Unsupervised classification

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```
packages<-c("FactoMineR", "factoextra", "xtable", "NbClust", "plyr","GGally", "ggcorrplot")
lapply(packages, library, character.only=TRUE)
```

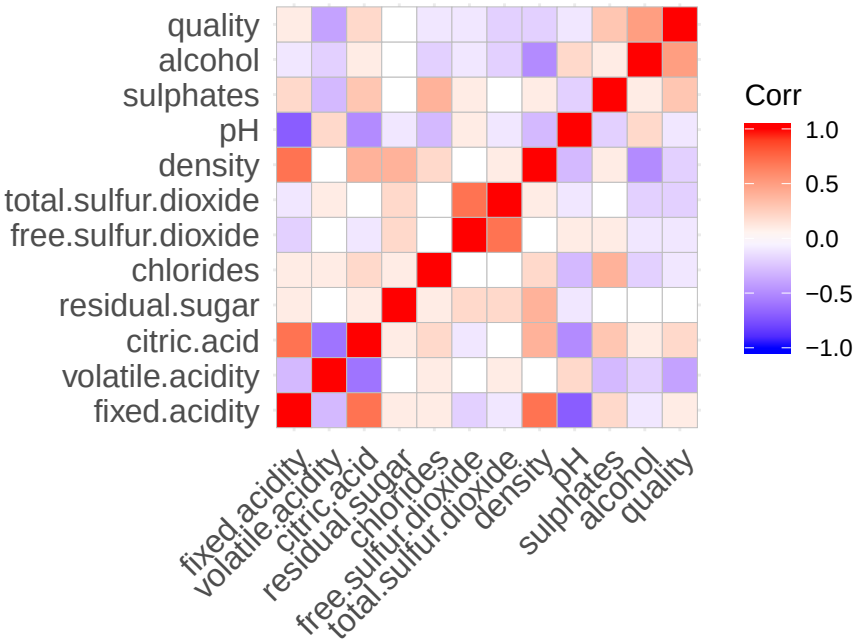
This dataset is a subset of the results of a chemical analysis of Italian wine. The analysis determined the quantities of 13 constituents of red wines. These are the variables:

- fixed acidity
- volatile acidity
- citric acid
- resigual sugar
- chlorides
- free.sulfur.dioxide
- total.sulfur.dioxide
- density
- ph
- sulphates
- alcohol
- quality

```
winequality.red <- read.csv("C:/Users/Andrea/Desktop/wine/winequality-red.csv", sep=";")
```

Looking into the data structure we can see a strong direct/inverse relation between some variables like fixed-volatile acidity, free-total sulfor dioxide and alcohol-quality.

```
corr <- round(cor(winequality.red), 1)
ggcorrplot(corr)
```



Kmeans

Number of cluster

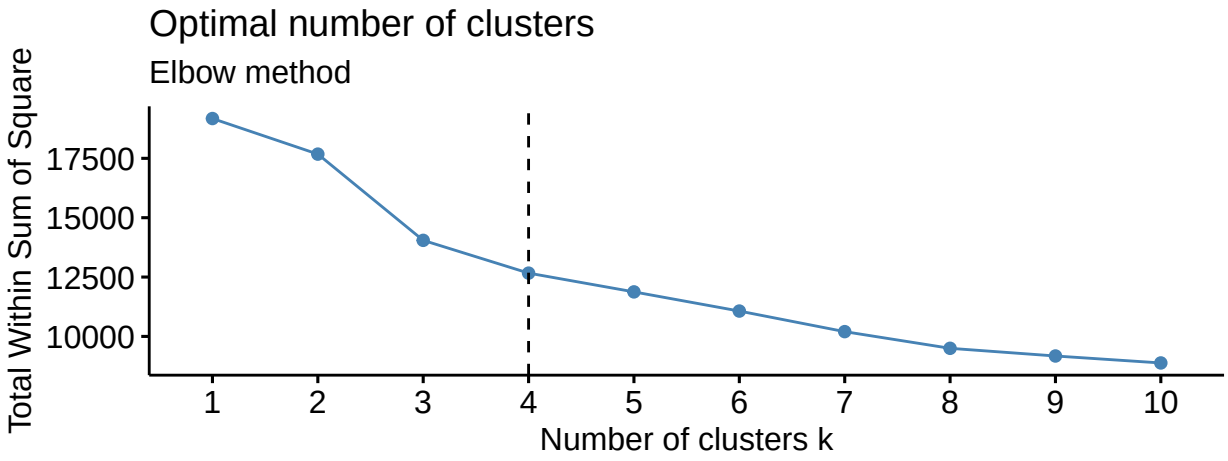
The data is standardized before clustering to obtain a better quality, efficient and accurate cluster result. The library *NbClust* is used to calculate the optimum number of clusters, we are going to use the Friedman index.

```
df<-scale(winequality.red)
res.wine<-NbClust(df, distance = "canberra", min.nc = 2, max.nc = 10, method = "kmeans", index = "friedm
res.wine$Best.nc
```

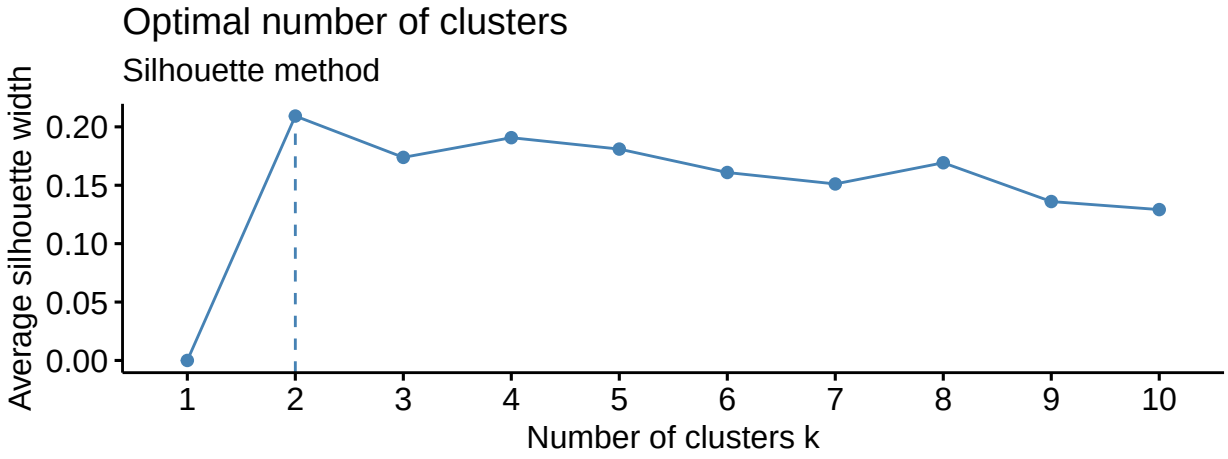
```
## Number_clusters     Value_Index
##          4.0000          3.7614
```

Another methods to select the number of cluster are plotted below.

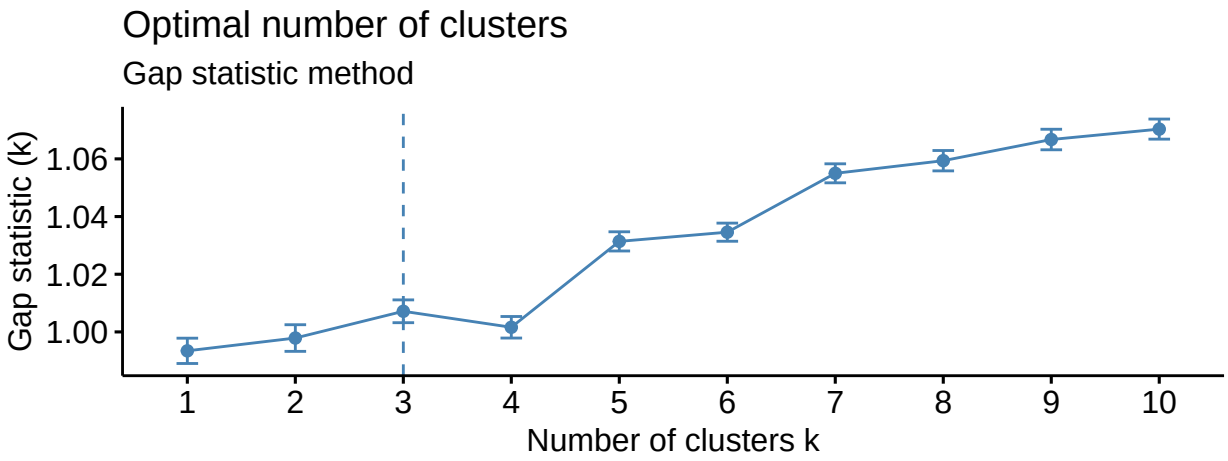
```
set.seed(21)
elbow<-fviz_nbclust(df, kmeans, method = "wss") +geom_vline(xintercept = 4, linetype = 2)+ labs(subtitle
```




```
Silhouette<-fviz_nbclust(df, kmeans, method = "silhouette")+
  labs(subtitle = "Silhouette method");Silhouette
```




```
gap<-fviz_nbclust(df, kmeans, nstart = 25,  method = "gap_stat",
  nboot = 50)+labs(subtitle = "Gap statistic method"); gap
```



After all of the results, I decided to use the mode and in this way, obtaining that the better number of clusters is 4.

Kmeans algorithm

No forget to set a seed to obtain every run the same results.

```
set.seed(10)
n_cluster<-4
kmedia2<-kmeans(df, n_cluster, nstart = 1000)
```

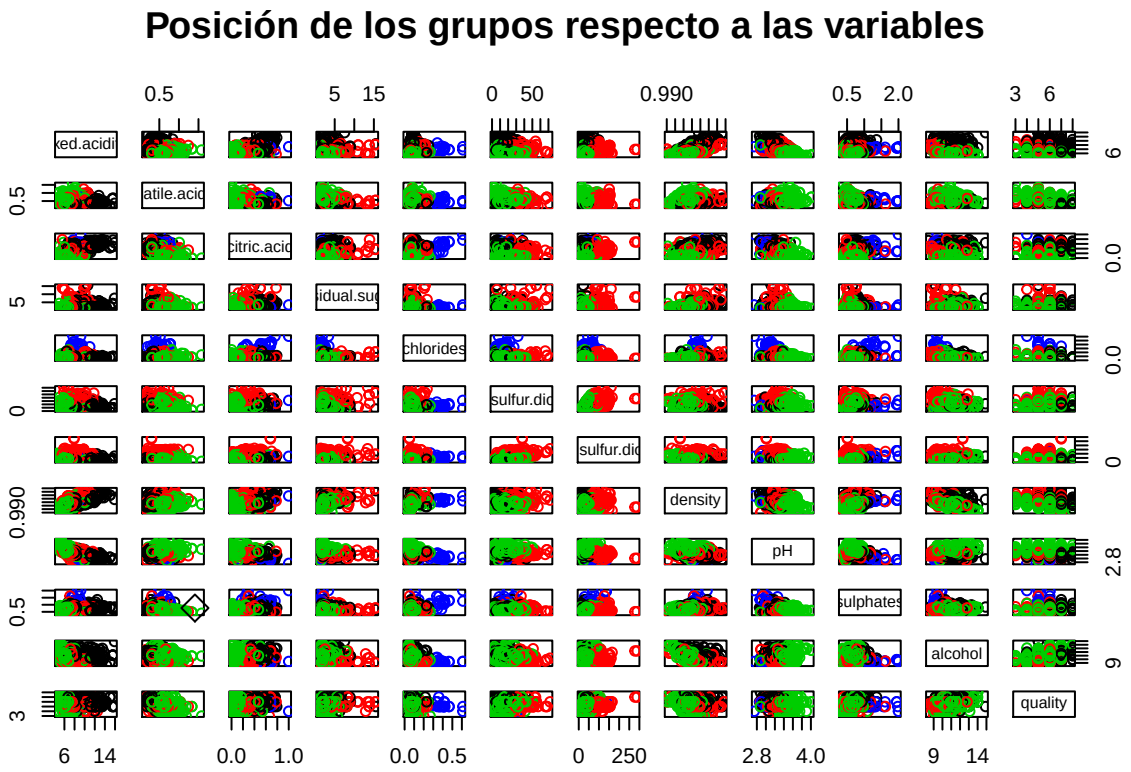
Let see the centroids

```
round(kmedia2$centers,2)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1          0.99            -0.78        1.01           0.06     -0.09
## 2         -0.05             0.03        0.12           0.37      0.00
## 3         -0.65             0.51       -0.80          -0.23     -0.17
## 4          0.08             0.02        1.14          -0.40      5.60
##   free.sulfur.dioxide total.sulfur.dioxide density    pH sulphates alcohol
## 1               -0.46                -0.53    0.36 -0.66      0.38    0.47
## 2                1.00                 1.26    0.32 -0.17     -0.20   -0.56
## 3               -0.24                -0.36   -0.43  0.61     -0.30    0.03
## 4               -0.07                 0.47    0.19 -1.69      3.72   -0.88
##   quality
## 1    0.63
## 2   -0.45
## 3   -0.16
## 4   -0.36
```

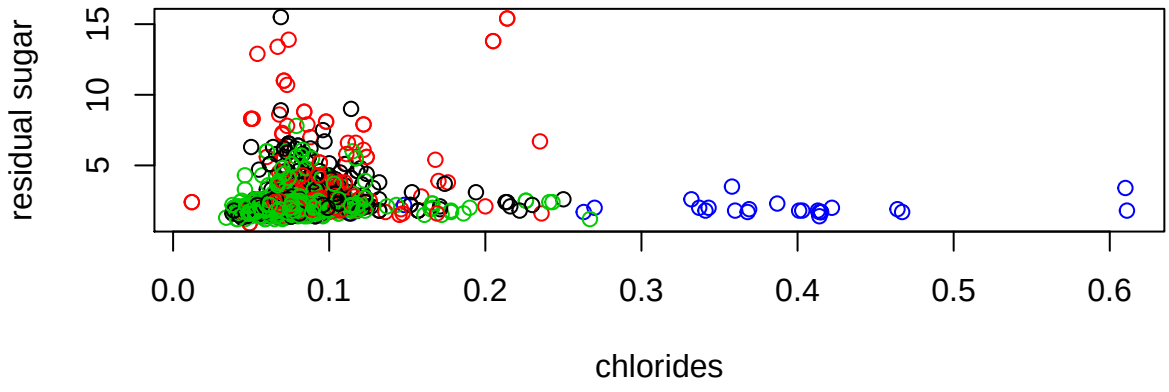
And the clusters over all of the variables are painted in the scatter plots when each color represents a different cluster.

```
plot(winequality.red, col=kmedia2$cluster,
     main="PosiciÃ³n de los grupos respecto a las variables")
points(kmedia2$centers, col = kmedia2$cluster, pch = 23, cex = 1.5)
```



Too see in detail one of the scatterplots

```
plot(winequality.red$chlorides, winequality.red$residual.sugar, col=kmedia2$cluster, xlab = "chlorides"
legend(0,100, legend=c('1', '2', '3', '4'),col=c("black","blue", "red","green" ),
pch = 18, cex = 1)
```



It is really imporant look into the withinss and beteens sum of squares.

```r
print(round(kmedia2$withinss,2))
```

```
## [1] 3749.95 3728.35 4704.79  478.21
```

```r
print(kmedia2$betweenss)
```

```
## [1] 6514.699
```

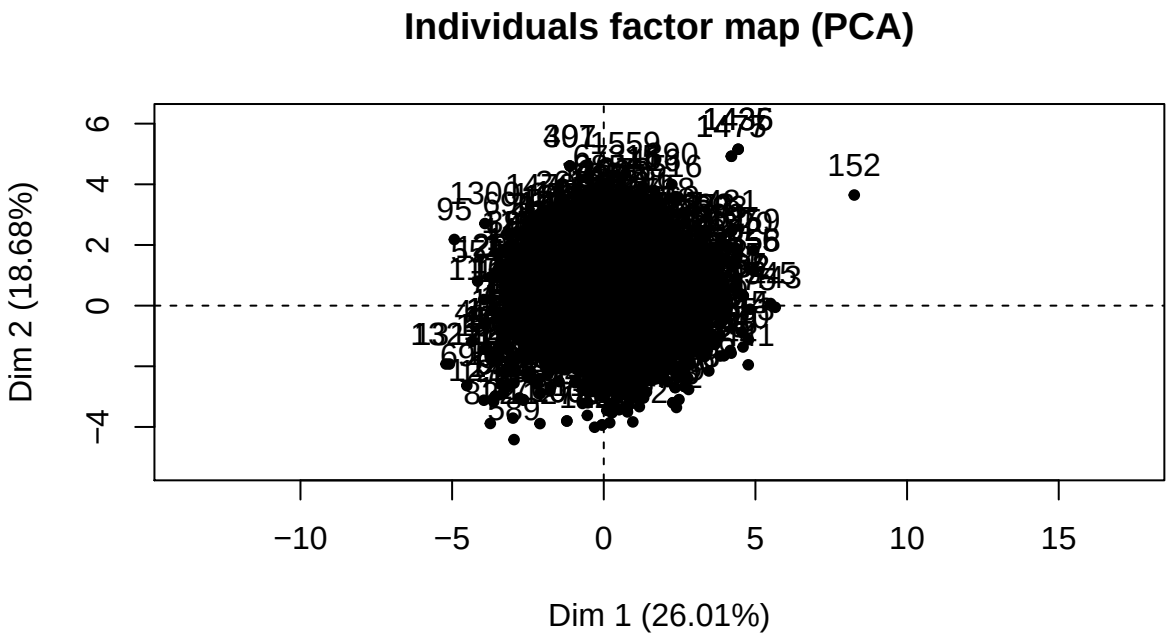
In this case, the sum of squares over the betweens is greater than the within, which means that the segmentation creates cluster different between them but internally the observations are similar, homogeneity inside and heterogeneity outside the clusters.

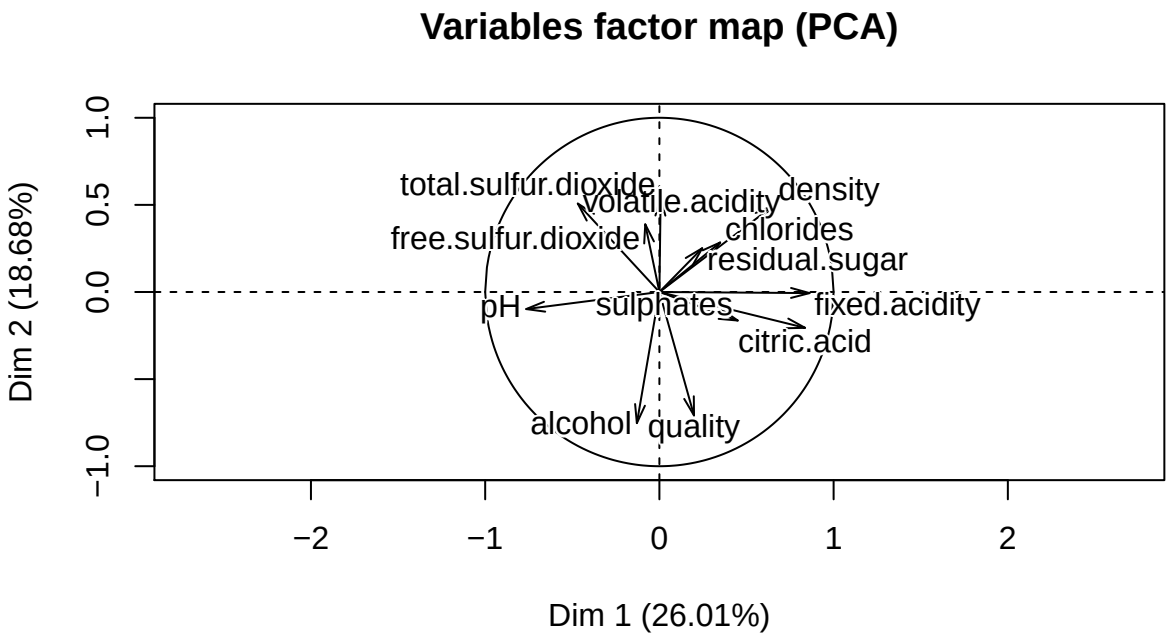
Hierarchichal Clustering

Principal Component Analysis

To use the function HCPC is necessary to run before a PCA, because the cluster are made over the space generated in the PCA.

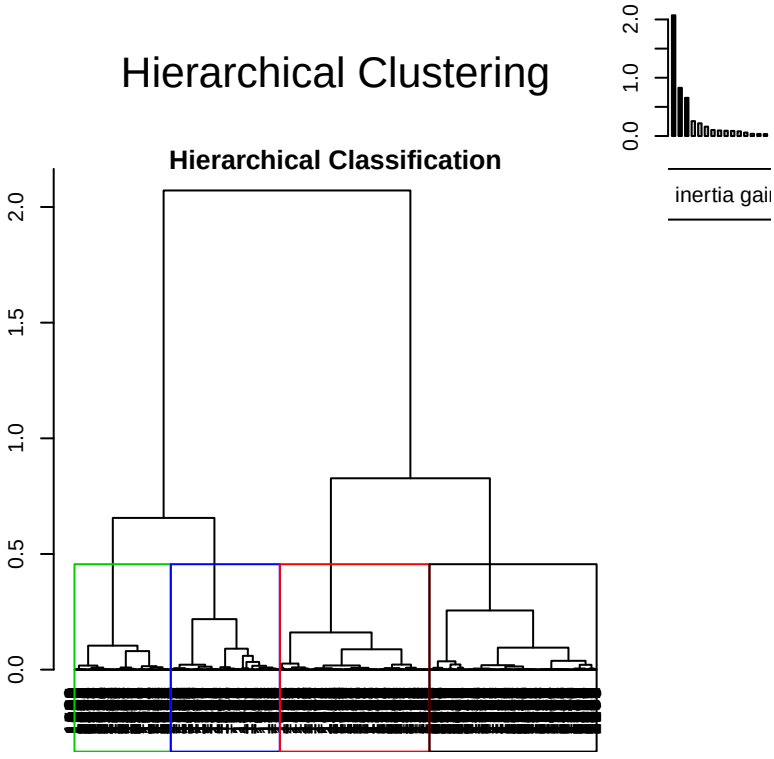
```r
res.PCA<-PCA(df, ncp = 2)
```

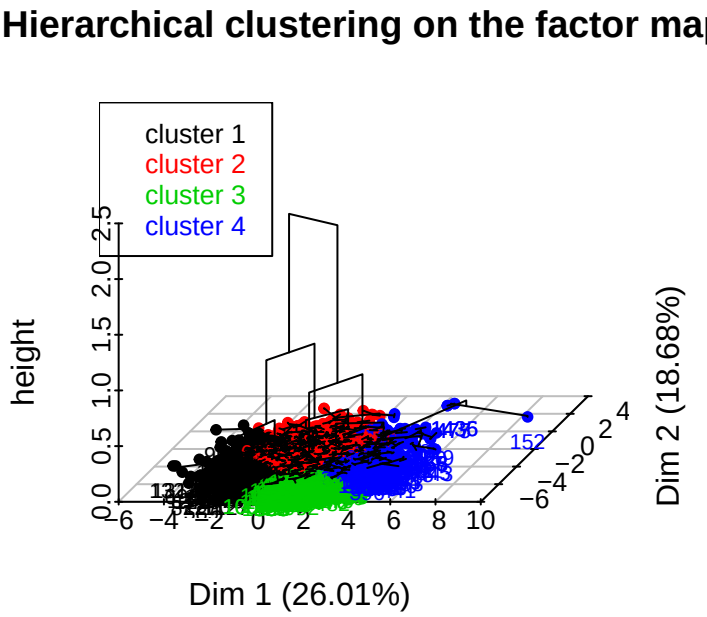


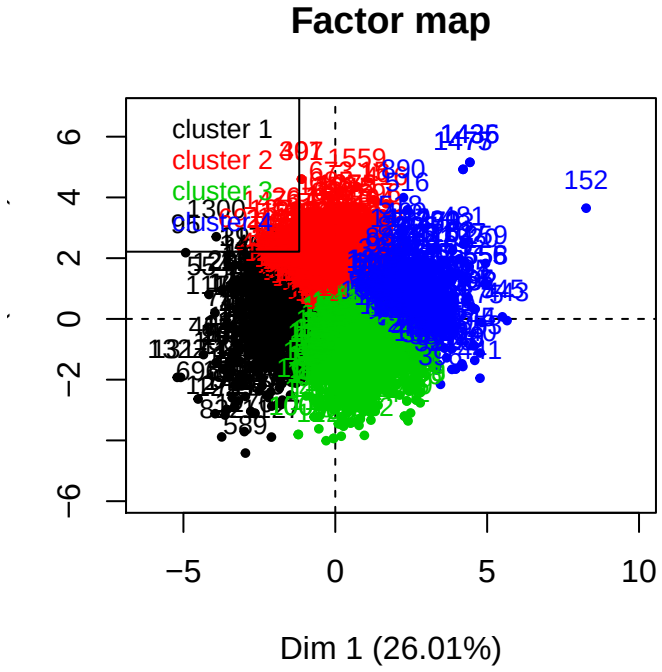


It is necessary to determine the minimum and the maximum number of possible clusters. If nb.clust=-1 the optimal number of clusters is used and if nb.clust is an integer it fixes the number of clusters. The indexed hierarchy is represented by a tree named a dendrogramm.

```
set.seed(10)
res.hcpc<-HCPC(res.PCA,  nb.clust = -1,min = 3, max = 6)
```







Facto investigate

Finally, a quickly way to have an analysis of your results is using the function Investigate which generate an extra file with the analysis.

```
library(FactoInvestigate)
Investigate(res.hcpc,document="pdf_document")
```

```
## -- creation of the .Rmd file (time spent : 0s) --
##
## -- saving data (time spent : 0.28s) --
##
## -- outputs compilation (time spent : 0.28s) --
```

```
## -- task completed (time spent : 5.66s) --
## This interpretation of the results was carried out automatically,
## it cannot match the quality of a personal interpretation
```

References

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