

DSA 5013-001 Homework 8

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December 09, 2018

These are the libraries used:

```
library(cluster) # silhouette model
library(rgl) # silhouette model
library(useful)
library(dplyr)
library(dbSCAN) #density based clustering
library(factoextra) #fviz_cluster
library(fpc) #Compute DBSCAN
```

Problem 1. Cluster Analysis

Problem 1a

Identify a data set for cluster analysis. The data set must have a minimum of 8 numeric variables and 500 observations.

We are using a red wine classification set from kaggle. (<https://www.kaggle.com/piyushgoyal443/red-wine-dataset/>) It contains 1599 observations and 11 numeric variables. We show that there is no missing data, remove X and the variable quality, then scale the data.

```
wine= read.csv("C:\\Users\\zackw\\Documents\\Classes\\Intelligent Data
Analytics\\HW\\HW8\\wineQualityReds.csv")

#finding missigness
propMissing = function (x) mean(is.na(x))
missing = apply(wine,2, propMissing)
missing

##           X      fixed.acidity      volatile.acidity
##           0              0              0
##      citric.acid      residual.sugar      chlorides
##           0              0              0
## free.sulfur.dioxide total.sulfur.dioxide      density
##           0              0              0
##           pH      sulphates      alcohol
##           0              0              0
##           quality
##           0

# delete variable x "it is row number"
wine$X = NULL
z= wine[,-c(12,12)]

#Scale the data
wineScaled = data.frame(scale(z))
```

Problem 1b

Briefly describe the data set.

The data contains information on red wine. It contains 1599 observations and 11 numeric variables. There is a 12th variable in the dataset named *quality* that ranges from 0-10. Ideally, the cluster data will be grouped together similar quality. The information about the 11 variables is given from the kaggle website.

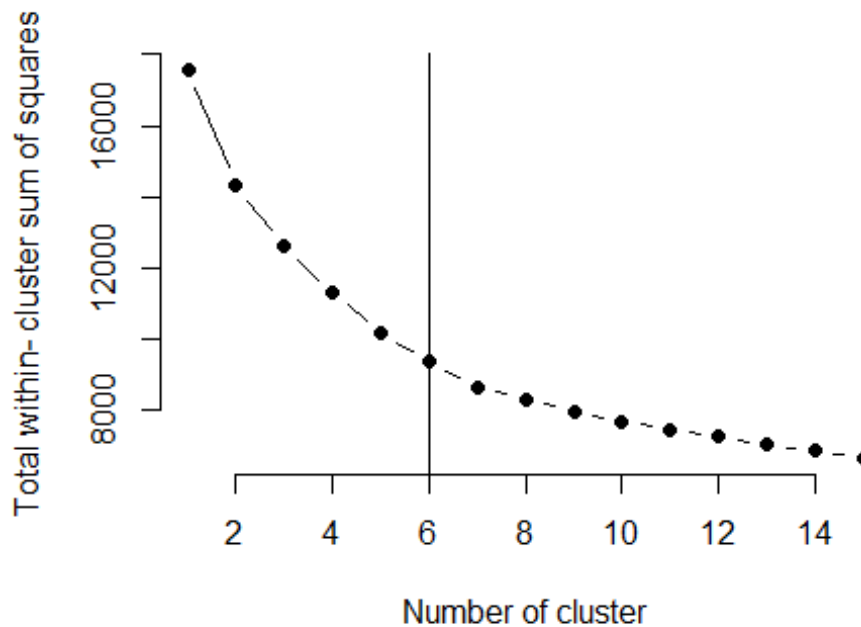
- 1 - fixed acidity: most acids involved with wine or fixed or nonvolatile (do not evaporate readily)
- 2 - volatile acidity: the amount of acetic acid in wine, which at too high of levels can lead to an unpleasant, vinegar taste
- 3 - citric acid: found in small quantities, citric acid can add 'freshness' and flavor to wines
- 4 - residual sugar: the amount of sugar remaining after fermentation stops, it's rare to find wines with less than 1 gram/liter and wines with greater than 45 grams/liter are considered sweet
- 5 - chlorides: the amount of salt in the wine
- 6 - free sulfur dioxide: the free form of S02 exists in equilibrium between molecular S02 (as a dissolved gas) and bisulfite ion; it prevents microbial growth and the oxidation of wine
- 7 - total sulfur dioxide: amount of free and bound forms of S02; in low concentrations, S02 is mostly undetectable in wine, but at free S02 concentrations over 50 ppm, S02 becomes evident in the nose and taste of wine
- 8 - density: the density of water is close to that of water depending on the percent alcohol and sugar content
- 9 - pH: describes how acidic or basic a wine is on a scale from 0 (very acidic) to 14 (very basic); most wines are between 3-4 on the pH scale
- 10 - sulphates: a wine additive which can contribute to sulfur dioxide gas (S02) levels, which acts as an antimicrobial and antioxidant
- 11 - alcohol: the percent alcohol content of the wine

Problem 1c

Perform a clustering analysis of this data set using:

- *Partitional Clustering (use statistical and/or rational reasoning to determine k)*

```
#kmeans
# elbow method
set.seed(7)
k.max = 15
data = wineScaled
wass = sapply(
  1:k.max, function(k){kmeans(data,k,nstart=50,iter.max=15)$tot.withinss})
plot(1:k.max, wass,
     type="b", pch=19, frame=F,
     xlab="Number of cluster",
     ylab="Total within- cluster sum of squares")
abline(v=6)
```

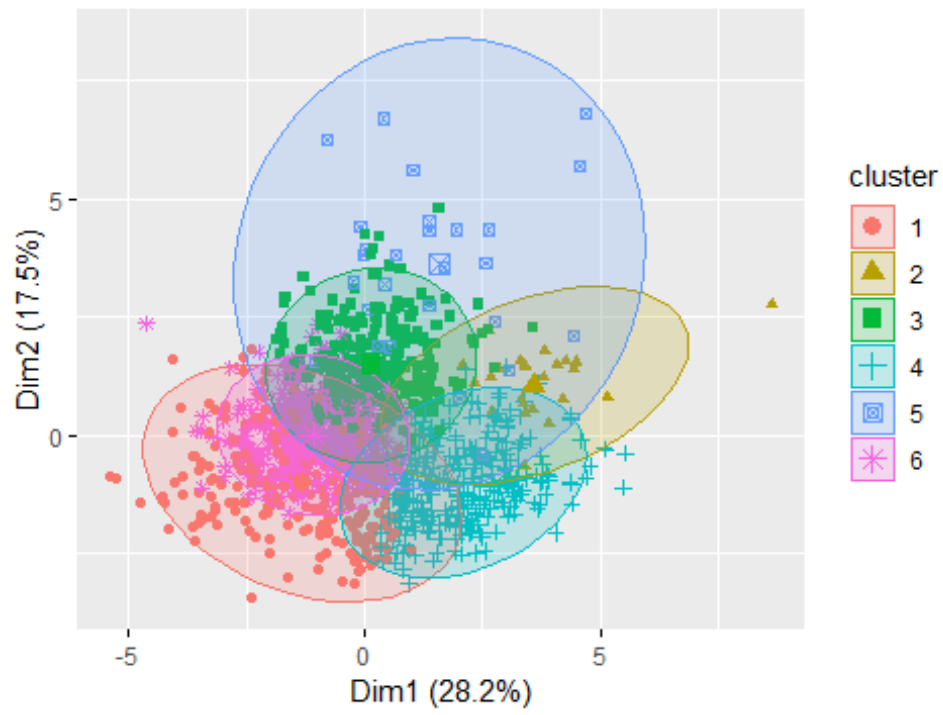


By using elbow method, we determine through the chart that $k = 6$ is the best number clusters

```
# choosing k=6 as clustering
winekm1= kmeans(wineScaled,6,nstart = 20)

# visualization of k-, means clustering
fviz_cluster(winekm1, data = wineScaled, geom = "point",
             stand = FALSE, frame.type = "norm")
```

Cluster plot

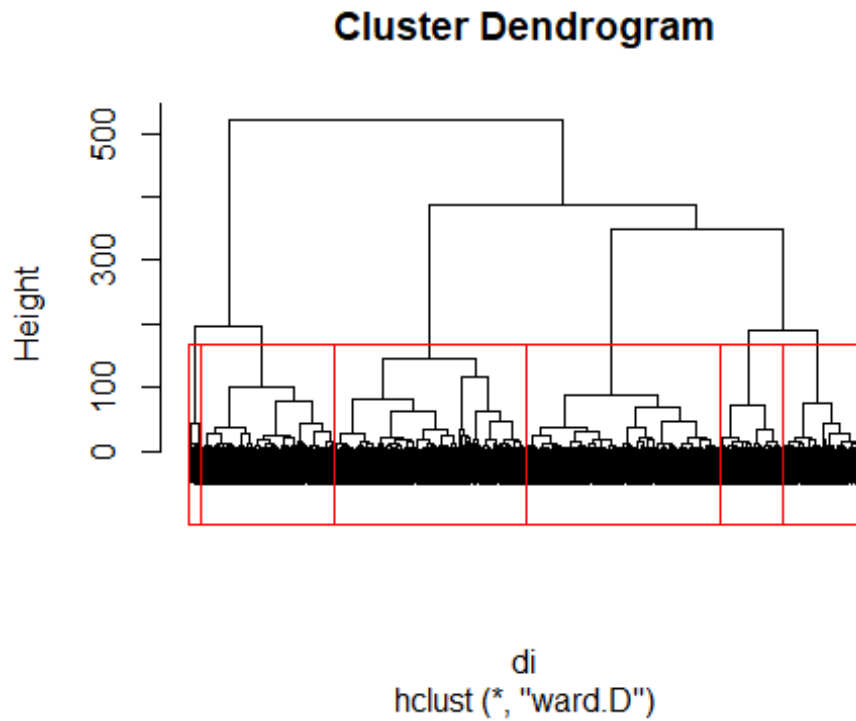


- Hierarchical Clustering (use statistical and/or rational reasoning to determine cut height)

```
# with hierarchical clustering
di <- dist(wineScaled, method="euclidean")

hc <- hclust(di, method="ward.D")
plot(hc, labels=FALSE)

rect.hclust(hc, k=6, border="red")
```

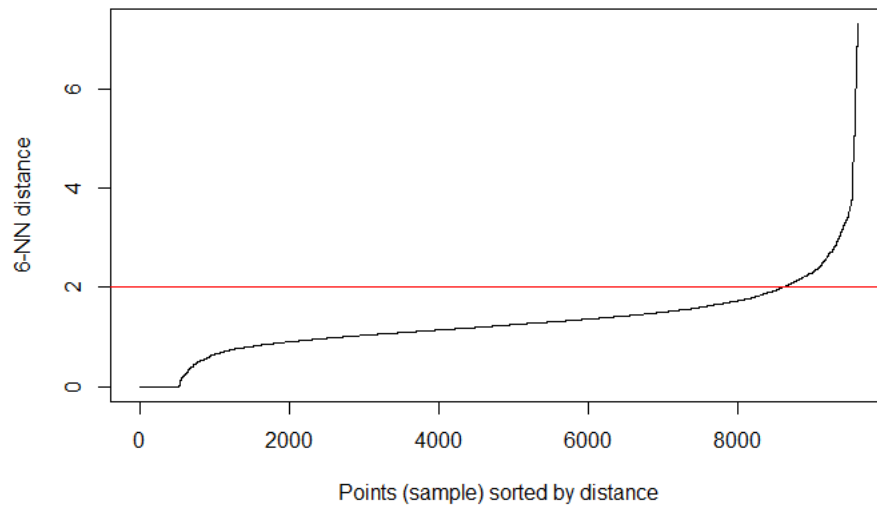


By observing the dendrogram, we estimate that 6 is the optimal cut height. So hierarchical base Clustering says that there are 6 clusters.

- *Density-Based Clustering (use statistical and/or rational reasoning to determine ϵ and min points)*

#3-density based clustering

```
winewmatrix= data.matrix(wineScaled)
kNNdistplot(winewmatrix, k=6)
abline(h=2, col="red")
```

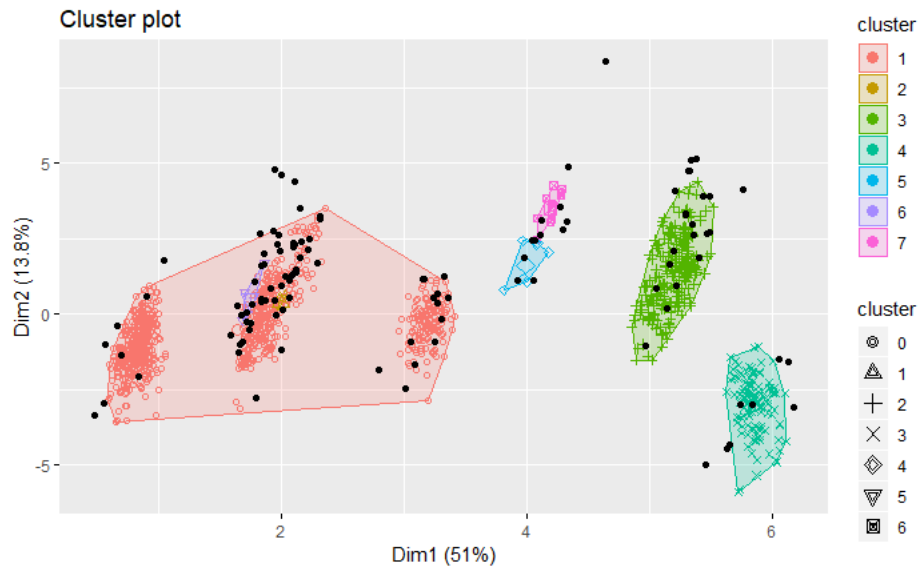


By looking at the knee chart, we estimate $\epsilon = 2$. Through experiments, we estimate that minPt = 5.

```
res <- dbscan(winevmatrix, eps=2, minPts = 5)

# Compute DBSCAN using fpc package
set.seed(123)
db <- fpc::dbscan(winevmatrix, eps = 2, MinPts = 5)

fviz_cluster(db, winevmatrix, stand = FALSE, frame = FALSE, geom = "point")
```



Density based clustering says there are 7 clusters.

Problem 1d

Provide a concise, statistical description of the final cluster results for each method.

Kmeans:

6 clusters

K-means clustering with 6 clusters of sizes 302, 28, 345, 365, 34, 525

```
winekm1$centers
```

```
##    fixed.acidity volatile.acidity citric.acid residual.sugar  chlorides
## 1  -0.69270212    -0.437750230 -0.14745270   -0.257678973 -0.416913732
## 2   0.09538646     0.002199115  1.18118314   -0.389750233  5.782950580
## 3  -0.06888024     0.056768744  0.07177018   -0.009945823 -0.030112762
## 4   1.33443302    -0.671842755  1.12280156    0.073230184 -0.007875253
## 5  -0.08560643    -0.034641327  0.41472600    4.960215800  0.296295201
## 6  -0.48355911     0.683722264 -0.83281214   -0.196596170 -0.062524449
##    free.sulfur.dioxide total.sulfur.dioxide    density      pH
## 1      0.12449435          -0.2294327 -1.24608499  0.6334369
## 2     -0.04950011           0.5101700  0.18001552 -1.7352487
## 3      0.98015875           1.2141818  0.24707145 -0.1281191
## 4     -0.56740982          -0.5433378  0.76180825 -0.8453491
## 5      1.74964380           1.6953018  1.22461740 -0.3253578
## 6     -0.43190355          -0.4251634 -0.06411318  0.4211518
##      sulphates    alcohol
## 1  0.13496581  1.2951673
## 2  3.66226647 -0.8694593
## 3 -0.17786196 -0.5665520
## 4  0.34646284  0.1742501
## 5 -0.02378189 -0.3637992
## 6 -0.39541164 -0.4239378
```

Hierarchical:

6 clusters

Cluster size:

```
> table(as.factor(wineScaled$hcluster))
```

```
 1    2    3    4    5    6
460 452 192  33 314 148
```

Density:

7 clusters

Cluster Size:

```
> table(res$cluster)
```

```
 0    1    2    3    4    5    6    7
130 1004    9  288  140    8    7   13
```


Problem 1e

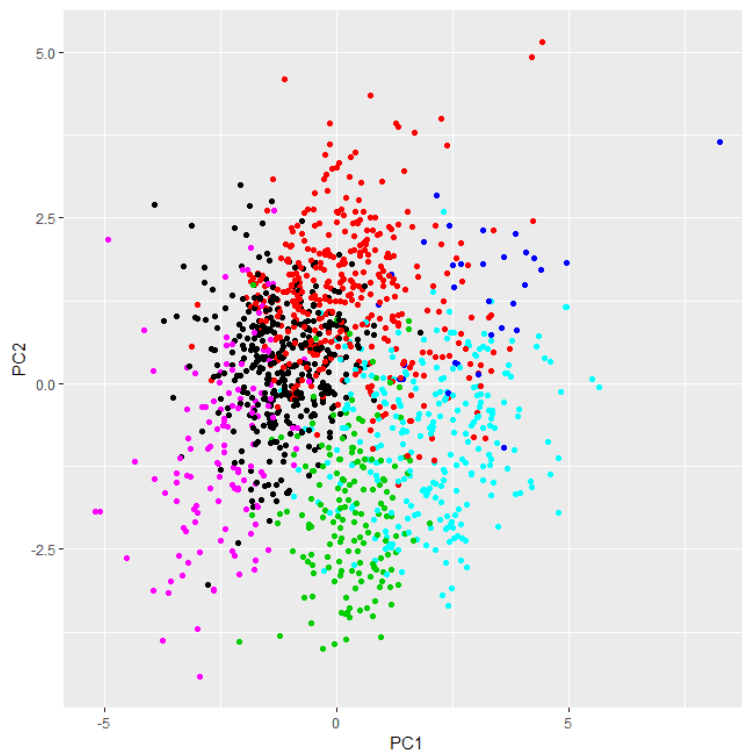
Identify the cluster solution you think is best and provide a rationale for your choice.

Hierarchical Clustering is the best solution. When looking at the three charts of the clusters: k-means clustering has significant overlap and density based clustering shows 6 clusters but reports 7 clusters and has two clusters within another cluster. Hierarchical clustering's dendrogram does not have any of these errors. Therefore we believe that hierarchical clustering to be the best method.

Problem 1f

Provide an interpretation of the clusters belonging to your preferred solution. This interpretation will require a subjective analysis of the clusters.

```
pcWine = prcomp(wine, scale. = T)
biplot(pcWine)
biplot(pcWine)
newData = pcWine$x
newData = newData[,1:2]
ggplot(data = newData, aes(x = PC1, y = PC2))
newData = as.data.frame(newData)
ggplot(data = newData, aes(x = PC1, y = PC2)) + geom_point(col = wineScaled$hcluster)
```



We plotted the 1st two principle components and it shows 6 clusters.