# Class 07

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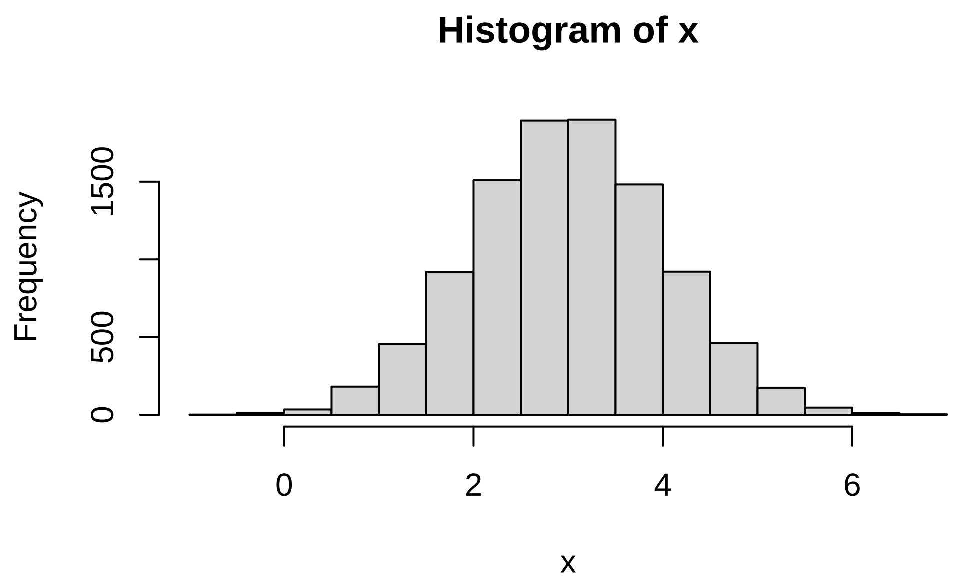
#Clustering

We will start today's lab with clustering methods, in particular so-called K-means. The main function for this in R is `kmeans()`.

Let's try it on some made up data where we know what the answer should be.

```r
x <- rnorm(10000,mean=3)
hist(x)
```



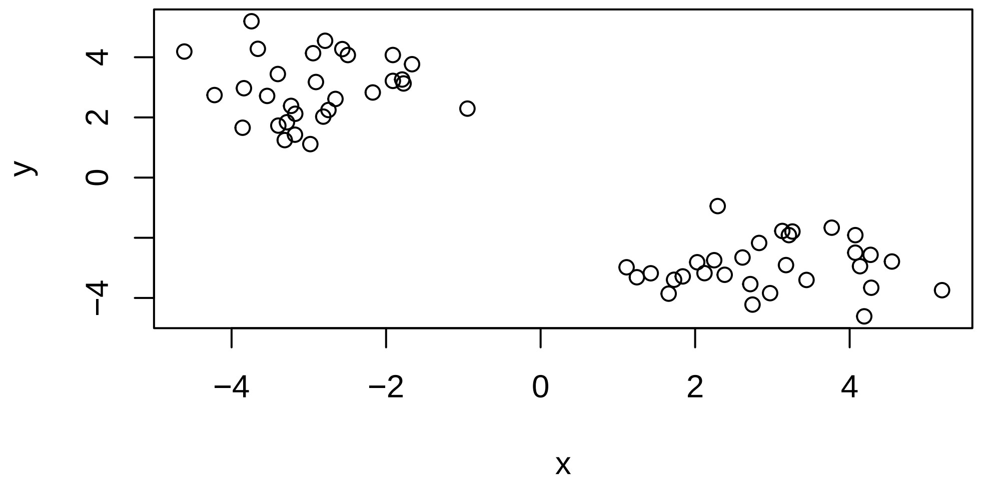
60 points

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

```
            x          y
[1,] 2.026536 -2.8131156
[2,] 2.292031 -0.9471092
[3,] 4.270506 -2.5665141
[4,] 1.839629 -3.2833284
[5,] 4.133919 -2.9448375
[6,] 2.742538 -4.2206130
```

We can pass this to the base R `plot()` for the function for a quick plot

```r
plot(x)
```



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

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

```
Cluster means:
          x         y
1  2.956482 -2.917354
2 -2.917354  2.956482

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] 53.67978 53.67978
 (between_SS / total_SS =  90.6 %)

Available components:

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

Q1.How many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q2. Cluster membership?

```
k$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
```

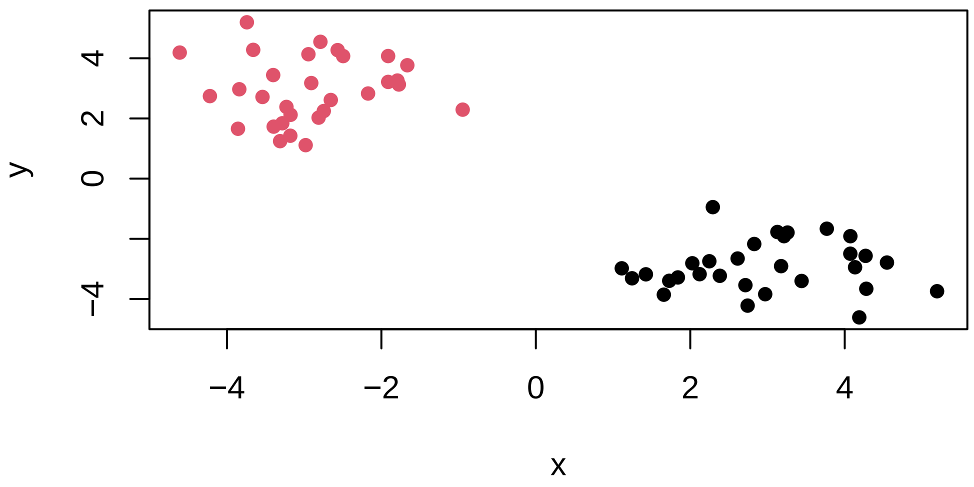
Q3. Cluster centers?

```
k$centers
```

```
          x         y
1  2.956482 -2.917354
2 -2.917354  2.956482
```

Q4. Plot my clustering results

```r
plot(x, col = k$cluster, pch=16)
```



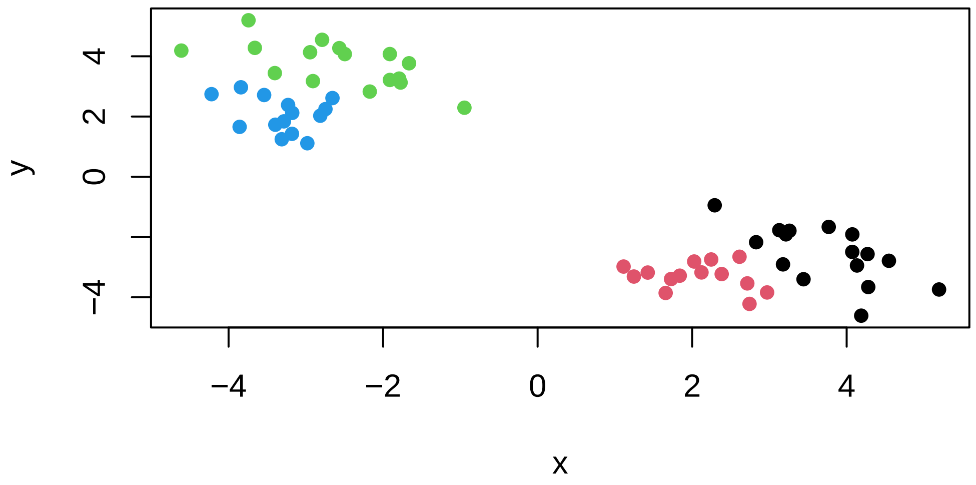
Q5. Cluster the data again into 4 groups

```r
k4<-kmeans(x, centers = 4, n = 20)
k4
```

```
K-means clustering with 4 clusters of sizes 16, 14, 16, 14

Cluster means:
          x         y
1  3.741822 -2.580840
2  2.058951 -3.301941
3 -2.580840  3.741822
4 -3.301941  2.058951

Clustering vector:
 [1] 2 1 1 2 1 2 2 1 2 1 1 1 2 1 1 1 2 1 2 1 2 2 1 2 2 2 1 1 1 2 4 3 3 3 4 4 4 3
[39] 4 4 3 4 3 4 3 3 3 4 3 3 3 4 3 4 4 3 4 3 3 4

Within cluster sum of squares by cluster:
```

```
[1] 21.58220  7.06899 21.58220  7.06899
 (between_SS / total_SS =  95.0 %)

Available components:

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

```
plot(x, col = k4$cluster, pch=16)
```



K-means is very popular mostly because it is fast and relatively straigtforward to run and undderstand. aIt has a big limitation in that you need to tell it how many groups (k, or centers) you want.

## Hierarchal clustering

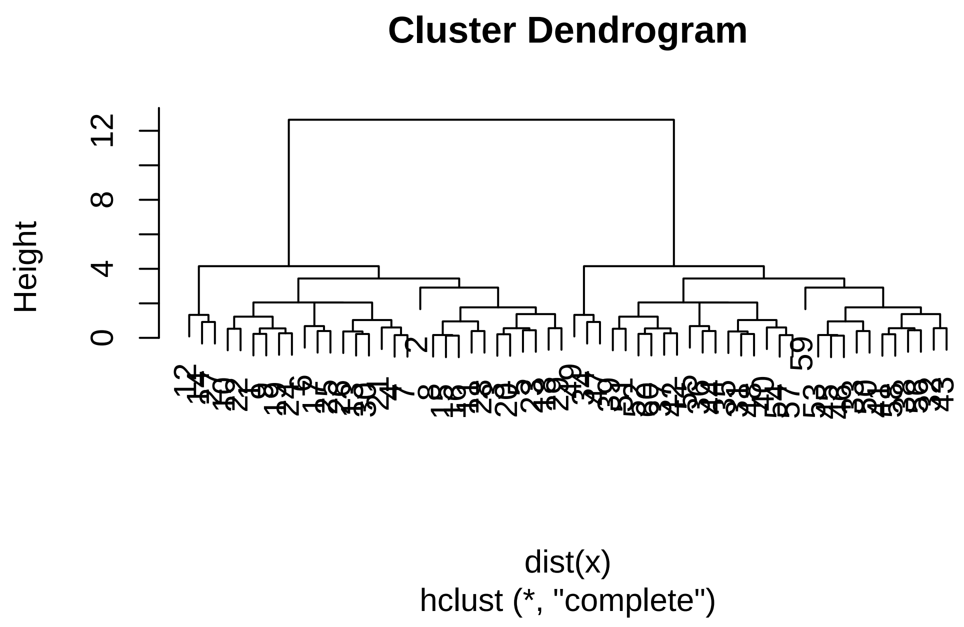
The main function in base R is called `hclust()`. You have to pass it in a "distance matrix" not just your input data.

You can generate a distance matrix with the `dist()` function.

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

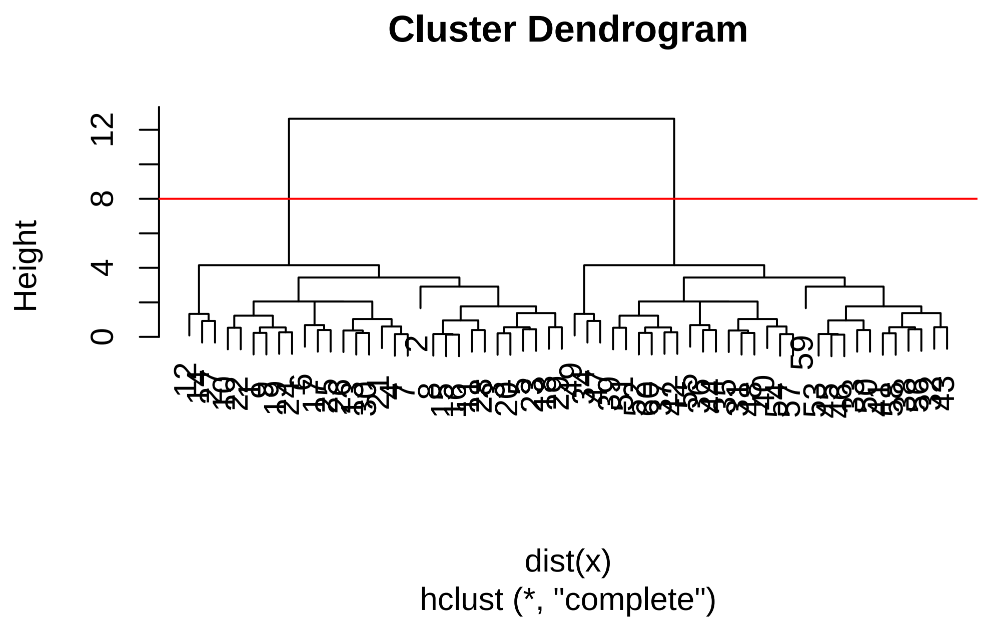
```
Call:
hclust(d = dist(x))

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

```
plot(hc)
```



To find the clusters (cluster membership vector) from a `hclust()` result we can "cut" the tree at a certain height that we like.

```
plot(hc)
abline(h=8, col = "red")
```



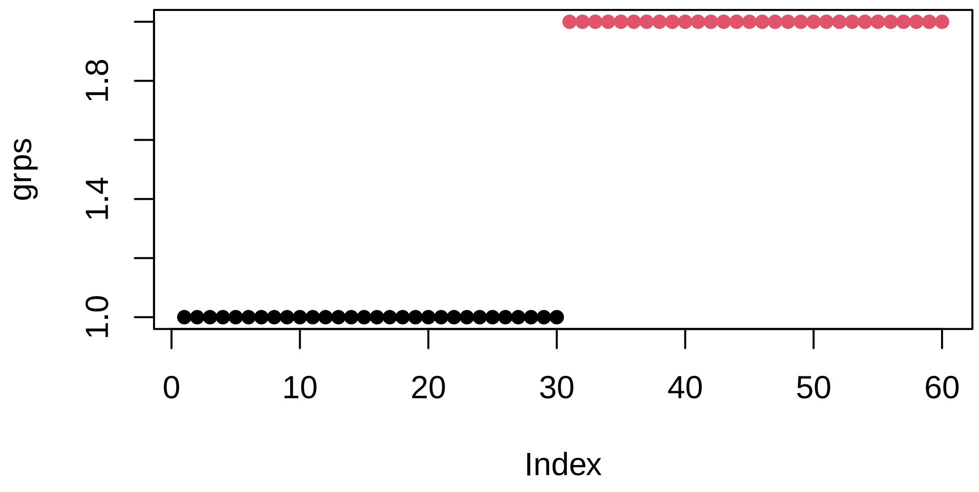
```r
grps <- cutree(hc, h=8)
```

```r
table(grps)
```

```
grps
 1  2 
30 30 
```

Q6. Plot our hclust results.

```r
plot(grps,col=grps, pch=16)
```



#Principal Component Analysis

##PCA of UK food data

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

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

```r
dim(x)
```

```
[1] 17  5
```

```r
head(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
```

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

```r
dim(x)
```

```
[1] 17  4
```

```r
x <- read.csv(url, row.names=1)
head(x)
```

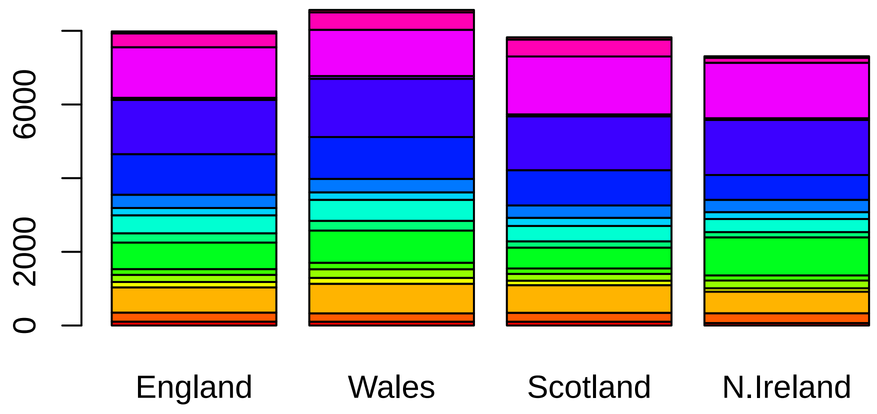
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
Fats_and_oils      193   235      184       209
Sugars             156   175      147       139
```

> 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?

Personally I prefer the csv rownames -1 one, since if you run the former way more than once, it will continue to remove columns. This for me resulted in me having 3 columns after having accidentally running the program more than once. For this reason also I believe the second way to be more robust.

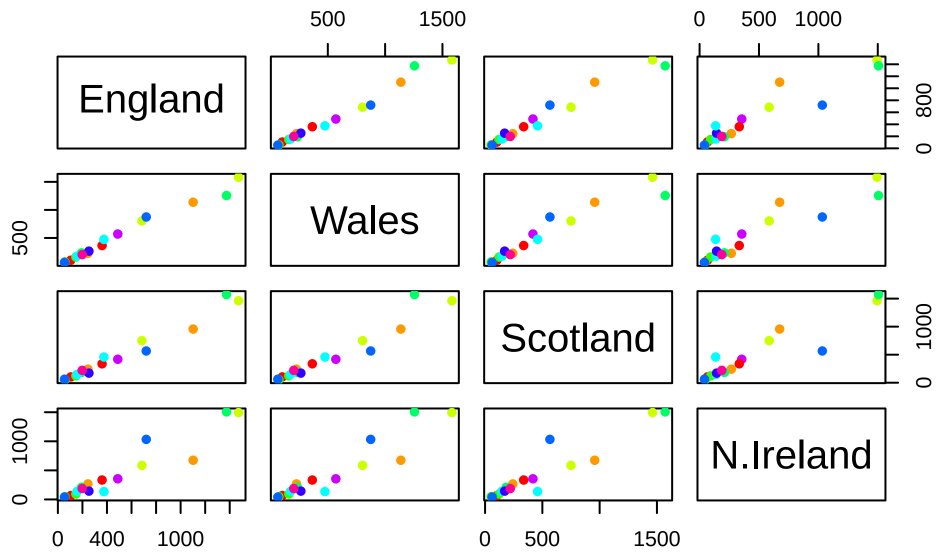
> Q3: Changing what optional argument in the above barplot() function results in the following plot?

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



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?

```
pairs(x, col=rainbow(10), pch=16)
```



```
#I think pairs() graphs two countries against each other. Each of the graphs represents a
```

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

A: N. Ireland clearly has different levels on consumption for many foodstuffs, as evidenced by the fact that the line of best fit between N. Ireland and the other countries does not perfectly line up on the diagonal or is not close to it.

## Principal Component Analysis (PCA)

PCA can help us make sense of these types of datasets. Let's see how it works.

The main function in base R is called `prcomp()`. In this case we want to first take the transpose of our input `x` so the columns are the food types and the countries are the rows.

```
head(t(x))
```

```
          Cheese Carcass_meat  Other_meat  Fish Fats_and_oils  Sugars
England      105          245         685   147           193     156
Wales        103          227         803   160           235     175
```

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

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

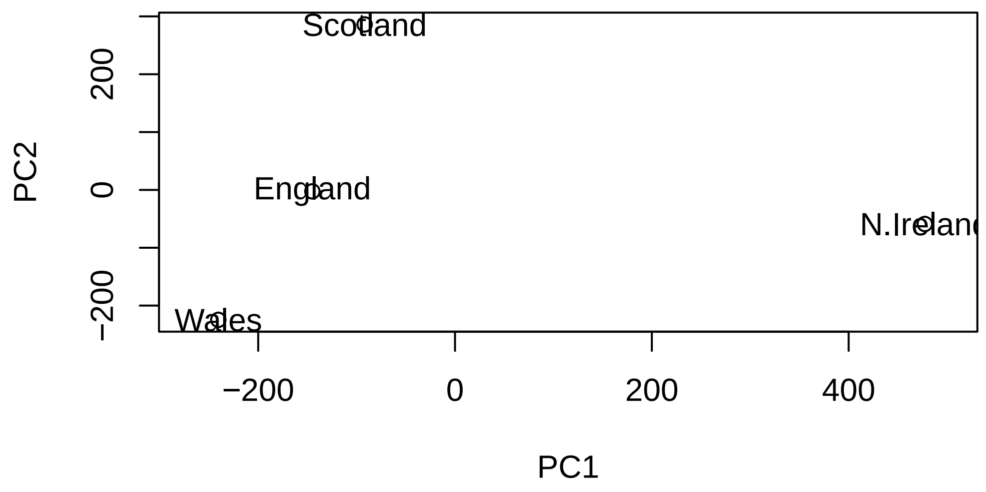
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 3.176e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
pca$x
```

```
                 PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -4.894696e-14
Wales     -240.52915 -224.646925 -56.475555  5.700024e-13
Scotland   -91.86934  286.081786 -44.415495 -7.460785e-13
N.Ireland  477.39164  -58.901862  -4.877895  2.321303e-13
```

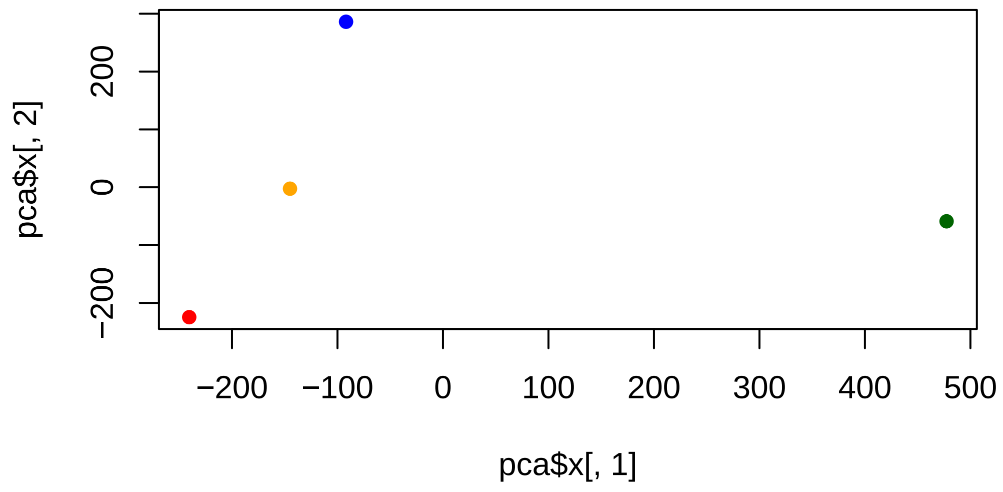
The "loadings" tell us how mjych the original variables (in our case the foods) contribute to the new variables i.e. the PCs >Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
plot(pca$x[,1], pca$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.

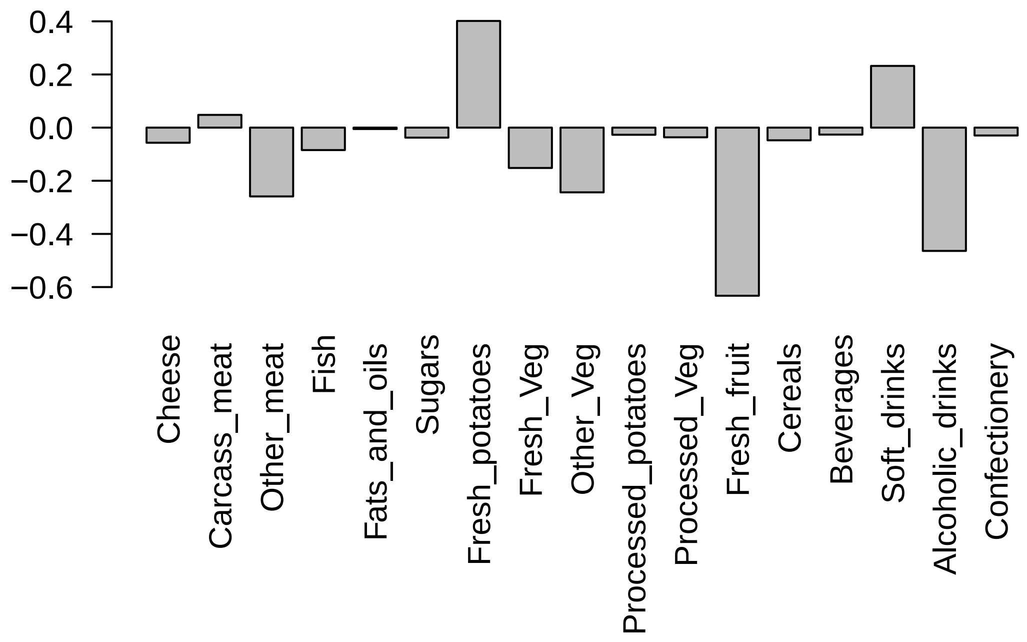
```
plot(pca$x[,1],pca$x[,2], col =c("orange","red","blue","darkgreen"), pch = 16)
```



```r
head(pca$rotation)
```

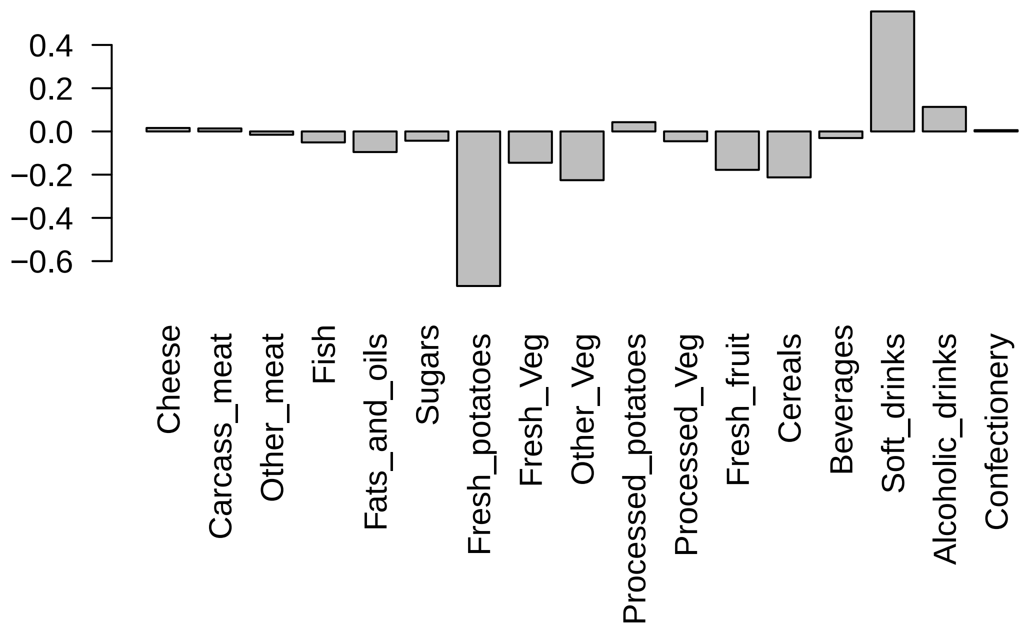
```
                      PC1         PC2         PC3          PC4
Cheese       -0.056955380  0.01601285  0.02394295 -0.694538519
Carcass_meat  0.047927628  0.01391582  0.06367111  0.489884628
Other_meat   -0.258916658 -0.01533114 -0.55384854  0.279023718
Fish         -0.084414983 -0.05075495  0.03906481 -0.008483145
Fats_and_oils -0.005193623 -0.09538866 -0.12522257  0.076097502
Sugars       -0.037620983 -0.04302170 -0.03605745  0.034101334
```

```r
par(mar=c(10, 3, 0.35, 0))
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?

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



Soft drinks and fresh potatoes feature prominently. PC2 shows us the rest of the variance not covered in PC1.