Class8

Jibin (PID: A53300326)

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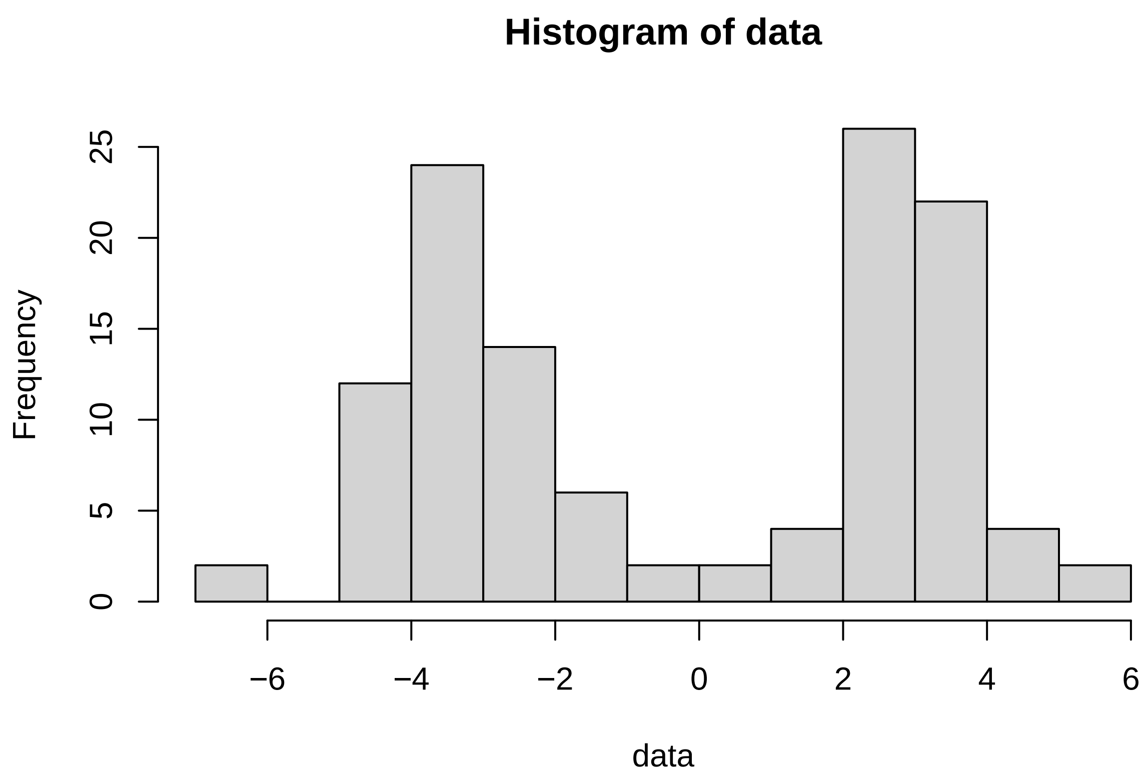
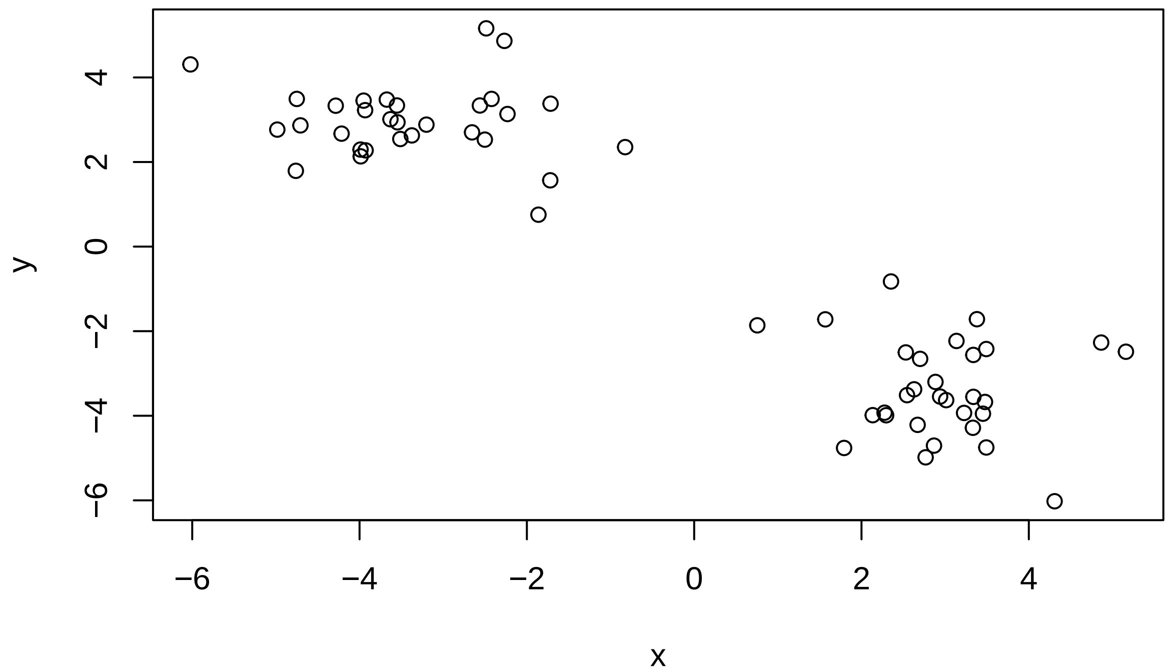
kmeans

```
tmp = c(rnorm(30,3), rnorm(30, -3))
data <-  cbind(x=tmp, y=rev(tmp))
hist(data)
```




```
plot(data)
```



Run `kmeans()` set k to 2 nstart 20. The thing with kmeans is you have to tell it how many clusters you want.

```
km <- kmeans(data, centers=2, nstart =20)
km
```

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##           x         y
## 1  2.956860 -3.375057
## 2 -3.375057  2.956860
##
## Clustering vector:
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
## [39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
##
## Within cluster sum of squares by cluster:
## [1] 61.99171 61.99171
##  (between_SS / total_SS =  90.7 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

Q. How many points are in each clusters?

```
km$size
```

```
## [1] 30 30
```

Q. What "component" of your result object details cluster assigment/membership?

```
km$cluster
```

```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
## [39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

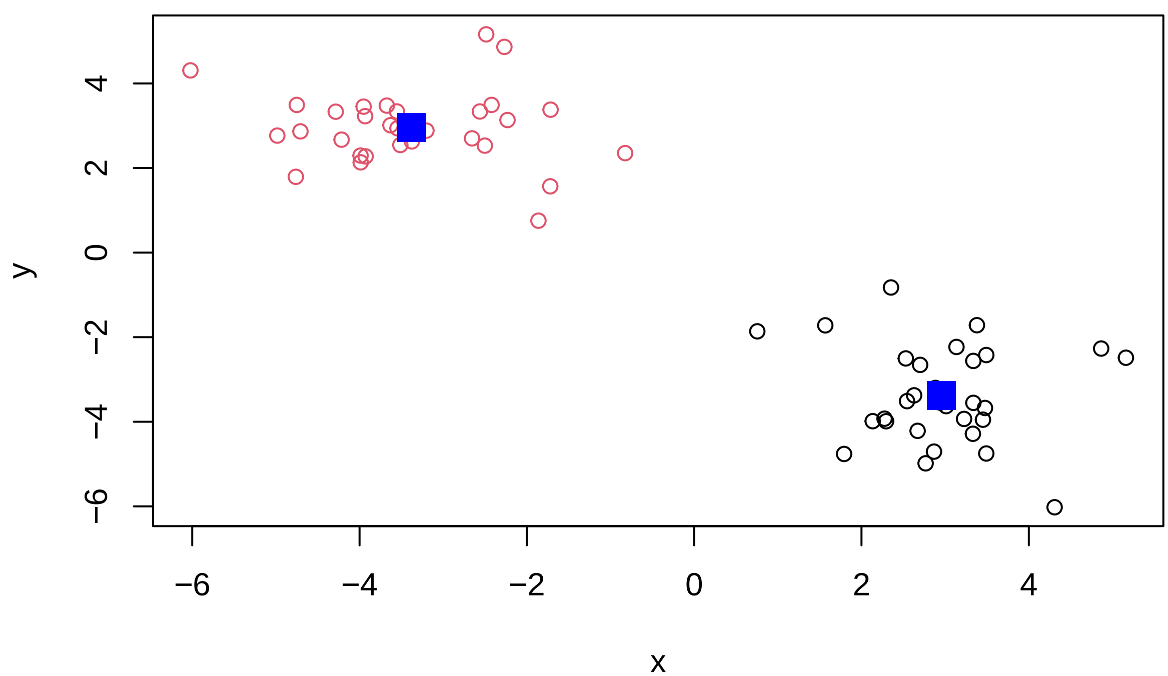
Q. What "component" of your result object details cluster center?

```
km$centers
```

```
##           x         y
## 1  2.956860 -3.375057
## 2 -3.375057  2.956860
```

Q. Plot x colored by the kmeans cluster assigment and add cluster centers as blue points?

```
plot(data, col=km$cluster)
points(km$centers, col="blue", pch=15, cex=2)
```



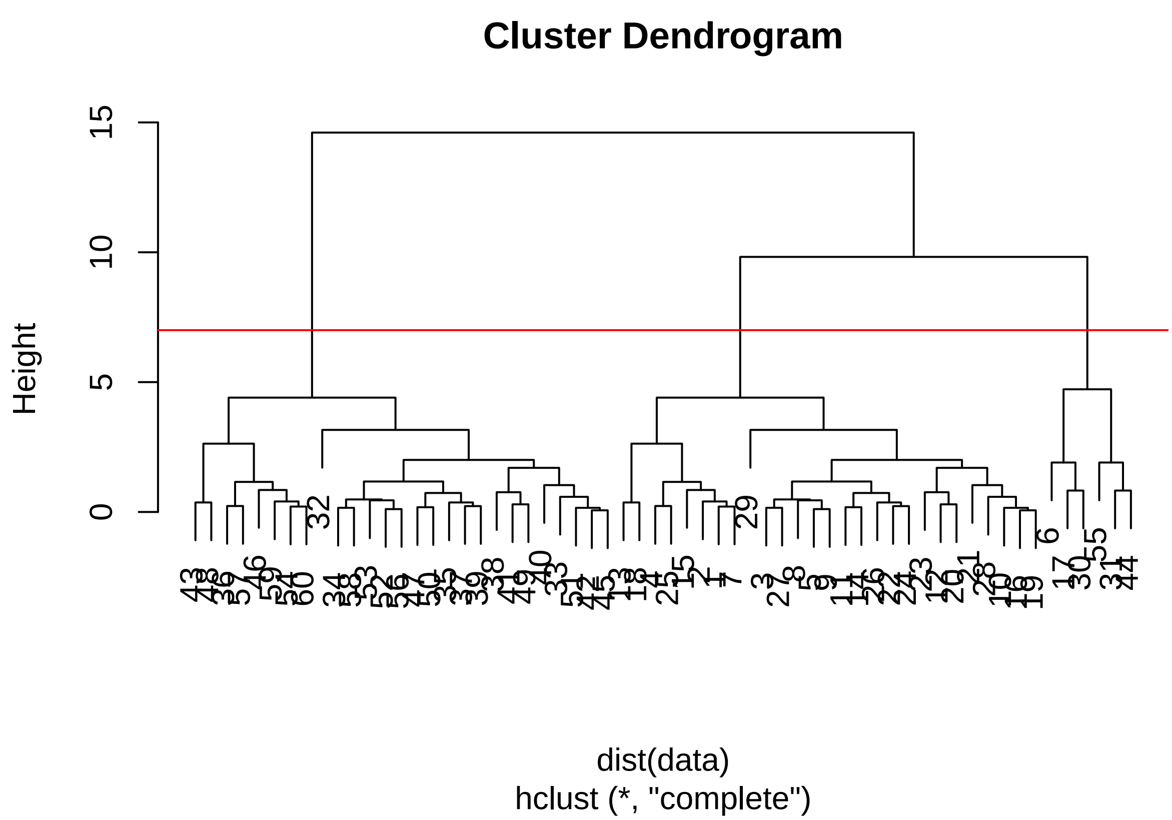
Hierarchical Clustering

We will use the hclust() function on the same data as before and see how this method works.

```
hc <- hclust(dist(data))
hc
```

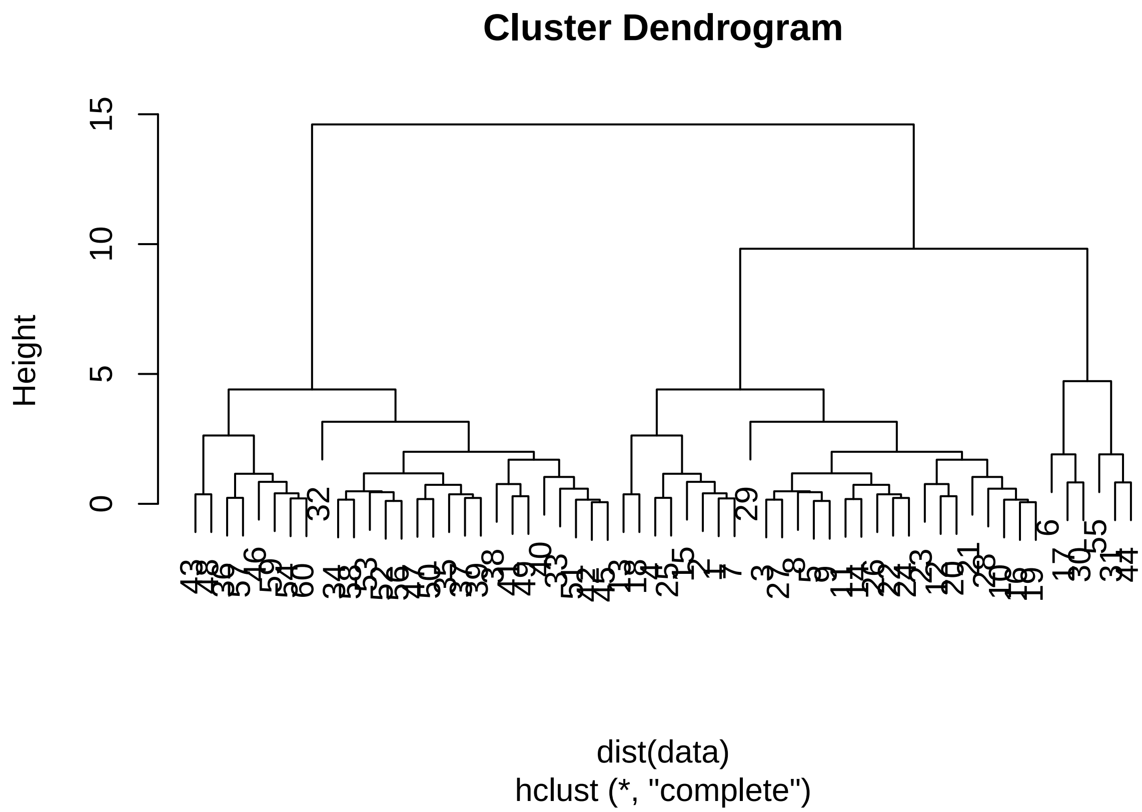
```
##
## Call:
## hclust(d = dist(data))
##
## Cluster method   : complete
## Distance         : euclidean
## Number of objects: 60
```

```
plot(hc)
abline(hc, h=7, col="red")
```



To find our membership vector we need to "cut" the tree and for this we use the `cutree()` function and tell it the height to cut at.

```
plot(hc)
```

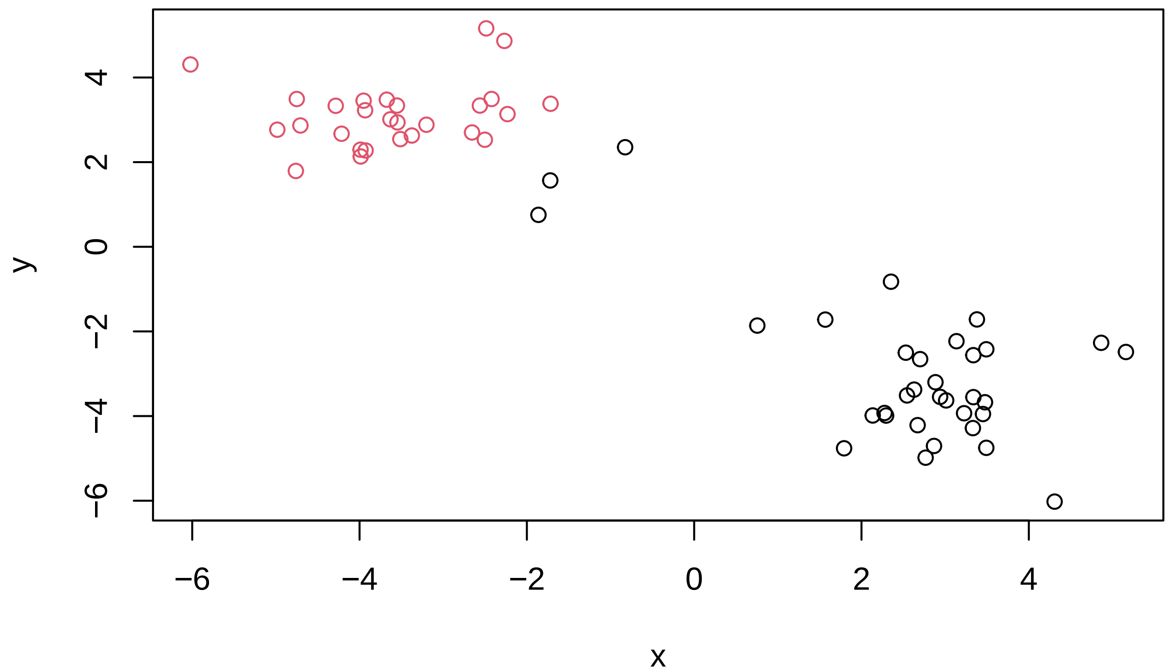



```
cutree(hc, h=7)
```

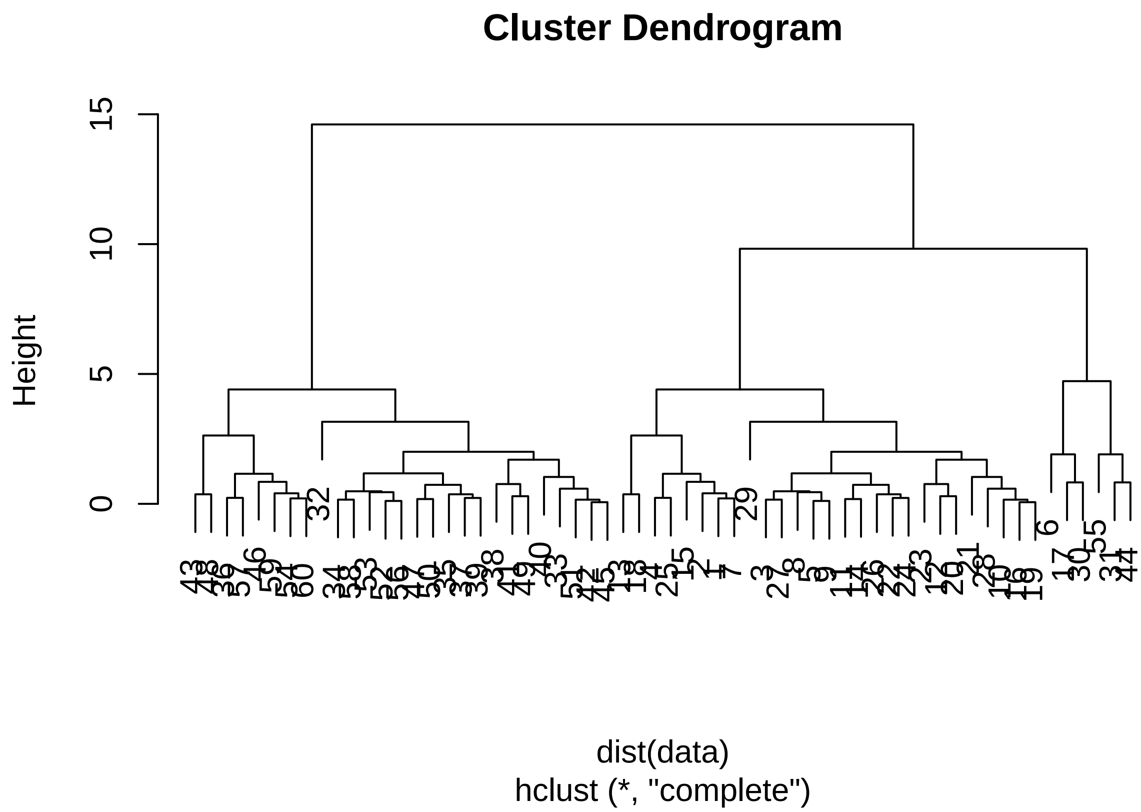
```
##  [1] 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 2 2 3 3 3 3 3 3 3
## [39] 3 3 3 3 3 2 3 3 3 3 3 3 3 3 3 3 2 3 3 3 3 3
```

```
grps <- cutree(hc, k=2)
```

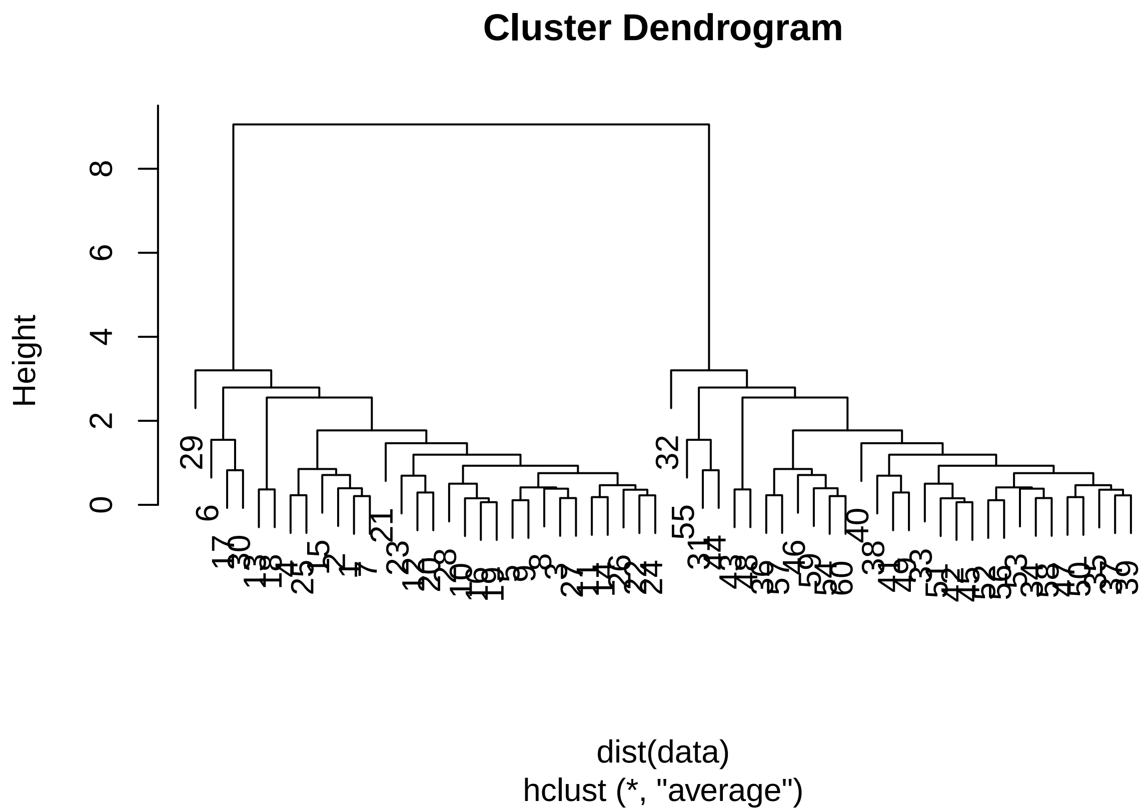
```
plot(data, col=grps)
```



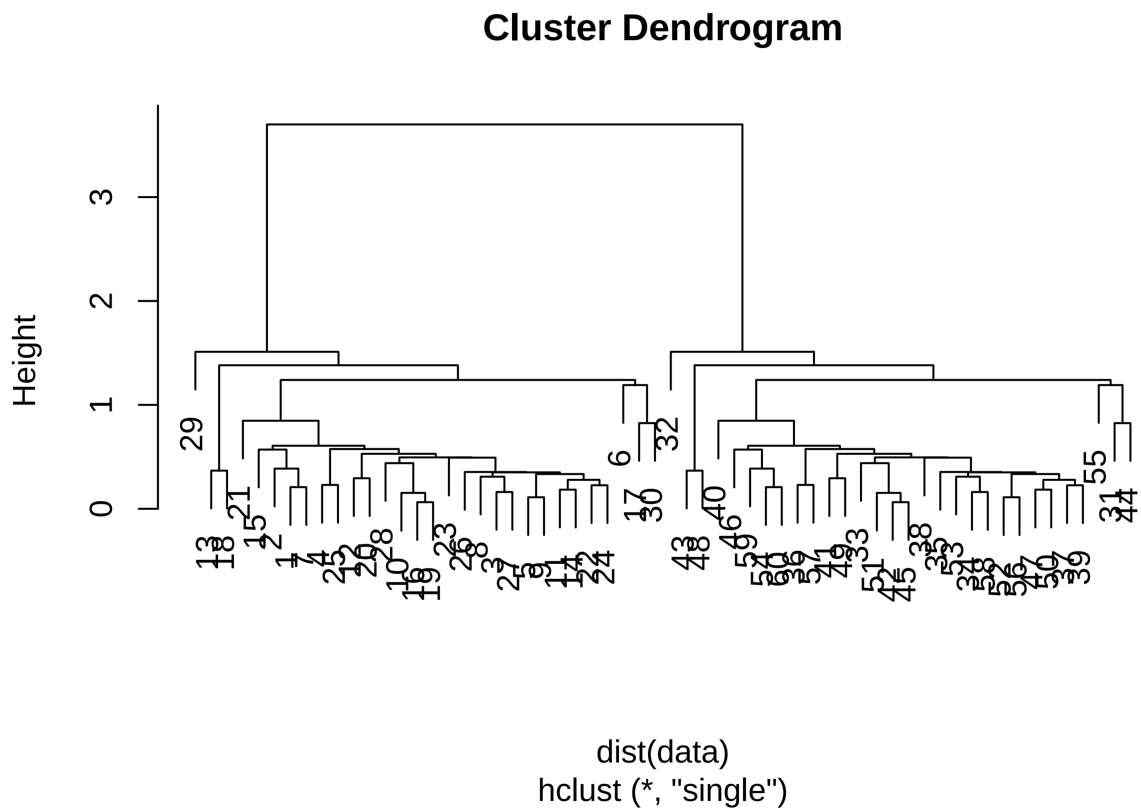

```
plot(hclust(dist(data), method="complete"))
```




```
plot(hclust(dist(data), method="average"))
```




```
plot(hclust(dist(data), method="single"))
```



Principal Component Analysis (PCA)

PCA is a super useful analysis method when you have lots of dimensions in your data

PCA of the UK_food

```r
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
```

how many rows and columns are in x?

```r
dim(x)
```

```
## [1] 17  5
```

```r
x
```

```
##                      X England Wales Scotland N.Ireland
## 1               Cheese     105   103      103        66
## 2        Carcass_meat      245   227      242       267
```

```
## 3          Other_meat      685   803      750        586
## 4                 Fish      147   160      122         93
## 5        Fats_and_oils      193   235      184        209
## 6               Sugars      156   175      147        139
## 7       Fresh_potatoes      720   874      566       1033
## 8            Fresh_Veg      253   265      171        143
## 9            Other_Veg      488   570      418        355
## 10 Processed_potatoes      198   203      220        187
## 11       Processed_Veg      360   365      337        334
## 12         Fresh_fruit     1102  1137      957        674
## 13             Cereals     1472  1582     1462       1494
## 14           Beverages       57    73       53         47
## 15         Soft_drinks     1374  1256     1572       1506
## 16    Alcoholic_drinks      375   475      458        135
## 17       Confectionery       54    64       62         41
```

```
rownames(x)<- x[,1]
x <- x[,1]
x
```

```
##  [1] "Cheese"                "Carcass_meat "        "Other_meat "
##  [4] "Fish"                  "Fats_and_oils "       "Sugars"
##  [7] "Fresh_potatoes "       "Fresh_Veg "           "Other_Veg "
## [10] "Processed_potatoes " "Processed_Veg "       "Fresh_fruit "
## [13] "Cereals "              "Beverages"            "Soft_drinks "
## [16] "Alcoholic_drinks "    "Confectionery "
```

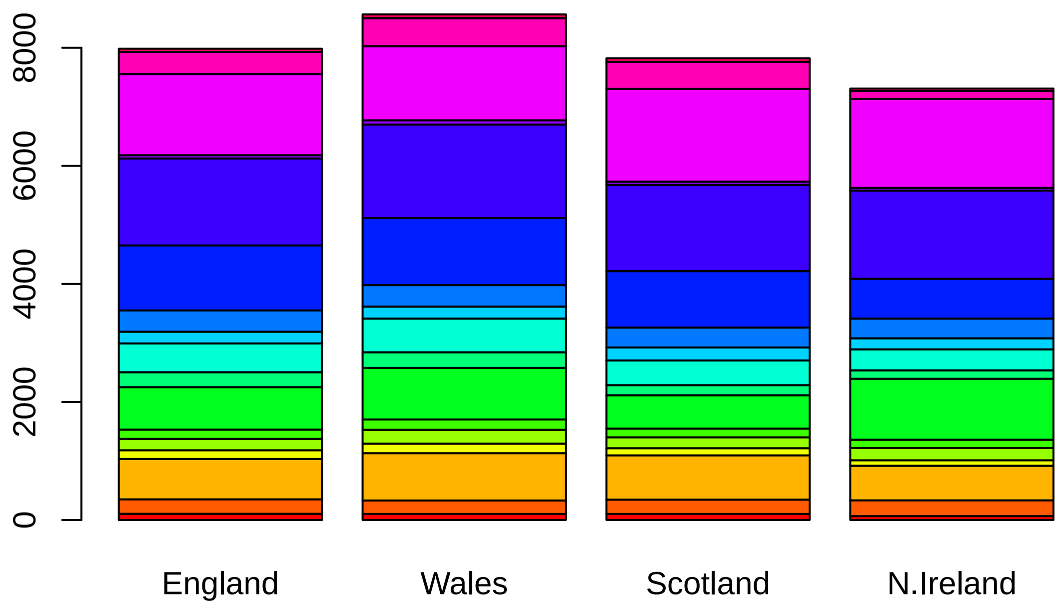
Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
x
```

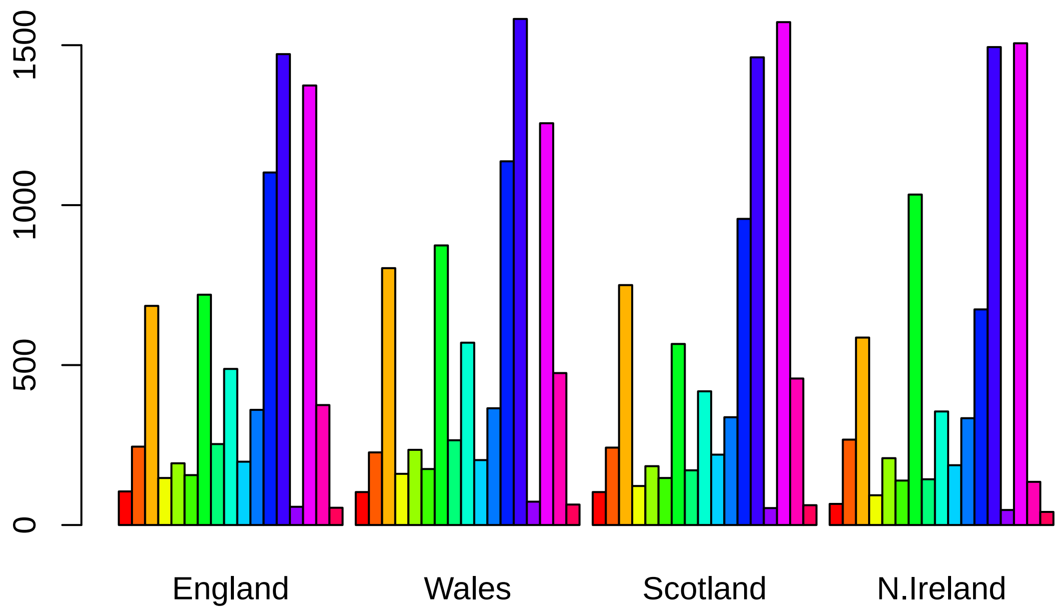
```
##                     England Wales Scotland N.Ireland
## Cheese                  105   103      103        66
## Carcass_meat            245   227      242       267
## Other_meat              685   803      750       586
## Fish                    147   160      122        93
## Fats_and_oils           193   235      184       209
## Sugars                  156   175      147       139
## Fresh_potatoes          720   874      566      1033
## Fresh_Veg               253   265      171       143
## Other_Veg               488   570      418       355
## Processed_potatoes      198   203      220       187
## Processed_Veg           360   365      337       334
## Fresh_fruit            1102  1137      957       674
## Cereals                1472  1582     1462      1494
## Beverages                57    73       53        47
## Soft_drinks            1374  1256     1572      1506
## Alcoholic_drinks        375   475      458       135
## Confectionery            54    64       62        41
```

Q3: Changing what optional argument in the above barplot() function results in the following plot?

```
barplot(as.matrix(x), col=rainbow(17),)
```

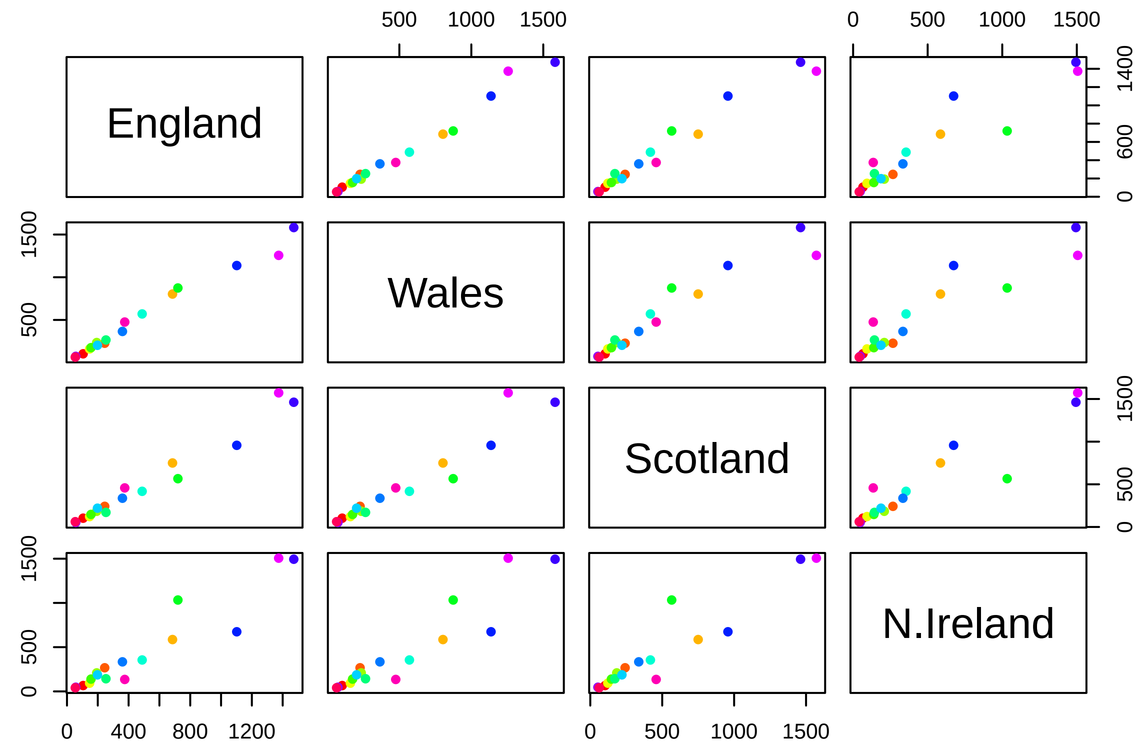



```
barplot(as.matrix(x), col=rainbow(17), beside=T)
```



Q5: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

```
mycol <- rainbow(nrow(x))
pairs(x, col=mycol, pch=16)
```



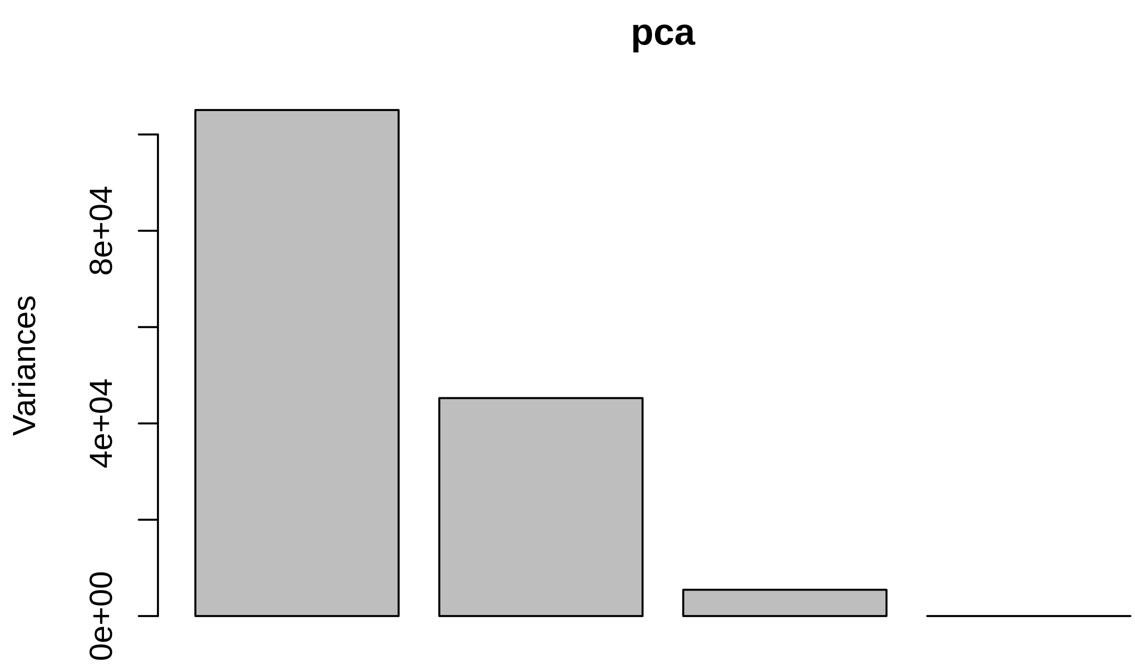
PCA to the rescue

Here we will use the base R function for PCA, which is called `prcomp()`. This function wants the transpose of the data.

```
pca <- prcomp(t(x))
summary(pca)
```

```
## Importance of components:
##                             PC1      PC2      PC3       PC4
## Standard deviation     324.1502 212.7478 73.87622 4.189e-14
## Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
## Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
plot(pca)
```



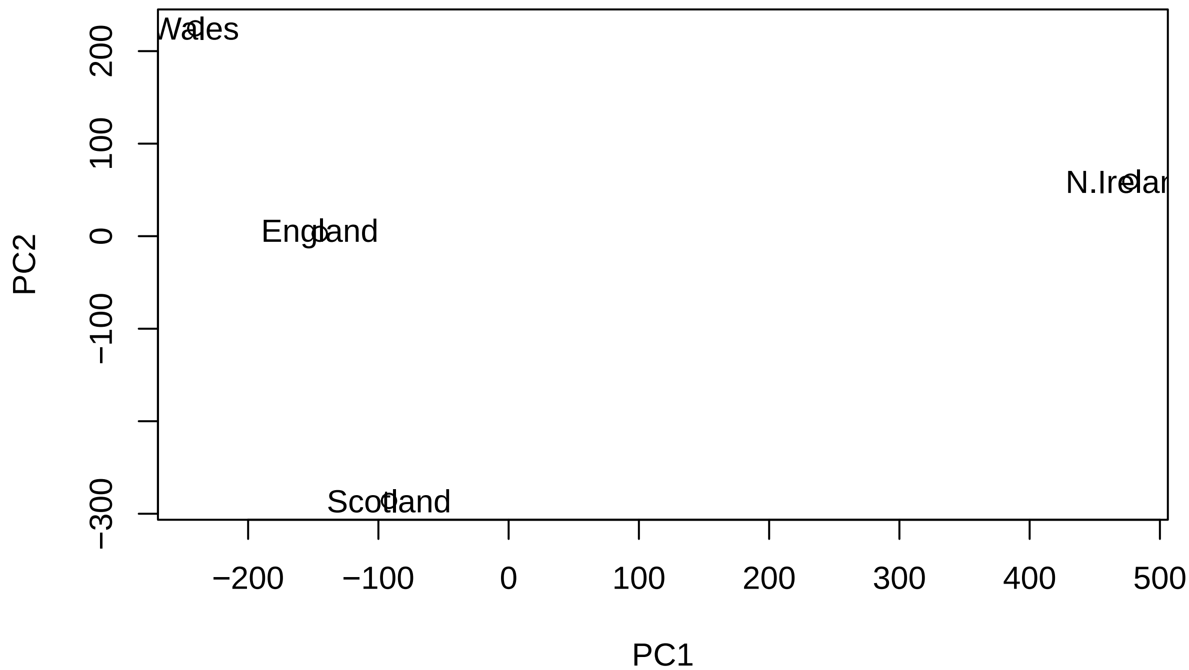
We want score plot (a.k.a, PCA plot). Basically of PC1 vs PC2

```
attributes(pca)
```

```
## $names
## [1] "sdev"     "rotation" "center"   "scale"    "x"
##
## $class
## [1] "prcomp"
```

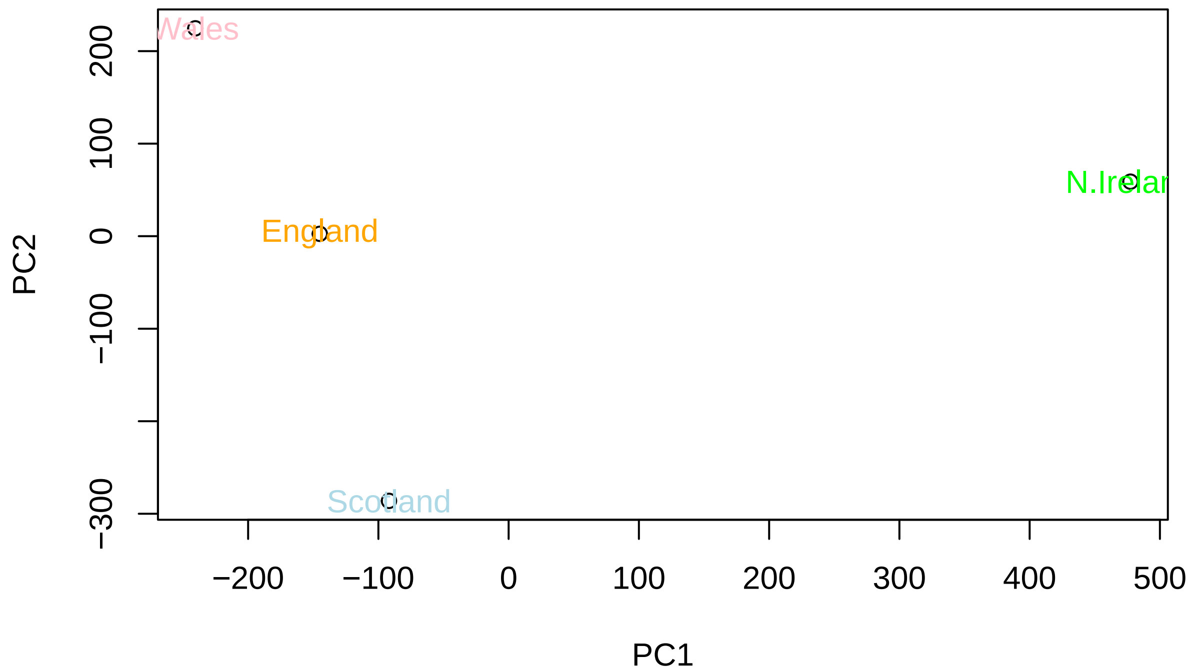
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points

```
plot(pca$x[,1:2])
text(pca$x[,1:2], labels = colnames(x))
```



Q8. Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

```
plot(pca$x[,1:2])
text(pca$x[,1:2], labels = colnames(x), col=c("orange", "pink", "light blue", "green"))
```

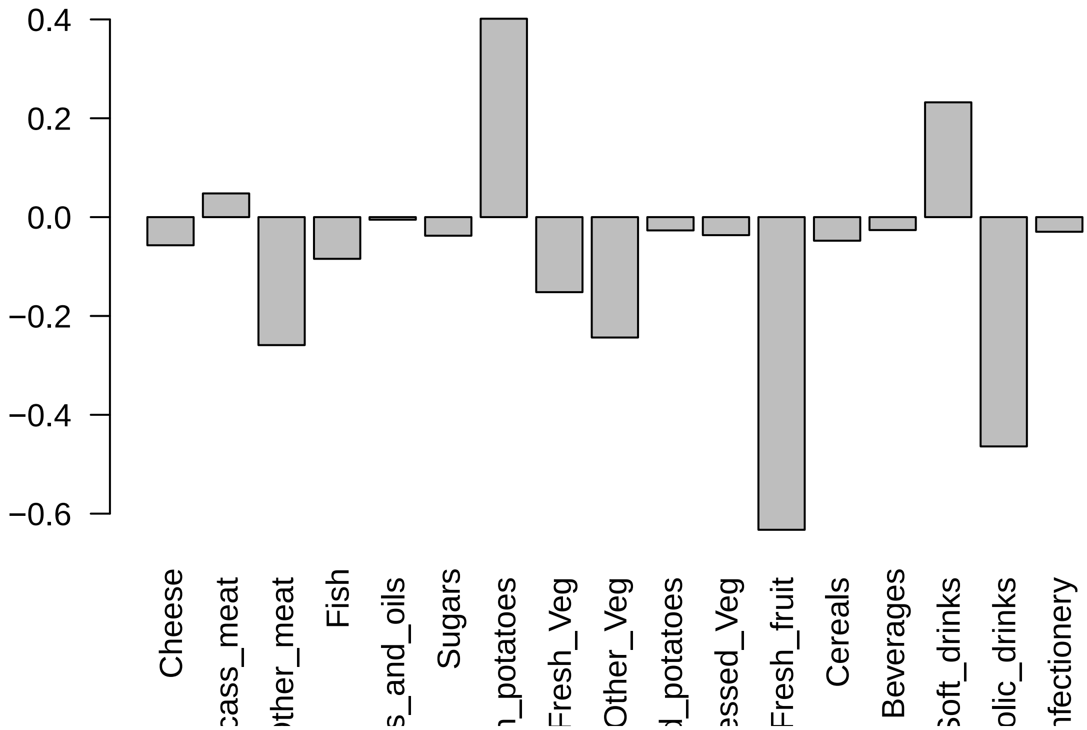


We can also examine the PCA "loading", which tell us how much the roifinal variable contribute to teach new PC...

```
pca$rotation
```

```
##                              PC1          PC2         PC3          PC4
## Cheese              -0.056955380 -0.016012850 -0.02394295 -0.691718038
## Carcass_meat         0.047927628 -0.013915823 -0.06367111  0.635384915
## Other_meat          -0.258916658  0.015331138  0.55384854  0.198175921
## Fish                -0.084414983  0.050754947 -0.03906481 -0.015824630
## Fats_and_oils       -0.005193623  0.095388656  0.12522257  0.052347444
## Sugars              -0.037620983  0.043021699  0.03605745  0.014481347
## Fresh_potatoes       0.401402060  0.715017078  0.20668248 -0.151706089
## Fresh_Veg           -0.151849942  0.144900268 -0.21382237  0.056182433
## Other_Veg           -0.243593729  0.225450923  0.05332841 -0.080722623
## Processed_potatoes  -0.026886233 -0.042850761  0.07364902 -0.022618707
## Processed_Veg       -0.036488269  0.045451802 -0.05289191  0.009235001
## Fresh_fruit         -0.632640898  0.177740743 -0.40012865 -0.021899087
## Cereals             -0.047702858  0.212599678  0.35884921  0.084667257
## Beverages           -0.026187756  0.030560542  0.04135860 -0.011880823
## Soft_drinks          0.232244140 -0.555124311  0.16942648 -0.144367046
## Alcoholic_drinks    -0.463968168 -0.113536523  0.49858320 -0.115797605
## Confectionery       -0.029650201 -0.005949921  0.05232164 -0.003695024
```

```
barplot(pca$rotation[,1], las=2)
```

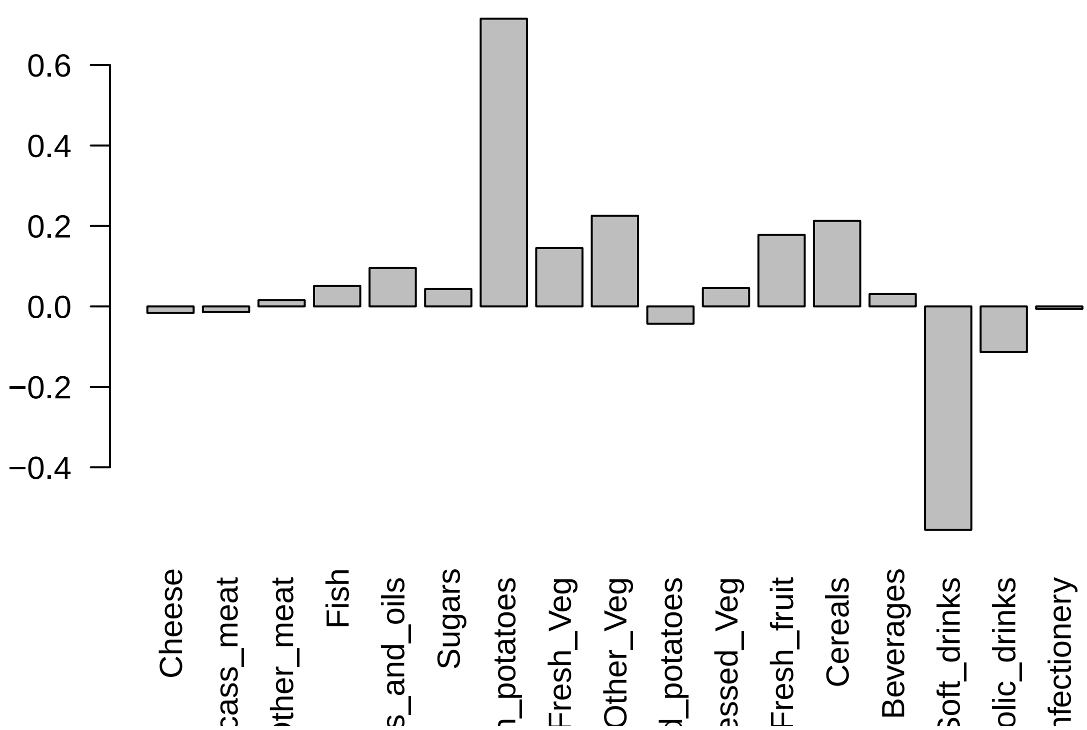


Q9: Generate a similar 'loadings plot' for PC2. What two food groups feature prominantely and what does PC2 maninly tell us about?

```
pca$rotation
```

```
##                             PC1          PC2         PC3          PC4
## Cheese              -0.056955380 -0.016012850 -0.02394295 -0.691718038
## Carcass_meat         0.047927628 -0.013915823 -0.06367111  0.635384915
## Other_meat          -0.258916658  0.015331138  0.55384854  0.198175921
## Fish                -0.084414983  0.050754947 -0.03906481 -0.015824630
## Fats_and_oils       -0.005193623  0.095388656  0.12522257  0.052347444
## Sugars              -0.037620983  0.043021699  0.03605745  0.014481347
## Fresh_potatoes       0.401402060  0.715017078  0.20668248 -0.151706089
## Fresh_Veg           -0.151849942  0.144900268 -0.21382237  0.056182433
## Other_Veg           -0.243593729  0.225450923  0.05332841 -0.080722623
## Processed_potatoes  -0.026886233 -0.042850761  0.07364902 -0.022618707
## Processed_Veg       -0.036488269  0.045451802 -0.05289191  0.009235001
## Fresh_fruit         -0.632640898  0.177740743 -0.40012865 -0.021899087
## Cereals             -0.047702858  0.212599678  0.35884921  0.084667257
## Beverages           -0.026187756  0.030560542  0.04135860 -0.011880823
## Soft_drinks          0.232244140 -0.555124311  0.16942648 -0.144367046
## Alcoholic_drinks    -0.463968168 -0.113536523  0.49858320 -0.115797605
## Confectionery       -0.029650201 -0.005949921  0.05232164 -0.003695024
```

```r
barplot(pca$rotation[,2], las=2)
```



One more PCA for today

```r
url2 <- "https://tinyurl.com/expression-CSV"
rna.data <- read.csv(url2, row.names=1)
head(rna.data)
```

```
##        wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
## gene1  439 458  408  429 420  90  88  86  90  93
## gene2  219 200  204  210 187 427 423 434 433 426
## gene3 1006 989 1030 1017 973 252 237 238 226 210
## gene4  783 792  829  856 760 849 856 835 885 894
## gene5  181 249  204  244 225 277 305 272 270 279
## gene6  460 502  491  491 493 612 594 577 618 638
```

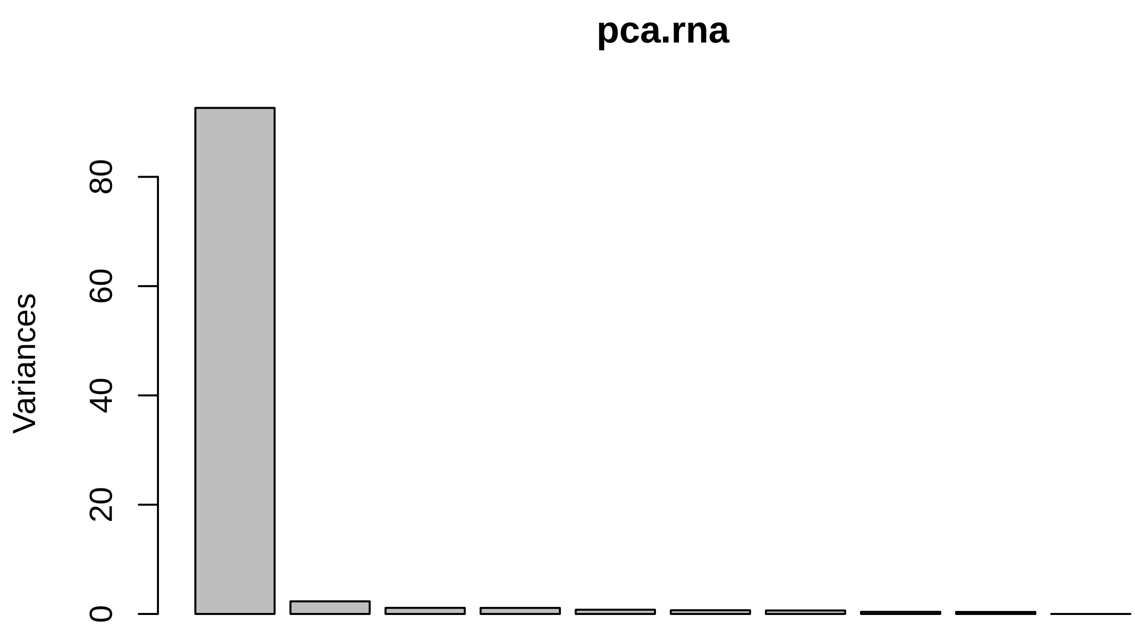
```r
dim(rna.data)
```

```
## [1] 100  10
```

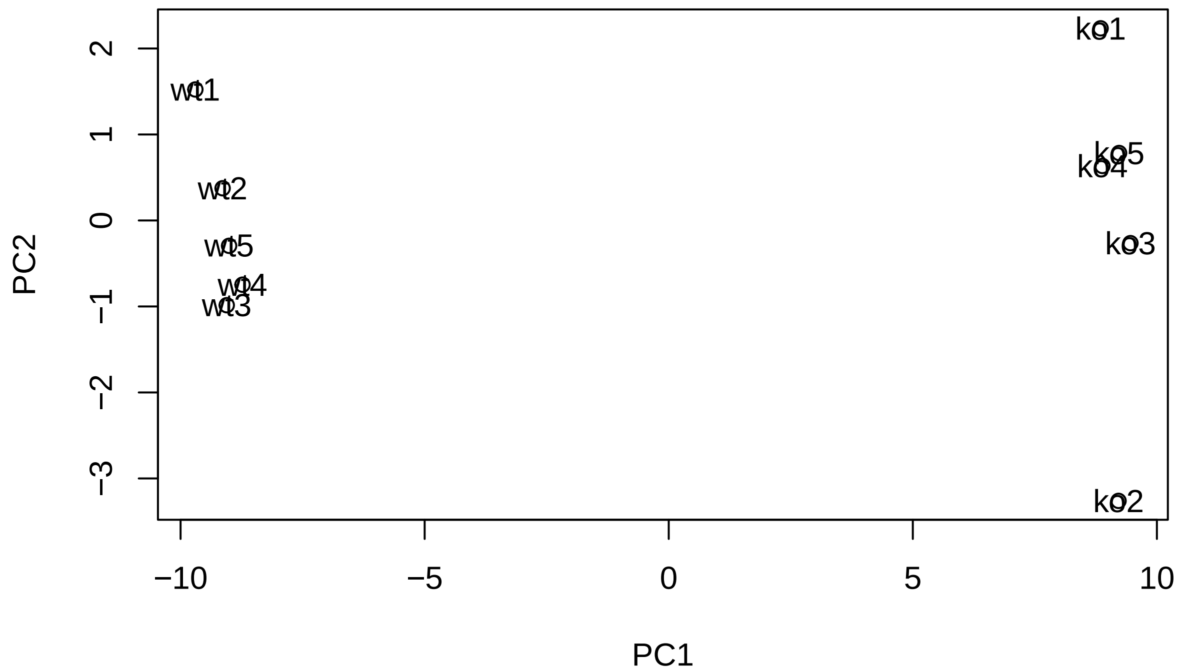
```
pca.rna <- prcomp(t(rna.data), scale=TRUE)
summary(pca.rna)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     9.6237 1.5198 1.05787 1.05203 0.88062 0.82545 0.80111
## Proportion of Variance 0.9262 0.0231 0.01119 0.01107 0.00775 0.00681 0.00642
## Cumulative Proportion  0.9262 0.9493 0.96045 0.97152 0.97928 0.98609 0.99251
##                            PC8     PC9      PC10
## Standard deviation     0.62065 0.60342 3.348e-15
## Proportion of Variance 0.00385 0.00364 0.000e+00
## Cumulative Proportion  0.99636 1.00000 1.000e+00
```

```
plot(pca.rna)
```




```
plot(pca.rna$x[,1:2])
text(pca.rna$x[,1:2], labels = colnames(rna.data))
```



ko1
wt1
ko5
ko4
wt2
ko3
wt5
wt4
wt3
ko2
−10
−5
0
5
10
PC1
2
1
0
−1
−2
−3
PC2