Assignment-5 Hierarchical Clustering

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R Markdown

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Hierarchical clustering

```r
rm(list = ls())
library(caret)
```

```
## Loading required package: lattice

## Loading required package: ggplot2
```

```r
library(ISLR)
library(factoextra)
```

```
## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```r
library(cluster)
library(NbClust)

#Loadinng the data
DFCereals<-read.csv("Cereals.csv")

#EDA of the data set
summary(DFCereals)
```

```
##      name               mfr                type              calories
##  Length:77          Length:77          Length:77          Min.   : 50.0
##  Class :character   Class :character   Class :character   1st Qu.:100.0
##  Mode  :character   Mode  :character   Mode  :character   Median :110.0
##                                                           Mean   :106.9
##                                                           3rd Qu.:110.0
##                                                           Max.   :160.0
##
##     protein           fat             sodium          fiber
##  Min.   :1.000   Min.   :0.000   Min.   :  0.0   Min.   : 0.000
##  1st Qu.:2.000   1st Qu.:0.000   1st Qu.:130.0   1st Qu.: 1.000
##  Median :3.000   Median :1.000   Median :180.0   Median : 2.000
##  Mean   :2.545   Mean   :1.013   Mean   :159.7   Mean   : 2.152
##  3rd Qu.:3.000   3rd Qu.:2.000   3rd Qu.:210.0   3rd Qu.: 3.000
##  Max.   :6.000   Max.   :5.000   Max.   :320.0   Max.   :14.000
##
##      carbo          sugars           potass          vitamins
##  Min.   : 5.0   Min.   : 0.000   Min.   : 15.00   Min.   :  0.00
##  1st Qu.:12.0   1st Qu.: 3.000   1st Qu.: 42.50   1st Qu.: 25.00
##  Median :14.5   Median : 7.000   Median : 90.00   Median : 25.00
##  Mean   :14.8   Mean   : 7.026   Mean   : 98.67   Mean   : 28.25
##  3rd Qu.:17.0   3rd Qu.:11.000   3rd Qu.:120.00   3rd Qu.: 25.00
##  Max.   :23.0   Max.   :15.000   Max.   :330.00   Max.   :100.00
##  NA's   :1      NA's   :1        NA's   :2
##      shelf           weight          cups           rating
##  Min.   :1.000   Min.   :0.50   Min.   :0.250   Min.   :18.04
##  1st Qu.:1.000   1st Qu.:1.00   1st Qu.:0.670   1st Qu.:33.17
##  Median :2.000   Median :1.00   Median :0.750   Median :40.40
##  Mean   :2.208   Mean   :1.03   Mean   :0.821   Mean   :42.67
##  3rd Qu.:3.000   3rd Qu.:1.00   3rd Qu.:1.000   3rd Qu.:50.83
##  Max.   :3.000   Max.   :1.50   Max.   :1.500   Max.   :93.70
##
```

```r
colMeans(is.na(DFCereals))
```

```
##       name        mfr       type   calories    protein        fat     sodium
## 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
##      fiber      carbo     sugars     potass   vitamins      shelf     weight
## 0.00000000 0.01298701 0.01298701 0.02597403 0.00000000 0.00000000 0.00000000
##       cups     rating
## 0.00000000 0.00000000
```

```r
#Median imputation of missing data
preProcess_1<-preProcess(DFCereals, method = c("medianImpute"))
ImputedDF<-predict(preProcess_1, DFCereals)

#No more NULL values presnt
colMeans(is.na(ImputedDF))
```

```
##     name      mfr     type calories  protein      fat   sodium    fiber
##        0        0        0        0        0        0        0        0
##    carbo   sugars   potass vitamins    shelf   weight     cups   rating
##        0        0        0        0        0        0        0        0
```

```r
#Scaling the DF
ImputedDF<-subset(ImputedDF, select= -c(1,2,3))
ImputedDF<-scale(ImputedDF)


# Compute with agnes and with different linkage methods
hc_single <- agnes(ImputedDF, method = "single")
```

```r
hc_complete<-agnes(ImputedDF, method="complete")
hc_average <- agnes(ImputedDF, method = "average")
hc_ward <- agnes(ImputedDF, method = "ward")

# Compare Agglomerative coefficients
print(hc_single$ac)
```

```
## [1] 0.6029274
```

```r
print(hc_complete$ac)
```

```
## [1] 0.8353216
```

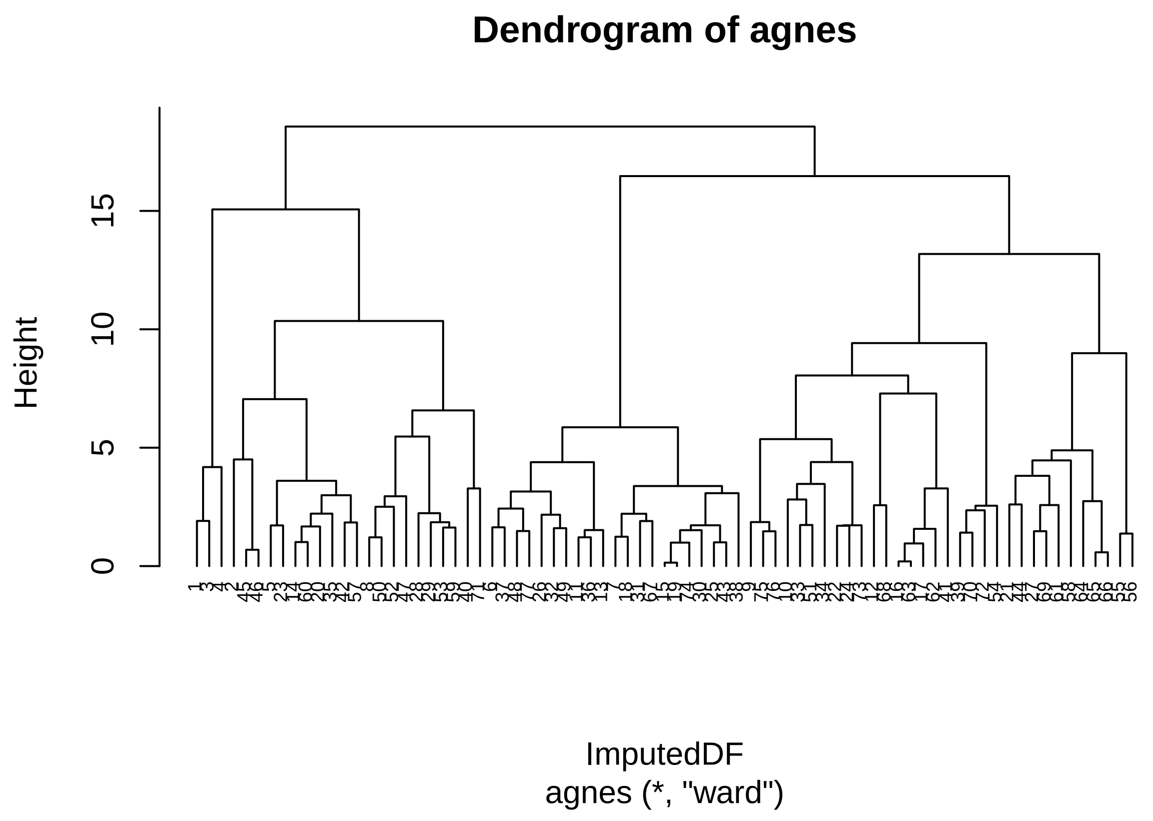
```r
print(hc_average$ac)
```

```
## [1] 0.7777555
```

```r
print(hc_ward$ac)
```

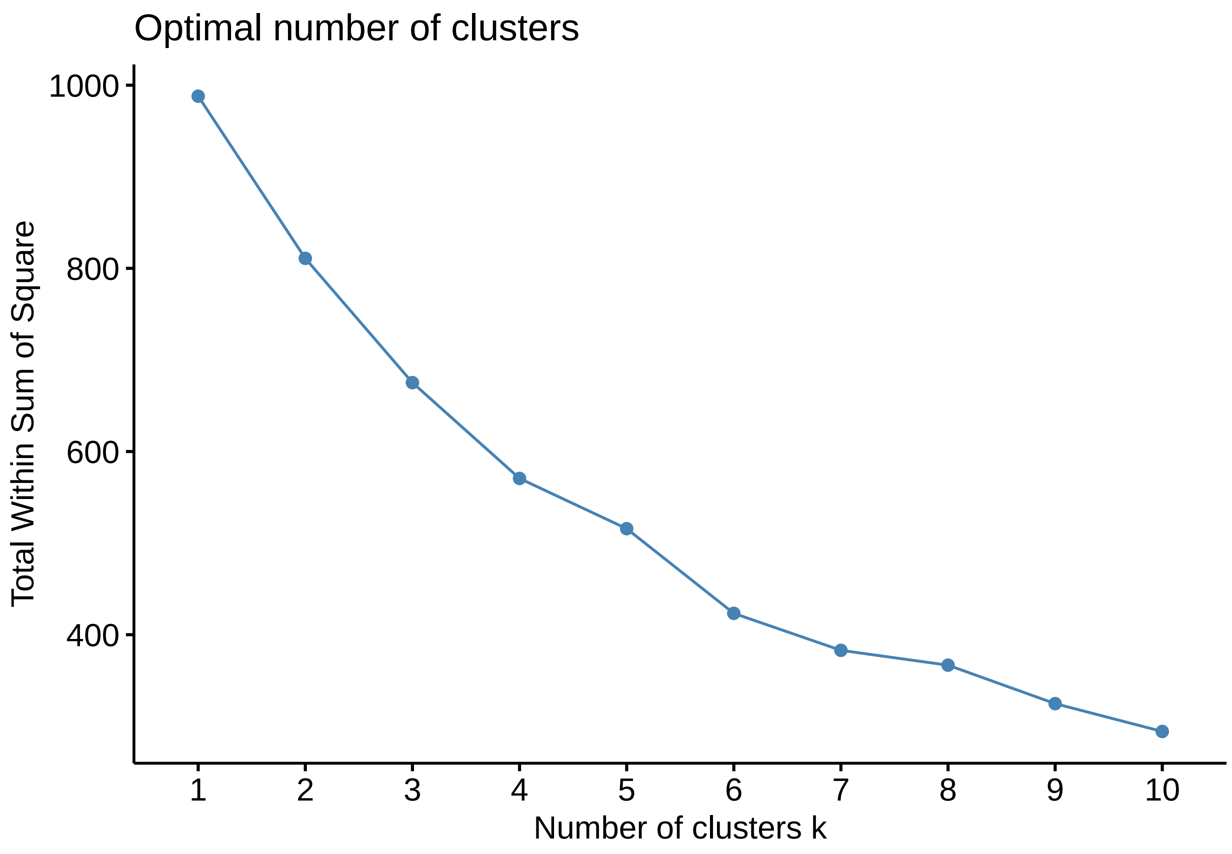
```
## [1] 0.9027089
```

```r
# The approach used by Ward describes the best clustering mechanism of the four approaches tested
#visualize the dendrogram
pltree(hc_ward, cex = 0.6, hang = -1, main = "Dendrogram of agnes")
```

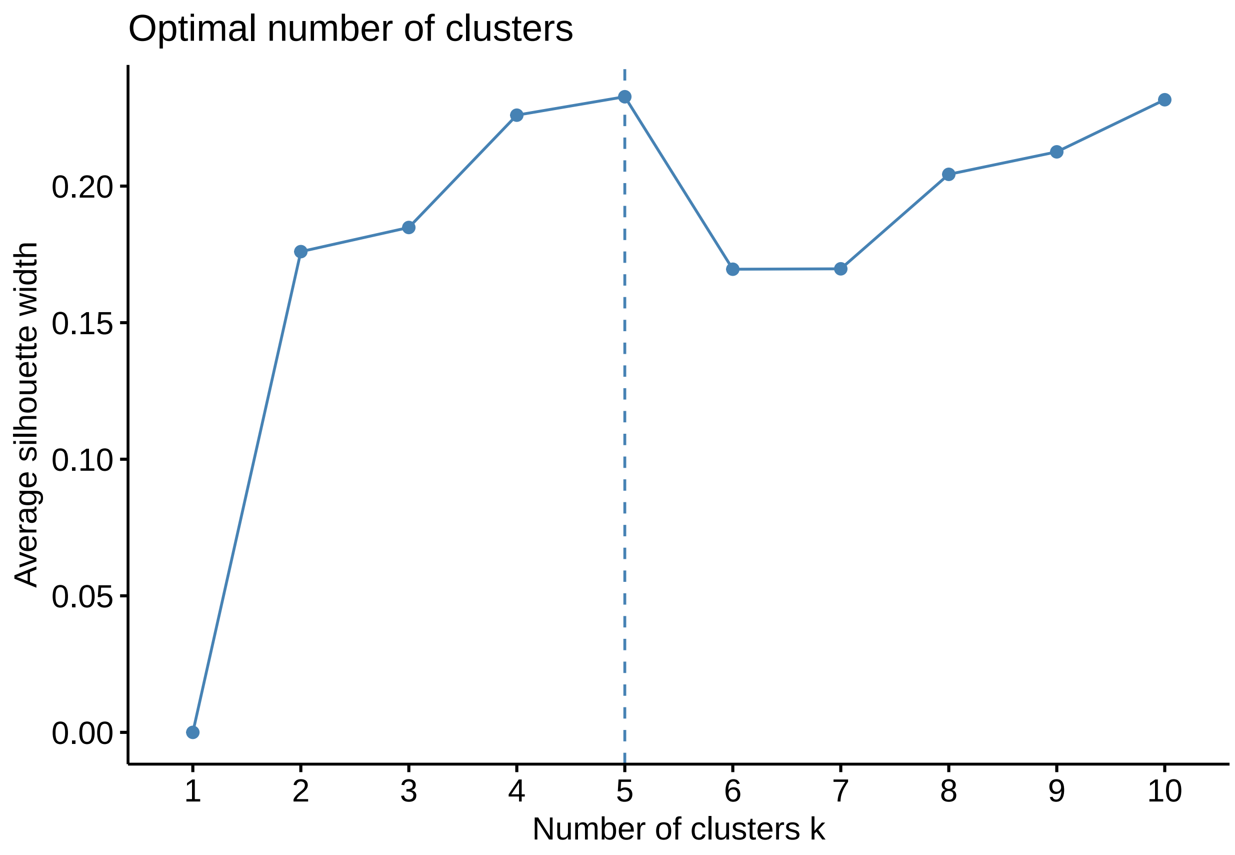


Q> Comment on differences between hierarchical Clustering and K-means

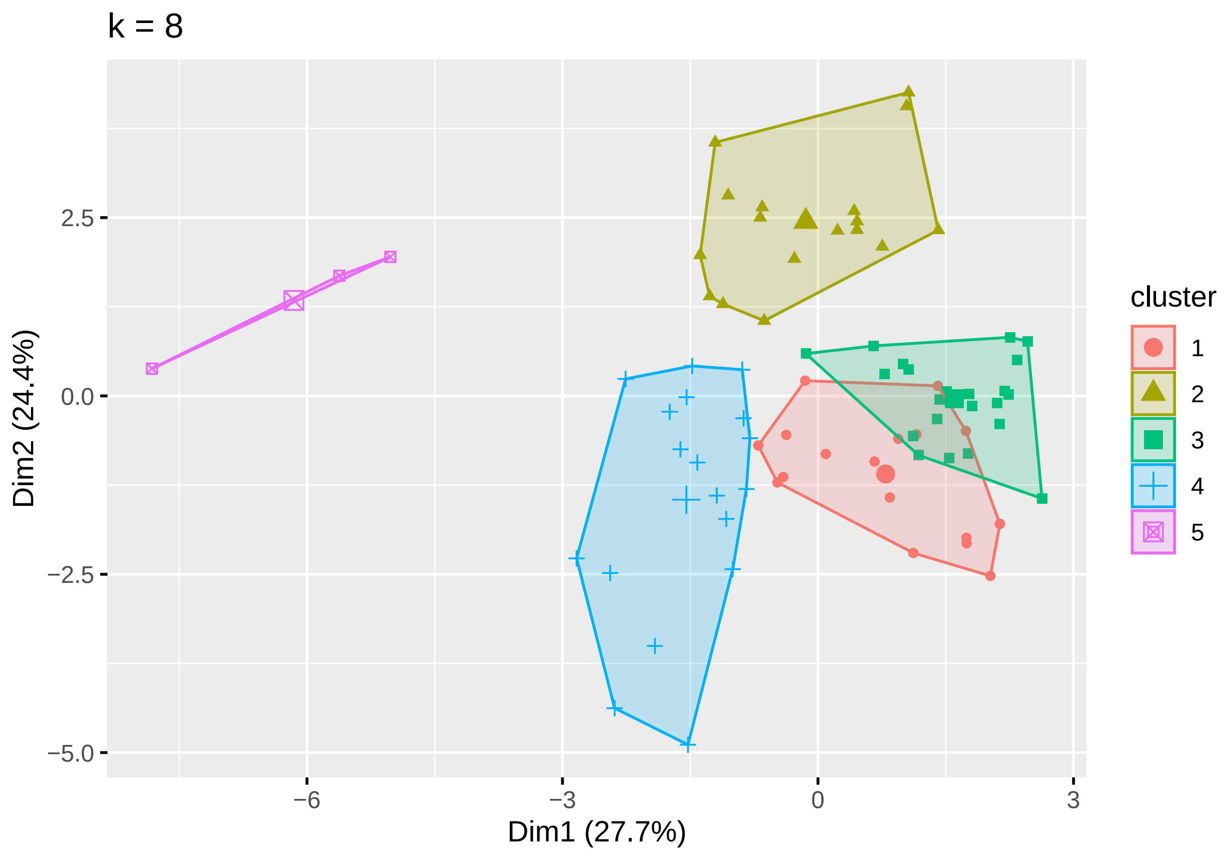
```r
set.seed(123)
#Finding optimal number of clusters - Elbow Method
fviz_nbclust(ImputedDF, kmeans, method = "wss")
```



```r
#Determining Optimal Cluster by Average Silhouette Method
fviz_nbclust(ImputedDF, kmeans, method = "silhouette")
```



```
#Silhouette method shows that 5 numbers of clusters would be optimum.

k8 <- kmeans(ImputedDF, centers = 5, nstart = 25)
fviz_cluster(k8, geom = "point",  data = ImputedDF) + ggtitle("k = 8")
```



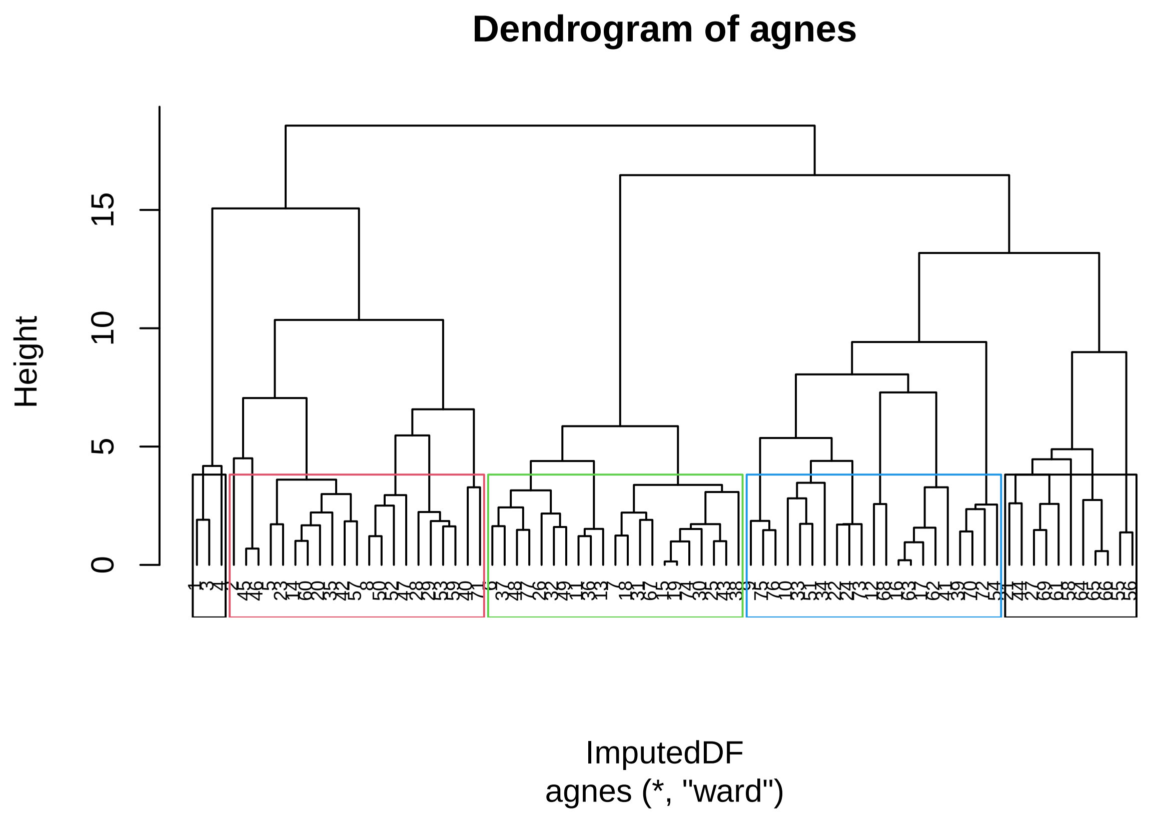
```r
# slicing the dendogram on the longest path, 5 is the optimal level of clusters.
# Cut tree into 5 groups
sub_grp <- cutree(hc_ward, k = 5)
C2 <- as.data.frame(cbind(ImputedDF,sub_grp))
head(C2)
```

```
##     calories    protein         fat     sodium       fiber      carbo
## 1 -1.8929836  1.3286071 -0.01290349 -0.3539844  3.29284661 -2.5243405
## 2  0.6732089  0.4151897  3.96137277 -1.7257708 -0.06375361 -1.7514808
## 3 -1.8929836  1.3286071 -0.01290349  1.1967306  2.87327158 -2.0091007
## 4 -2.9194605  1.3286071 -1.00647256 -0.2346986  4.97114672 -1.7514808
## 5  0.1599704 -0.4982277  0.98066557  0.4810160 -0.48332864 -0.2057614
## 6  0.1599704 -0.4982277  0.98066557  0.2424445 -0.27354112 -1.1074310
##       sugars     potass   vitamins      shelf     weight       cups     rating
## 1 -0.2358694  2.6126578 -0.1453172  0.9515734 -0.1967771 -2.1100340  1.8321876
## 2  0.2239266  0.5260824 -1.2642598  0.9515734 -0.1967771  0.7690100 -0.6180571
## 3 -0.4657674  3.1882648 -0.1453172  0.9515734 -0.1967771 -2.1100340  1.1930986
## 4 -1.6152574  3.3321665 -0.1453172  0.9515734 -0.1967771 -1.3795303  3.6333849
## 5  0.2239266 -0.1214755 -0.1453172  0.9515734 -0.1967771 -0.3052601 -0.5894990
## 6  0.6837226 -0.4092790 -0.1453172 -1.4507595 -0.1967771 -0.3052601 -0.9365625
##   sub_grp
## 1       1
## 2       2
## 3       1
## 4       1
## 5       2
## 6        3
```

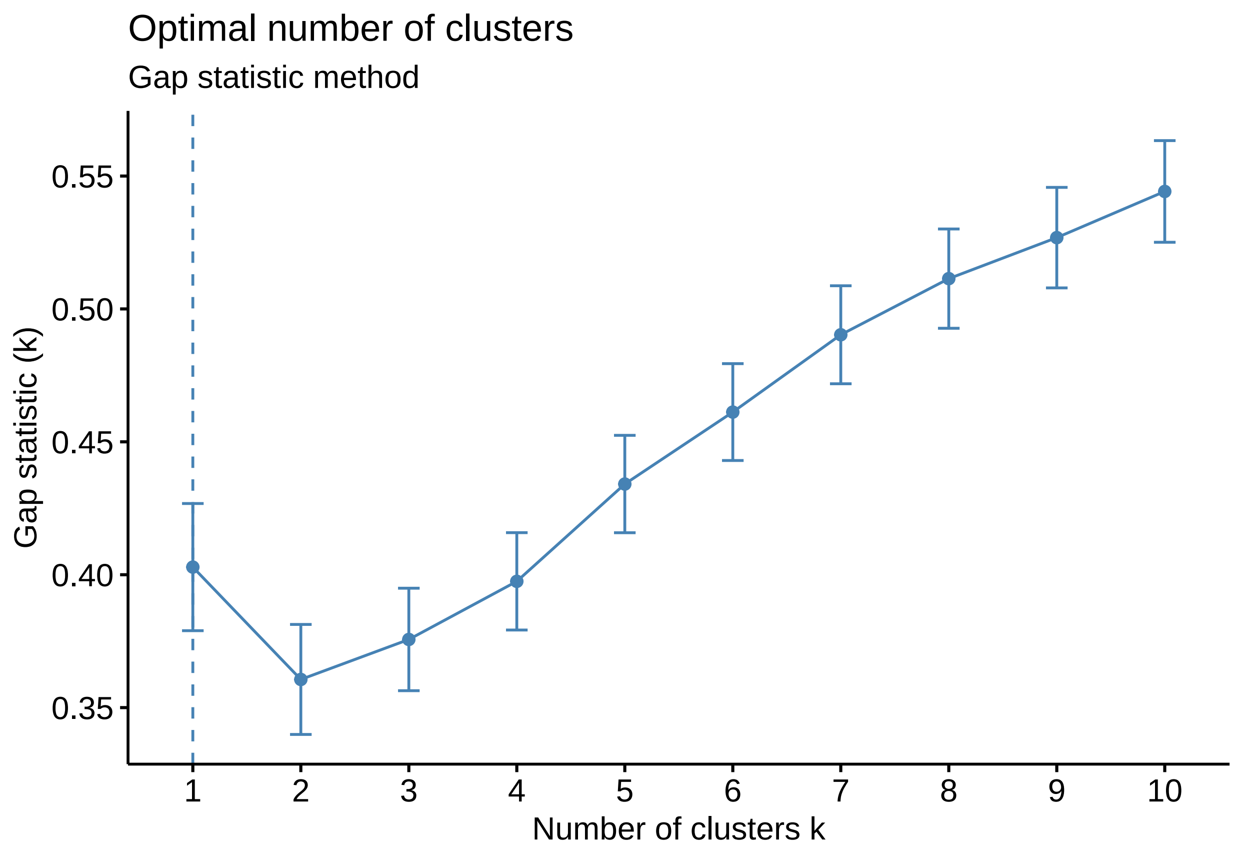
```
# Number of members in each cluster
table(sub_grp)
```

```
## sub_grp
##  1  2  3  4  5
##  3 21 21 21 11
```

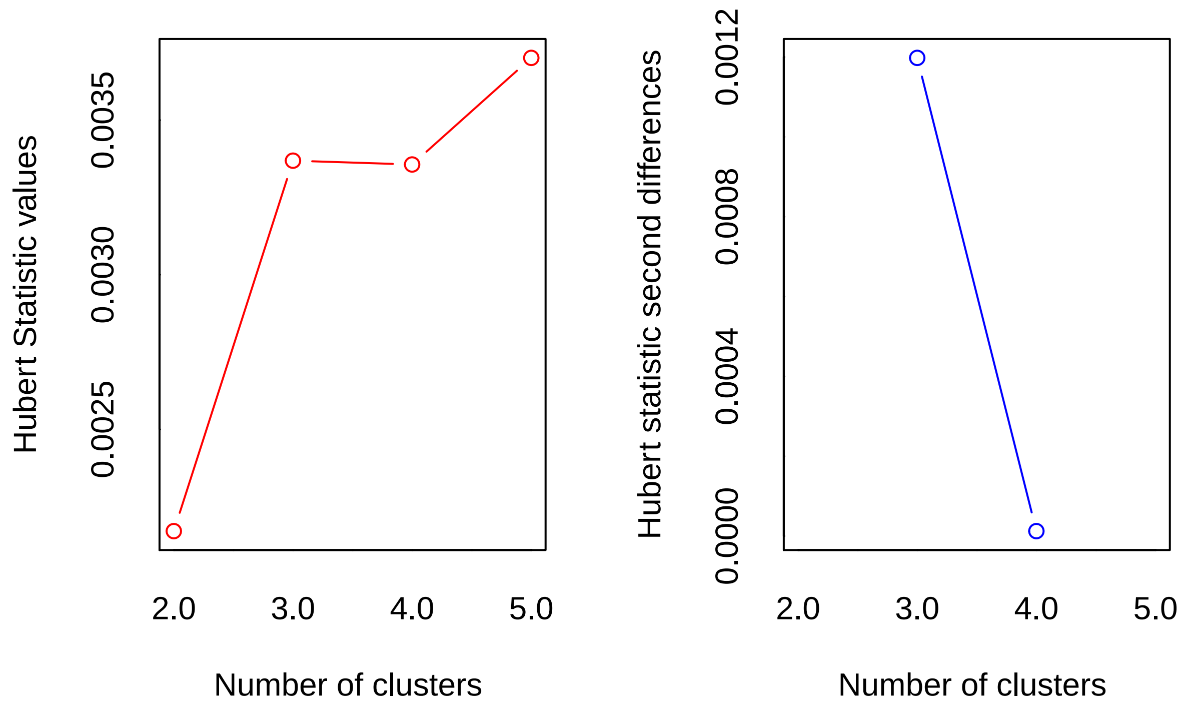
```
#plot dendrogram
pltree(hc_ward, cex = 0.6, hang = -1, main = "Dendrogram of agnes")
rect.hclust(hc_ward, k = 5, border = 1:4)
```



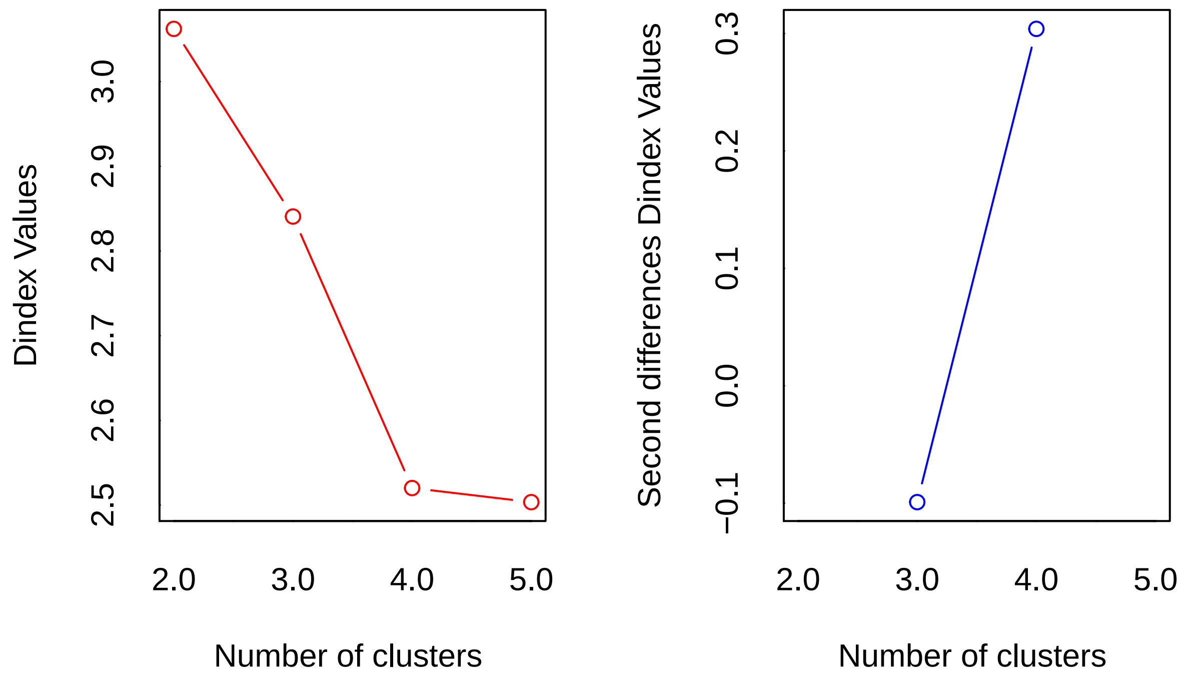
```
# Gap statistic
set.seed(42)
fviz_nbclust(ImputedDF, kmeans,
  nstart = 25,
  method = "gap_stat",
  nboot = 500
) + # reduce it for lower computation time (but less precise results)
  labs(subtitle = "Gap statistic method")
```



```r
#The optimal number of clusters is the one that maximizes the gap statistic. This method suggests only

#Three methods do not necessarily lead to the same result. Here, all 3 approaches suggest a different n

#A fourth alternative is to use the NbClust() function, which provides 30 indices for choosing the best
nbclust_out <- NbClust(
  data = ImputedDF,
  distance = "euclidean",
  min.nc = 2, # minimum number of clusters
  max.nc = 5, # maximum number of clusters
  method = "kmeans" # one of: "ward.D", "ward.D2", "single", "complete", "average", "mcquitty", "median
)
```



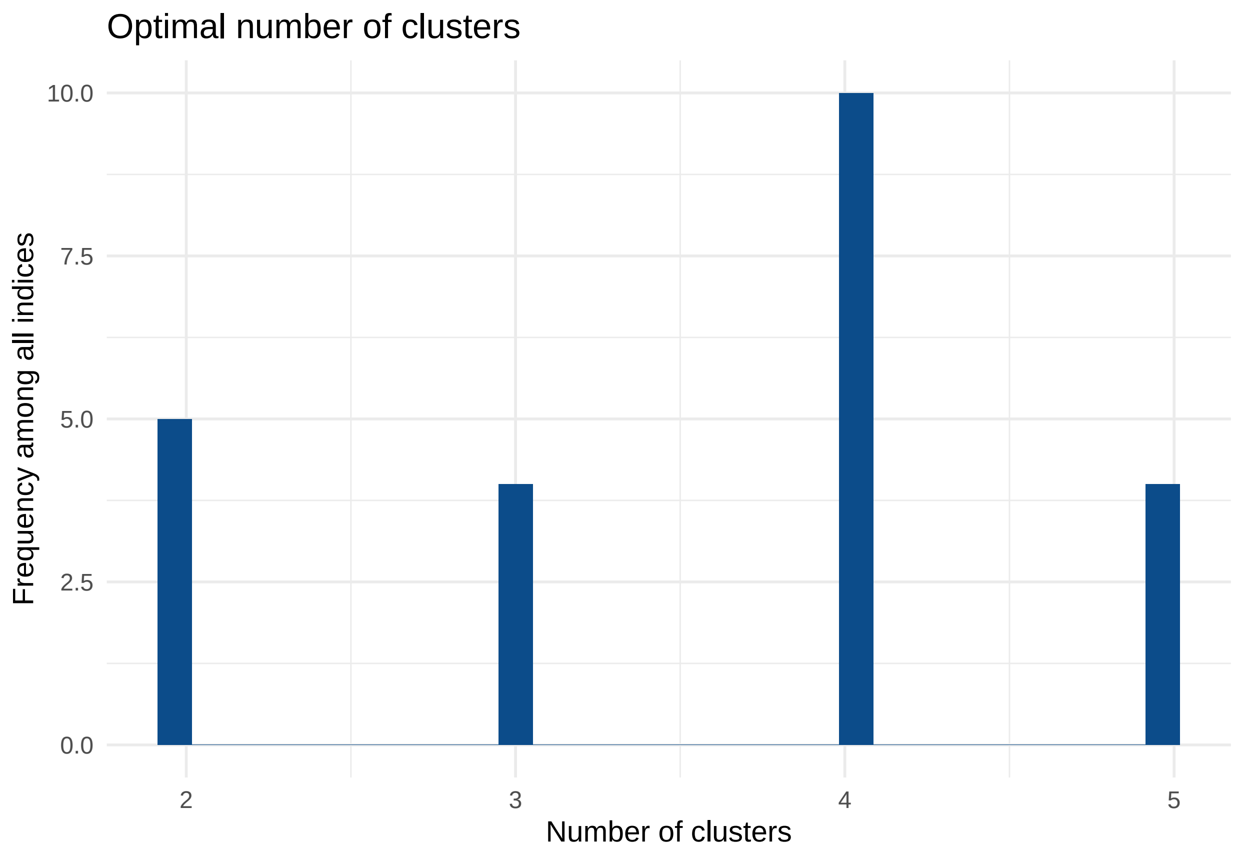
```
## *** : The Hubert index is a graphical method of determining the number of clusters.
##                 In the plot of Hubert index, we seek a significant knee that corresponds to a
##                 significant increase of the value of the measure i.e the significant peak in Hubert
##                 index second differences plot.
##
```



```
## *** : The D index is a graphical method of determining the number of clusters.
##                 In the plot of D index, we seek a significant knee (the significant peak in Dindex
##                 second differences plot) that corresponds to a significant increase of the value of
##                 the measure.
##
## *******************************************************************
## * Among all indices:
## * 5 proposed 2 as the best number of clusters
## * 4 proposed 3 as the best number of clusters
## * 10 proposed 4 as the best number of clusters
## * 4 proposed 5 as the best number of clusters
##
##                    ***** Conclusion *****
##
## * According to the majority rule, the best number of clusters is  4
##
##
## *******************************************************************
```

```
# create a dataframe of the optimal number of clusters
nbclust_plot <- data.frame(clusters = nbclust_out$Best.nc[1, ])
# select only indices which select between 2 and 5 clusters
nbclust_plot <- subset(nbclust_plot, clusters >= 2 & clusters <= 5)

# create plot
```

```
ggplot(nbclust_plot) +
  aes(x = clusters) +
  geom_histogram(bins = 30L, fill = "#0c4c8a") +
  labs(x = "Number of clusters", y = "Frequency among all indices", title = "Optimal number of clusters
  theme_minimal()
```

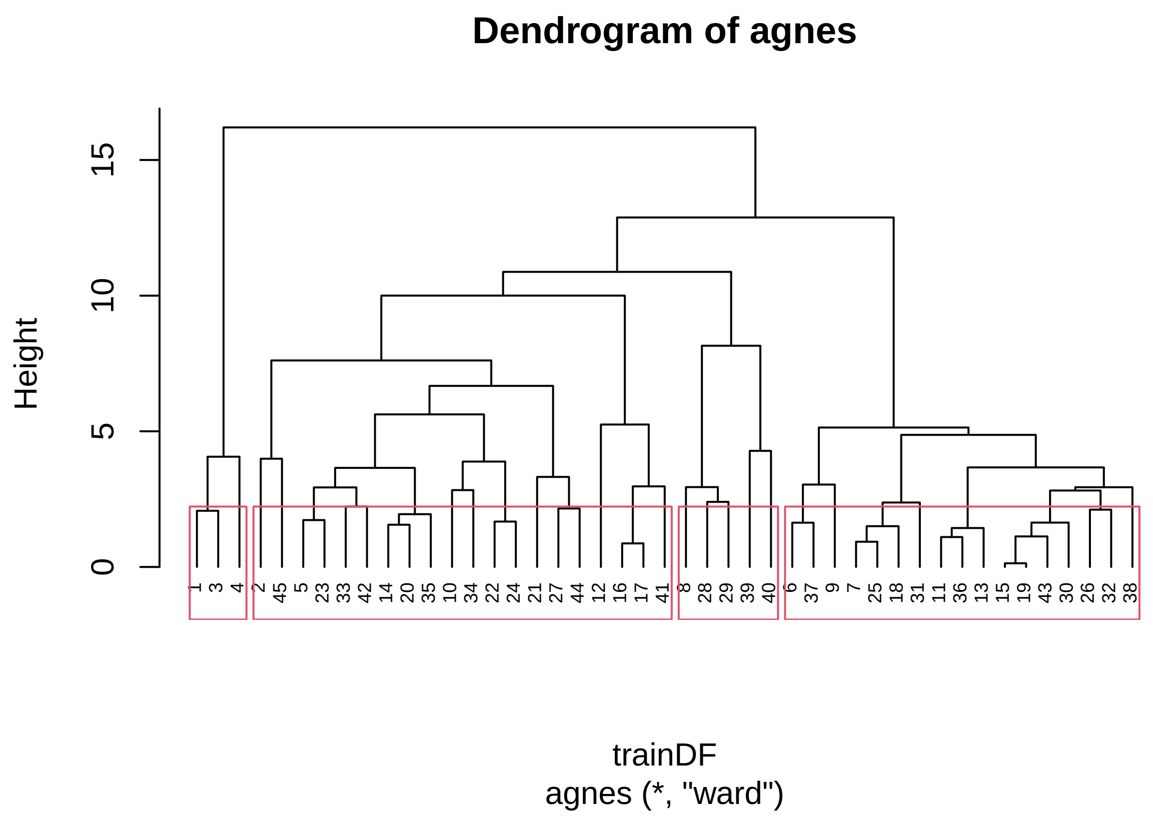


```
#Based on all 30 indices, the best number of clusters is 4 clusters.
# I would choose 4 clusters.
```

Q> Comment on the structure of the clusters and on their stability.

```
library(caret)
DF<-ImputedDF

# Cluster partition
trainDF<-DF[1:45,] # Partition A
testDF<-DF[46:77,] # Partition B
trainDF <- scale(trainDF)
testDF<-scale(testDF)

# The approach used earlier describes that ward is the best clustering mechanism
hc_train <- agnes(trainDF, method = "ward")

#visualize the dendrogram
```

```r
pltree(hc_train, cex = 0.6, hang = -1, main = "Dendrogram of agnes")
rect.hclust(hc_train, k = 4)
```



```r
CWcut <- cutree(hc_train, k = 4)
CWtotal <- as.data.frame( cbind(trainDF,CWcut))
head(CWtotal)
```

```
##     calories    protein        fat     sodium       fiber       carbo
## 1 -2.2902757  1.3899279 -0.1190407 -0.5218048  2.74720044 -2.27995823
## 2  0.7589079  0.4964028  3.4521808 -2.0963468 -0.07044104 -1.51239124
## 3 -2.2902757  1.3899279 -0.1190407  1.2581124  2.39499525 -1.76824691
## 4 -3.5099491  1.3899279 -1.0118461 -0.3848881  4.15602117 -1.51239124
## 5  0.1490712 -0.3971223  0.7737647  0.4366121 -0.42264622  0.02274273
## 6  0.1490712 -0.3971223  0.7737647  0.1627787 -0.24654363 -0.87275209
##         sugars      potass   vitamins      shelf     weight        cups
## 1 -0.44514757  2.45188569 -0.1330313  0.9770643 -0.3068967 -1.8861150
## 2  0.05564345  0.51266701 -1.6296338  0.9770643 -0.3068967  0.7128963
## 3 -0.69554308  2.98684257 -0.1330313  0.9770643 -0.3068967 -1.8861150
## 4 -1.94752061  3.12058179 -0.1330313  0.9770643 -0.3068967 -1.2266644
## 5  0.05564345 -0.08915948 -0.1330313  0.9770643 -0.3068967 -0.2568840
## 6  0.55643446 -0.35663792 -0.1330313 -1.6092824 -0.3068967 -0.2568840
##       rating CWcut
## 1  1.9353757     1
## 2 -0.4509040     2
## 3  1.3129704     1
## 4  3.6895518     1
## 5 -0.4230914     2
## 6 -0.7610947     3
```

```
CWclust1 <- CWtotal[CWtotal$CWcut==1,]
 colMeans(CWclust1)
```

```
##   calories    protein        fat     sodium      fiber      carbo     sugars 
## -2.6968335  1.3899279 -0.4166425  0.1171398  3.0994056 -1.8535321 -1.0294038 
##     potass   vitamins      shelf     weight       cups     rating      CWcut 
##  2.8531034 -0.1330313  0.9770643 -0.3068967 -1.6662981  2.3126327  1.0000000
```

```
CWclust2 <- CWtotal[CWtotal$CWcut==2,]
 colMeans(CWclust2)
```

```
##     calories      protein          fat       sodium        fiber        carbo 
##  0.027103854  0.451726576  0.148800897 -0.189781762 -0.088051296  0.444904567 
##       sugars       potass     vitamins        shelf       weight         cups 
## -0.683023300  0.004457974 -0.282691581  0.265818965 -0.306896708  0.053445672 
##       rating        CWcut 
##  0.377687667  2.000000000
```

```
CWclust3 <- CWtotal[CWtotal$CWcut==3,]
 colMeans(CWclust3)
```

```
##   calories    protein        fat     sodium      fiber      carbo     sugars 
##  0.1490712 -0.8701650 -0.1190407  0.1144552 -0.5262360 -0.3685659  0.8952049 
##     potass   vitamins      shelf     weight       cups     rating      CWcut 
## -0.6359169 -0.1330313 -0.7725232 -0.3068967  0.2861930 -0.8097474  3.0000000
```

```
CWclust4 <- CWtotal[CWtotal$CWcut==4,]
 colMeans(CWclust4)
```

```
##    calories     protein         fat      sodium       fiber       carbo 
##  1.00284261  0.31769781  0.05952036  0.29969545  0.28176415  0.58562518 
##      sugars      potass    vitamins       shelf      weight        cups 
##  0.30603895  0.43242348  1.66289165  0.97706430  2.45517366 -0.18705985 
##      rating       CWcut 
## -0.14518909  4.00000000
```

```
CWmeans1 <- rbind(colMeans(CWclust1),colMeans(CWclust2),colMeans(CWclust3),colMeans(CWclust4))
head(CWmeans1)
```

```
##         calories    protein         fat     sodium      fiber      carbo
## [1,] -2.69683350  1.3899279 -0.41664251  0.1171398  3.0994056 -1.8535321
## [2,]  0.02710385  0.4517266  0.14880090 -0.1897818 -0.0880513  0.4449046
## [3,]  0.14907120 -0.8701650 -0.11904072  0.1144552 -0.5262360 -0.3685659
## [4,]  1.00284261  0.3176978  0.05952036  0.2996954  0.2817641  0.5856252
##          sugars      potass   vitamins      shelf     weight        cups
## [1,] -1.0294038 2.853103352 -0.1330313  0.9770643 -0.3068967 -1.66629812
## [2,] -0.6830233 0.004457974 -0.2826916  0.2658190 -0.3068967  0.05344567
## [3,]  0.8952049 -0.635916878 -0.1330313 -0.7725232 -0.3068967  0.28619295
## [4,]  0.3060390  0.432423477  1.6628917  0.9770643  2.4551737 -0.18705985
##          rating CWcut
## [1,]  2.3126327     1
## [2,]  0.3776877     2
## [3,] -0.8097474     3
## [4,] -0.1451891     4
```

Q> The elementary public schools would like to choose a set of cereals to include in their daily cafeterias. Every day a different cereal is offered, but all cereals should support a healthy diet. For this goal, you are requested to find a cluster of "healthy cereals." Should the data be normalized? If not, how should they be used in the cluster analysis?

```r
#install.packages("hrbrthemes")
library(GGally)
```

```
## Registered S3 method overwritten by 'GGally':
##   method from
##   +.gg   ggplot2
```

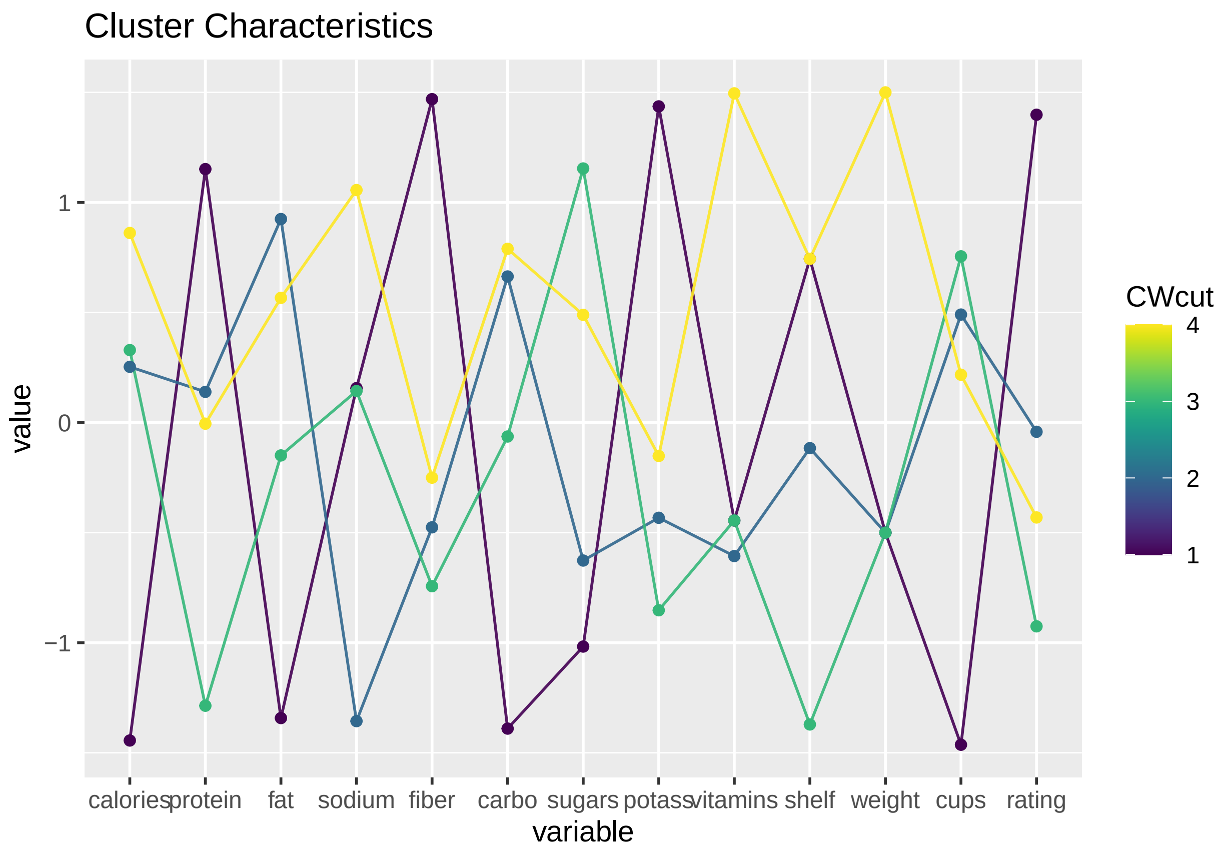
```r
library(ggplot2)
library(hrbrthemes)
```

```
## NOTE: Either Arial Narrow or Roboto Condensed fonts are required to use these themes.

##       Please use hrbrthemes::import_roboto_condensed() to install Roboto Condensed and

##       if Arial Narrow is not on your system, please see https://bit.ly/arialnarrow
```

```r
library(viridis)
```

```
## Loading required package: viridisLite
```

```r
#ggparcoord(cbind(c(1:4),CWmeans),columns = 2:14,groupColumn = 1,showPoints = TRUE,title = " Charter of
ggparcoord(CWmeans1,
           columns = 1:13, groupColumn = 14,
           showPoints = TRUE,
           title = "Cluster Characteristics",
           alphaLines = 0.9
) +
  scale_color_viridis(discrete=FALSE)
```



```
# Based on the characteristics of the cluster, it is clear that Cluster 1 is the strongest with low cal
###In general,when we use the distance metric algorithm the data should be normalized,because the data
```

Q> How do you compare hierarchical clustering and k-means? What are they main advantages of hierarchical clustering compared to k-means?

Ans: Clustering is a subjective statistical analysis and there can be more than one appropriate algorithm, depending on the dataset at hand or the type of problem to be solved. So choosing between k-means and hierarchical clustering is not always easy. If the cluster size is known or if we know that there is a specific number of clusters in our dataset (for example if we would like to distinguish diseased and healthy patients depending on some characteristics but we do not know in which group patients belong to), we should probably opt for the k-means clustering as this technique is used when the number of groups is specified in advance. If the number of groups or clusters in the dataset is unknown (for instance in marketing when trying to distinguish clients without any prior belief on the number of different types of customers), then we should probably opt for the hierarchical clustering to determine in how many clusters the data should be divided.