Unsupervised Learning Homework

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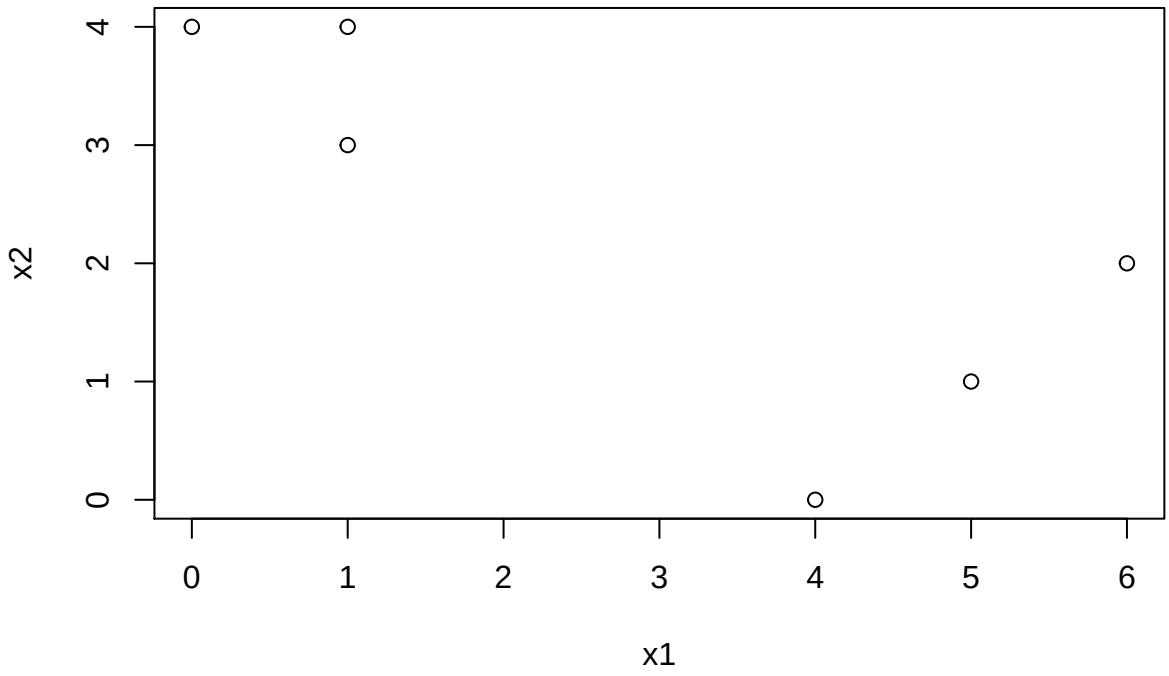
Problem 3

(a)

```
x1 <- c(1,1,0,5,6,4)
x2 <- c(4,3,4,1,2,0)
df <- data.frame(x1,x2)
plot(x1, x2)
```

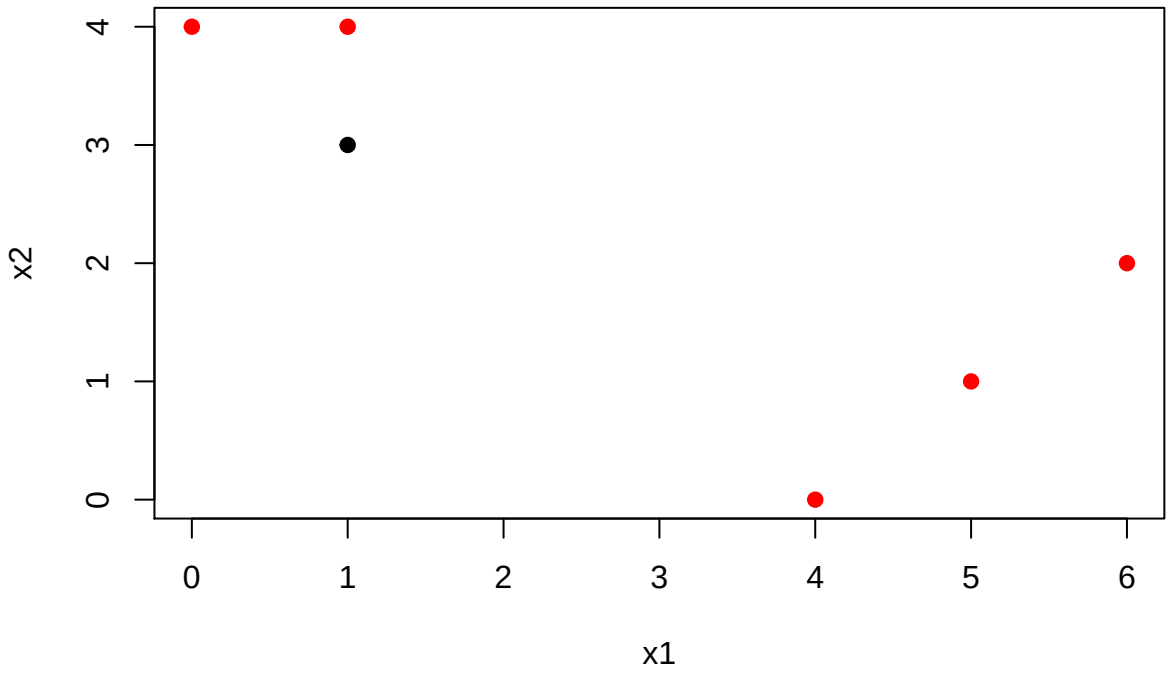


(b)

```
set.seed(99)
in_clusters <- sample(2, nrow(df), replace = TRUE)
in_clusters
```

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

```
plot(x1, x2, col = in_clusters, pch = 20, cex = 1.5)
```




```
df1 <- data.frame(df, in_clusters)
```

(c)

From the plot in (b), we can calculate the centroids as follows:

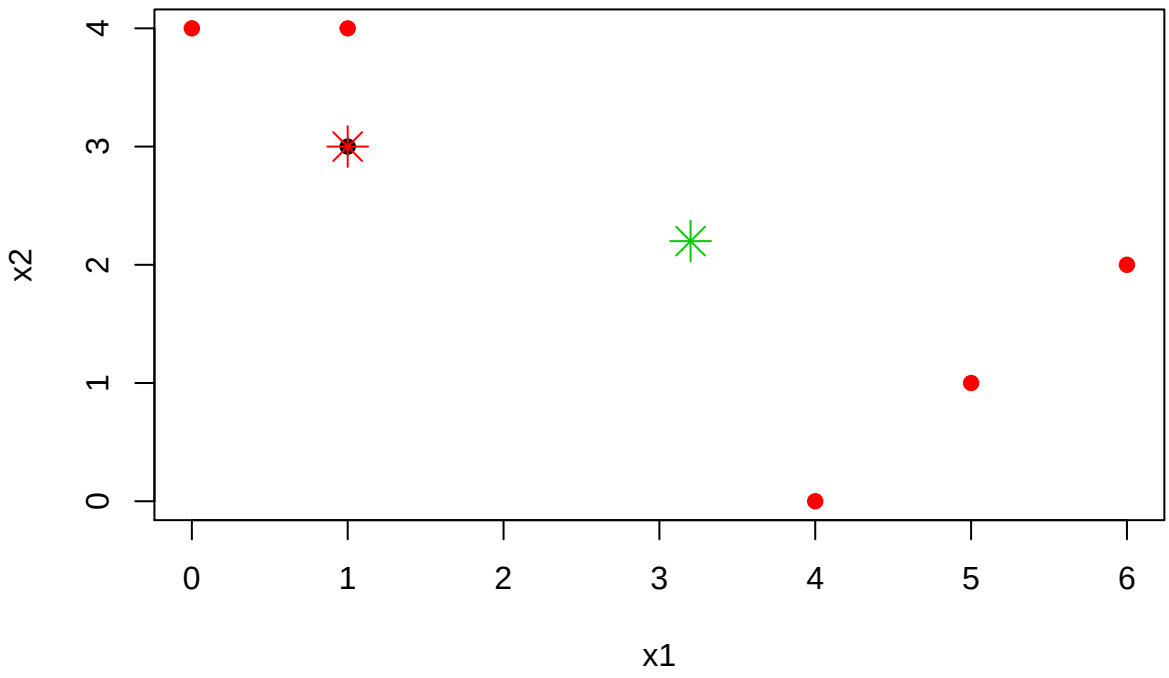
```
cent_1 <- c(mean(df1[df1$in_clusters == 1,1]), mean(df1[df1$in_clusters == 1,2]))
cent_2 <- c(mean(df1[df1$in_clusters == 2,1]), mean(df1[df1$in_clusters == 2,2]))

print(paste0("Centroid for cluster 1 is: ", "(", cent_1[1], ",", cent_1[2], ")"))
```

```
## [1] "Centroid for cluster 1 is: (1,3)"
```

```
print(paste0("Centroid for cluster 2 is: ", "(", cent_2[1], ",", cent_2[2], ")"))
```

```
## [1] "Centroid for cluster 2 is: (3.2,2.2)"
```

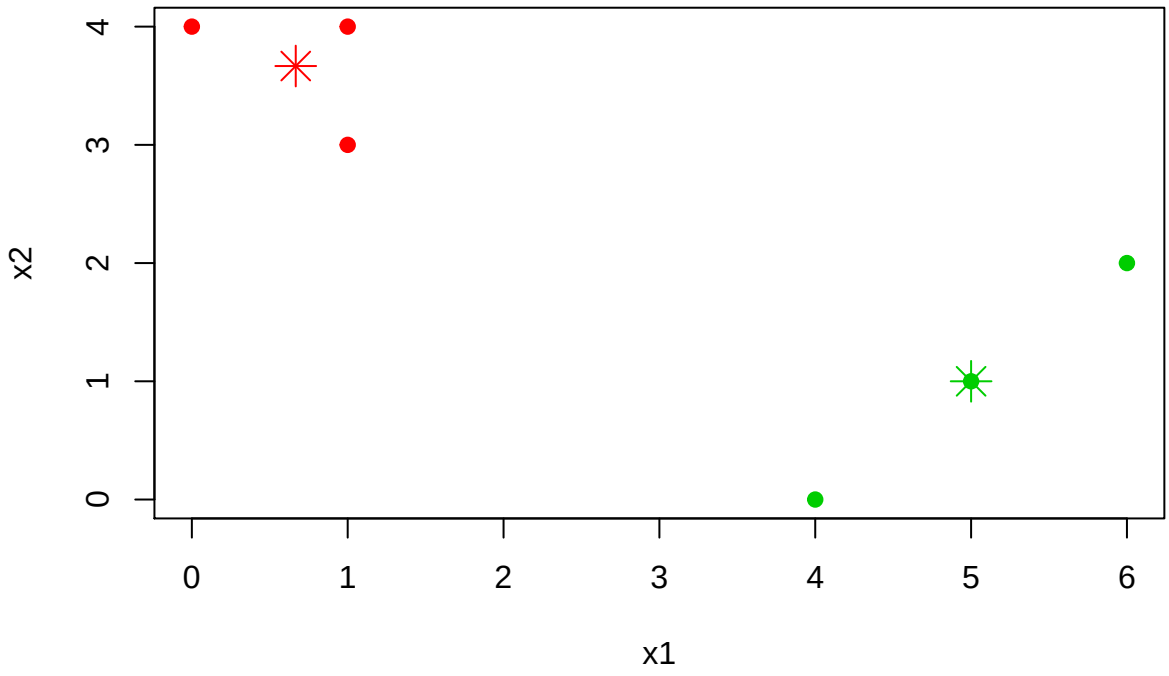
```
plot(x1, x2, col = in_clusters, pch = 20, cex = 1.5)
points(cent_1[1], cent_1[2], pch = 8, cex = 2, col = 2)
points(cent_2[1], cent_2[2], pch = 8, cex = 2, col = 3)
```



(d)

```
euc_dist <- function(v,z){
  sqrt(sum((v-z)^2))
}

df1$updated_cluster <- c()

for (i in 1:nrow(df1)) {
  d1 <- euc_dist(c(df1[i,1],df1[i,2]), c(cent_1[1], cent_1[2]))
  d2 <- euc_dist(c(df1[i,1],df1[i,2]), c(cent_2[1], cent_2[2]))

  if (d1 <= d2){
    df1$updated_cluster[i] <- 1
  }else {
    df1$updated_cluster[i] <- 2
  }
}

updated_centroid1 <- c(mean(df1[df1$updated_cluster == 1,1]), mean(df1[df1$updated_cluster == 1,2]))
updated_centroid2 <- c(mean(df1[df1$updated_cluster == 2,1]), mean(df1[df1$updated_cluster == 2,2]))
```

```
plot(x1, x2, col = df1$updated_cluster+1, pch = 20, cex = 1.5)
points(updated_centroid1[1], updated_centroid1[2], pch = 8, cex = 2, col = 2)
points(updated_centroid2[1], updated_centroid2[2], pch = 8, cex = 2, col = 3)
```

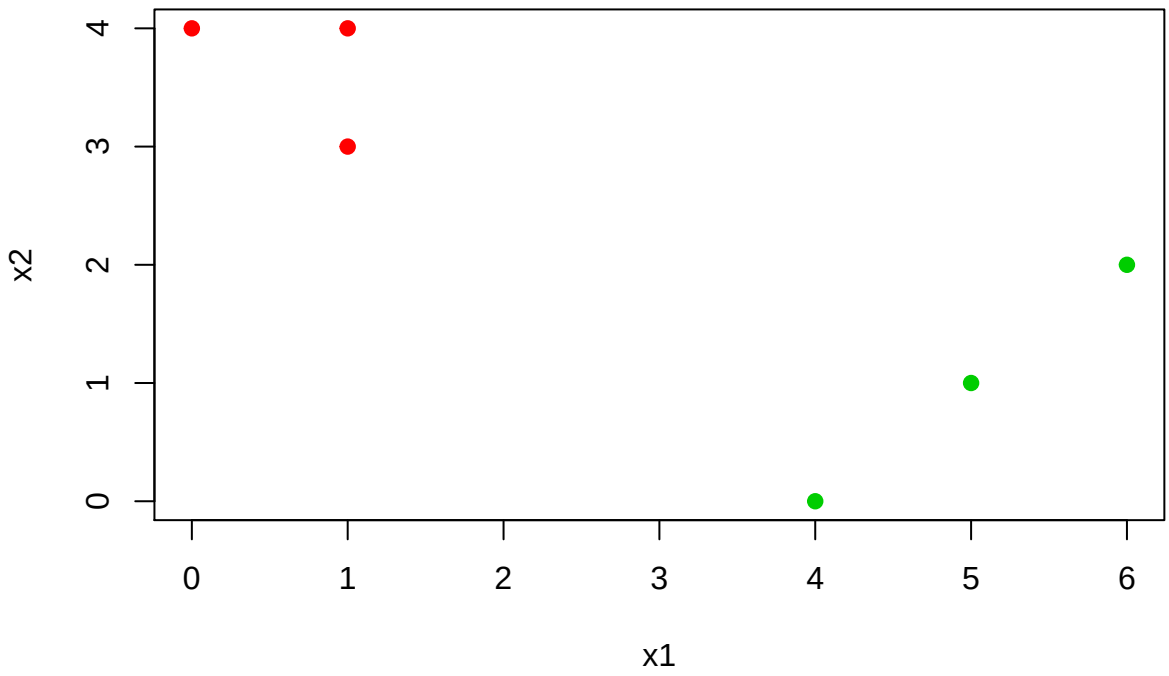


(e)

Assigning each observation to the centroid it is closest to, we do not find a change in the clusters. The algorithm stops with the above step.

(f)

```
plot(x1, x2, col = df1$updated_cluster+1, pch = 20, cex = 1.5)
```



Problem 5

Left: The left side plot shows unscaled variables. In this case, the number of socks becomes more important than the number of computers. With K = 2, the K-Means clustering will result in two clusters separately for soks and computer purchases. Center: Since the variables are scaled, in this case, the piurchase of computers becomes as important as socks. Here, the K-Means clustering will produce two clusters - one of people who have purchased a computer and the other of people who haven't. Right: In this case, K-Means clustering will produce clusters of socks purchases and computer purchases separately because there is a huge difference in the price of socks and computers.

Problem 6

(a)

The first principal component explains 10% of the variation means that 90% of the information in the original data is lost in projecting the tissue sample observations onto the first principal component. Or, 90% of the vraiation in the original data is not containe din the first principal component.

(b)

Since each patient sample was run on either of the machines A and B, the machine used could be used as a feature in the PCA. We could check if there is an improvement in the PVE after adding the machine used as a feature.

(c)

```
set.seed(9)
control <- matrix(rnorm(50*1000), ncol = 50)
treatment <- matrix(rnorm(50*1000), ncol = 50)

x <- cbind(control, treatment)
x[1,] <- seq(-18, 18 -.36, .36)
pca <- prcomp(scale(x))
summary(pca)$importance[,1]
```

```
##     Standard deviation Proportion of Variance  Cumulative Proportion
##               3.159783               0.099840               0.099840
```

The proportion of variance explained by the first principal component is 9.98%. Including the machine used (A and B) as a feature in the data, coding 0 for A and 10 for B, we get results as below: the PVE increased to 11.5%.

```
X <- rbind(x, c(rep(0,50), rep(10, 50)))
pca_out <- prcomp(scale(X))
summary(pca_out)$importance[,1]
```

```
##     Standard deviation Proportion of Variance  Cumulative Proportion
##               3.391937               0.115050               0.115050
```

Problem 8

(a)

```
#The sdev approach to PVE
data("USArrests")

pca_usa <- prcomp(USArrests, scale. = TRUE)
pca_usa$sdev
```

```
## [1] 1.5748783 0.9948694 0.5971291 0.4164494
```

```
#To get the variance
pca_var <- pca_usa$sdev^2
pca_var
```

```
## [1] 2.4802416 0.9897652 0.3565632 0.1734301
```

```r
#To get the PVE
pve <- pca_var/sum(pca_var)
pve
```

```
## [1] 0.62006039 0.24744129 0.08914080 0.04335752
```

(b)

```r
#The prcomp PVE approach
usa_scaled <- scale(USArrests)

loadings <- pca_usa$rotation
sum_var <- sum(apply(as.matrix(usa_scaled)^2, 2, sum))
apply((as.matrix(usa_scaled) %*% loadings)^2, 2, sum)/ sum_var
```

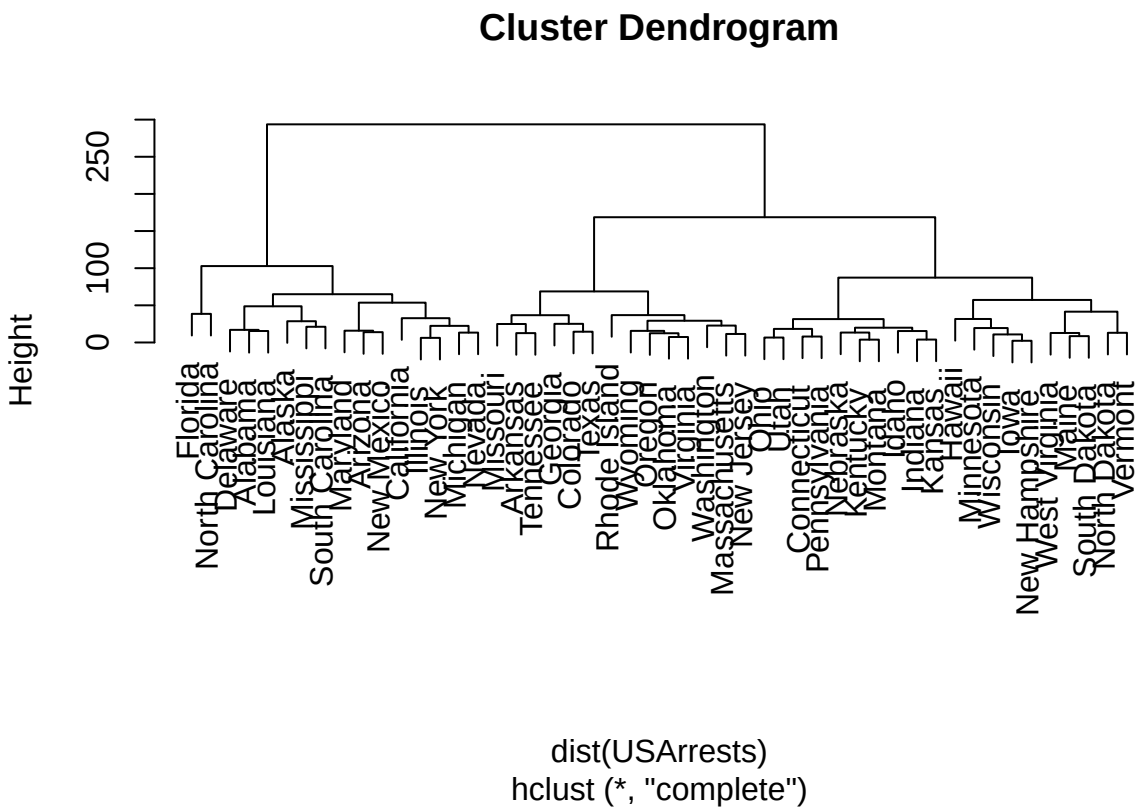
```
##        PC1        PC2        PC3        PC4
## 0.62006039 0.24744129 0.08914080 0.04335752
```

The PVE for each principal component form both the approaches is the same.

Problem 9

(a)

```r
set.seed(9)

hc.complete <- hclust(dist(USArrests), method = "complete")
plot(hc.complete)
```



(b)

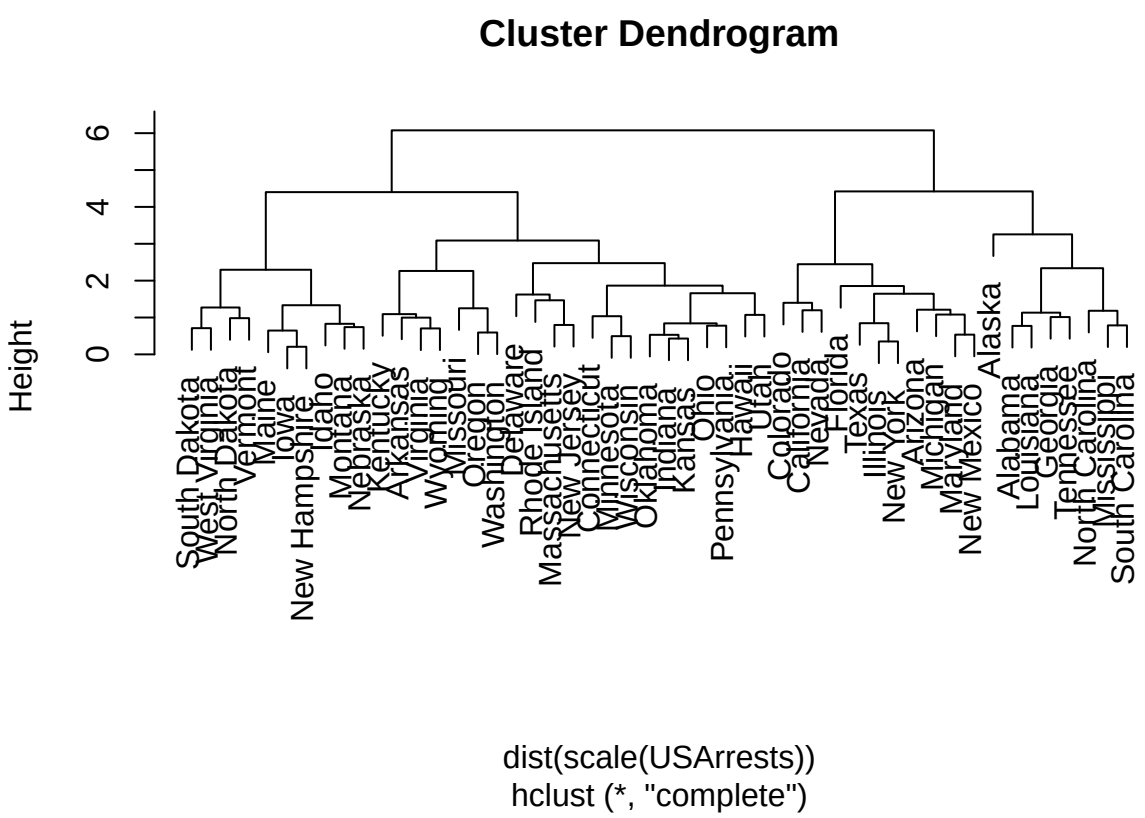
```
hc_cut <- cutree(hc.complete, 3)
clusters <- split(data.frame(names(hc_cut), hc_cut), as.factor(hc_cut))
clusters
```

```
## $`1`
##                 names.hc_cut. hc_cut
## Alabama               Alabama      1
## Alaska                 Alaska      1
## Arizona               Arizona      1
## California         California      1
## Delaware             Delaware      1
## Florida               Florida      1
## Illinois             Illinois      1
## Louisiana           Louisiana      1
## Maryland             Maryland      1
## Michigan             Michigan      1
## Mississippi       Mississippi      1
## Nevada                 Nevada      1
## New Mexico         New Mexico      1
## New York             New York      1
## North Carolina North Carolina      1
## South Carolina South Carolina      1
```

```
##
## $`2`
##                names.hc_cut. hc_cut
## Arkansas            Arkansas      2
## Colorado            Colorado      2
## Georgia              Georgia      2
## Massachusetts Massachusetts      2
## Missouri            Missouri      2
## New Jersey       New Jersey      2
## Oklahoma            Oklahoma      2
## Oregon                Oregon      2
## Rhode Island    Rhode Island      2
## Tennessee          Tennessee      2
## Texas                  Texas      2
## Virginia            Virginia      2
## Washington       Washington      2
## Wyoming              Wyoming      2
##
## $`3`
##                names.hc_cut. hc_cut
## Connecticut      Connecticut      3
## Hawaii                Hawaii      3
## Idaho                  Idaho      3
## Indiana              Indiana      3
## Iowa                    Iowa      3
## Kansas                Kansas      3
## Kentucky            Kentucky      3
## Maine                  Maine      3
## Minnesota          Minnesota      3
## Montana              Montana      3
## Nebraska            Nebraska      3
## New Hampshire New Hampshire      3
## North Dakota    North Dakota      3
## Ohio                    Ohio      3
## Pennsylvania    Pennsylvania      3
## South Dakota    South Dakota      3
## Utah                    Utah      3
## Vermont              Vermont      3
## West Virginia West Virginia      3
## Wisconsin          Wisconsin      3
```

(c)

```r
hc_scaled <- hclust(dist(scale(USArrests)), method = "complete")
plot(hc_scaled)
```



(d)

```
hc_scaled_cut <- cutree(hc_scaled, 3)
clusters_scaled <- split(data.frame(names(hc_scaled_cut), hc_scaled_cut), as.factor(hc_scaled_cut))
clusters_scaled
```

```
## $`1`
##                names.hc_scaled_cut. hc_scaled_cut
## Alabama                     Alabama             1
## Alaska                       Alaska             1
## Georgia                     Georgia             1
## Louisiana                 Louisiana             1
## Mississippi             Mississippi             1
## North Carolina       North Carolina             1
## South Carolina       South Carolina             1
## Tennessee                 Tennessee             1
##
## $`2`
##            names.hc_scaled_cut. hc_scaled_cut
## Arizona                  Arizona             2
## California            California             2
## Colorado                Colorado             2
## Florida                  Florida             2
## Illinois                Illinois             2
```

```
## Maryland               Maryland             2
## Michigan               Michigan             2
## Nevada                   Nevada             2
## New Mexico           New Mexico             2
## New York               New York             2
## Texas                     Texas             2
##
## $`3`
##               names.hc_scaled_cut. hc_scaled_cut
## Arkansas                  Arkansas             3
## Connecticut            Connecticut             3
## Delaware                  Delaware             3
## Hawaii                      Hawaii             3
## Idaho                       Idaho              3
## Indiana                    Indiana             3
## Iowa                          Iowa             3
## Kansas                     Kansas              3
## Kentucky                  Kentucky             3
## Maine                        Maine             3
## Massachusetts        Massachusetts             3
## Minnesota                Minnesota             3
## Missouri                  Missouri             3
## Montana                    Montana             3
## Nebraska                  Nebraska             3
## New Hampshire        New Hampshire             3
## New Jersey              New Jersey             3
## North Dakota          North Dakota             3
## Ohio                          Ohio             3
## Oklahoma                 Oklahoma              3
## Oregon                     Oregon              3
## Pennsylvania          Pennsylvania             3
## Rhode Island          Rhode Island             3
## South Dakota          South Dakota             3
## Utah                          Utah             3
## Vermont                   Vermont              3
## Virginia                  Virginia             3
## Washington              Washington             3
## West Virginia        West Virginia             3
## Wisconsin                Wisconsin             3
## Wyoming                    Wyoming             3
```

```
table(hc_cut, hc_scaled_cut)
```

```
##       hc_scaled_cut
## hc_cut  1  2  3
##      1  6  9  1
##      2  2  2 10
##      3  0  0 20
```

Scaling the variables affect the clusters obtained. It is better to scale the variables because they are measured on different units. For example, Assault is measured on a higher scale and will contribute most to the first principal component because of higher variance. Therefore, to obtain better results, all the variables need to be scaled prior to performing the clustering.

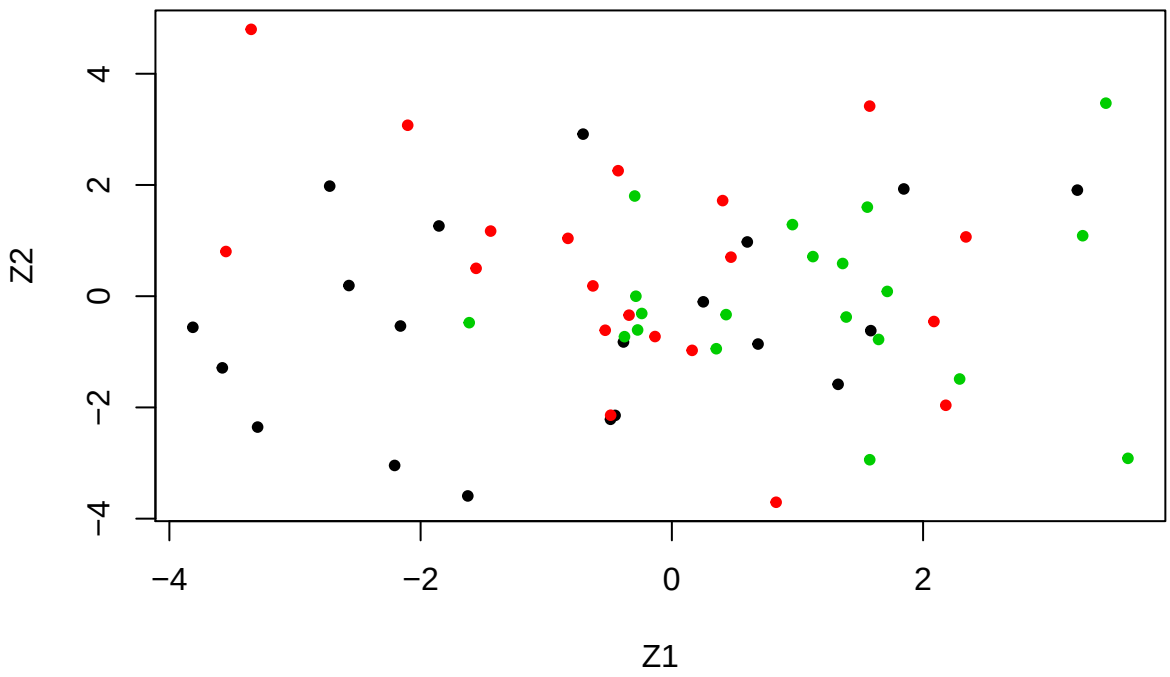
Problem 10

(a)

```
set.seed(9)

sim_data <- matrix(sapply(1:3, function(x) rnorm(20*50, mean = 0, sd = 0.001)), ncol = 50)
class <- unlist(lapply(1:3, FUN = function(x) rep(x,20)))

sim_data <- data.frame(sim_data)
sim_data$true_labels <- c(rep(1,20), rep(2,20), rep(3,20))
```

(b)

```
sim_pca <- prcomp(sim_data, scale. = TRUE, center = TRUE)
plot(sim_pca$x[,1:2], col = class, xlab = "Z1", ylab = "Z2", pch = 20)
```



(c)

```
set.seed(9)

sim_kmeans <- kmeans(sim_data, 3)
table(sim_data$true_labels, sim_kmeans$cluster)
```

```
##
##      1  2  3
##   1 20  0  0
##   2  0 20  0
##   3  0  0 20
```

K-Means performs well in this case. It clusters the observations correctly.

(d)

```
set.seed(9)

sim_kmeans2 <- kmeans(sim_data, 2)
table(sim_data$true_labels, sim_kmeans2$cluster)
```

```
##
##      1  2
##   1 20  0
##   2  0 20
##   3  0 20
```

All the observations from the third cluster are absorbed into cluster 2.

(e)

```
set.seed(9)

sim_kmeans4 <- kmeans(sim_data, 4)
table(sim_data$true_labels, sim_kmeans4$cluster)
```

```
##
##      1  2  3  4
##   1  0  0 20  0
##   2 10 10  0  0
##   3  0  0  0 20
```

K-Means with K = 4 doesn't perform as well as the above two.

(f)

```
set.seed(9)
```

```
km_out <- kmeans(sim_pca$x[,1:2], 3)
table(sim_data$true_labels, km_out$cluster)
```

```
##
##      1  2  3
##   1  7  9  4
##   2  6  9  5
##   3  1 11  8
```

Using the first two principal components also does not seem to improve the results. There are many miclassified observations.

(g)

```
set.seed(9)

km_out_1 <- kmeans(scale(sim_data), 3)
table(sim_data$true_labels, km_out_1$cluster)
```

```
##
##      1  2  3
##   1 10  6  4
##   2  9  8  3
##   3  4  7  9
```

Scaling the variables did not improve the results much.

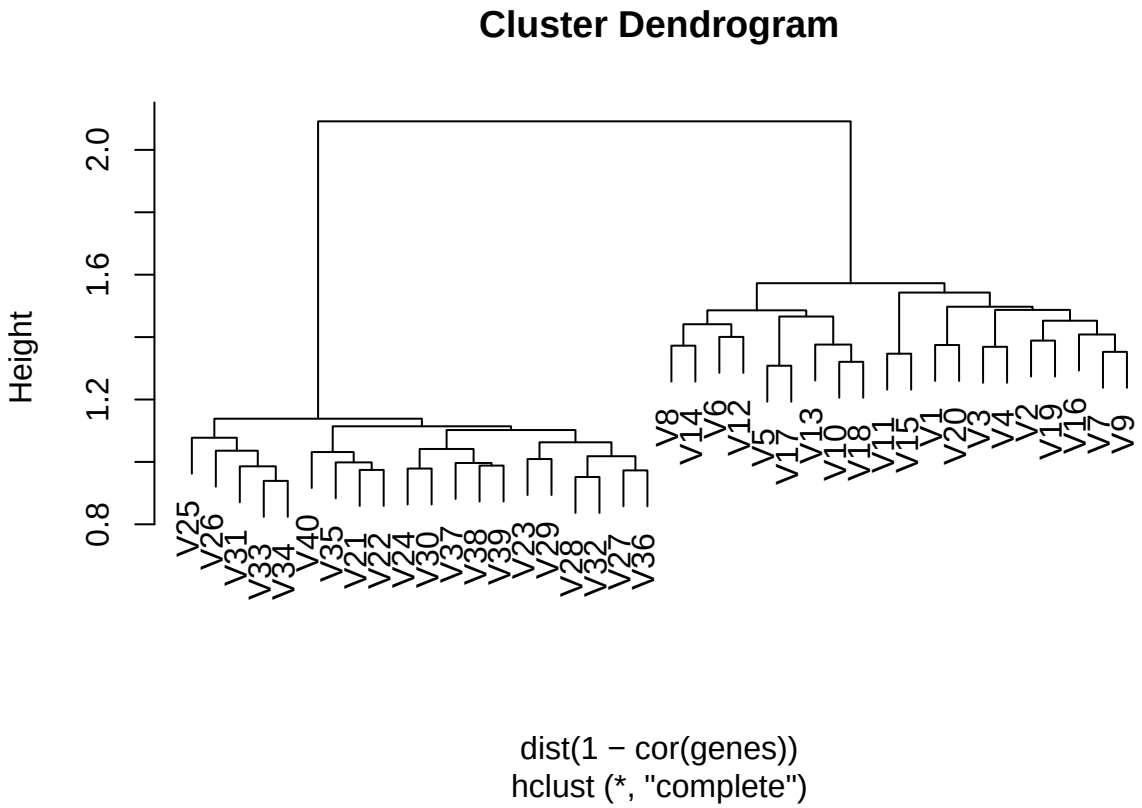
Problem 11

(a)

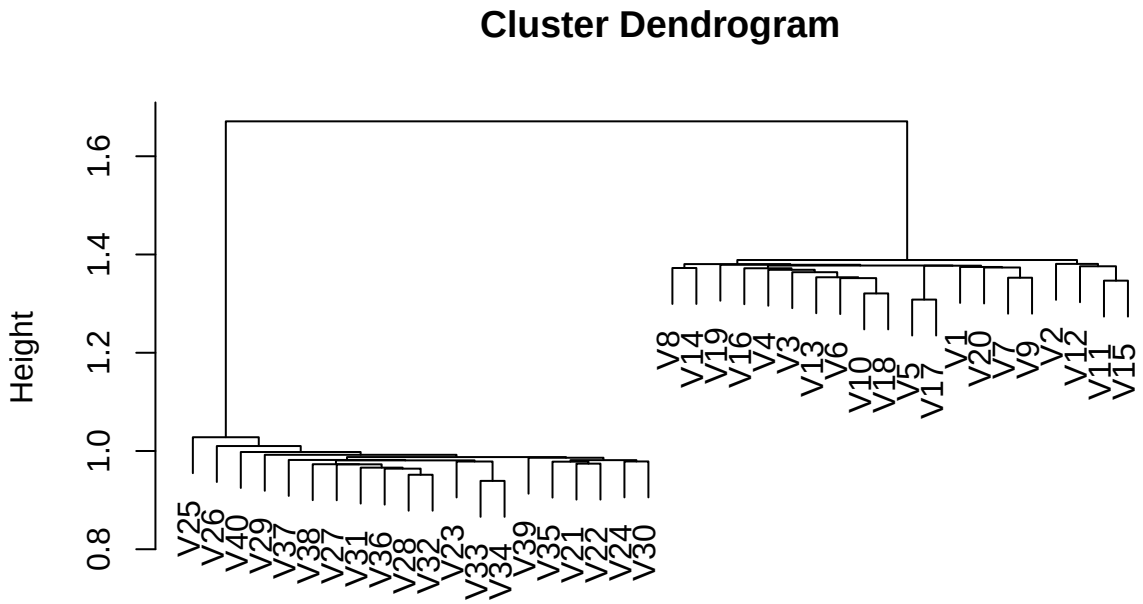
```
library(readr)
genes <- read.csv("C:/Users/GP/Desktop/MEGHA/SemII/MA679 - Appl Stat Learning/Homework/MA679---Stat-Mach
```

(b)

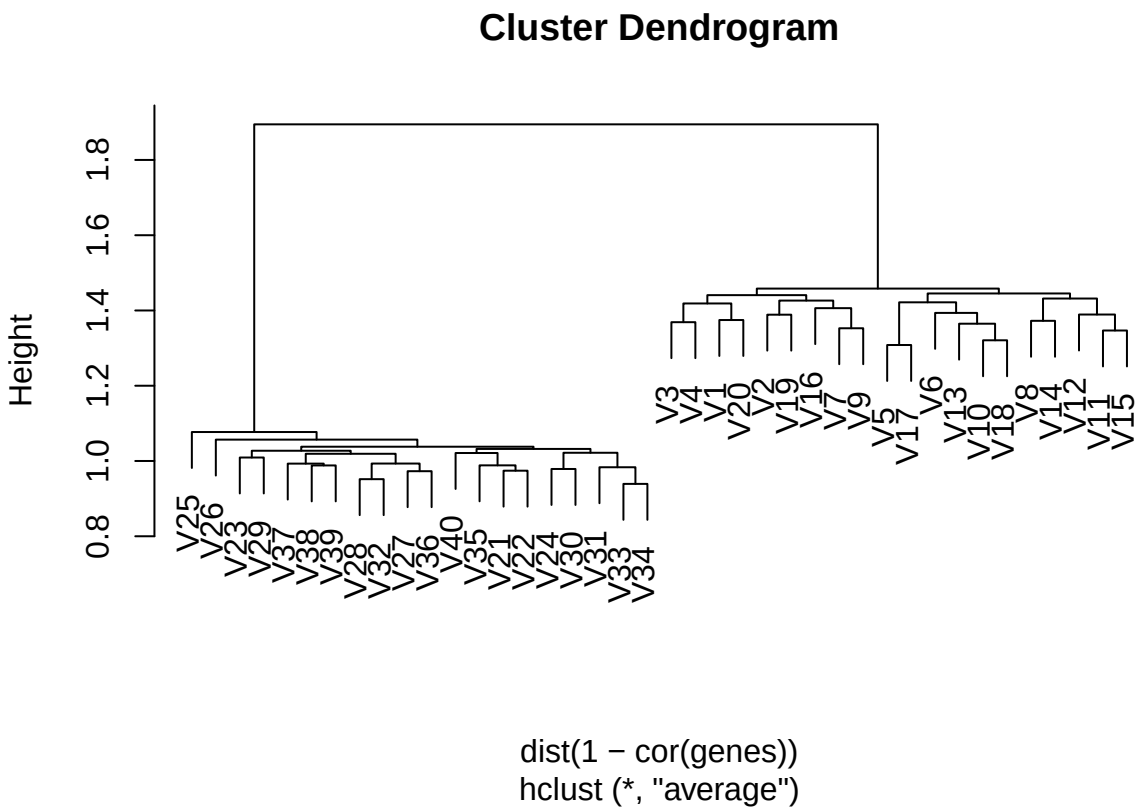
```
#complete linkage
hc_complete <- hclust(dist(1 - cor(genes)), method = "complete")
plot(hc_complete)
```




```
#single linkage
hc_single <- hclust(dist(1 - cor(genes)), method = "single")
plot(hc_single)
```




```r
#average linkage
hc_average <- hclust(dist(1 - cor(genes)), method = "average")
plot(hc_average)
```



All the three linkage methods give similar results.

(c)

To determine which genes differ the most across the two groups, we can perform PCA.

```
pca_genes <- prcomp(t(genes))
head(order(abs(rowSums(pca_genes$rotation)), decreasing = TRUE))
```

```
## [1] 865  68 911 428 624  11
```

The above are the genes that differ the most across the two groups.