Class 7: Machine Learning

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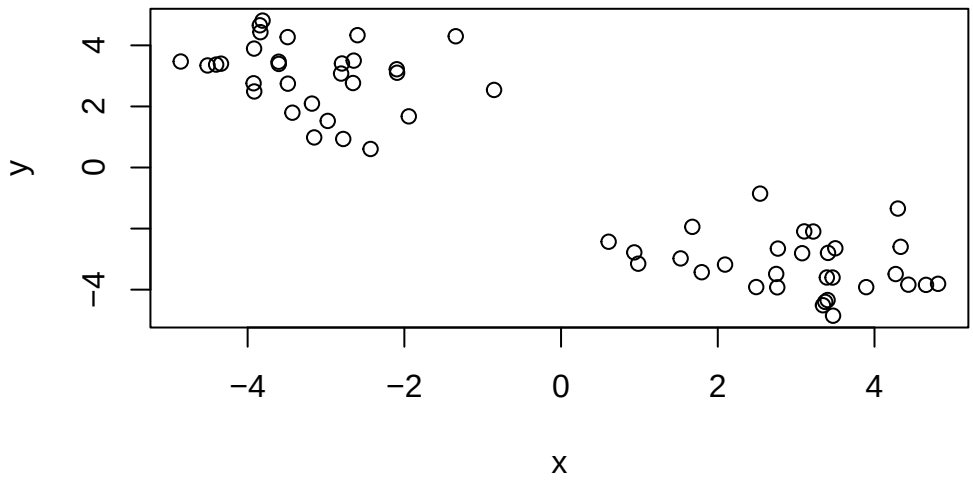
Example of K-means clustering

First step is to make up some data with a known structure, so we know what the answer should be.

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



Now we have some structured data in x. Let's see if k-means is able to identify the two groups.

```
k <- kmeans (x, centers = 2, nstart = 20)
k
```

```
K-means clustering with 2 clusters of sizes 30, 30

Cluster means:
          x         y
1  3.011910 -3.177176
2 -3.177176  3.011910

Clustering vector:
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

Within cluster sum of squares by cluster:
[1] 61.87937 61.87937
 (between_SS / total_SS =  90.3 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

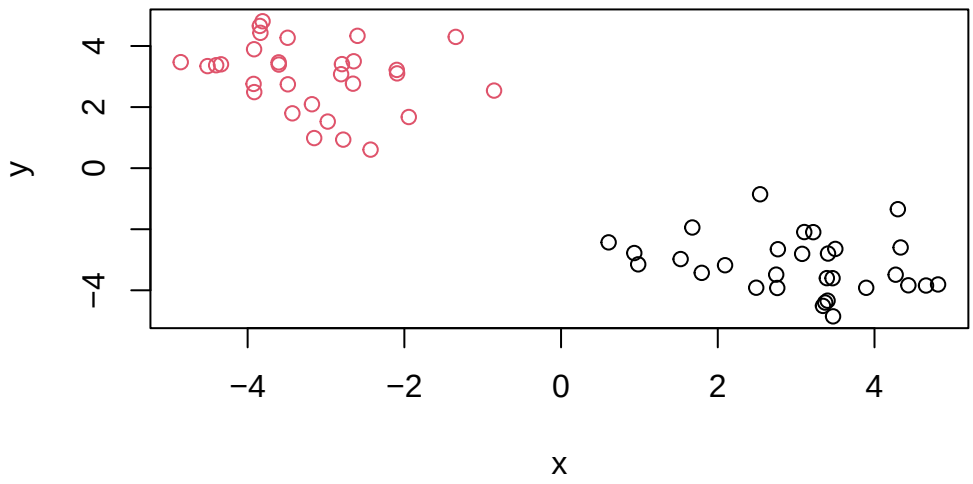
Let's explore k:

```
k$centers
```

```
          x         y
1  3.011910 -3.177176
2 -3.177176  3.011910
```

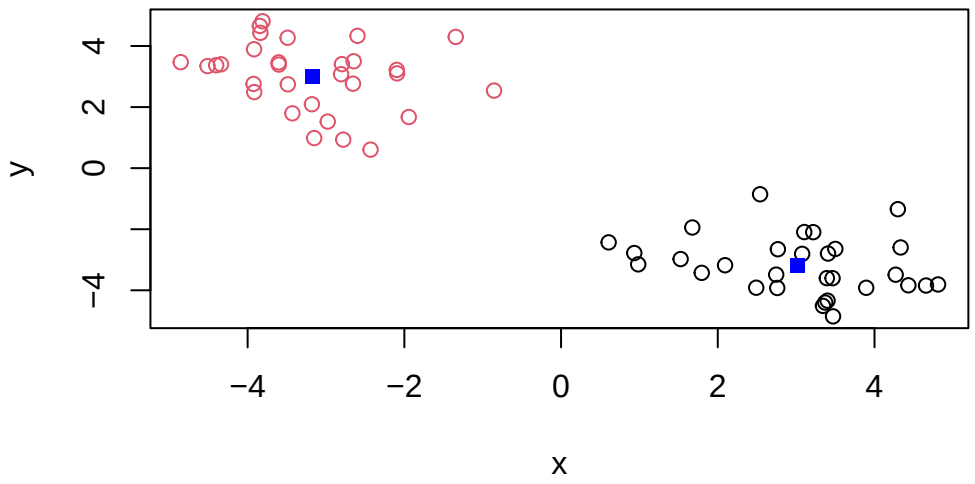
Adding colors to each clusters:

```
plot(x, col = k$cluster)
```



Adding the clusters centers:

```
plot(x, col = k$cluster)
points(k$centers, col = 'blue', pch = 15)
```



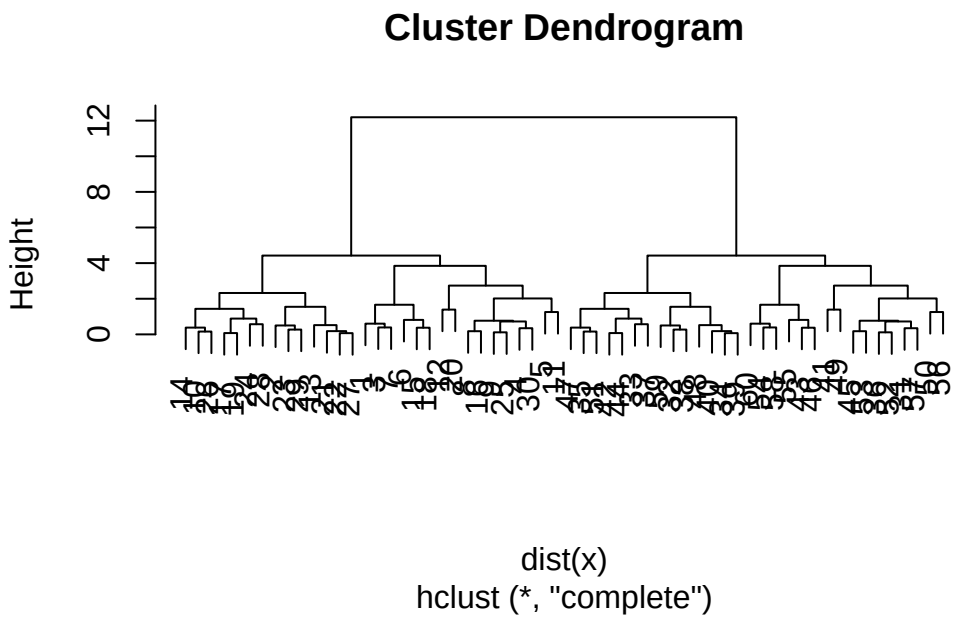
Example of Hierarchical Clustering

Let's use the same data as before, which we stored in 'x'. We will use the 'hclust()' function.

```
clustering <- hclust(dist(x))
clustering
```

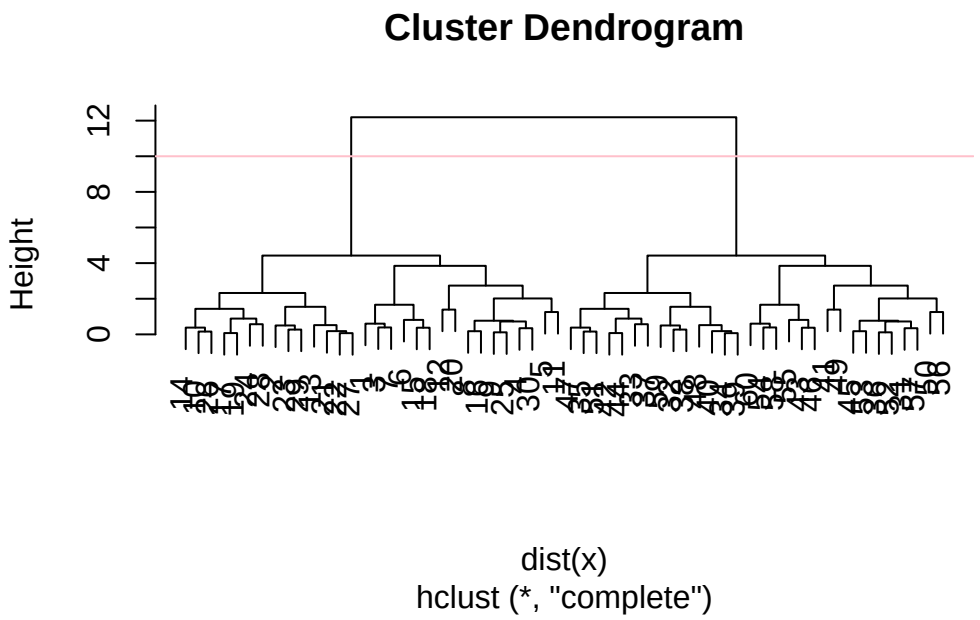
```
Call:
hclust(d = dist(x))

Cluster method   : complete
Distance         : euclidean
Number of objects: 60
```

```
plot(clustering)
```



Let's add an horizontal line.

```
plot(clustering)
abline(h = 10, col = 'pink')
```



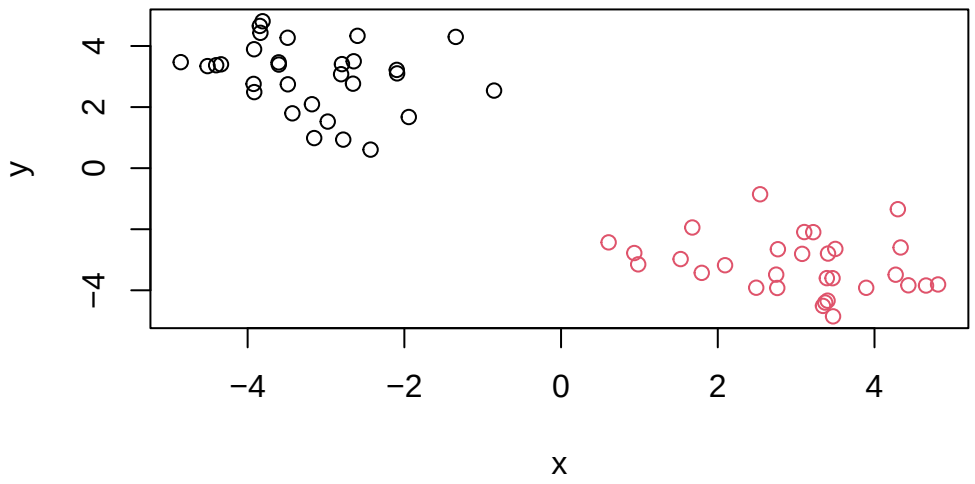
To get our results (i.e., membership vector), we need to cut the tree. The function for doing that is cutree().

```
subgroups <- cutree(clustering, h=10)
subgroups
```

```
 [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 2 2
```

Plotting this...

```
plot(x, col = subgroups)
```



You can also "cut" your tree with a number of clusters you want:

```
cutree(clustering, k = 2)
```

```
 [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 2
```

Principle Component Analysis (PCA)

PCA of UK Food

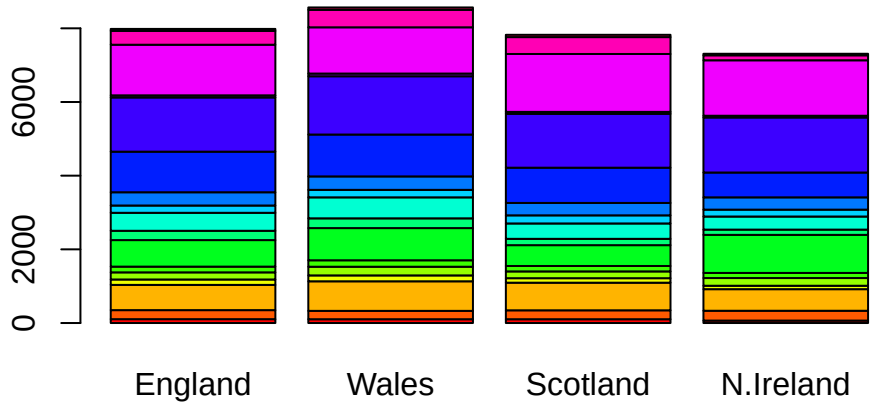
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
head(x)
```

```
              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
```

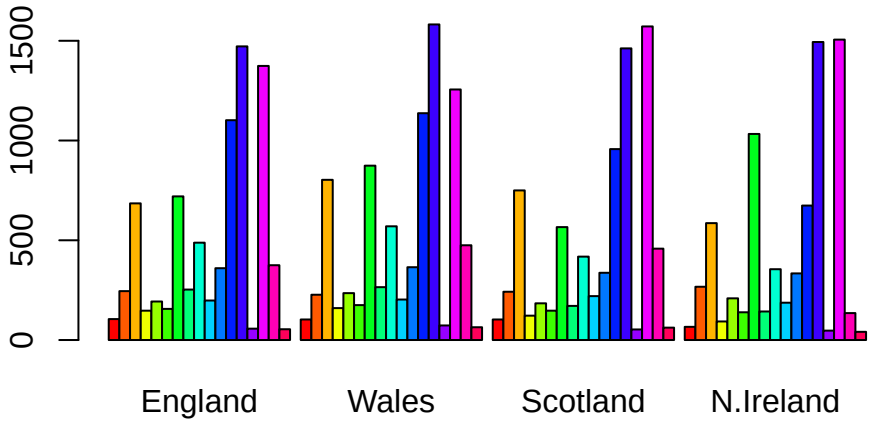
Now we can generate some basic visualizations.

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



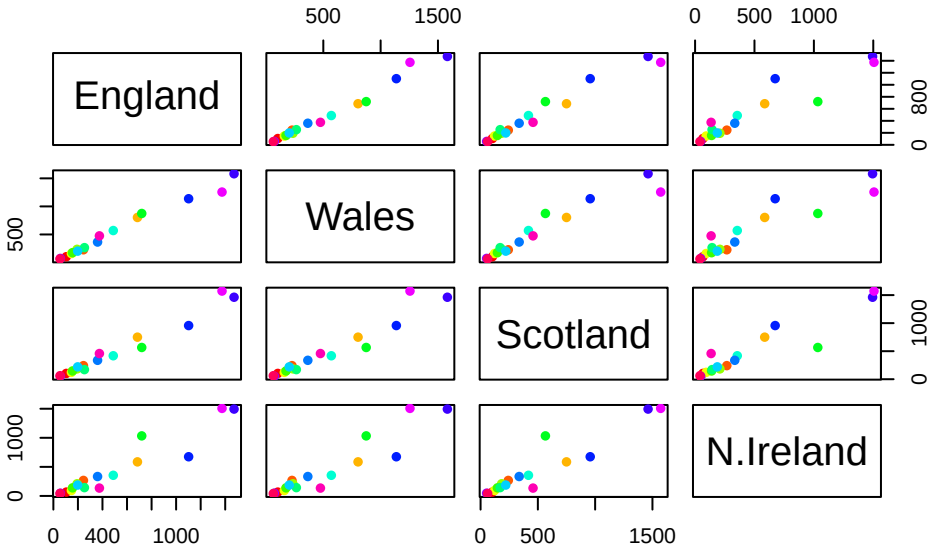
Refining our barplot:

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



Other visualizations that can be useful...

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



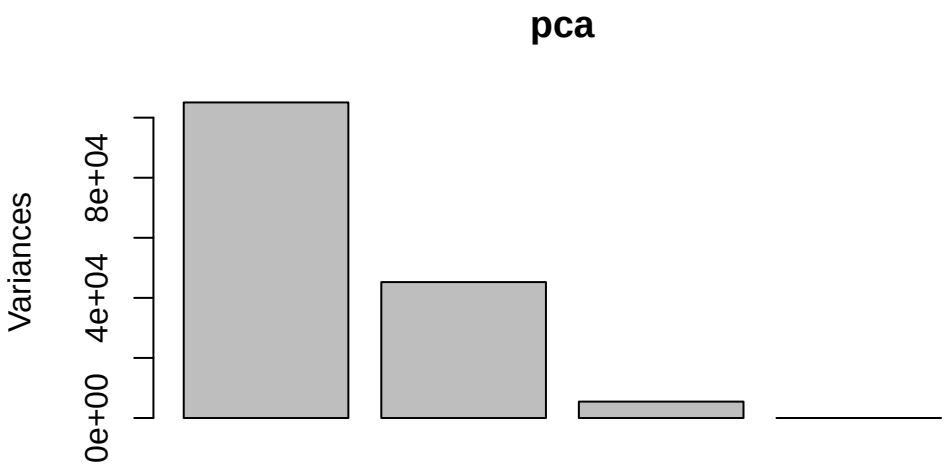
Applying PCA... using the command "prcomp()". This function expects the transpose of our data (flipping rows and columns).

```
#transpose_matrix <- t(x)
#pca <- prcomp(transpose_matrix)

#combining the two lines to make the code shorter
pca <- prcomp(t(x))
summary(pca)
```

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 5.552e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

Let's plot the PCA results.

```
plot(pca)
```



We need to access the results of the PCA analysis:

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

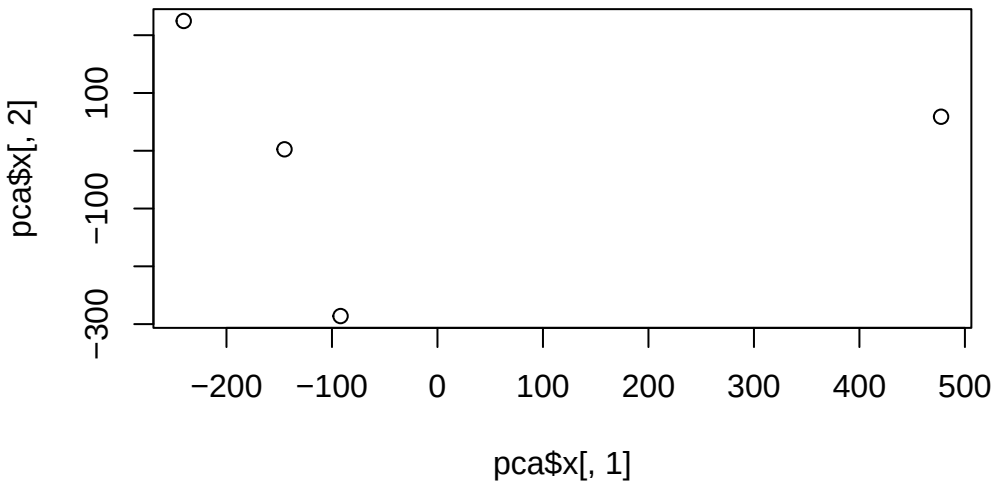
We can explore the pca$x dataframe

```
pca$x
```

```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  1.042460e-14
Wales     -240.52915  224.646925   56.475555  9.556806e-13
Scotland   -91.86934 -286.081786   44.415495 -1.257152e-12
N.Ireland  477.39164   58.901862    4.877895  2.872787e-13
```

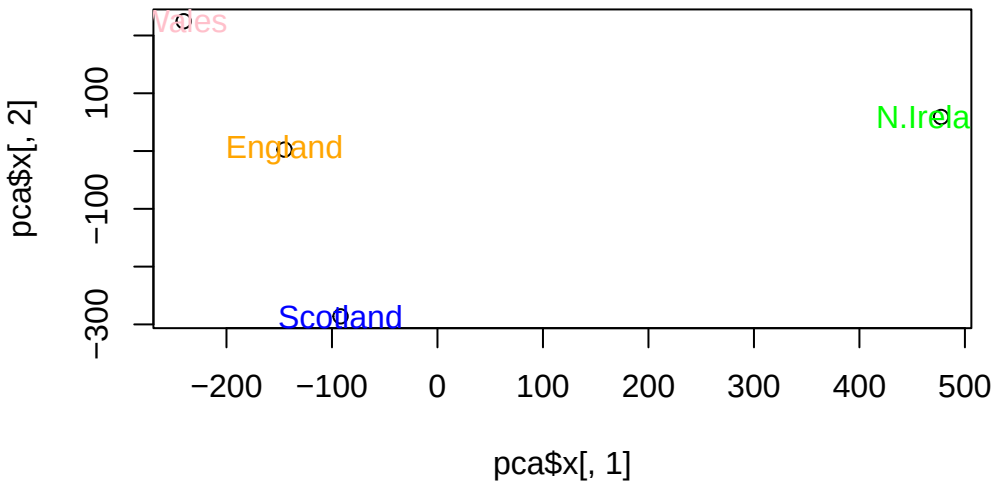
Plotting:

```
plot( x = pca$x[,1], y = pca$x[,2] )
```

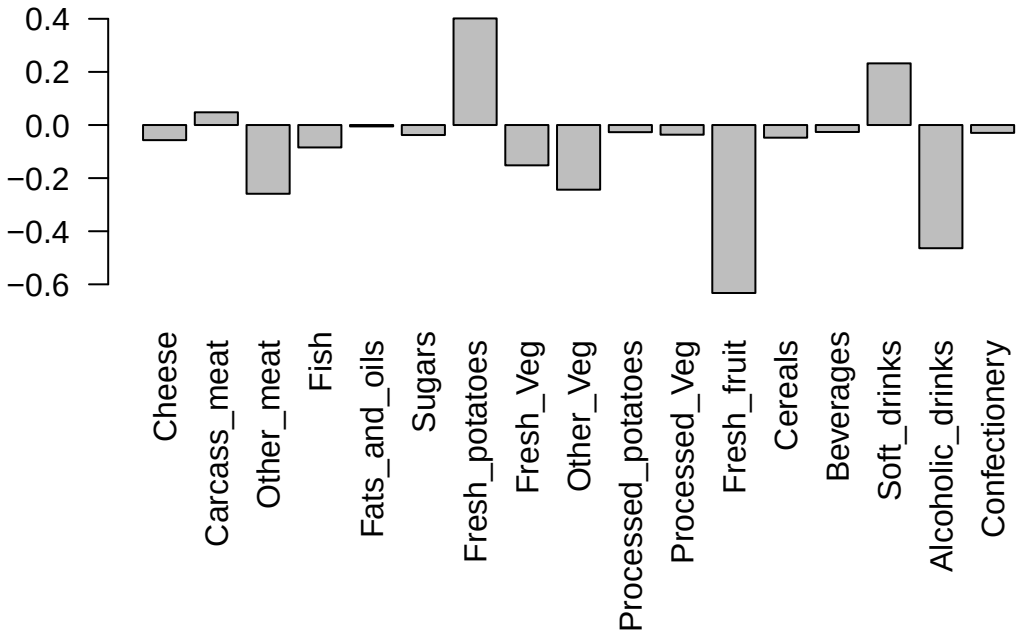


Adding colors and labels...

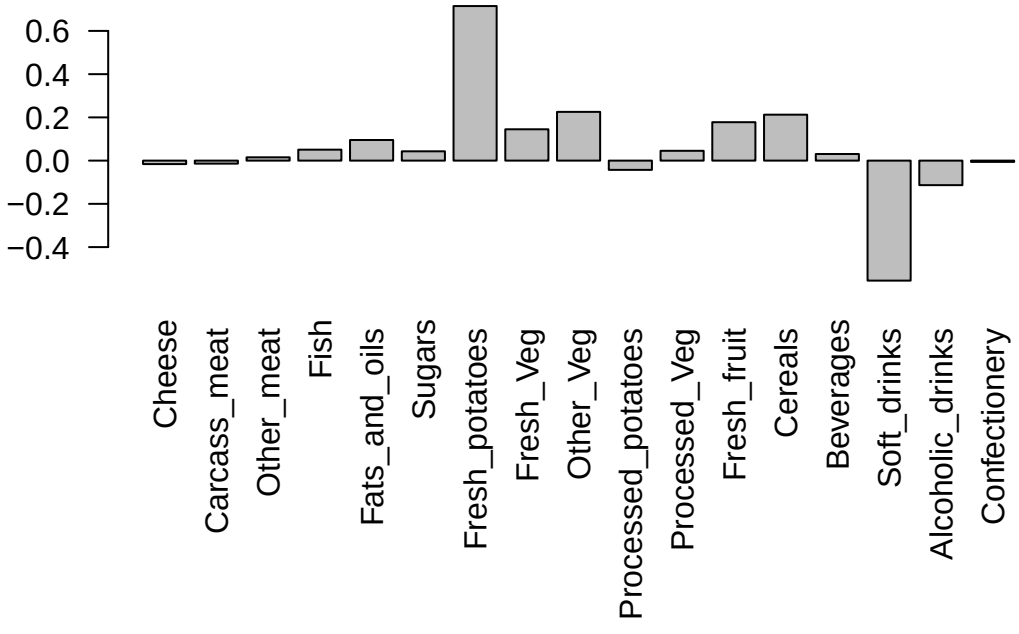
```
plot( x = pca$x[,1], y = pca$x[,2] )
colors_countries <- c('orange', 'pink', 'blue', 'green')
text( x = pca$x[,1], y = pca$x[,2], colnames(x), col = colors_countries )
```




```
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```




```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```



PCA of RNA-seq data

Loading the data...

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

Q10: How many genes and samples are in this data set?

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

```
[1] 100  10
```

Answer: There are 100 genes and 10 samples.

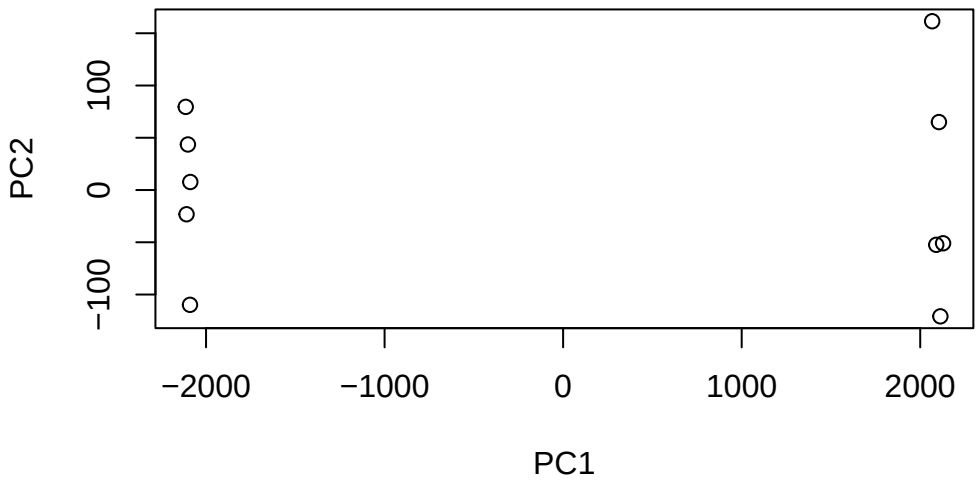
Applying PCA...

```
pca_rna = prcomp(t(rna.data))
summary(pca_rna)
```

```
Importance of components:
                            PC1     PC2      PC3      PC4      PC5      PC6
Standard deviation     2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
Proportion of Variance    0.9917  0.0016  0.00144  0.00122  0.00098  0.00093
Cumulative Proportion     0.9917  0.9933  0.99471  0.99593  0.99691  0.99784
                           PC7      PC8      PC9      PC10
Standard deviation     65.29428 59.90981 53.20803 2.715e-13
Proportion of Variance  0.00086  0.00073  0.00057 0.000e+00
Cumulative Proportion   0.99870  0.99943  1.00000 1.000e+00
```

Plotting principle components 1 and 2.

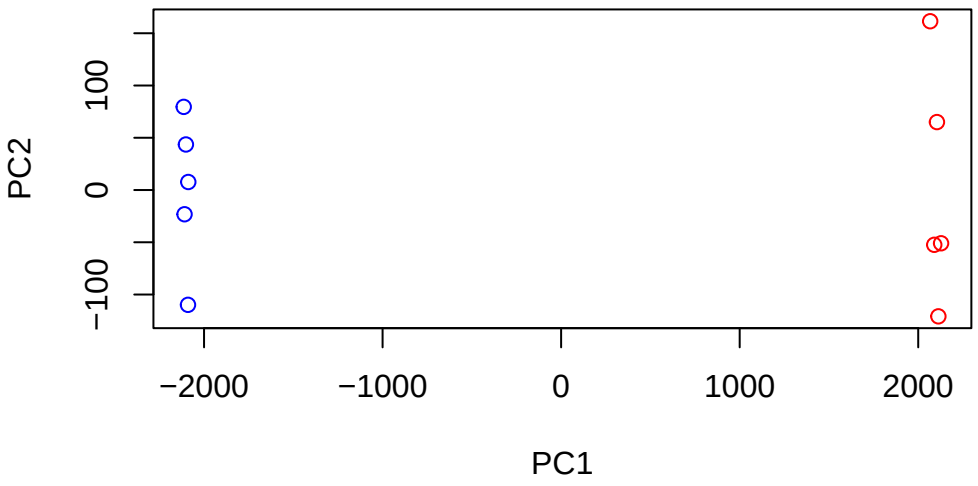
```
plot(pca_rna$x[,1], pca_rna$x[,2], xlab='PC1', ylab='PC2')
```



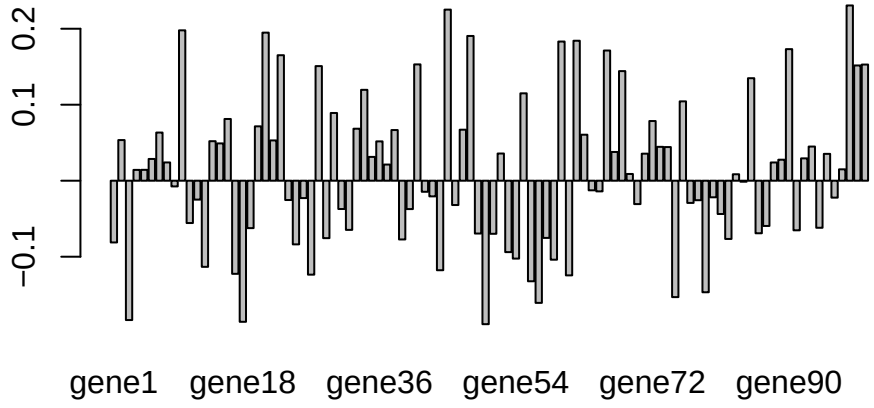

```
#colnames(rna.data)
cols_samples <- c(rep('blue', 5), rep('red', 5))
cols_samples
```

```
[1] "blue" "blue" "blue" "blue" "blue" "red"  "red"  "red"  "red"  "red"
```

```
#using cols_samples to plot
plot(pca_rna$x[,1], pca_rna$x[,2], xlab='PC1', ylab='PC2', col = cols_samples )
```




```
barplot( pca_rna$rotation[,1])
```



```
sort (pca_rna$rotation[,1])
```

```
      gene50       gene18        gene3       gene57       gene75       gene79
-0.188796985 -0.185668500 -0.183374164 -0.160771014 -0.153164404 -0.146803635
      gene56       gene61       gene27       gene17       gene44       gene13
-0.132330117 -0.124572881 -0.123615228 -0.122536548 -0.117808971 -0.113357525
      gene59       gene54       gene53       gene25        gene1       gene39
-0.103935563 -0.102503320 -0.093979884 -0.083761992 -0.081247810 -0.077306742
      gene82       gene29       gene58       gene51       gene49       gene86
-0.076658760 -0.075605635 -0.075274651 -0.069855142 -0.069530208 -0.069165267
      gene91       gene32       gene19       gene94       gene87       gene11
-0.065288752 -0.064721235 -0.062411218 -0.061938300 -0.059547317 -0.055698801
      gene81       gene40       gene31       gene46       gene70       gene77
-0.043780416 -0.037323670 -0.037219970 -0.031990529 -0.030784982 -0.029225446
      gene78       gene24       gene12       gene26       gene96       gene80
-0.025639741 -0.025407507 -0.024870802 -0.022868107 -0.022293151 -0.021824860
      gene43       gene42       gene65       gene64        gene9       gene84
-0.020617052 -0.014550791 -0.014052839 -0.012639567 -0.007495075 -0.001289937
      gene83       gene69        gene4        gene5       gene97       gene37
 0.008504287  0.008871890  0.014242602  0.014303808  0.014994546  0.021280555
      gene88        gene8       gene89        gene6       gene92       gene35
 0.024015925  0.024026657  0.027652967  0.028634131  0.029394259  0.031349942
      gene95       gene71       gene52       gene67       gene74       gene73
 0.035342407  0.035589259  0.035802086  0.037840851  0.044286948  0.044581700
      gene93       gene15       gene36       gene14       gene22        gene2
 0.044940861  0.049090676  0.051765605  0.052004194  0.053013523  0.053465569
      gene63        gene7       gene38       gene47       gene33       gene20
 0.060529157  0.063389255  0.066665407  0.067141911  0.068437703  0.071571203
      gene72       gene16       gene30       gene76       gene55       gene34
 0.078551648  0.081254592  0.089150461  0.104435777  0.114988217  0.119604059
      gene85       gene68       gene28       gene99      gene100       gene41
 0.134907896  0.144227333  0.150812015  0.151678253  0.152877246  0.153077075
      gene23       gene66       gene90       gene60       gene62       gene48
 0.165155192  0.171311307  0.173156806  0.183139926  0.184203008  0.190495289
      gene21       gene10       gene45       gene98
 0.194884023  0.197905454  0.225149201  0.230633225
```

Questions

Q1. How many rows and columns are in your new data frame named `x`? What R functions could you use to answer this questions?

There are 17 rows and 4 columns in the new data frame named x.

R function used: dim(x)

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?

I prefer the row.names =1 better because it gives a straightforward direction as to putting column #1 as the name of the row. I think this approach is better than the other one because if we replace x to another value than the x from before would be replaced.

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

Adding beside=T in the barplot() function.

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?

The code displays a matrix of scatterplots. The diagonal shows the names of the variables of the data. The points in the scatterplot represents the differences or similarities between the two compared variables. If a given point lies on the diagonal, it means that the two variables are correlated.

Q6. What is the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

Based on the data set, people in Northern Ireland eat more fresh potatoes than other countries of the UK, and there is a lower amount of people who consume alcoholic drinks.

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

```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], 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(x = pca$x[,1], y = pca$x[,2])

colors_countries <- c('orange', 'pink', 'blue', 'green')

text(x = pca$x[,1], y = pca$x[,2], colnames(x), col = colors_countries)

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

PC2 mainly tell us about the second most variation in the data. The two food groups are fresh potatoes and soft drinks.

Q10: How many genes and samples are in this data set?

There are 100 genes and 10 samples in this data set.