

EXAM

Advanced Statistical Analysis and Machine Learning

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Exercise C

Let consider the files data1 and data2.

For data1, we want to explain the development while in data2, we want to explain the Grade. By considering the nature of the variables, create several models and give the best one.

C.1. DATA 1

C.1.1. Loading of libraries

```
library(ggplot2)
library(ggpubr)
library(Matrix)
library(glmnet)
```

C.1.2. Importation of the data

```
set.seed(3333)
D1 = read.csv('data1.csv', header=TRUE, sep=';')
dim(D1)
## [1] 12
head(D1)
##
                  Treatment Psychologist Development
     Children
## 1
                    placebo
                                        2
                                                  36.8
## 2
            2 produit actif
                                                  93.7
                                        1
## 3
            3
                                                  56.6
                    placebo
                                        1
                                                  37.7
## 4
            4
                    placebo
                                        1
                                        2
## 5
            5 produit actif
                                                  70.3
## 6
                    placebo
                                        1
                                                  24.2
str(D1)
## 'data.frame':
                    12 obs. of 4 variables:
```

```
## 'data.frame': 12 obs. of 4 variables:
## $ Children : int 1 2 3 4 5 6 7 8 9 10 ...
## $ Treatment : chr "placebo" "produit actif" "placebo" "placebo" ...
## $ Psychologist: int 2 1 1 1 2 1 2 2 1 2 ...
## $ Development : num 36.8 93.7 56.6 37.7 70.3 24.2 42.5 50.9 71.8 72.5 ...
```

We have at our disposal a small dataset containing two qualitative explanatory variables associated with a quantitative response variable.

As a first step, we convert the type of the qualitative variables ("Treatment" and "Psychologist") into factors.

```
D1$Psychologist = as.factor(D1$Psychologist)
D1$Psychologist

## [1] 2 1 1 1 2 1 2 2 1 2 1 2

## Levels: 1 2

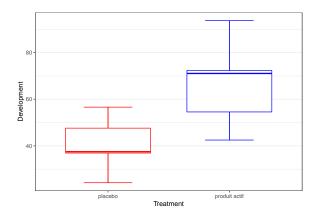
D1$Treatment = as.factor(D1$Treatment)
D1$Treatment

## [1] placebo produit actif placebo produit actif
```

Elimination of the column "Children".

```
D1$Children = NULL
```

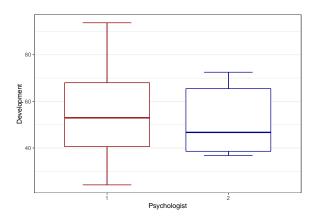
C.1.4. Visualization of the data



The above figure represents the boxplots of the explanatory variable "Treatment" with respect to the response variable "Development".

We see that our boxplots for the modality "placebo" and "produit actif" are different: the median of the modality "produit actif" is bigger than the median of the modality "placebo", and the observations of the modality "produit actif" are distributed at a higher level than the observations of the modality "placebo".

 \Rightarrow We can anticipate that there will be some influence of the variable "Treatment" onto the response variable "Development".



The above figure represents the boxplots of the explanatory variable "Psychologist" with respect to the response variable "Development".

We can note that the two boxplots are quiet at the same level and present the same dispersion.

 \Rightarrow We have the impression that there will be no influence of the factor "Psychologist" onto the response variable "Development".

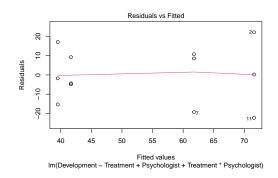
C.1.5. Assumption

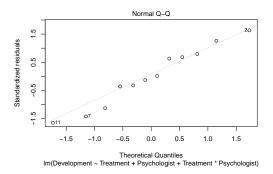
The goal in this step is to check the gaussianity of the noise.

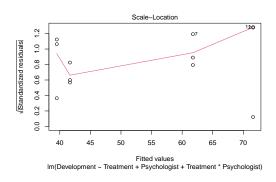
```
L1.c = lm(Development ~ Treatment + Psychologist + Treatment * Psychologist
          , data=D1)
summary(L1.c)
##
## Call:
## lm(formula = Development ~ Treatment + Psychologist + Treatment *
##
      Psychologist, data = D1)
##
## Residuals:
##
      Min
                1Q
                   Median
                                3Q
                                       Max
## -22.300 -7.475
                   -0.800
                             9.608
                                    22.100
##
## Coefficients:
##
                                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                                          39.500
                                                      9.580
                                                              4.123 0.00333 **
## Treatmentproduit actif
                                          32.100
                                                     13.548
                                                              2.369
                                                                     0.04530 *
## Psychologist2
                                           2.167
                                                     13.548
                                                              0.160 0.87691
## Treatmentproduit actif:Psychologist2 -12.000
                                                     19.160
                                                            -0.626 0.54857
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 16.59 on 8 degrees of freedom
## Multiple R-squared: 0.4992, Adjusted R-squared: 0.3114
## F-statistic: 2.658 on 3 and 8 DF, p-value: 0.1196
```

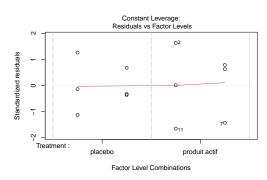
- From the "summary(L1.c)" we note that there is some symmetry of the "Residuals" with respect to the median and the median is close to 0.

plot(L1.c)









- In the "Residuals vs Fitted" plot presents some symmetry. Thus, we can consider that the noise is centered. The homoscedasticity can be retained.
- In the "Normal Q-Q" plot we can see that the cloud of points is distributed along the line. We can accept the gaussianity of the noise.

For further checking, we perform Kolmogorov test:

```
sres1 = rstandard(L1.c)
ks.test(sres1, 'pnorm')

##

## One-sample Kolmogorov-Smirnov test
##
## data: sres1
## D = 0.15227, p-value = 0.9048
## alternative hypothesis: two-sided
```

The p-value of the Kolmogorov-Smirnov test is equal to $0.9048 > 0.05 \implies$ we accept the gaussianity of the noise.

With the gaussianity of the noise being checked, we can now investigate all the elements provided by the "lm" function.

From the "summary(L1.c)" we can see that the p-value of the model is equal to 0.1196 > 0.05.

- \Rightarrow We accept H_0 in this test (all the coefficients are null).
- ⇒ We cannot consider a linear model between all the explanatory variables and the response variable.

By looking at the column "Pr(> |t|)", some p-values are bigger than 0.05 while others are smaller than 0.05.

 \Rightarrow we have to perform variable selection to improve our model.

C.1.6. ANOVA model

We begin by performing ANOVA for the complete model: additive model with cross effect

```
## Analysis of Variance Table
##
## Response: Development
##
## Df Sum Sq Mean Sq F value Pr(>F)
## Treatment 1 2043.63 2043.63 7.4222 0.02607 *
## Psychologist 1 44.08 44.08 0.1601 0.69953
```

```
## Treatment:Psychologist 1 108.00 108.00 0.3922 0.54857
## Residuals 8 2202.71 275.34
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

The application of the ANOVA procedure shows a p-value for the cross effect (Treatment:Psychologist) equal to $0.54857 > 0.05 \Rightarrow$ the cross effect has no influence on the response variable.

In this case, we construct the additive model:

##

(Intercept)

```
L1.a = lm(Development ~ Treatment + Psychologist, data=D1)
anova(L1.a)
## Analysis of Variance Table
## Response: Development
               Df Sum Sq Mean Sq F value Pr(>F)
## Treatment
                1 2043.63 2043.63 7.9597 0.0200 *
## Psychologist 1 44.08
                            44.08 0.1717 0.6883
## Residuals 9 2310.71 256.75
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
- For the row "Treatment" we have p-value = 0.0200 < 0.05
⇒ "Treatment" has an influence on the response variable "Development".
- For the row "Psychologist" we have p-value = 0.6883 > 0.05
⇒ "Psychologist" has no influence on the response variable "Development".
We have to consider a model with only the factor "Treatment" to take a conclusion.
L1.Treatment = lm(Development ~ Treatment, data=D1)
anova(L1.Treatment)
## Analysis of Variance Table
##
## Response: Development
             Df Sum Sq Mean Sq F value Pr(>F)
## Treatment 1 2043.6 2043.63 8.6786 0.01464 *
## Residuals 10 2354.8 235.48
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
summary(L1.Treatment)
##
## Call:
## lm(formula = Development ~ Treatment, data = D1)
## Residuals:
       Min
                  1Q Median
                                    ЗQ
                                             Max
## -24.1833 -6.9333 0.3667
                                6.9417 27.0167
## Coefficients:
```

Estimate Std. Error t value Pr(>|t|)

6.265 6.478 7.09e-05 ***

40.583

```
## Treatmentproduit actif 26.100 8.860 2.946 0.0146 *
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 15.35 on 10 degrees of freedom
## Multiple R-squared: 0.4646, Adjusted R-squared: 0.4111
## F-statistic: 8.679 on 1 and 10 DF, p-value: 0.01464
```

We can conclude that the best model with ANOVA method is: Development ~ Treatment.

C.1.7. Step by step strategies: backward strategy

- We start by the complete model and suppress the variable which has the biggest p-value.
- We repeat the first step and stop once the biggest p-value becomes small (p-value $< \alpha$).

```
\mbox{\it\#} The linear model with all the explanatory variables and the cross effect L1.c
```

```
##
## Call:
## lm(formula = Development ~ Treatment + Psychologist + Treatment *
       Psychologist, data = D1)
##
## Coefficients:
##
                             (Intercept)
                                                         Treatmentproduit actif
##
                                  39.500
                                                                         32.100
##
                          Psychologist2 Treatmentproduit actif:Psychologist2
##
                                   2.167
                                                                        -12.000
```

• We apply the backward strategy with AIC criterion

```
L1.B.AIC = step(L1.c, direction='backward')
```

```
## Start: AIC=70.55
## Development ~ Treatment + Psychologist + Treatment * Psychologist
##
##
                           Df Sum of Sq
                                           RSS
                                                  AIC
                                108 2310.7 69.125
## - Treatment:Psychologist 1
## <none>
                                        2202.7 70.550
##
## Step: AIC=69.12
## Development ~ Treatment + Psychologist
##
##
                                        AIC
                 Df Sum of Sq
                                 RSS
## - Psychologist 1
                     44.08 2354.8 67.352
## <none>
                              2310.7 69.125
## - Treatment
                      2043.63 4354.3 74.728
##
## Step: AIC=67.35
## Development ~ Treatment
##
##
              Df Sum of Sq
                              RSS
                                     AIC
## <none>
                           2354.8 67.352
## - Treatment 1
                    2043.6 4398.4 72.849
```

L1.B.AIC

##

```
## Call:
## lm(formula = Development ~ Treatment, data = D1)
## Coefficients:
##
              (Intercept) Treatmentproduit actif
##
                    40.58
   • We apply the backward strategy with Fisher criterion
L1.B.Fisher = step(L1.c, direction='backward', test='F')
## Start: AIC=70.55
## Development ~ Treatment + Psychologist + Treatment * Psychologist
                           Df Sum of Sq
                                          RSS
                                                  AIC F value Pr(>F)
## - Treatment:Psychologist 1 108 2310.7 69.125 0.3922 0.5486
                                        2202.7 70.550
## <none>
##
## Step: AIC=69.12
## Development ~ Treatment + Psychologist
##
##
                 Df Sum of Sq
                                 RSS
                                        AIC F value Pr(>F)
## - Psychologist 1 44.08 2354.8 67.352 0.1717 0.6883
## <none>
                              2310.7 69.125
## - Treatment
                      2043.63 4354.3 74.728 7.9597 0.0200 *
                 1
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Step: AIC=67.35
## Development ~ Treatment
##
              Df Sum of Sq
                              RSS
                                     AIC F value Pr(>F)
## <none>
                           2354.8 67.352
## - Treatment 1
                    2043.6 4398.4 72.849 8.6786 0.01464 *
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
L1.B.Fisher
##
## Call:
## lm(formula = Development ~ Treatment, data = D1)
## Coefficients:
##
              (Intercept) Treatmentproduit actif
##
                    40.58
                                           26.10
```

We can conclude that the model resulting from the backward strategy is: Development ~ Treatment.

C.1.8. Step by step strategies: forward strategy

We create a linear model with just the intercept.

```
L1.1 = lm(D1$Development ~ 1, data=D1)
```

- We start by comparing all the models of dimension 1 and we keep the best variable associated to the smallest p-value.

- We repeat the first step and stop when the smallest p-value becomes too big (p-value> α). We stop at the step before.
 - We apply the forward strategy with AIC criterion

```
L1.F.AIC = step(L1.1, scope=list(L1.1, L1.c), direction='forward')
## Start: AIC=72.85
## D1$Development ~ 1
L1.F.AIC
##
## Call:
## lm(formula = D1$Development ~ 1, data = D1)
## Coefficients:
## (Intercept)
##
         53.63
    • We apply the forward strategy with Fisher criterion
L1.F.Fisher = step(L1.1, scope=list(L1.1, L1.c), direction='forward', test='F')
## Start: AIC=72.85
## D1$Development ~ 1
L1.F.Fisher
##
## Call:
## lm(formula = D1$Development ~ 1, data = D1)
## Coefficients:
## (Intercept)
         53.63
```

The model provided by the forward strategy is Development \sim (Intercept) and thus will not be retained.

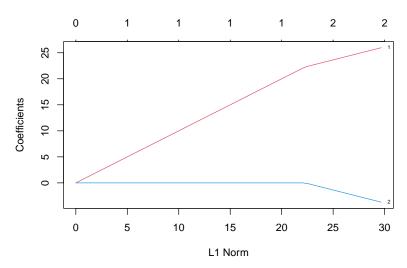
C.1.9. Lasso method

We are going to perform the Lasso method, the solution of which solves a penalized least squared criterion \Rightarrow we can write: $\widehat{\beta}_{Lasso,\lambda} = \min_{\beta} ||Y - X\beta||^2 + \lambda \sum_{i} |\beta_i|$

The penalty cost in the "glmnet" function is $\frac{1-\alpha}{2} \|\beta\|_2^2 + \alpha \|\beta\|_1$ with $\alpha \in [0,1]$ where $\|\beta\|_2^2$ is the penalty term for Ridge and $\|\beta\|_1$ is the penalty term for Lasso.

```
\Rightarrow We take \alpha = 1 to perform Lasso.
```

```
X1 = data.matrix(D1[, -3])
Y1 = D1$Development
D1.Lasso = glmnet(X1, Y1, alpha=1)
plot(D1.Lasso, col=c(2, 4), label=TRUE)
```



This graph gives the trajectories of the β_i obtained for different values of λ with respect to the \mathcal{L}_1 norm of the β vector.

When we decrease λ (increase the \mathcal{L}_1 norm), some coefficients become different from 0 but not all at the same time.

 \Rightarrow We obtain many models, one for each value of λ and we select the best value of λ .

To perform this, we apply 'cv.glmnet' function to compute the cross validation error for each model. Then we keep the best model presenting the lowest error.

Since we have a small dataset, we will take the number of the splitting in K-folds "nfolds = 3" (by default nfolds = 10).

```
D1.Lasso.cv = cv.glmnet(X1, Y1, alpha=1, nfolds=3)
##
## Call: cv.glmnet(x = X1, y = Y1, nfolds = 3, alpha = 1)
##
## Measure: Mean-Squared Error
##
##
       Lambda Index Measure
                                 SE Nonzero
## min 3.233
                 16
                      334.2 74.77
                      382.2 174.03
                                          0
## 1se 13.050
                  1
```

In order to delete the instability due to the search of a minimum, we look for the "1se" row and not the "min".

```
D1.best.Lambd = D1.Lasso.cv$lambda.1se
D1.best.Lambd
```

```
## [1] 13.05
```

We plug the λ of the "1se" row into the "glmnet" function to obtain the best model for the Lasso.

```
D1.best.Lasso = glmnet(X1, Y1, alpha=1, lambda=D1.best.Lambd)
coefficients(D1.best.Lasso)

## 3 x 1 sparse Matrix of class "dgCMatrix"

## s0

## (Intercept) 5.363333e+01

## Treatment 1.275321e-14

## Psychologist .
```

We can conclude that the best model with Lasso method is: Development \sim Treatment.

Since the Lasso is a biased model we will only consider the information about the selected variables and not the estimated coefficients it provides.

To obtain an unbiased model we apply classical ordinary squared to the selected variables by the Lasso.

C.1.10. Conclusion

All the considered approaches: ANOVA method, Step by Step method and Lasso method suggest the same model that is Development ~ Treatment.

Applying the "lm" function, we obtain the below parameters for this model:

```
L1.best = lm(Development ~ Treatment, data=D1)
L1.best
##
## Call:
## lm(formula = Development ~ Treatment, data = D1)
##
## Coefficients:
##
              (Intercept)
                          Treatmentproduit actif
##
                    40.58
summary(L1.best)
##
## Call:
## lm(formula = Development ~ Treatment, data = D1)
##
## Residuals:
##
       Min
                  1Q
                     Median
                                    3Q
                                            Max
                      0.3667
                                        27.0167
## -24.1833 -6.9333
                                6.9417
##
## Coefficients:
##
                          Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                            40.583
                                        6.265
                                                6.478 7.09e-05 ***
## Treatmentproduit actif
                            26.100
                                        8.860
                                                2.946
                                                        0.0146 *
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 15.35 on 10 degrees of freedom
## Multiple R-squared: 0.4646, Adjusted R-squared: 0.4111
## F-statistic: 8.679 on 1 and 10 DF, p-value: 0.01464
```

C.2. DATA 2

C.2.1. Loading of libraries

```
library(ggplot2)
library(ggpubr)
library(MASS)
library(leaps)
library(Matrix)
library(glmnet)
library(dplyr)
library(VSURF)
```

```
C.2.2. Importation of the data
set.seed(3333)
D2 = read.csv('data2.csv', header=TRUE, sep=';')
dim(D2)
## [1] 16 6
head(D2)
##
    Product Sugar Acid Bitter Pulpy Grade
## 1
        1 6.21 7.08 2.00 2.54 4.97
## 2
          2 7.75 3.29 1.54 2.26 6.98
## 3
          3 7.21 4.38 1.79 2.58 4.58
## 4
          4 8.33 2.79 1.63 2.71 6.45
          5 4.87 7.71
## 5
                        1.96 1.70 4.33
          6 5.09 7.50
                        2.13 2.42 4.26
## 6
str(D2)
## 'data.frame':
                   16 obs. of 6 variables:
## $ Product: int 1 2 3 4 5 6 7 8 9 10 ...
## $ Sugar : num 6.21 7.75 7.21 8.33 4.87 5.09 6.04 6.09 6.08 6.17 ...
## $ Acid : num 7.08 3.29 4.38 2.79 7.71 7.5 6.58 5.13 5.5 5.58 ...
## $ Bitter : num 2 1.54 1.79 1.63 1.96 2.13 2.04 2 2.09 2.13 ...
## $ Pulpy : num 2.54 2.26 2.58 2.71 1.7 2.42 2.04 2.42 2.46 2.48 ...
   $ Grade : num 4.97 6.98 4.58 6.45 4.33 4.26 6.16 6.26 5.83 5.74 ...
```

We have at our disposal a small dataset containing four quantitative explanatory variables associated with a quantitative response variable.

As we have a small dataset, a false correlation phenomenon may occur.

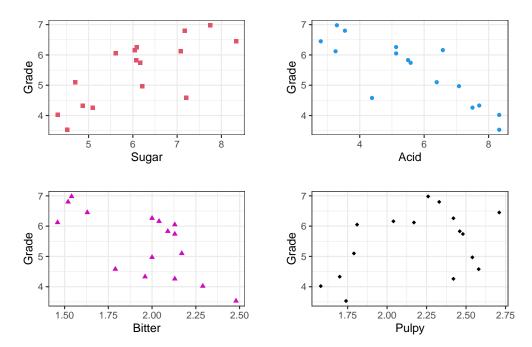
C.2.3. Preparation of the data

• Elimination of the column "Product"

```
D2$Product = NULL
```

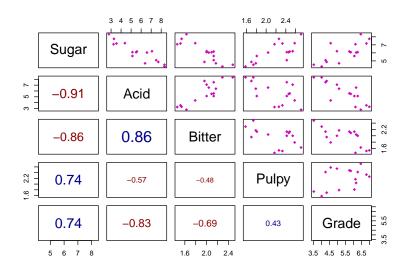
C.2.4. Visualization of the data

• Scatter plot:



• pairs plot:

```
# Correlation panel
panel.cor <- function (x, y) {
    usr = par('usr'); on.exit(par(usr))
    par(usr = c(0, 1, 0, 1))
    r = round(cor(x, y), digits=2)
    txt = pasteO('', r)
    cex.cor = 0.6 / strwidth(txt)
    text(0.5, 0.5, txt, cex=abs(cex.cor*r), col=c('darkred', 'darkblue')[floor(r)+2])
}
# Customize upper panel
panel.plot <- function (x, y) {
    points(x, y, pch=18, col=6)
}
# Create the plots
pairs(D2, lower.panel=panel.cor, upper.panel=panel.plot)</pre>
```



We can see that there is high correlation between some explanatory variables.

⇒ We need probably to perform variable selection.

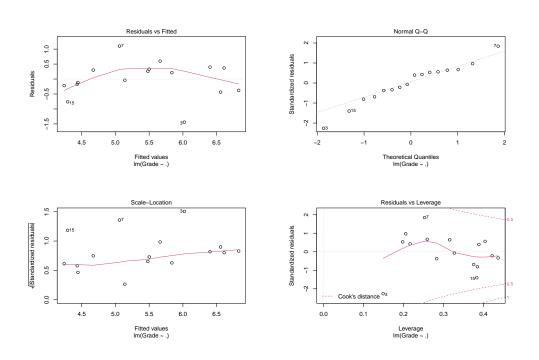
C.2.5. Assumption

The goal in this step is to check the gaussianity of the noise.

```
L2.c = lm(Grade ~ ., data=D2)
summary(L2.c)
##
## Call:
## lm(formula = Grade ~ ., data = D2)
##
## Residuals:
##
                  1Q
                       Median
                                     3Q
                      0.08703
## -1.44199 -0.25923
                               0.33864
                                        1.10096
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                 7.5091
                            4.8970
                                     1.533
                                              0.1534
## Sugar
                            0.5589
                                              0.8605
                 0.1006
                                     0.180
## Acid
                -0.4973
                            0.2624
                                    -1.895
                                              0.0846 .
                 0.3869
                            1.3644
                                     0.284
                                              0.7820
## Bitter
## Pulpy
                -0.2816
                            0.8537
                                    -0.330
                                              0.7477
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6914 on 11 degrees of freedom
## Multiple R-squared: 0.6883, Adjusted R-squared: 0.575
## F-statistic: 6.073 on 4 and 11 DF, p-value: 0.00786
```

- From the "summary(L2.c)" we note that there is some symmetry of the "Residuals" with respect to the median and the median is close to 0.

plot(L2.c)



- In the "Normal Q-Q" plot, we note that the main part of the points are quiet close to the line, which suggests the gaussianity of the noise.

- However, in the "Residuals vs Fitted" plot, the distribution of the residuals does not conform perfectly with a gaussian behaviour.

For further checking, we perform Kolmogorov test:

```
# Kolmogorov-Smirnov test
sres = rstandard(L2.c)
ks.test(sres, 'pnorm')

##
## One-sample Kolmogorov-Smirnov test
##
## data: sres
## D = 0.15354, p-value = 0.7919
## alternative hypothesis: two-sided
```

The Kolmogorov-Smirnov test returns a p-value of 0.7919. We will try to find a transformation of the response variable to improve the gaussianity test.

Possible transformations include applying the square root, the reciprocal or the logarithmic functions to the data.

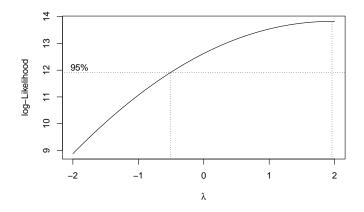
To find the best transformation we are going to use the "Box-Cox" transformation which is defined by:

$$y(\lambda) = \begin{cases} \frac{y^{\lambda} - 1}{\lambda} & \text{if } \lambda \neq 0\\ \log(y) & \text{if } \lambda = 0 \end{cases}$$

where y is a list of n strictly positive numbers and λ is the transformation constant.

We are going to perform a "Box-Cox" transformation in R by using the "boxcox" function from the "MASS" package. By using the "boxcox" function we can compute the best λ associated with the best transformation of the response variable.

```
# Application of the function "boxcox":
bc = boxcox(Grade ~ ., data=D2)
```



```
# Saving of the best lambda:
Lambda = bc$x[which.max(bc$y)]
Lambda
## [1] 1.959596
\Rightarrow We find \lambda = 1.959 \neq 0 \Rightarrow we apply the transformation y = \frac{y^{\lambda} - 1}{1}
# Transformation of the response variable:
D2.t = D2[,1:4]
D2.t$Grade.t = (D2$Grad^Lambda - 1) / Lambda
# Creation of the model
new.L2.c = lm(Grade.t ~ ., data=D2.t)
summary(new.L2.c)
##
## Call:
## lm(formula = Grade.t ~ ., data = D2.t)
##
## Residuals:
       Min
                1Q Median
                                 3Q
## -7.3523 -1.2286 0.1371 1.7154 5.0220
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 22.1352 24.0297 0.921 0.3767
                0.9939 2.7428 0.362 0.7239
## Sugar
                -2.3154
## Acid
                           1.2877 -1.798 0.0996 .
                2.1414
                            6.6952 0.320 0.7551
## Bitter
                -2.3584
## Pulpy
                            4.1893 -0.563 0.5848
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 3.393 on 11 degrees of freedom
## Multiple R-squared: 0.695, Adjusted R-squared: 0.5841
## F-statistic: 6.267 on 4 and 11 DF, p-value: 0.007028
  We perform the Kolmogorov-Smirnov test:
# Kolmogorov-Smirnov test
sres2 = rstandard(new.L2.c)
ks.test(sres2, 'pnorm')
##
##
   One-sample Kolmogorov-Smirnov test
##
## data: sres2
## D = 0.11213, p-value = 0.9742
## alternative hypothesis: two-sided
  The p-value of the Kolmogorov-Smirnov test is equal to 0.9742 > 0.05 \implies we accept the gaussianity
```

of the noise.

With the gaussianity of the noise being checked, we can now investigate all the elements provided by the "lm" function.

From the "summary(new.L2.c)" we can see that the p-value of the model is equal to 0.007028 < 0.05.

 \Rightarrow We accept H_1 in this test (at least one of the coefficients is not null).

⇒ We can consider a linear model between all the explanatory variables and the response variable.

By looking at the column "Pr(>|t|)", we can see that all the p-values are big but as we have a high correlation between some explanatory variables, we need to perform variable selection to improve our model.

C.2.6. Adjusted R-squared

```
L2.AR2 = leaps(D2.t[,-5], D2.t$Grade.t, method='adjr2', nbest=1)
L2.AR2
## $which
##
         1
              2
## 1 FALSE TRUE FALSE FALSE
## 2 FALSE TRUE FALSE TRUE
## 3 TRUE TRUE FALSE TRUE
## 4 TRUE TRUE TRUE TRUE
##
## $label
                                   "2"
                                                  "3"
                                                                 "4"
## [1] "(Intercept)" "1"
##
## $size
## [1] 2 3 4 5
##
## $adjr2
## [1] 0.6630176 0.6430580 0.6152232 0.5841111
  We can see that the biggest value of the "adjr2" is obtained by the first model.
id.max.adjr2 = which(L2.AR2$adjr2==max(L2.AR2$adjr2))
L2.AR2.Coeff = L2.AR2$which[id.max.adjr2,]
L2.AR2.Coeff
             2
                   3
       1
## FALSE TRUE FALSE FALSE
names(D2.t[,-5])[which(L2.AR2.Coeff==TRUE)]
```

We can conclude that the best model according to the "adjusted R-squared" procedure is: Grade.t \sim Acid.

C.2.7. backward-AIC

[1] "Acid"

```
L2.B.AIC = step(new.L2.c, direction='backward')
## Start: AIC=43.1
## Grade.t ~ Sugar + Acid + Bitter + Pulpy
##
##
           Df Sum of Sq
                           RSS
## - Bitter 1
                  1.178 127.81 41.248
## - Sugar 1
                  1.512 128.15 41.289
## - Pulpy 1
                  3.648 130.28 41.554
## <none>
                        126.64 43.099
## - Acid
                 37.223 163.86 45.223
##
## Step: AIC=41.25
## Grade.t ~ Sugar + Acid + Pulpy
```

```
##
##
       Df Sum of Sq RSS
## - Sugar 1 0.635 128.45 39.327
## - Pulpy 1
              2.646 130.46 39.575
               127.81 41.248
## <none>
## - Acid 1 36.104 163.92 43.228
##
## Step: AIC=39.33
## Grade.t ~ Acid + Pulpy
        Df Sum of Sq RSS
## - Pulpy 1 2.145 130.59 37.592
## <none>
                   128.45 39.327
## - Acid 1 216.507 344.95 53.133
##
## Step: AIC=37.59
## Grade.t ~ Acid
        Df Sum of Sq
##
                     RSS AIC
## <none>
                    130.59 37.592
## - Acid 1 284.62 415.22 54.099
L2.B.AIC
##
## Call:
## lm(formula = Grade.t ~ Acid, data = D2.t)
## Coefficients:
## (Intercept)
                    Acid
      27.392
##
                   -2.348
```

We can conclude that the best model with the "backward-AIC" procedure is: Grade.t ~ Acid.

C.2.8. backward-Fisher

```
L2.B.Fisher = step(new.L2.c, direction='backward', test='F')
## Start: AIC=43.1
## Grade.t ~ Sugar + Acid + Bitter + Pulpy
##
          Df Sum of Sq
                         RSS
                              AIC F value Pr(>F)
## - Bitter 1 1.178 127.81 41.248 0.1023 0.75508
## - Sugar 1 1.512 128.15 41.289 0.1313 0.72394
## - Pulpy 1
                3.648 130.28 41.554 0.3169 0.58476
## <none>
                      126.64 43.099
## - Acid 1 37.223 163.86 45.223 3.2334 0.09962 .
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Step: AIC=41.25
## Grade.t ~ Sugar + Acid + Pulpy
    Df Sum of Sq RSS AIC F value Pr(>F)
## - Sugar 1 0.635 128.45 39.327 0.0596 0.81129
## - Pulpy 1 2.646 130.46 39.575 0.2484 0.62720
## <none>
                     127.81 41.248
```

```
## - Acid 1 36.104 163.92 43.228 3.3898 0.09045 .
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Step: AIC=39.33
## Grade.t ~ Acid + Pulpy
##
         Df Sum of Sq RSS AIC F value
                                             Pr(>F)
## - Pulpy 1 2.145 130.59 37.592 0.2171 0.6489372
## <none>
                    128.45 39.327
## - Acid 1 216.507 344.95 53.133 21.9125 0.0004297 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Step: AIC=37.59
## Grade.t ~ Acid
##
                      RSS AIC F value Pr(>F)
       Df Sum of Sq
              130.59 37.592
## <none>
## - Acid 1
            284.62 415.22 54.099 30.513 7.497e-05 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
L2.B.Fisher
##
## Call:
## lm(formula = Grade.t ~ Acid, data = D2.t)
## Coefficients:
## (Intercept)
                     Acid
       27.392
                   -2.348
```

We can conclude that the best model with the "backward-Fisher" procedure is: Grade.t ~ Acid.

C.2.9. forward-AIC

We create a linear model with just the intercept:

```
new.L2.1 = lm(D2.t$Grade ~ 1, data=D2.t)
L2.F.AIC = step(new.L2.1, scope=list(new.L2.1, new.L2.c), direction='forward')
## Start: AIC=54.1
## D2.t$Grade ~ 1
```

The model provided by the "forward-AIC" strategy is Grade.t \sim (Intercept) and thus will not be retained.

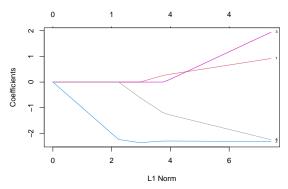
C.2.10. forward-Fisher

D2.t\$Grade ~ 1

The model provided by the "forward-Fisher" strategy is Grade.t \sim (Intercept) and thus will not be retained.

C.2.11. LASSO

```
X2 = data.matrix(D2.t[,-5])
Y2 = D2.t$Grade
D2.Lasso = glmnet(X2, Y2, alpha=1)
plot(D2.Lasso, col=c(2,4,6,8), label=TRUE)
```



This graph gives the trajectories of the β_i obtained for different values of λ with respect to the \mathcal{L}_1 norm of the β vector.

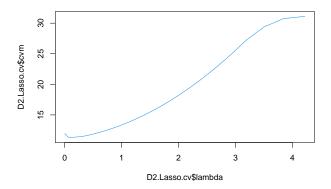
When we decrease λ (increase the \mathcal{L}_1 norm), some coefficients become different from 0 but not all at the same time.

 \Rightarrow We obtain many models, one for each value of λ and we select the best value of λ .

To perform this, we apply 'cv.glmnet" function to compute the cross validation error for each model. Then we keep the best model presenting the lowest error.

Since we have a small dataset, we will take the number of the splitting in K-folds "nfolds = 3" (by default nfolds = 10).

```
# Cross validation error
D2.Lasso.cv = cv.glmnet(X2, Y2, alpha=1, nfolds=3)
D2.Lasso.cv
##
## Call: cv.glmnet(x = X2, y = Y2, nfolds = 3, alpha = 1)
##
## Measure: Mean-Squared Error
##
##
       Lambda Index Measure
                               SE Nonzero
                      11.27 4.929
## min 0.093
                 42
## 1se
        1.516
                      15.53 0.875
                                         1
plot(D2.Lasso.cv$lambda, D2.Lasso.cv$cvm, type='1', col=4)
```



In order to delete the instability due to the search of a minimum, we look for the "1se" row and not the "min".

```
# Saving the best lambda from "1se" row:
D2.best.Lambd = D2.Lasso.cv$lambda.1se
# Selection of the variables associated with the best lambda:
D2.best.Lasso = glmnet(X2, Y2, alpha=1, lambda=D2.best.Lambd)
coefficients(D2.best.Lasso)

## 5 x 1 sparse Matrix of class "dgCMatrix"
## s0
## (Intercept) 22.618734
## Sugar .
## Acid -1.504126
## Bitter .
## Pulpy .
```

We can conclude that the best model with Lasso method is: Grade.t ~ Acid.

C.2.12. Initial results

All the previous procedures return the same model: Grade.t \sim Acid. However since we have a small dataset we need to apply Bagging so that the dataset can appear more populated than it really is.

This is the objective of the next section in which we combine Bagging with the computation of the testing error.

C.2.13. Computation of the testing error with Bagging

• Computation of the testing error

To compute the testing error using Bagging, we repeat the following steps (100 times): - We split te initial dataset at random into learning sample and testing sample.

- We use the learning sample to create the linear model using the set of the explanatory variables determined by each of the considered procedures (Adjusted R squared, step by step backward, step by step forward, Lasso, VSURF)
 - We use the testing sample to compute the error for all the created models.

The below code implements all these steps.

```
# Initialization
n.row = dim(D2.t)[1]
n.col = dim(D2.t)[2]
n.learn = floor(2 * n.row / 3)
u = 1 : n.row
k = 100

df.best.L2b = data.frame()
df.error = data.frame(ind=integer(), Procedure=character(), Error=double())

for (i in 1:k){
    #---- Splitting the dataset into learning and testing datasets
    1 = sample(u, n.learn, replace=FALSE)
    D.learn = D2.t[1,]
    D.test = D2.t[-1,]
    X.learn = D.learn[, -5]
    X.learn = data.matrix(X.learn)
```

```
df.X.learn = as.data.frame(X.learn)
Y.learn = D.learn$Grade.t
X.test = D.test[, -5]
Y.test = D.test$Grade.t
#---- Creation of the model with all the explanatory variables -----
L2b.split.c = lm(Grade.t ~ ., data=D.learn)
#---- Creation of the model with only the intercept -----
L2b.split.1 = lm(Grade.t ~ 1, data=D.learn)
#-----#
                   ---- Adjusted R squared ----
#----#
cat(' \n #### Adjusted R squared ####################### ', i, ' # \n')
#---- Variables selection ------
D2b.best.AdjR2 = leaps(df.X.learn, Y.learn, method='adjr2', nbest=1)
# Selection of the index of the biggest adjusted R squared:
id.max.adjr2 = which(D2b.best.AdjR2$adjr2==max(D2b.best.AdjR2$adjr2))
# Selection of the variables:
Coef.D2b.best.AdjR2 = D2b.best.AdjR2$which[id.max.adjr2,]
# Storing the names of the selected variables:
nm.Coef.best.AdjR2 = names(df.X.learn)[which(Coef.D2b.best.AdjR2==TRUE)]
#---- Creation of the model with the selected variables -----
# Concatenating the names of the variables in a string:
formula.Coef.best.AdjR2 = paste(nm.Coef.best.AdjR2, collapse = '+')
# Storing the formula of the model in a string:
str.L2b.AdjR2 = sprintf('Grade.t ~ %s', formula.Coef.best.AdjR2)
# Computing the model with the selected variables:
best.L2b.AdjR2 = do.call('lm', list(str.L2b.AdjR2, quote(D.learn)))
#---- Prediction ------
Y.prdc.AdjR2 = predict(best.L2b.AdjR2, newdata=D.test)
#---- Computation of the error -----
err.AdjR2 = (1 / nrow(X.test)) * sum((Y.test - Y.prdc.AdjR2)^2)
# Storing the error in a data frame:
df.err.AdjR2 = data.frame(ind=i, Procedure='AdjR2', Error=err.AdjR2)
df.error = bind_rows(df.error, df.err.AdjR2)
#---- Saving the coefficients of the best model ------
Coef.best.L2b.AdjR2 = best.L2b.AdjR2$coefficients
# Storing the coefficients in a data frame:
df.Coef.AdjR2 = data.frame(as.list(Coef.best.L2b.AdjR2))
df.Coef.AdjR2 = data.frame(id=i, Procedure='AdjR2', df.Coef.AdjR2)
df.best.L2b = bind_rows(df.best.L2b, df.Coef.AdjR2)
#---- Deletion of the intermediate variables -----
rm(D2b.best.AdjR2, id.max.adjr2, Coef.D2b.best.AdjR2, nm.Coef.best.AdjR2
   , formula.Coef.best.AdjR2, str.L2b.AdjR2, best.L2b.AdjR2, Y.prdc.AdjR2
   , err.AdjR2, df.err.AdjR2, Coef.best.L2b.AdjR2, df.Coef.AdjR2)
```

```
---- Step by step "Backward" method with AIC test ----
#----#
cat(' \n #### Backward - AIC ###################### ', i, ' # \n')
#---- Variables selection -----
L2b.Back.AIC = step(L2b.split.c, direction='backward')
# formula of the model with the selected variables:
L2b.Back.AIC.formula = L2b.Back.AIC$call$formula
#---- Creation of the model with the selected variables -----
best.L2b.Back.AIC = lm(L2b.Back.AIC.formula, data=D.learn)
#---- Prediction -----
Y.prdc.Back.AIC = predict(best.L2b.Back.AIC, newdata=X.test)
#---- Computation of the error -----
err.Back.AIC = (1 / nrow(X.test)) * sum((Y.test - Y.prdc.Back.AIC)^2)
# Storing the error in a data frame:
df.err.Back.AIC = data.frame(ind=i, Procedure='Backword_AIC', Error=err.Back.AIC)
df.error = bind_rows(df.error, df.err.Back.AIC)
#---- Saving the coefficients of the best model -----
Coef.best.L2b.Back.AIC = best.L2b.Back.AIC$coefficients
# Storing the coefficients in a data frame:
df.Coef.Back.AIC = data.frame(as.list(Coef.best.L2b.Back.AIC))
df.Coef.Back.AIC = data.frame(id=i, Procedure='Backword_AIC', df.Coef.Back.AIC)
df.best.L2b = bind_rows(df.best.L2b, df.Coef.Back.AIC)
#---- Deletion of the intermediate variables -----
rm(L2b.Back.AIC, L2b.Back.AIC.formula, best.L2b.Back.AIC, Y.prdc.Back.AIC
  , err.Back.AIC, df.err.Back.AIC, Coef.best.L2b.Back.AIC, df.Coef.Back.AIC)
# ---- Step by step "Forward" method with AIC test ----
cat(' \n ##### Forward - AIC ######################## ', i, ' # \n')
#---- Variables selection ------
L2b.Forw.AIC = step(L2b.split.c, scope=list(L2b.split.1, L2b.split.c)
               , direction='forward')
L2b.Forw.AIC.formula = L2b.Forw.AIC$call$formula
#---- Creation of the model with the selected variables -----
best.L2b.Forw.AIC = lm(L2b.Forw.AIC.formula, data=D.learn)
#---- Prediction ------
Y.prdc.Forw.AIC = predict(best.L2b.Forw.AIC, newdata=D.test)
#---- Computation of the error
err.Forw.AIC = (1 / nrow(X.test)) * sum((Y.test - Y.prdc.Forw.AIC)^2)
# Storing the error in a data frame:
df.err.Forw.AIC = data.frame(ind=i, Procedure='Forward_AIC', Error=err.Forw.AIC)
df.error = bind_rows(df.error, df.err.Forw.AIC)
```

```
#---- Saving the coefficients of the best model -----
 Coef.best.L2b.Forw.AIC = best.L2b.Forw.AIC$coefficients
 # Storing the coefficients in a data frame:
 df.Coef.Forw.AIC = data.frame(as.list(Coef.best.L2b.Forw.AIC))
 df.Coef.Forw.AIC = data.frame(id=i, Procedure='Forward_AIC', df.Coef.Forw.AIC)
 df.best.L2b = bind_rows(df.best.L2b, df.Coef.Forw.AIC)
 #---- Deletion of the intermediate variables -----
 rm(L2b.Forw.AIC, L2b.Forw.AIC.formula, best.L2b.Forw.AIC, Y.prdc.Forw.AIC
    , err.Forw.AIC, df.err.Forw.AIC, Coef.best.L2b.Forw.AIC, df.Coef.Forw.AIC)
  ---- LASSO ----
  cat(' \n ##### LASSO ############################### ', i, ' # \n')
  #---- Variables selection -----
  # Computing of the cross validation error
 D2b.Lasso.cv = cv.glmnet(X.learn, Y.learn, alpha=1, nfolds=3)
  # Storing the best lambda from "1se" row:
 D2b.best.Lambd = D2b.Lasso.cv$lambda.1se
  # Selection of variables:
 D2b.best.Lasso = glmnet(X.learn, Y.learn, alpha=1, lambda=D2b.best.Lambd)
 Coef.D2b.best.Lasso = coefficients(D2b.best.Lasso)
  # Selecting the names of variables whose coefficients are not null:
 nm.Coef.best.Lasso = names(which(Coef.D2b.best.Lasso[,1]!=0))
 # Rename the "(Intercept)" as "1":
 nm.Coef.best.Lasso[1] = '1'
 #---- Creation of the model with the selected variables -----
 # Concatenating the names of the variables in a string:
 formula.Coef.best.Lasso = paste(nm.Coef.best.Lasso, collapse = '+')
  # Storing the formula of the model in a string:
 str.L2b.Lasso = sprintf('Grade.t ~ %s', formula.Coef.best.Lasso)
  # Computing the model with the selected variables:
 best.L2b.Lasso = do.call('lm', list(str.L2b.Lasso, quote(D.learn)))
  #---- Prediction ------
 Y.prdc.Lasso = predict(best.L2b.Lasso, newdata=D.test)
  #---- Computation of the error ------
 err.Lasso = (1 / nrow(X.test)) * sum((Y.test - Y.prdc.Lasso)^2)
  # Storing the error in a data frame:
 df.err.Lasso = data.frame(ind=i, Procedure='LASSO', Error=err.Lasso)
 df.error = bind_rows(df.error, df.err.Lasso)
 #---- Saving the coefficients of the best model ------
 Coef.best.L2b.Lasso = best.L2b.Lasso$coefficients
 # Storing the coefficients in a data frame:
 df.Coef.Lasso = data.frame(as.list(Coef.best.L2b.Lasso))
 df.Coef.Lasso = data.frame(id=i, Procedure='LASSO', df.Coef.Lasso)
 df.best.L2b = bind_rows(df.best.L2b, df.Coef.Lasso)
 #---- Deletion of the intermediate variables -----
 rm(D2b.Lasso.cv, D2b.best.Lambd, D2b.best.Lasso, Coef.D2b.best.Lasso
```

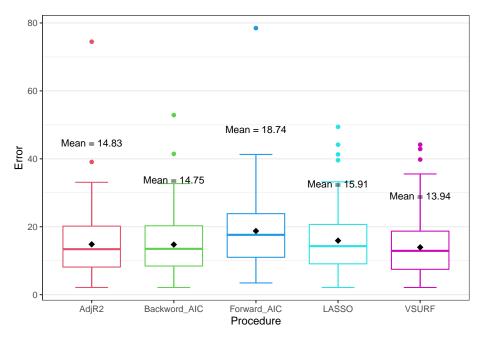
```
, nm.Coef.best.Lasso, formula.Coef.best.Lasso, str.L2b.Lasso, best.L2b.Lasso
   , Y.prdc.Lasso, err.Lasso, df.err.Lasso, Coef.best.L2b.Lasso, df.Coef.Lasso)
         ---- VSURF: Variable Selection Using Random Forests ----
cat(' \n ##### VSURF ############################## ', i, ' # \n')
#---- Variables selection -----
Var.Selec.VSURF = VSURF(df.X.learn, Y.learn)
# Storing the names of the selected variables:
nm.Coef.VSURF = colnames(df.X.learn[Var.Selec.VSURF$varselect.pred])
#---- Creation of the model with the selected variables -----
# Add the "Intercept" to the names of the selected variables:
nm.Coef.VSURF = c('1', nm.Coef.VSURF)
# Concatenating the names of the variables in a string:
formula.Coef.best.VSURF = paste(nm.Coef.VSURF, collapse = '+')
# Storing the formula of the model in a string:
str.L2b.VSURF = sprintf('Grade.t ~ %s', formula.Coef.best.VSURF)
# Computing the model with the selected variables:
best.L2b.VSURF = do.call('lm', list(str.L2b.VSURF, quote(D.learn)))
#---- Prediction ------
Y.prdc.VSURF = predict(best.L2b.VSURF, newdata=D.test)
#---- Computation of the error ------
err.VSURF = (1 / nrow(X.test)) * sum((Y.test - Y.prdc.VSURF)^2)
# Storing the error in a data frame:
df.err.VSURF = data.frame(ind=i, Procedure='VSURF', Error=err.VSURF)
df.error = bind_rows(df.error, df.err.VSURF)
#---- Saving the coefficients of the best model -----
Coef.best.L2b.VSURF = best.L2b.VSURF$coefficients
# Storing the coefficients in a data frame:
df.Coef.VSURF = data.frame(as.list(Coef.best.L2b.VSURF))
df.Coef.VSURF = data.frame(id=i, Procedure='VSURF', df.Coef.VSURF)
df.best.L2b = bind_rows(df.best.L2b, df.Coef.VSURF)
#---- Deletion of the intermediate variables -----
rm(Var.Selec.VSURF, nm.Coef.VSURF, formula.Coef.best.VSURF, str.L2b.VSURF
  , best.L2b.VSURF, Y.prdc.VSURF, err.VSURF, df.err.VSURF, Coef.best.L2b.VSURF
   , df.Coef.VSURF)
```

The above code returns the coefficients of all models for each learning sample in the variable "df.best.L2b" as well as their associated testing error stored in the variable "df.error".

To compare between all procedures we compute the average of their testing errors and select the one that presents the lowest average.

The obtained results are displayed in the below boxplot.

They show that the "VSURF" is the procedure that presents the lowest average testing error.



```
# Extraction of the mean for each procedure:
list.mean.error = df.error %>%
  group_by(Procedure) %>%
  summarise(mean_error=mean(Error))
list.mean.error
```

```
## # A tibble: 5 x 2
##
     Procedure mean_error
##
     <chr>>
                        <dbl>
## 1 AdjR2
                        14.8
## 2 Backword_AIC
                        14.8
## 3 Forward_AIC
                        18.7
## 4 LASSO
                        15.9
## 5 VSURF
                        13.9
```

• Creation of the model

The best model is obtained by averaging all the coefficients associated with the models of the procedure "VSURF".

The below code implements this step and provides the best model.

```
# Storing the index of the smallest mean:
id.min.error = which.min(as.data.frame(list.mean.error)[,2])
id.min.error
## [1] 5
 \textit{\# Replacement of the "NA" values by 0 in the data frame "df.best.L2b"} : \\
df.best.L2b[is.na(df.best.L2b)] = 0
# Computation of the mean of each coefficient:
list.mean.coeff = df.best.L2b %>%
  group_by(Procedure) %>%
  summarise(Intercept=mean(X.Intercept.)
            , Sugar=mean(Sugar)
            , Acid=mean(Acid)
            , Bitter=mean(Bitter)
            , Pulpy=mean(Pulpy))
# The best model
best.model = list.mean.coeff[id.min.error,]
best.model
## # A tibble: 1 x 6
## Procedure Intercept
                                   Sugar
                                                                    Pulpy
                                              Acid
                                                        Bitter
##
                                   <dbl>
   <chr>
                                                                    <dbl>
                        <dbl>
                                             <dbl>
                                                        <dbl>
## 1 VSURF
                         23.7
                                   0.388
                                             -2.01
                                                        -0.102
                                                                   -0.186
```