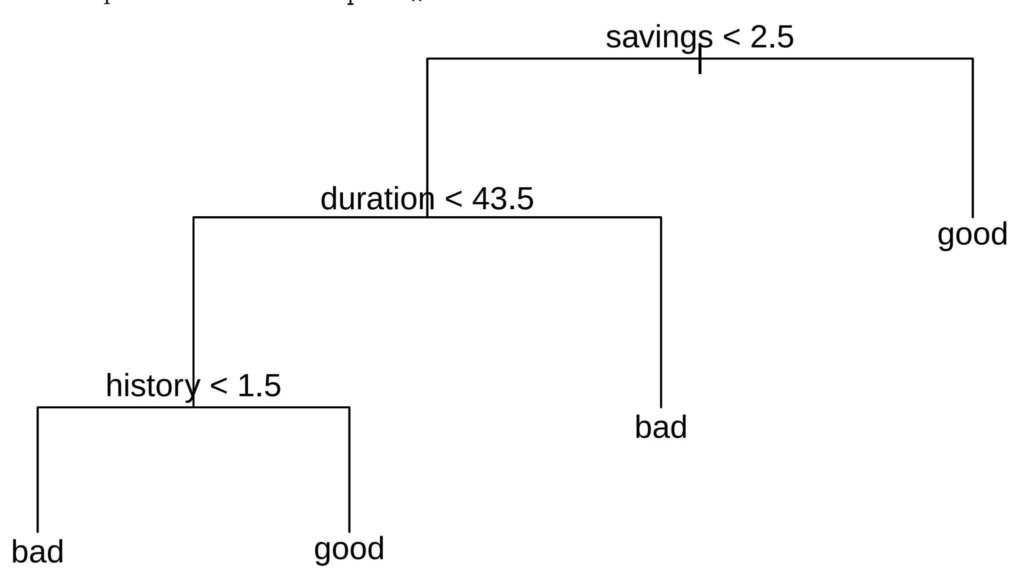
In `summary(fit)` we have obtained that the number of terminal nodes is 15, so we have used the `prune.tree()` function with the fitted model (using the deviance) in the **tree** argument and values $2, 3, \ldots, 15$ in the **best** argument. So, 14 different trees with $2, 3, \ldots, 15$ terminal nodes in each one has been considered and the deviance of each model has been calculated with the `deviance()` function.

Then, the results obtained are shown in the plot below:



Validation data graph: It appears that a tree with 4 leaves has the lowest deviance of the considered trees. More precisely the deviance when we have a tree of size 4 is 285.9425 and it's the smallest.

We can draw the optimal tree with the `plot()` function



This three has depth 3 and 4 terminal nodes and the variables used are: duration, history and savings.

Finally, we will estimate the misclassification rate for the test data:

```
## [1] 0.256
```

We have reduced the misclassification rate (compared to the tree chosen in question 2). Now, only 25.6% of the observations are classificated wrongly.

4. Use training data to perform classification using Naïve Bayes and report the confusion matrices and misclassification rates for the training and for the test data. Compare the results with those from step 3.

We have fitted the required model using the training data and the function `naiveBayes()` from the package **e1071**.

- Confusion matrices.

```
##       fitted_test
##         bad good
##   bad    46   30
##   good   49  125
```

```
##       fitted_train
##         bad good
##   bad    95   52
##   good   98  255
```

- Misclassification rates.

```
## For the test data: 0.316
```

```
## For the training data: 0.3
```

The misclassification rate for the test data using Naive Bayes is bigger than the one obtained by the optimal tree computed in question three. More precisely, the misclassification rate of Naive Bayes for the test data is 0.316 whereas for the optimal tree is 0.256.

5. Use the optimal tree and the Naïve Bayes model to classify the test data by using the following principle:

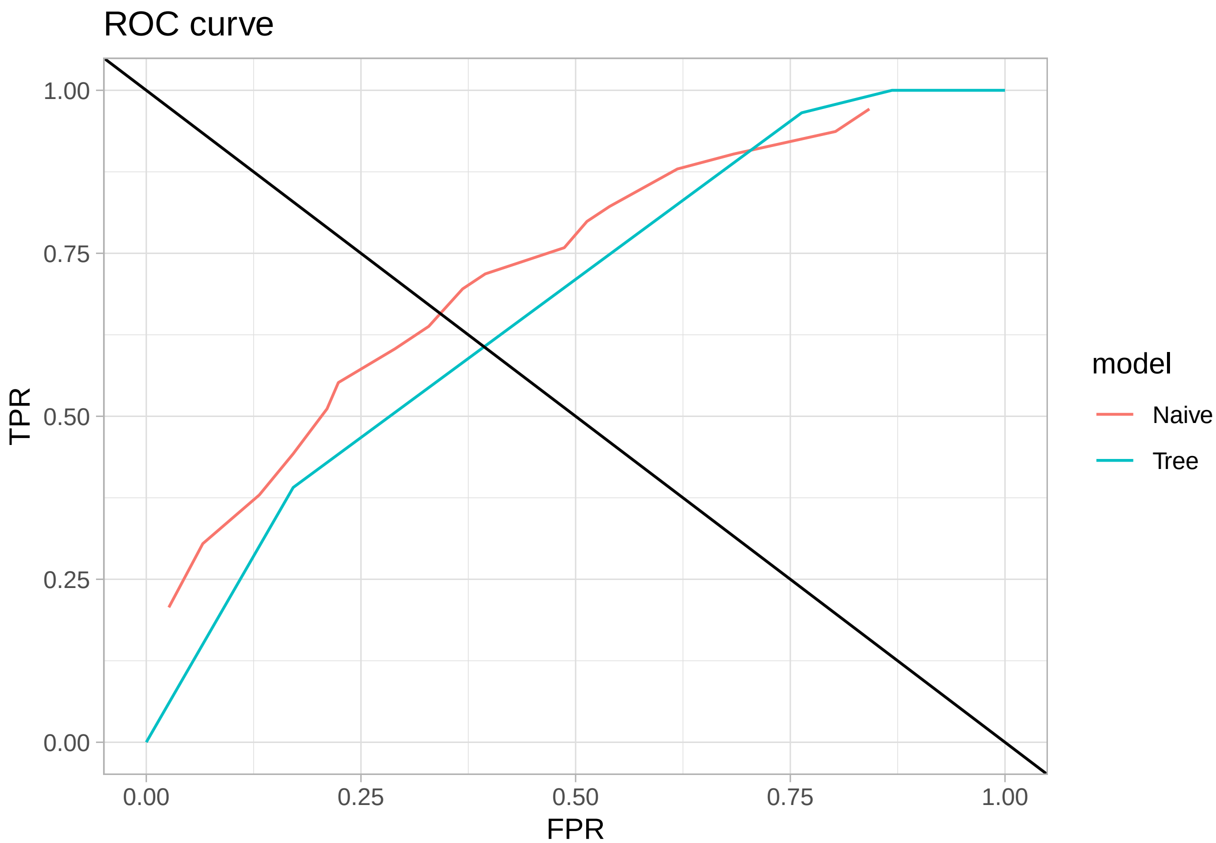
$$\hat{Y} = 1 \text{ if } p(Y = \text{‘good’}|X) > \pi, \text{ otherwise } \hat{Y} = 0$$

where $\pi = 0.05, 0.1, 0.15, ...0.9, 0.95$**. Compute the TPR and FPR values for the two models and plot the corresponding ROC curves. Conclusion?**

- Table TPR and FPR values:

```
##      pi model    TPR    FPR   pi model    TPR    FPR
## 1  0.05 Naive 0.9713 0.8421 0.05  Tree 1.0000 1.0000
## 2  0.10 Naive 0.9368 0.8026 0.10  Tree 1.0000 1.0000
## 3  0.15 Naive 0.9253 0.7632 0.15  Tree 1.0000 1.0000
## 4  0.20 Naive 0.9023 0.6842 0.20  Tree 1.0000 0.8684
## 5  0.25 Naive 0.8793 0.6184 0.25  Tree 1.0000 0.8684
## 6  0.30 Naive 0.8218 0.5395 0.30  Tree 1.0000 0.8684
## 7  0.35 Naive 0.7989 0.5132 0.35  Tree 0.9655 0.7632
## 8  0.40 Naive 0.7586 0.4868 0.40  Tree 0.9655 0.7632
## 9  0.45 Naive 0.7356 0.4342 0.45  Tree 0.9655 0.7632
## 10 0.50 Naive 0.7184 0.3947 0.50  Tree 0.9655 0.7632
## 11 0.55 Naive 0.6954 0.3684 0.55  Tree 0.9655 0.7632
## 12 0.60 Naive 0.6379 0.3289 0.60  Tree 0.9655 0.7632
## 13 0.65 Naive 0.6034 0.2895 0.65  Tree 0.9655 0.7632
## 14 0.70 Naive 0.5517 0.2237 0.70  Tree 0.9655 0.7632
## 15 0.75 Naive 0.5115 0.2105 0.75  Tree 0.3908 0.1711
## 16 0.80 Naive 0.4425 0.1711 0.80  Tree 0.3908 0.1711
## 17 0.85 Naive 0.3793 0.1316 0.85  Tree 0.0000 0.0000
## 18 0.90 Naive 0.3046 0.0658 0.90  Tree 0.0000 0.0000
## 19 0.95 Naive 0.2069 0.0263 0.95  Tree 0.0000 0.0000
```

- Plot of FPR vs TPR (ROC curve).



We know that the best classifier is the one that has the biggest area under the ROC curve. From the plot we can see that the greatest ares is under the Naive Bayes curve, therefore we can conclude that compared to the decision tree, Naive Bayes classifier is a better model. For the same False Positive rate, in most cases Bayes model has a higher True Positive Rate.

6. Repeat Naïve Bayes classification as it was in step 4 but use the following loss matrix:

$$L = \begin{pmatrix} 0 & 1 \\ 10 & 0 \end{pmatrix}$$

and report the confusion matrix for the training and test data. Compare the results with the results from step 4 and discuss how the rates has changed and why.

Rule to classify an observation:

$$\frac{P(C_1|x)}{P(C_2|x)} > \frac{L_{21}}{L_{12}} \rightarrow \text{predict } y \text{ as } C_1$$

In our case:

$$\frac{P(\text{“good"}|x)}{P(\text{“bad"}|x)} > 10 \rightarrow \text{predict } y \text{ as “good"}$$

- Confusion matrices.

```
##       fitted_class_test
##        bad good
##   bad   71    5
##   good 122   52
```

```
##       fitted_class_train
##        bad good
```

```
##    bad  137    10
##    good 263    90
```

In this case, the number of good customers predicted as good has been reduced in comparison to the confusion matrices in question (4) which happened because when using the loss matrix, our rule to classify a customer as "good" is "the propability to classify a customer as good has to be 10 times higher than the probability of being bad". So we are being more strict.

- Misclassification rates.

```
## For the test data: 0.508
```

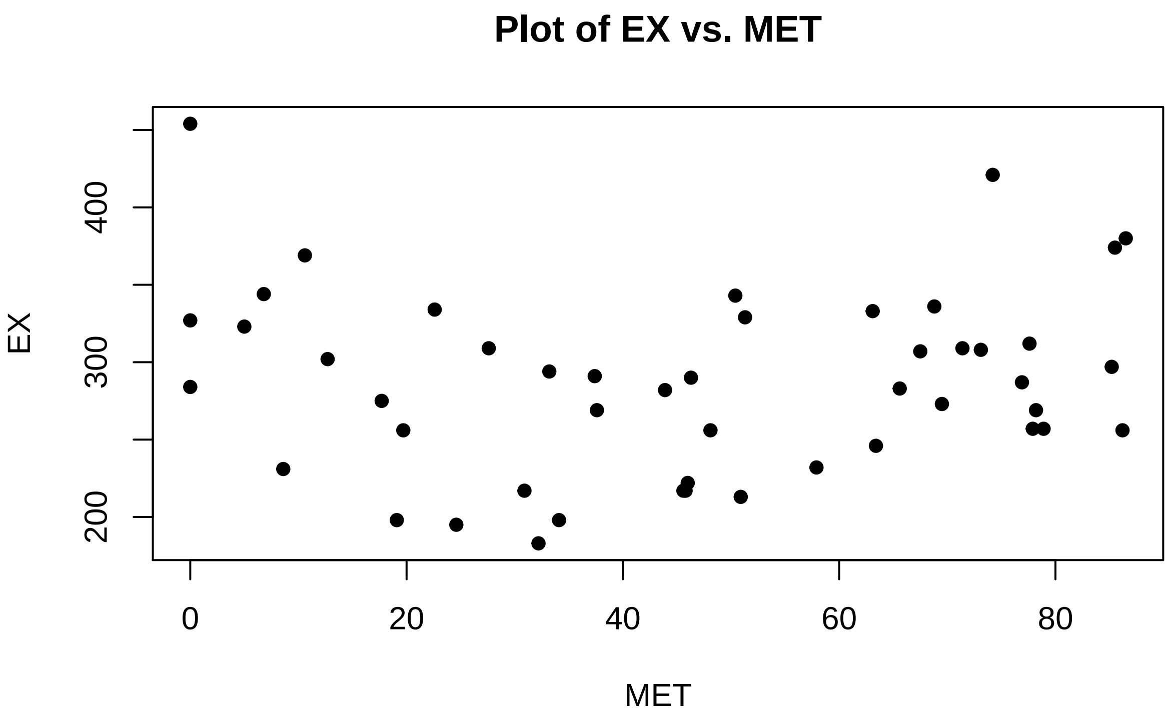
```
## For the training data: 0.546
```

The misclassification rate for the train data is bigger when following the loss matrix than it was on question 4. Now the misclassification rate for the train data is 0.546 whereas previously it was 0.3.

The misclassification rate for the test data is also bigger when following the loss matrix than it was on question 4. Now the misclassification rate for the train data is 0.508 whereas previously it was 0.316.

Assignment 3. Uncertainty estimation.

1. Reorder your data with respect to the increase of MET and plot EX versus MET. Discuss what kind of model can be appropriate here. Use the reordered data in steps 2-5.



The observations (black dots) are quite sparsed in the plot, so a linear regression model wouldn't be appropiate. But if we want to perform some kind of regression, quadratic model would be a viable option.

However, the best option seems to be fitting a regression tree, because the target variable is numeric.

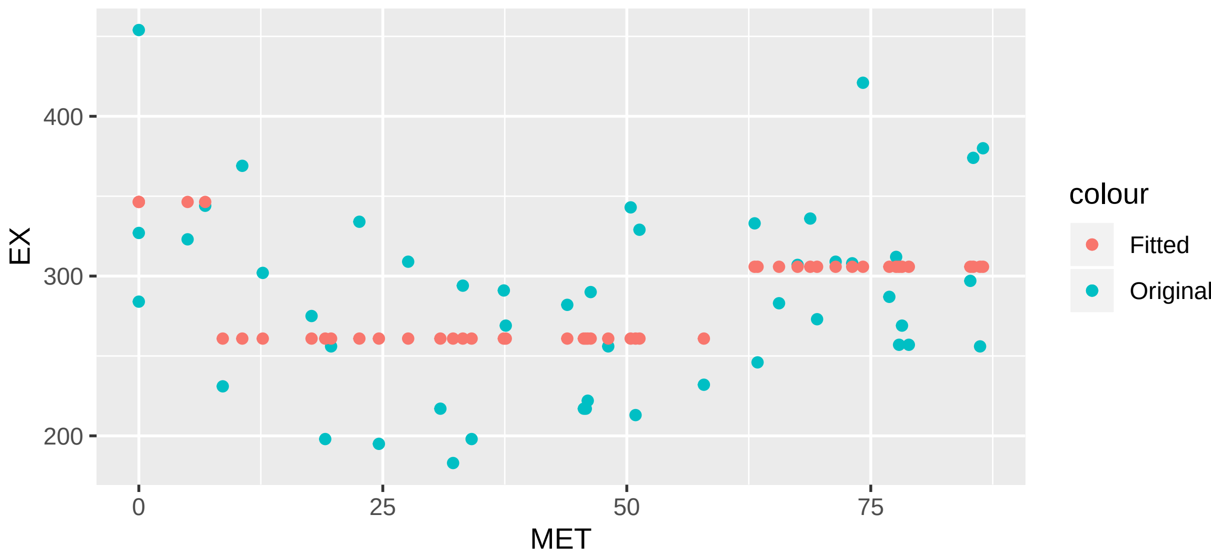
2. Use package tree and fit a regression tree model with target EX and feature MET in which the number of the leaves is selected by cross-validation, use the entire data set and set minimum number of observations in a leaf equal to 8 (setting minsize in tree.control). Report the selected tree. Plot the original and the fitted data and histogram of residuals. Comment on the distribution of the residuals and the quality of the fit.

In order to fit the regression tree with at least 8 observations in each leaf, it has been used the option `minsize` in the control argument. Then, the `cv.tree` function has been used to selet the optimal number of leaves by cross-validation. This value can be seen executing the following code: `cv.tree$size[which(cv.tree$dev==min(cv.tree$dev))]`.

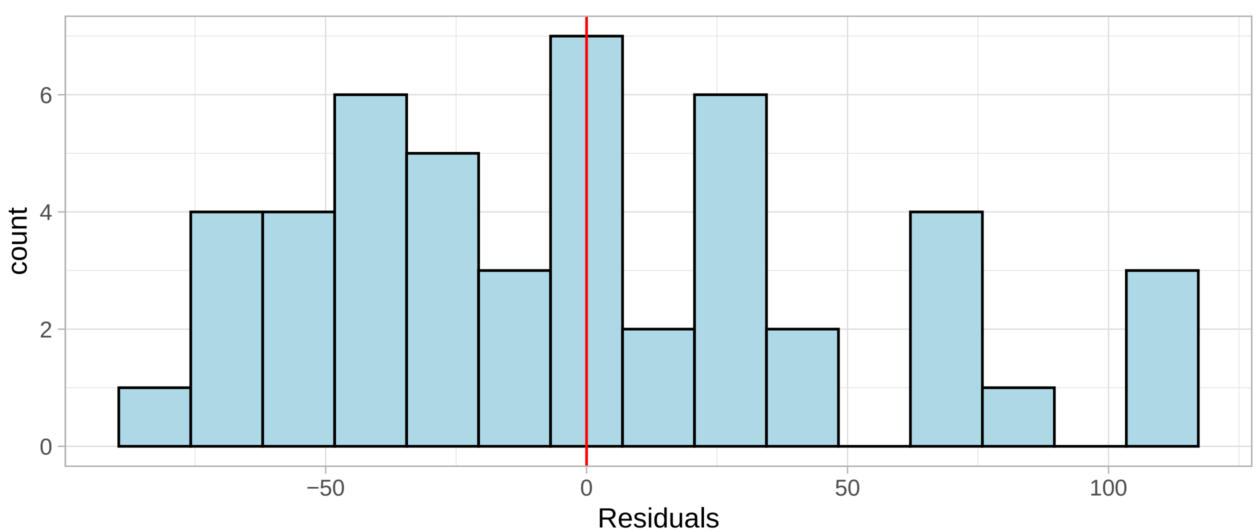
So the optimal number of leaves is 3 (the size of the tree) and we can report this tree:

```
##
## Regression tree:
## snip.tree(tree = fit, nodes = 7:6)
## Number of terminal nodes:  3
## Residual mean deviance:  2698 = 121400 / 45
## Distribution of residuals:
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  -77.88  -43.88   -4.88    0.00   30.13  115.20
```

We will plot the original and the fitted data:



The fit of the tree model doesn't look so good. The histogram of the residuals is the following:



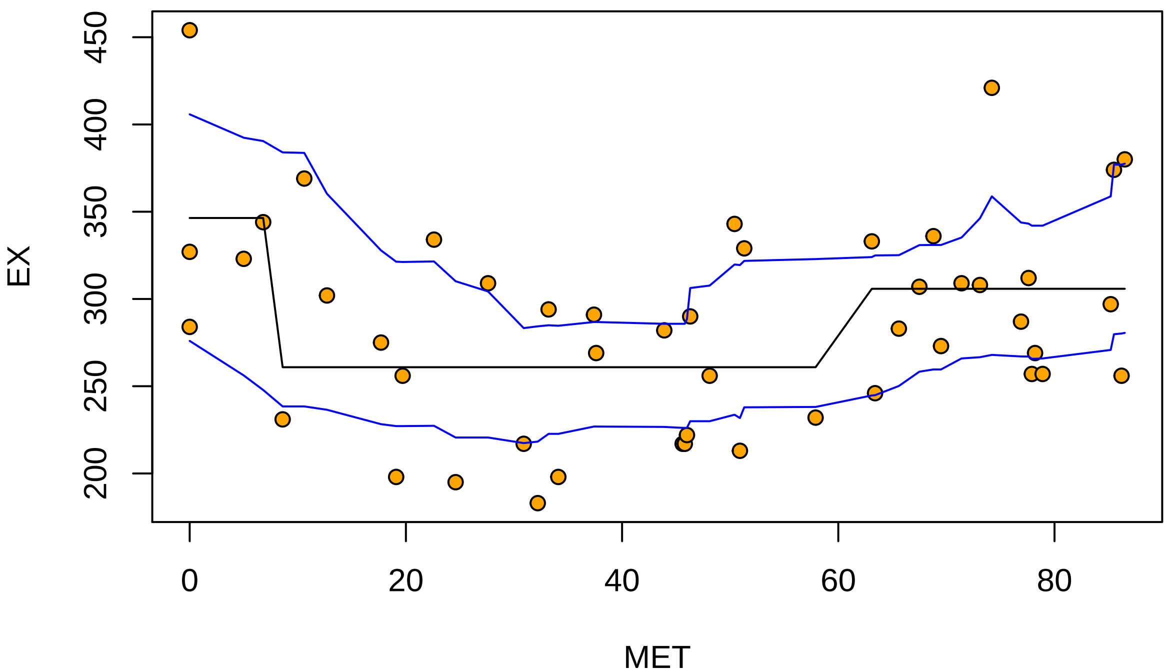
Looking at the histogram of residuals we can conclude that they don't look normal at all.

3. Compute and plot the 95% confidence bands for the regression tree model from step 2 (fit a regression tree with the same settings and the same number of leaves as in step 2 to the resampled data) by using a non-parametric bootstrap. Comment whether the band is smooth or bumpy and try to explain why. Consider the width of the confidence band and comment whether results of the regression model in step 2 seem to be reliable.

We have used the `boot()` function in order to generate 1000 bootstrap replicates. The statistic of interest in our case is the vector of predictions obtained in each regression tree (fitted with all the bootstrap sample).

Once we have had the 1000 vectors of predictions the `envelope()` function has been used to compute the confidence bands.

Then we can plot the observations with the estimate line (in black) and the confidence intervals (blue lines):



We observe that the bands' shapes are bumpy: the lines are rising and falling irregularly.

Also, the width of the confidence band is quite wide, but it does not include most of the points. We only have 48 observations and many of them are outside the 95% confidence band which is an indication that our model is not good, as we saw in step (2). If the model would fit well the data, then 95% of the observations would be inside of the confidence bands.

The width of the confidence band is wide because we don't have many observations. If we had considered more data points, the confidence bands would be near the curve (fitted black line). Generally, larger sample sizes tend to produce narrower confidence intervals.

4. Compute and plot the 95% confidence and prediction bands the regression tree model from step 2 by using a parametric bootstrap, assume $Y \sim N(\mu_i, \sigma^2)$ where μ_i are labels in the tree leaves and σ^2 is the residual variance. Consider the width of the confidence band and comment whether results of the regression model in step 2 seem to be reliable. Does it look like only 5% of data are outside the prediction band? Should it be?

Steps followed to compute parametric bootstrap confidence and prediction bands:

1. Compute value MLE that estimates model parameters from the data: the maximum likelihoood estimates of the parameters in our case are computed with the function `prune.tree()` because our tree regression model is pruned with only 3 leaves.

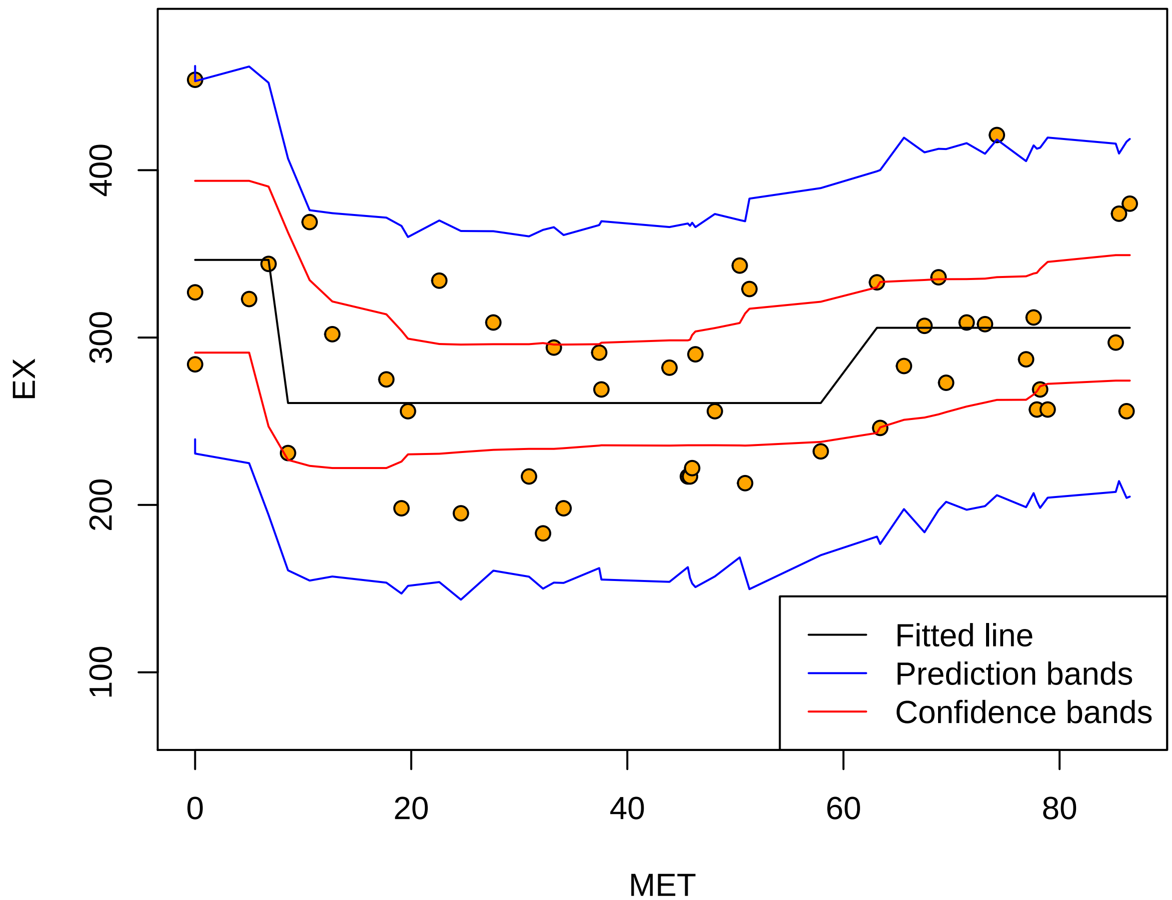
2. Write function "ran.gen" that depends on data and MLE and which generates new data. This function returns new values for the target variable "EX", generated from a normal distribution of μ = predictions of MLE and σ = residuals of MLE.

3. Write function "statistic" that depend on data which will be generated by ran.gen and should return the estimator. In this case two different statistics have been computed: prediction and confidence.

4. Make bootstrap for each statistic. We have used the `boot()`function for this in order to generate 1000 parametric bootstrap replicates of each statistic.

5. Compute the confidence and prediction bands with `envelope()`.

So, the plot of the 95% confidence and prediction bands:



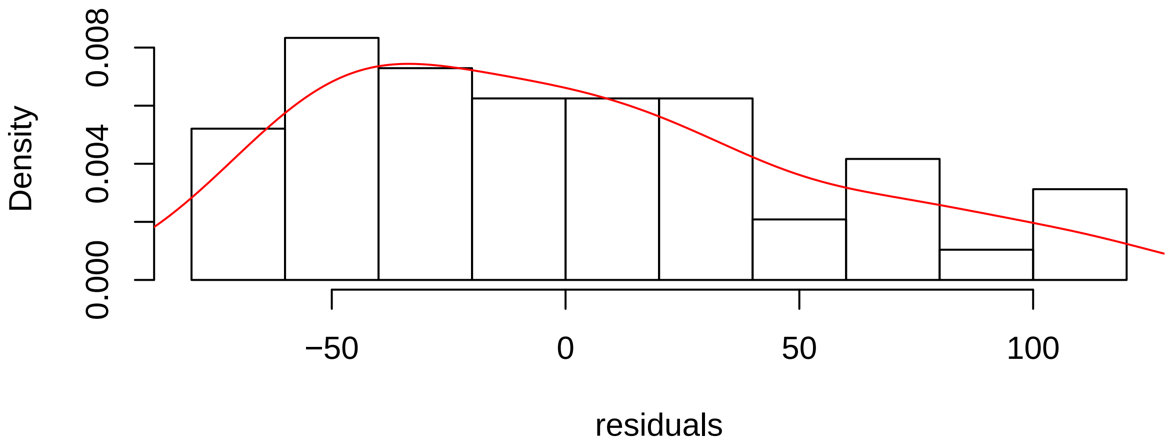
From the plot we observe that the prediction bands are quite wider than the confidence bands and that almost all the points are inside these bands. This is totally normal because the 95% confidence bands enclose the area that contains the true curve (at 95% confidence) while the 95% prediction bands takes in the area that one can **expect** to enclose 95% of future data points.

Also, we can see that there are only 1 point is outside the prediction bands (given that we have 48 points, that is the 1.2%), this is less than 5% and it is expected to be like this because only a maximum of 5% of new points can be outside given that the prediction bands are at 95% level.

Regarding the confidence bands, we see that they are a bit smoother than the ones using non-parametric bootstap. Still, many points (more than 5%) are outside the confidence bands so, again, the results of the regression model in step (2) don't seem to be reliable.

5. Consider the histogram of residuals from step 2 and suggest what kind of bootstrap is actually more appropriate here.

If we draw the density curve in the histogram of the residuals, we obtain the following plot:



Which makes us think that a Gamma distribution could be appropiate in this case. Then, the paramteric-bootstrap assuming that the target variable (EX) has a Gamma distribution would be a better option.

Assignment 4. Principal components.

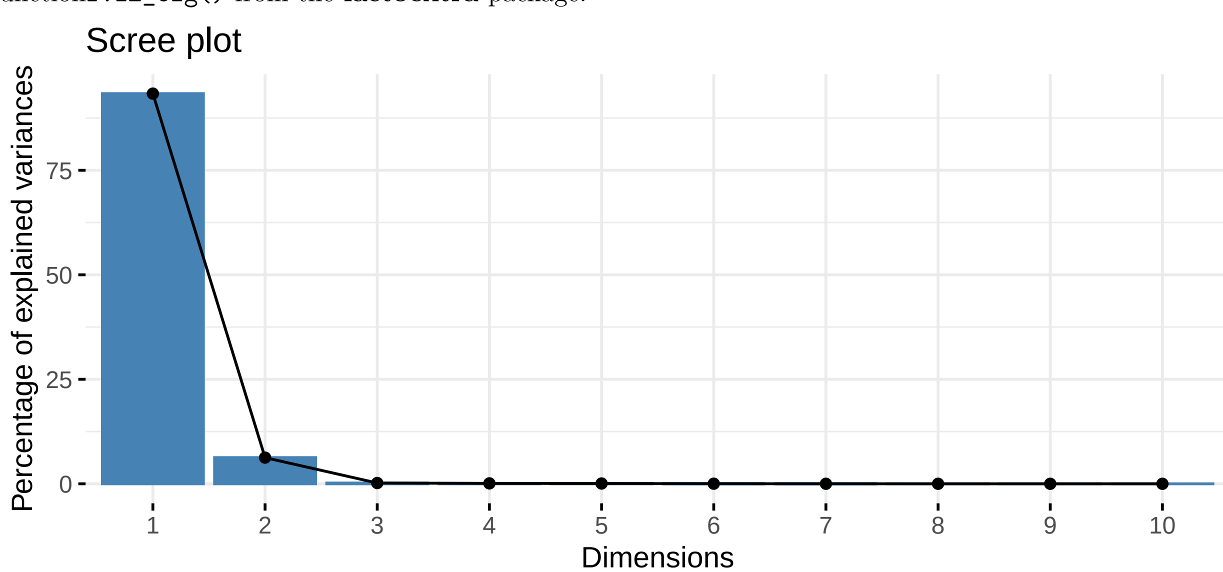
1. Conduct a standard PCA by using the feature space and provide a plot explaining how much variation is explained by each feature.

The Principal Component Analysis for all the different near-infrared spectra levels (variables 750 to 1000 from the original data frame) has been performed with the `prcomp()` function. In the following table it is possible to see how much variation is explained by each of the first five principal components as well as the cumulative proportion of variance.

```
##                            PC1     PC2     PC3     PC4     PC5
## Standard deviation     0.12206 0.03162 0.00544 0.00401 0.00330
## Proportion of Variance 0.93332 0.06263 0.00185 0.00101 0.00068
## Cumulative Proportion  0.93332 0.99596 0.99781 0.99882 0.99950
```

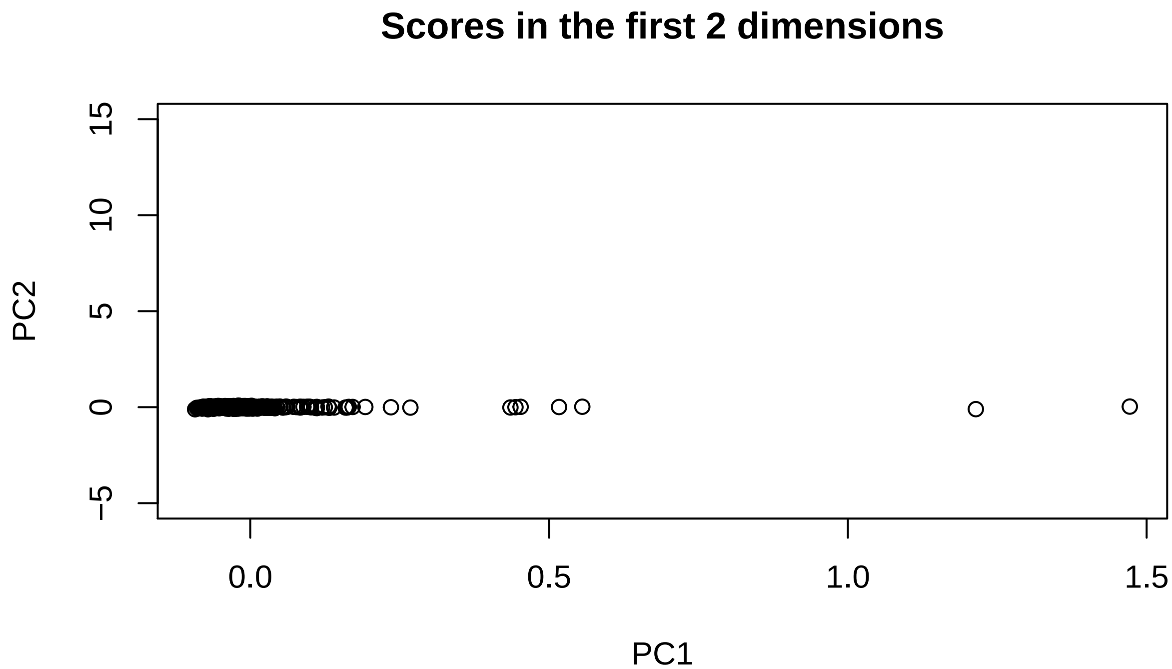
From the table we can observe that the first two principal components explain 99.6% of the total variance.

Also, we will plot the percentage of explained variation for each dimension (PC1 to PC10) with the function`fviz_eig()` from the **factoextra** package:



Again, we see that the first principal component explains more than 90% of the variance. Also, it is made evident that we should only extract 2 PC's in order to explain almost all the variation in our data (nearly without losing information).

Finally, we will plot the scores in in the coordinates (PC1, PC2).

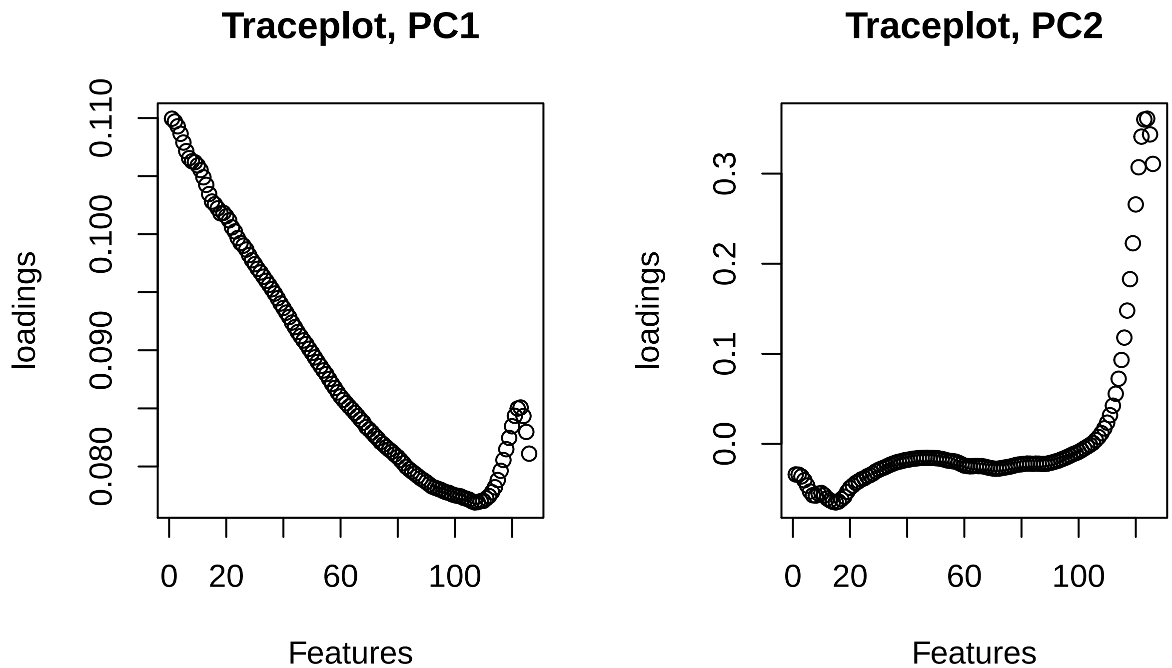


According to this plot there are unusual diesel fuels (outliers), those with high values in the x axis (PC1).There are two diesel fuels with very big scores compared to the others (1.4718634 & 1.2141754) which we can see on the far right part of the scores plot. Those are the more significant, but we can observe around 4 more fuels having quite big scores (0.5555528 0.5166276 0.4523158 0.4437367), those who are around in the middle of the plot.

More or less we can say that the unusual diesel fuels have a PC1 score greater than 0.4.

2. Make trace plots of the loadings of the components selected in step 1. Is there any principle component that is explained by mainly a few original features?

Since in question (1) we selected PC1 and PC2, now we will make a trace plot for each one:




```
## Variables with higest loadings in PC1:

##      X750      X752      X754      X756      X758      X760
## 0.1099439 0.1096993 0.1092886 0.1086458 0.1078912 0.1071514

## Variables with higest loadings in PC2:

##      X996      X994      X998      X992     X1000      X990
## 0.3609749 0.3601228 0.3435218 0.3410492 0.3108059 0.3070516
```

However, the variables with highest loadings don't differ too much from the rest (as observed in the PC1 plot), so we can't choose only a few original features that explain PC1.

Regarding the traceplot for PC2, we can observe that PC2 is basically explained by the 124th (X996) and 123th (X994) variables which have the biggest loadings (0.3609748774 and 0.3601227691, respectively)

3. Perform Independent Component Analysis with the number of components selected in step 1 (set seed 12345). Check the documentation for the fastICA method in R and do the following:

a. Compute $W' = K \cdot W$ and present the columns of W' in form of the trace plots. Compare with the trace plots in step 2 and make conclusions. What kind of measure is represented by the matrix W'?

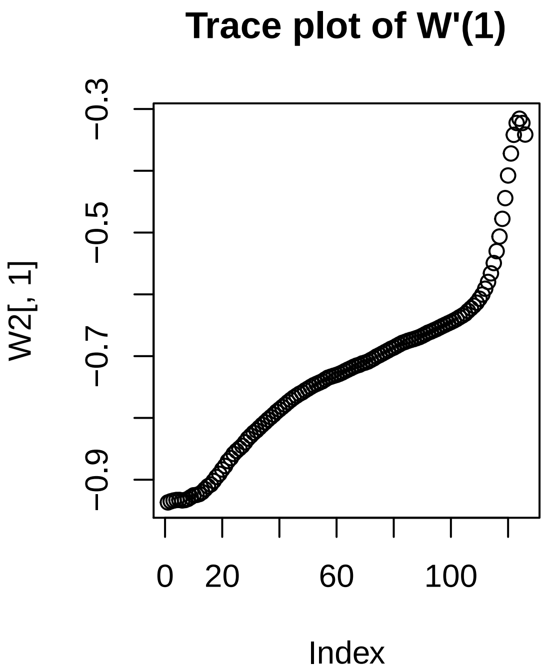
Matrix definitions, obtained from `fastICA()` function:

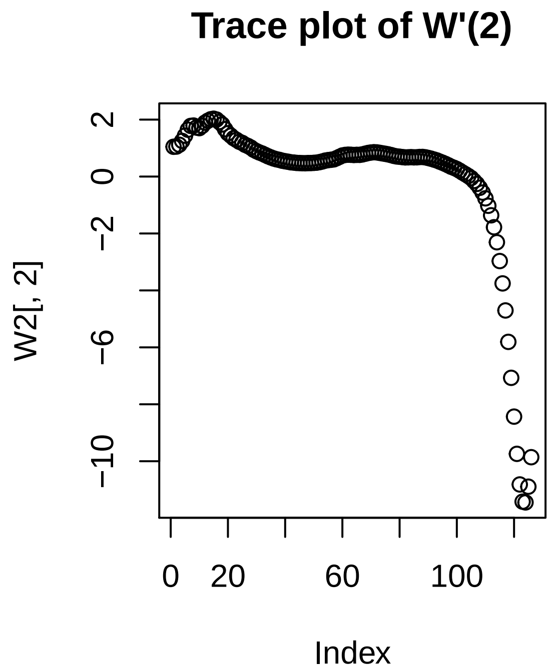
```
K: pre-whitening matrix that projects data onto the first n.comp principal components.
W: estimated un-mixing matrix that maximizes the non-gaussianity of the sources.
```

We use `fastica()` with the data frame containung the variables 750 to 1000 from the original data set (*NIRspectra*) and indicating in the **n.comp** argument that the number of components to be extracted is 2.

So, the output W matrix is a 2x2 matrix and K has 126 rows and 2 columns. Then, when computing $W' = K \cdot W$ we only need to use the command "%*%" and the obtained matrix (W') will have 126x2 dimensions.

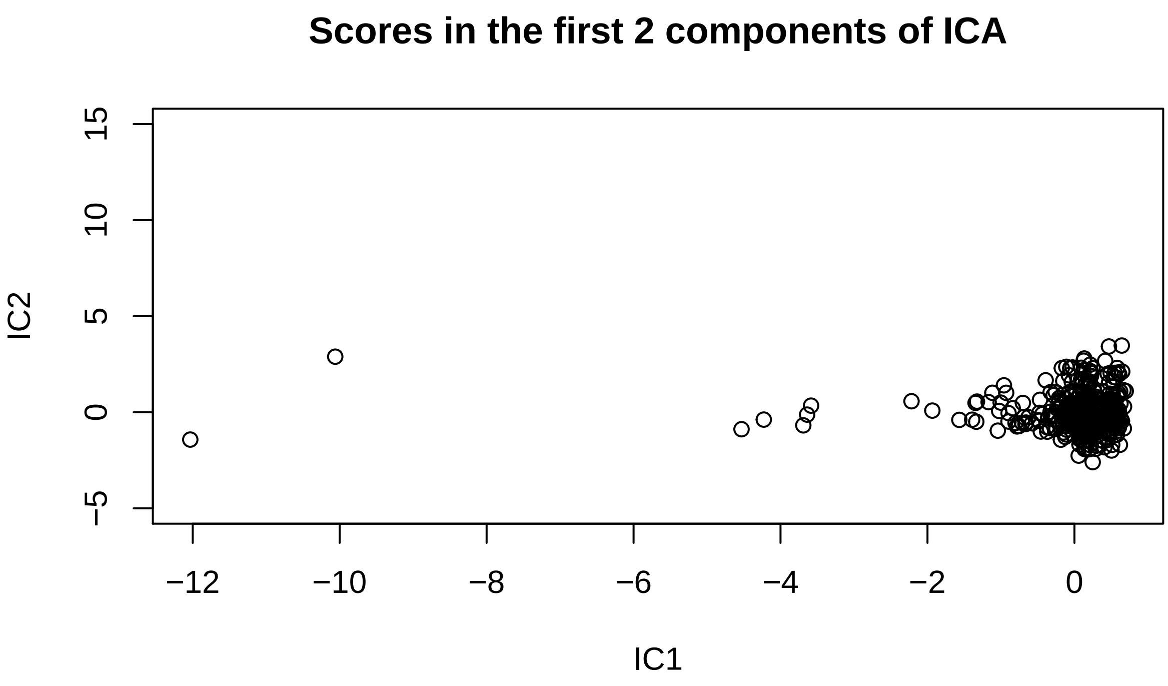
We will plot the W' values in each principal component, which represent the loadings of the variables in the Independent Component Analysis:





If we compare these two trace plots with the ones obtained in step (2) we observe that the loadings in ICA are the reversed PCA loadings.

b. Make a plot of the scores of the first two latent features and compare it with the score plot from step 1.



Again, we can observe that the plot in ICA is the reversed image of the PCA's scores plot. So, we still observe some unusual diesel fuels values.

Appendix

```r
## ----- ASSIGNMENT 2 ----- ##
# Changing the version:
RNGversion('3.5.1')

# Importing the data:
library(readxl)
data <- read_excel("creditscoring.xls")
data$good_bad <- as.factor(data$good_bad)

# Dividing it into training, validation and test sets:
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]

id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.25))
valid=data[id2,]

id3=setdiff(id1,id2)
test=data[id3,]
library(tree)

# 2.1. Fitting the models.
fit_dev = tree(good_bad~., data=train, split = "deviance") # Impurity measure: Deviance
fit_gini = tree(good_bad~., data=train, split = "gini") # Impurity measure: Gini index

# 2.2. Predictions.
## For the test data:
fitted_dev_test <- predict(fit_dev, newdata = test, type = "class")
fitted_gini_test <- predict(fit_gini, newdata = test, type = "class")

## For the training data:
fitted_dev_train <- predict(fit_dev, newdata = train, type = "class")
fitted_gini_train <- predict(fit_gini, newdata = train, type = "class")

# 2.3. Misclassification rates.
## For the test data:
mis_rate_dev_test <- mean(fitted_dev_test != test$good_bad)
mis_rate_gini_test <- mean(fitted_gini_test != test$good_bad)

## For the training data:
mis_rate_dev_train <- mean(fitted_dev_train != train$good_bad)
mis_rate_gini_train <- mean(fitted_gini_train != train$good_bad)
data.frame(cbind("Test data"=mis_rate_dev_test,"Training data"=mis_rate_dev_train))
data.frame(cbind("Test data"=mis_rate_gini_test,"Training data"=mis_rate_gini_train))
library(ggplot2)

# 3.1. Fitting the model
fit = tree(good_bad~., data=train, split = "deviance")
# summary(fit) -> Number of terminal nodes is 12
```

```r
# 3.2. Pruning trees with difference depths
trainScore=rep(0,15)
testScore=rep(0,15)

for(i in 2:15) {
  prunedTree=prune.tree(fit,best=i)
  pred=predict(prunedTree, newdata=valid, type="tree")

  trainScore[i]=deviance(prunedTree)
  testScore[i]=deviance(pred)
}
# 3.3. Plot of deviance vs. depth
df <- data.frame(depth=2:15, score= c(trainScore[2:15],testScore[2:15]), data= rep(c("Train", "Validati

ggplot(df, aes(x = depth, y = score, group = data, color = data)) + geom_point() + geom_line() + ggtitl
# 3.4. Optimal tree.
finalTree=prune.tree(fit, best=4)
{plot(finalTree)
text(finalTree, pretty=0)}
# 3.5. Misclassification rate for the test data.
fitted_best_test=predict(finalTree, newdata=test, type="class") # predictions
# table(fitted_best_test, test$good_bad) confussion matrix
mean(fitted_best_test != test$good_bad) # error rate
library(e1071)

# 4.1. Fitting the model.
fit_naive=naiveBayes(good_bad~., data=train)

# 4.2. Predictions.
fitted_test <- predict(fit_naive, newdata = test, type = "class") # For the test data
fitted_train <- predict(fit_naive, newdata = train, type = "class") # For the training data
# 4.3. Confusion matrices.
table(test$good_bad, fitted_test)
table(train$good_bad, fitted_train)
# 4.4. Misclassification rates.
cat("For the test data:", mean(fitted_test != test$good_bad),"\n")
cat("For the training data:", mean(fitted_train != train$good_bad),"\n")
# 5.1. Classification models:
## Naive Bayes model
fit_naive=naiveBayes(good_bad~., data=train)

## Optimal tree (4 terminal nodes)
fit = tree(good_bad~., data=train, split = "deviance")
fit_optimal=prune.tree(fit, best=4)

# 5.2. Predictions:
## Naive Bayes
fitted_naive <- predict(fit_naive, newdata = test, type="raw") # type raw to get probabilities

## Optimal tree
fitted_tree <- predict(fit_optimal, newdata = test)

# 5.3. Classification using the principle.
```

```r
pi <- seq(0.05, 0.95, by=0.05)

fitted_naive_class <- data.frame(matrix(ncol = length(pi), nrow = nrow(test)))
fitted_tree_class <- data.frame(matrix(ncol = length(pi), nrow = nrow(test)))
colnames(fitted_naive_class) <- pi
colnames(fitted_tree_class) <- pi

for(i in 1:length(pi)){
  fitted_naive_class[,i] <- ifelse(fitted_naive[,2] > pi[i], 1, 0)
  fitted_tree_class[,i] <- ifelse(fitted_tree[,2] > pi[i], 1, 0)
}

# 5.4. Computation of TPR and FPR: TPR=TP/(TP+FN) and FPR=FP/(FP+TN)
library(EvaluationMeasures)
real_values <- ifelse( test$good_bad == "good", 1, 0)

result <- data.frame(matrix(ncol = 4, nrow = length(pi)*2))
colnames(result) <- c("pi", "model", "TPR", "FPR")
result$pi <- rep(pi,2)
result$model <- rep(c("Naive", "Tree"),each=length(pi))

for(i in 1:ncol(fitted_naive_class)){
  result[i,3] <- EvaluationMeasures.TPR(Real= real_values, Predicted = fitted_naive_class[,i], Positive
  result[i+19,3] <- EvaluationMeasures.TPR(Real= real_values, Predicted = fitted_tree_class[,i], Positi

  result[i,4] <- EvaluationMeasures.FPR(Real= real_values, Predicted = fitted_naive_class[,i], Positive
  result[i+19,4] <- EvaluationMeasures.FPR(Real= real_values, Predicted = fitted_tree_class[,i], Positi
}
cbind(result[1:19,], result[20:38,])
# 5.5. ROC curve.
ggplot(result, aes(x = FPR, y=TPR)) + geom_line(aes(colour = model)) + geom_abline(intercept=1, slope =
  ggtitle("ROC curve") + theme_light()
# 6.1. Naive Bayes model.
fit =naiveBayes(good_bad~., data=train)

# 6.2. Predictions
# Probabilities (type= "raw")
fitted_prob_test <- predict(fit_naive, newdata = test, type="raw") # test data
fitted_prob_train <- predict(fit_naive, newdata = train, type="raw") # training data

# 6.3. Classification using the loss matrix.
fitted_class_test <- ifelse(fitted_prob_test[,2]/fitted_prob_test[,1] > 10, "good", "bad")
fitted_class_train <- ifelse(fitted_prob_train[,2]/fitted_prob_train[,1] > 10, "good", "bad")
# 6.4. Confusion matrices.
table(test$good_bad, fitted_class_test)
table(train$good_bad, fitted_class_train)
# 6.5. Misclassification rates.
cat("For the test data:", mean(fitted_class_test != test$good_bad),"\n")
cat("For the training data:", mean(fitted_class_train != train$good_bad),"\n")
## ----- ASSIGNMENT 3 ----- ##
# Importing the data:
data <- read.table("State.csv", header=TRUE, sep=";", dec=",")
```

```r
# Data reordered by MET
data <- data[order(data$MET),]

# Plot
plot(data$MET, data$EX, xlab="MET", ylab="EX", main="Plot of EX vs. MET", pch=19, cex=0.85)
# 2.1. Fitting a regression tree model.
fit <- tree(EX~ MET , data=data, control=tree.control(nobs= nrow(data), minsize = 8))

# 2.2. Selecting the optimal number of leaves by cross-validation.
set.seed(12345)
cv.tree=cv.tree(fit)

# 2.3. Fitting the optimal regression tree.
best.size <- cv.tree$size[which(cv.tree$dev==min(cv.tree$dev))]
fit_optimal <- prune.tree(fit, best=best.size)
summary(fit_optimal)
# 2.4. Plot of the original and the fitted data.
ggplot()+ geom_point(mapping = aes(x=data$MET,y=data$EX,color='Original'))+
  geom_point(mapping = aes(x=data$MET,y=predict(fit_optimal,newdata = data),color='Fitted'))+
  labs(y="EX",x='MET')
# 2.5 Histogram of residuals.
pred <- predict(fit_optimal, newdata = data)
resid <- data$EX-pred
df <- as.data.frame(resid)

ggplot(df, aes(x=resid)) + geom_histogram(color="black", fill="lightblue", bins=15)+ theme_light() + xla
# 3. Non-parametric bootstrap CI
library(boot)

# 3.1. First we need to compute bootstrap samples
f=function(data, ind){
  # extract bootstrap sample
  data1 = data[ind,]

  # fit regression tree model
  fit = tree(EX~ MET , data=data1, control=tree.control(nobs= nrow(data1), minsize = 8))
  fit_optimal <- prune.tree(fit, best=3)

  # predict values from the original data
  predictions = predict(fit_optimal, newdata=data)

  return(predictions)
}

# 3.2. And now we can make bootstrap:
res=boot(data, f, R=1000)

# 3.3. Bootstrap cofidence bands
e=envelope(res) #compute confidence bands

# 3.4. Plotting the predicted line and 95% confidence bands
fit <- tree(EX~ MET , data=data, control=tree.control(nobs= nrow(data), minsize = 8))
cv.tree=cv.tree(fit)
```

```
fit_optimal <- prune.tree(fit, best=3)

predictions =predict(fit_optimal)

{plot(data$MET, data$EX, xlab="MET", ylab="EX", pch=21, bg="orange")
points(data$MET,predictions,type="l") #plot fitted line
#plot cofidence bands
points(data$MET,e$point[2,], type="l", col="blue")
points(data$MET,e$point[1,], type="l", col="blue")}
# 4. Parametric bootstrap confidence and prediction bands
# 4.1. Compute value mle that estimates model parameters from the data:
fit <- tree(EX~ MET , data=data, control=tree.control(nobs= nrow(data), minsize = 8))
cv.tree=cv.tree(fit)
mle <- prune.tree(fit, best=3)

# 4.2. Write function ran.gen that depends on data and mle and which generates new data.
rng=function(data, mle) {
  data1=data.frame(Ex=data$EX, MET=data$MET)
  n=length(data$EX)

  #generate new EX (mle$residuals doesn't exist for prune.tree)
  data1$EX=rnorm(n,predict(mle, newdata=data1),sd(residuals(mle)))
  return(data1)
}

# 4.3. Write function "statistic" that depend on data which will be generated by ran.gen and should ret
# 4.3.1. Bootstrap samples for prediction bands
f_pred=function(data1){
  #fit linear model
  fit = tree(EX~ MET , data=data1, control=tree.control(nobs= nrow(data1), minsize = 8))
  fit_optimal <- prune.tree(fit, best=3)

  #predict values for all MET values from the original data
  n=length(data$EX)
  predictions_pred = rnorm(n,predict(fit_optimal, newdata=data), sd(residuals(mle)))
  return(predictions_pred)
}

# 4.3.2. Bootstrap samples for condicence bands
f_conf=function(data1){
  # fit regression tree model
  fit = tree(EX~ MET , data=data1, control=tree.control(nobs= nrow(data1), minsize = 8))
  fit_optimal <- prune.tree(fit, best=3)

  # predict values from the original data
  predictions_conf = predict(fit_optimal, newdata=data)

  return(predictions_conf)
}

# 4.4 Now we can make bootstrap for each statistic:
res_pred=boot(data, statistic=f_pred, R=1000, mle=mle, ran.gen=rng, sim="parametric")
res_conf=boot(data, statistic=f_conf, R=1000, mle=mle, ran.gen=rng, sim="parametric")
```

```
# 4.5. Parametric bootstrap bands
e_pred=envelope(res_pred) # compute prediction bands
e_conf=envelope(res_conf) # compute confidence bands

# 4.5. Plotting the predicted line and 95% confidence and prediction bands
estimated_line =predict(fit_optimal)

{plot(data$MET, data$EX, xlab="MET", ylab="EX", pch=21, bg="orange", ylim=c(70,480))
points(data$MET,estimated_line,type="l") #plot fitted line
#plot prediction bands
points(data$MET,e_pred$point[2,], type="l", col="blue")
points(data$MET,e_pred$point[1,], type="l", col="blue")
#plot confidence bands
points(data$MET,e_conf$point[2,], type="l", col="red")
points(data$MET,e_conf$point[1,], type="l", col="red")
legend("bottomright",legend=c("Fitted line","Prediction bands", "Confidence bands"), lty = c(1,1,1), col
dens = density(resid)
hist(resid, freq=F, xlab="residuals", main=NULL) #probability densities
lines(dens,col="red")
## ----- ASSIGNMENT 4 ----- ##
# Importing the data:
data4 <- read.table("NIRspectra.csv", header=TRUE, sep=";", dec=",")

# Standard PCA
data_pca <- data4[,-127] #  the feature space
pca <- prcomp(data_pca)
round(summary(pca)$importance[,1:5],5)
# Plot of the variation explained by each PC.
library(factoextra)
fviz_eig(pca)
plot(pca$x[,1], pca$x[,2], ylim=c(-5,15), xlab="PC1", ylab="PC2", main="Scores in the first 2 dimension
U= pca$rotation
par(mfrow=c(1,2))
plot(U[,1], main="Traceplot, PC1", xlab="Features",ylab="loadings")
plot(U[,2],main="Traceplot, PC2", xlab="Features", ylab="loadings")

cat("Variables with higest loadings in PC1:\n")
head(sort(U[,1], decreasing = TRUE))
cat("Variables with higest loadings in PC2:\n")
head(sort(U[,2], decreasing = TRUE))
library(fastICA)
set.seed(12345)

ICA <- fastICA(data_pca,2)
W2 <- ICA$K %*% ICA$W

par(mfrow=c(1,2))
plot(W2[,1], main = "Trace plot of W'(1)")
plot(W2[,2], main = "Trace plot of W'(2)")
plot(ICA$S[,1], ICA$S[,2],ylim=c(-5,15), xlab="IC1", ylab="IC2", main="Scores in the first 2 components
```