Class 07: Machine Learning 1

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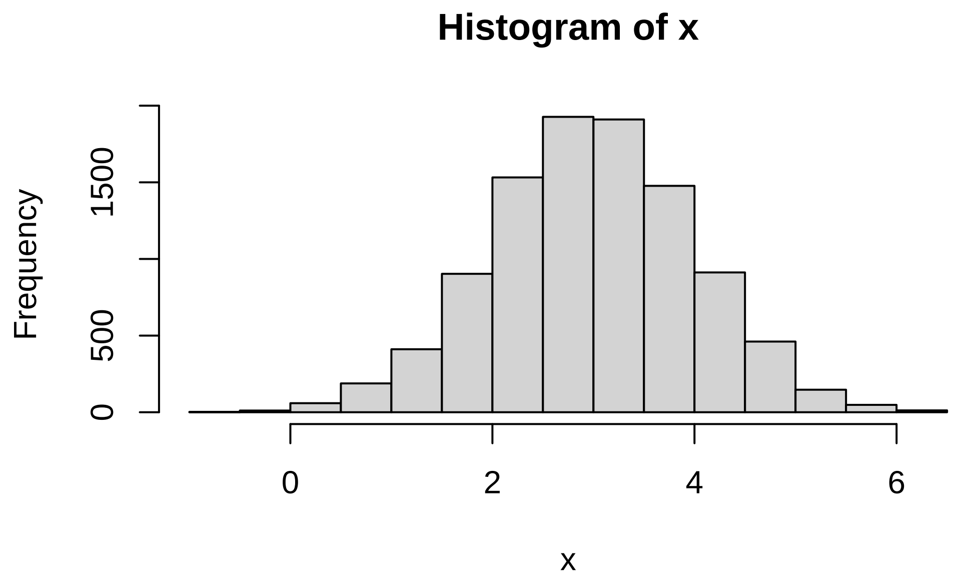
Clustering

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)
```



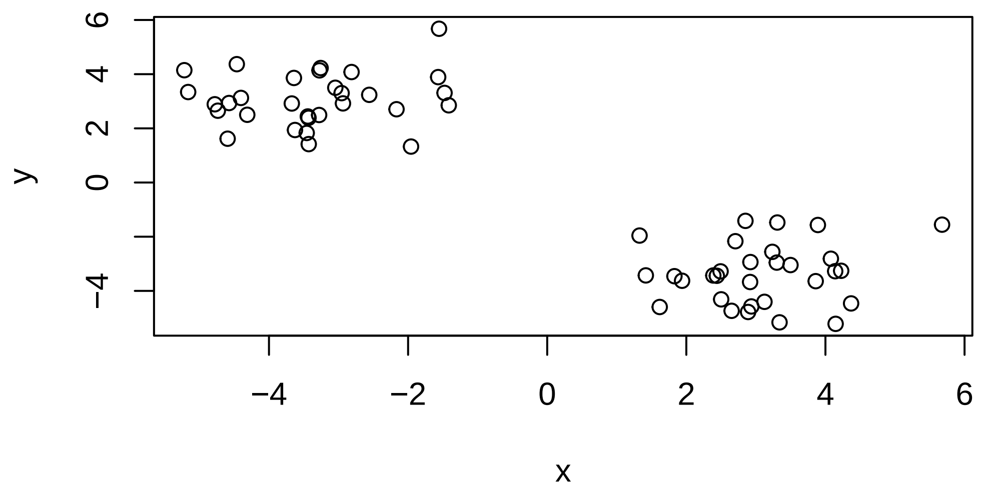
60 points

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

```
            x         y
[1,] 1.327587 -1.957994
[2,] 4.368673 -4.462531
[3,] 3.891283 -1.567629
[4,] 4.226020 -3.257913
[5,] 4.146358 -5.217173
[6,] 2.388003 -3.431526
```

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

```
plot(x)
```



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

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

```
Cluster means:
          x         y
1  3.066975 -3.373335
2 -3.373335  3.066975

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] 63.17707 63.17707
 (between_SS / total_SS =  90.8 %)

Available components:

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

Q1. How many points are in each cluster?

```r
k$size
```

```
[1] 30 30
```

Q2. Cluster membership?

```r
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
```

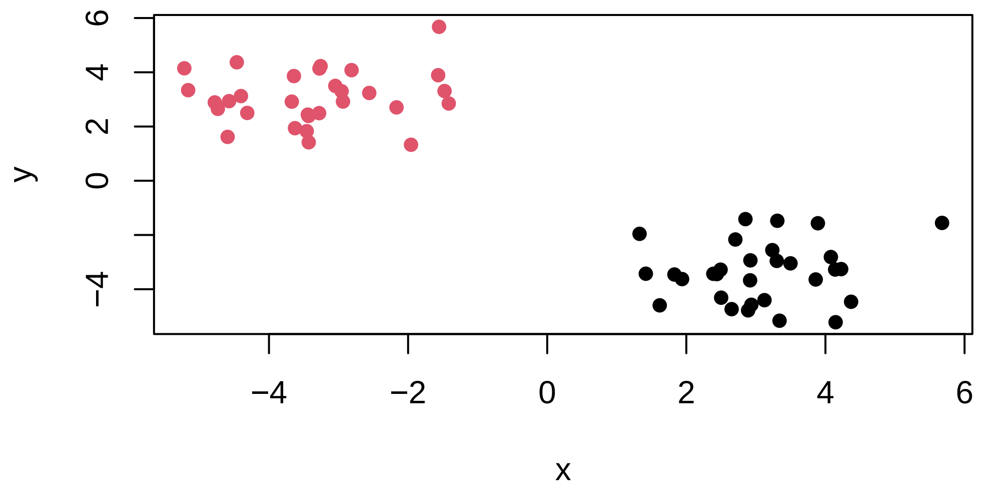
Q3. Cluster centers?

```r
k$centers
```

```
          x         y
1  3.066975 -3.373335
2 -3.373335  3.066975
```

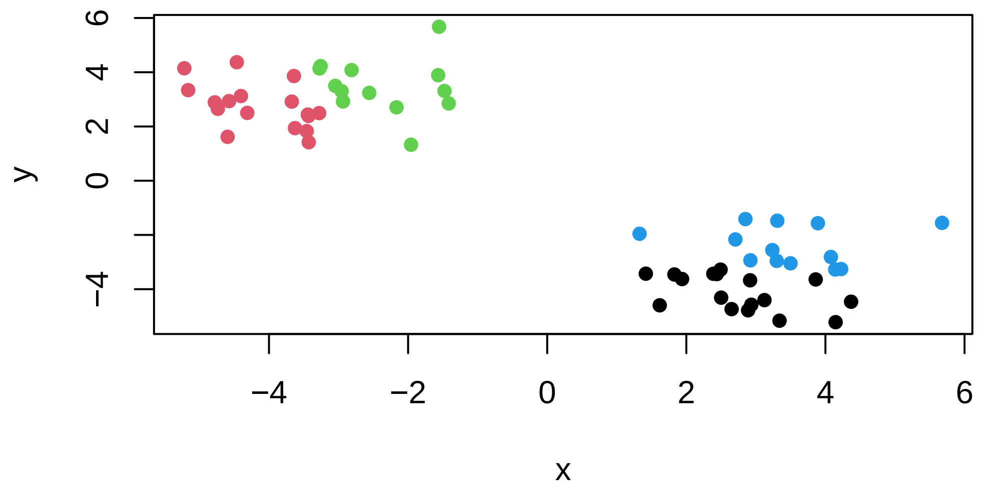
Q4. Plot my clustering results.

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



Q5. Cluster the data again with `kmeans()` into 4 groups and plot the results.

```r
k4 <- kmeans(x, centers = 4, nstart = 20)
plot(x, col = k4$cluster, pch = 16)
```



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

Hierarchical 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
```

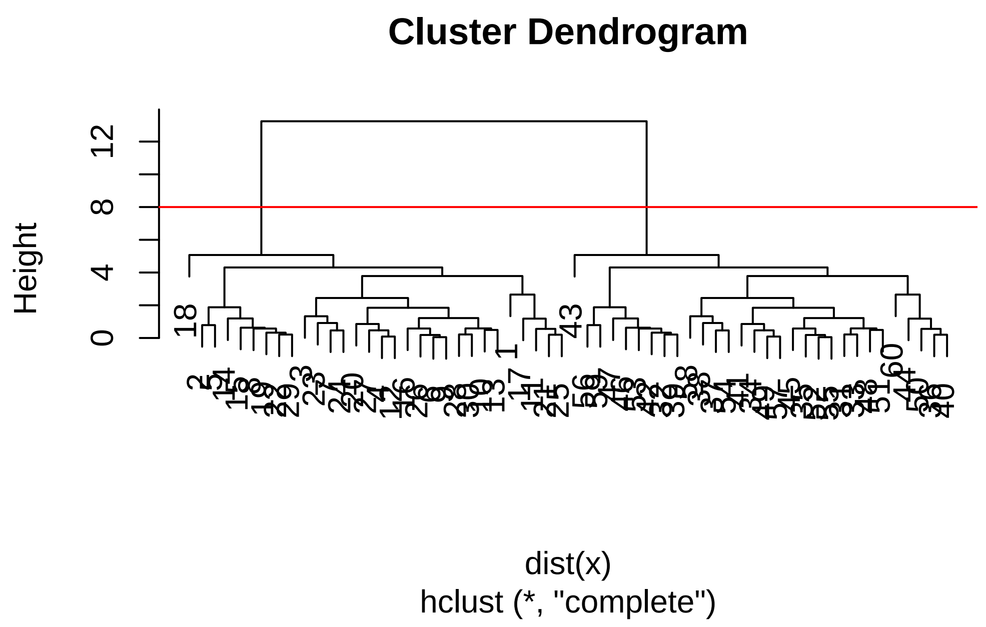
```

Call:
hclust(d = dist(x))

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

To find the clusters (cluster membership vector) from a `hclust()` result we can “cut” the tree at a certain height that we like. For this we use the `cutree()` function.

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



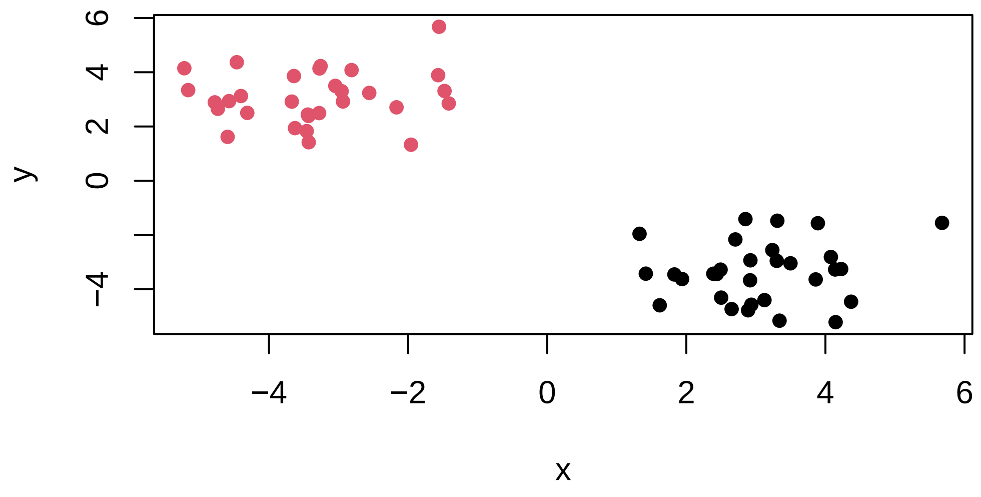
```
grps <- cutree(hc, h=8)
```

```
table(grps)
```

```
grps
 1  2 
30 30 
```

> Q6. Plot our hclust results.

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



Principal Component Analysis

PCA of UK food data

Suppose that we are examining the following data, from the UK's 'Department for Environment, Food and Rural Affairs' (DEFRA), showing the consumption in grams (per person, per week) of 17 different types of food-stuff measured and averaged in the four countries of the United Kingdom in 1997.

Lets see how PCA can help with conventional analysis.

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

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

```
dim(x)
```

```
[1] 17  5
```

Preview the first 6 rows:

```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
```

Here it appears that the row-names are incorrectly set as the first column of our x data frame (rather than set as proper row-names). This is very common error. Lets try to fix this up with the following code, which sets the rownames() to the first column and then removes the troublesome first column (with the -1 column index):

```r
# Note how the minus indexing works
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
```

Check the dimensions again; Notice how we now have 4 columns instead of 5.

```r
dim(x)
```

```
[1] 17  4
```

An alternative approach to setting the correct row-names in this case would be to read the data file again and this time set the row.names argument of read.csv() to be the first column (i.e. use argument setting row.names=1), see below:

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

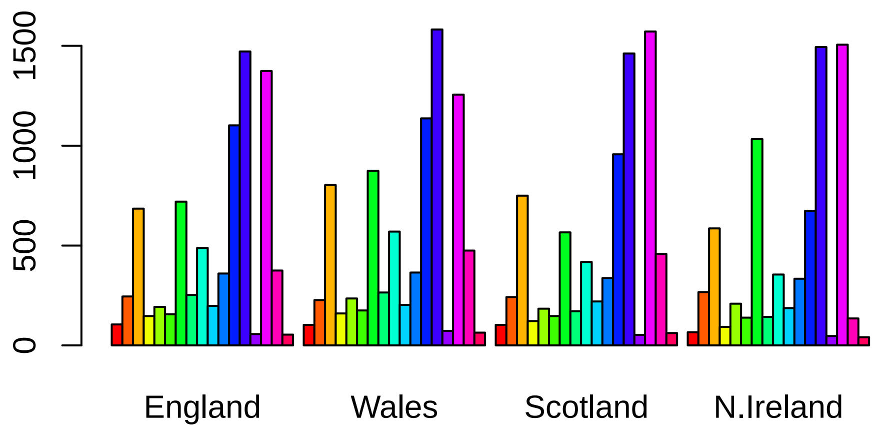
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
Fats_and_oils      193   235      184       209
Sugars  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

The second approach is definitely better because it avoids overwriting the dataset; Everytime you run the code with the [-1] syntax, it deletes a column from the dataset.

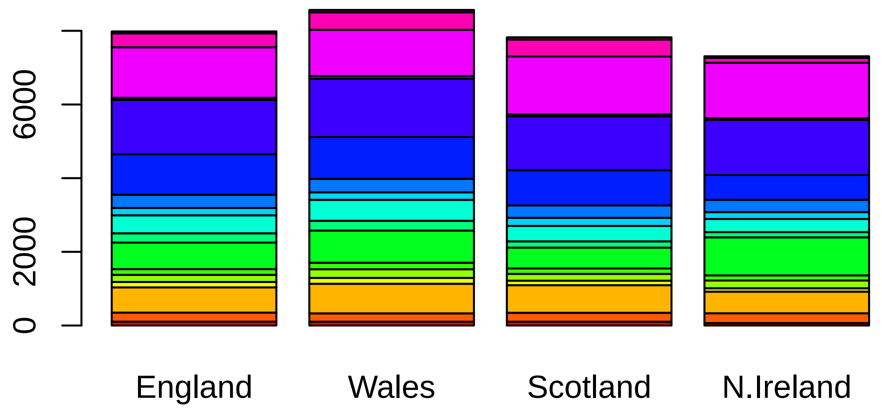
A cursory glance over the numbers in this table does not reveal much of anything. Indeed in general it is difficult to extract meaning in regard to major differences and trends from any given array of numbers. Generating regular bar-plots and various pairwise plots does not help too much either:

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



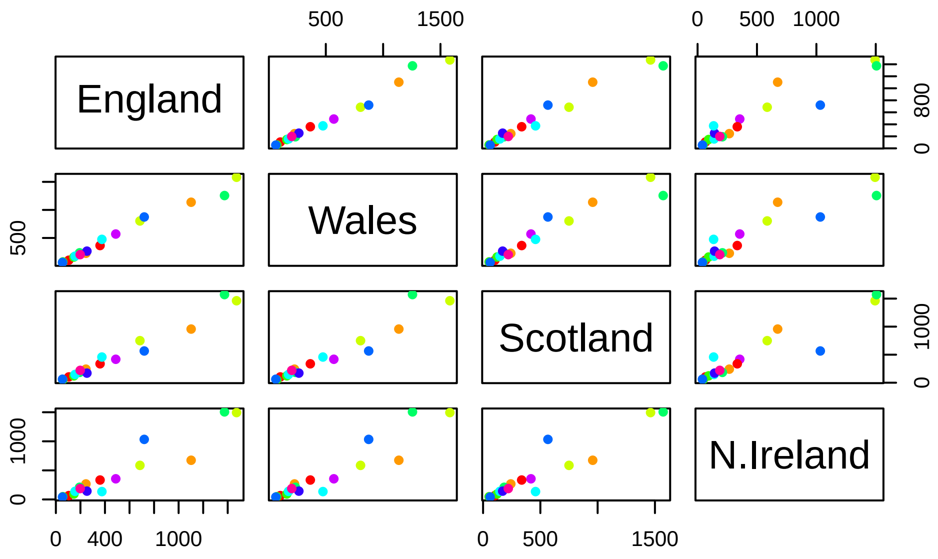
Q3: Changing what optional argument in the above barplot() function results in the following plot?

```
barplot(as.matrix(x), beside=F, 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)
```



The plot where each country intersects represents a comparison plot between the two countries. For example, the plot below England plots the x-axis of England against the y-axis of Wales. If points lie on the diagonal of the plot, that means that the data from the two countries being compared are very similar.

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

When plotted against N. Ireland, points lie off of the diagonal, suggesting a greater difference in the food consumption in this country.

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 `t()` of our input `x` so the columns are the food types and the countries are the rows.

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

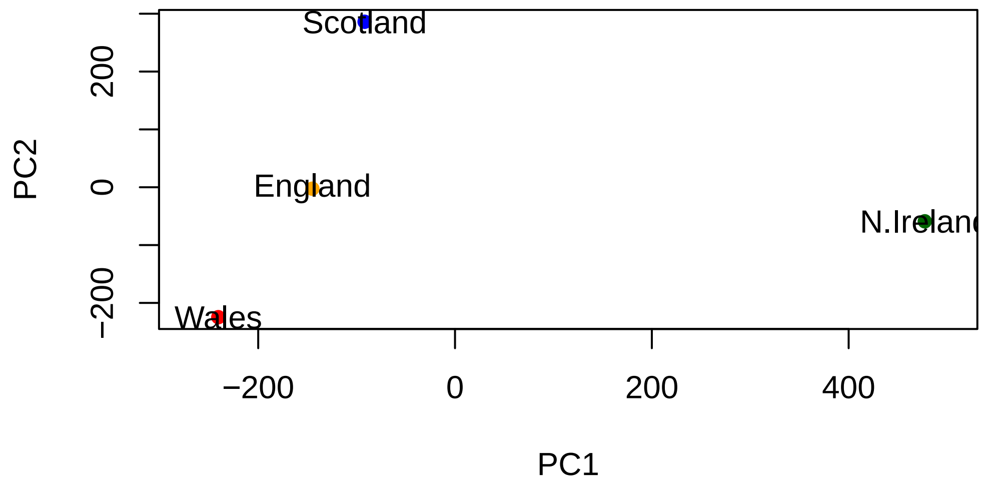
```
          Cheese Carcass_meat  Other_meat  Fish Fats_and_oils  Sugars
England      105          245         685   147           193     156
Wales        103          227         803   160           235     175
Scotland     103          242         750   122           184     147
N.Ireland     66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

```r
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
```

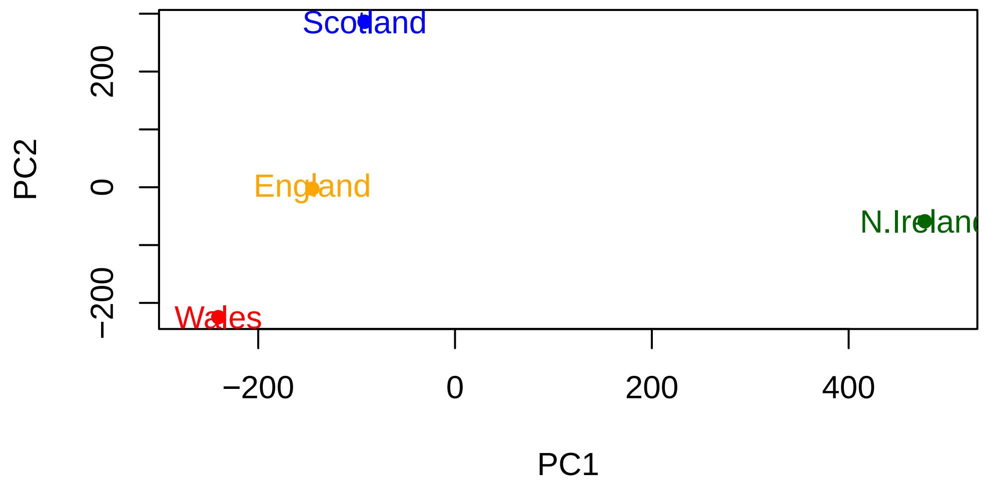
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```r
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], col=c("orange", "red", "blue", "darkgreen"), pch=16, xlab="PC1"
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, xlab="PC1"
text(pca$x[,1], pca$x[,2], colnames(x), col=c("orange", "red", "blue", "darkgreen"))
```



Below we can use the square of pca$sdev , which stands for “standard deviation”, to calculate how much variation in the original data each PC accounts for.

```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

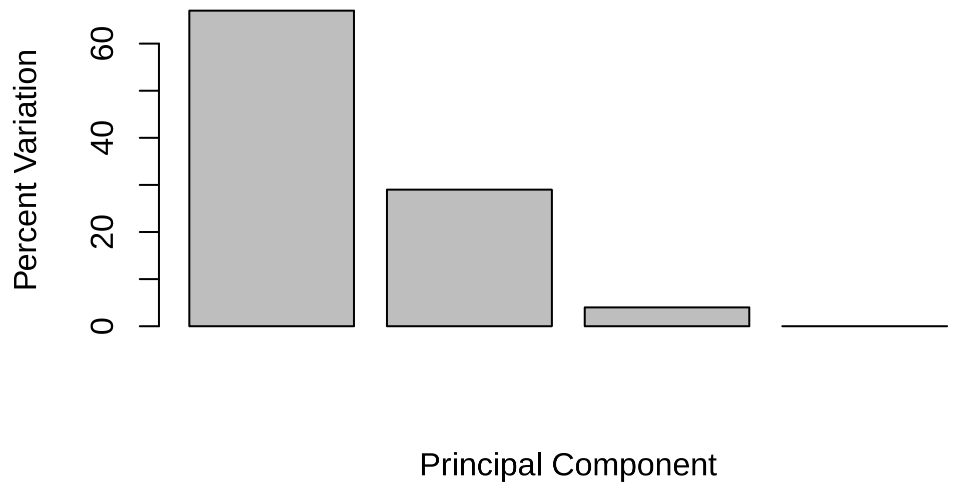
```
[1] 67 29  4  0
```

```
## or the second row here...
z <- summary(pca)
z$importance
```

```
                             PC1       PC2      PC3          PC4
Standard deviation     324.15019 212.74780 73.87622 3.175833e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

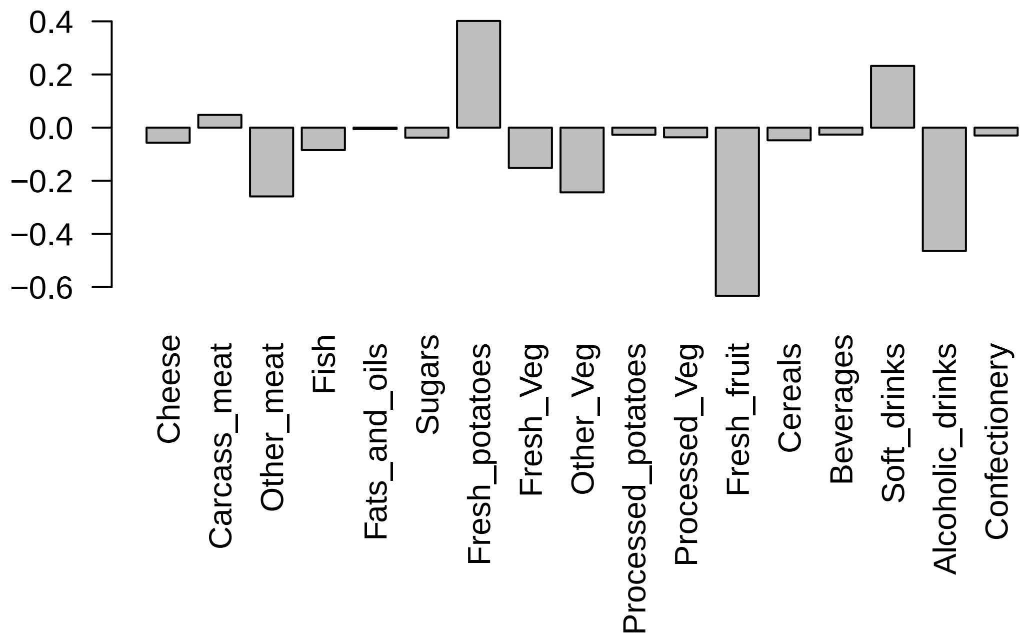
This information can be summarized in a plot of the variances (eigenvalues) with respect to the principal component number (eigenvector number), which is given below.

```
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```



We can also consider the influence of each of the original variables upon the principal components (typically known as loading scores). This information can be obtained from the prcomp() returned $rotation component. It can also be summarized with a call to biplot(), see below:

```
## 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 )
```

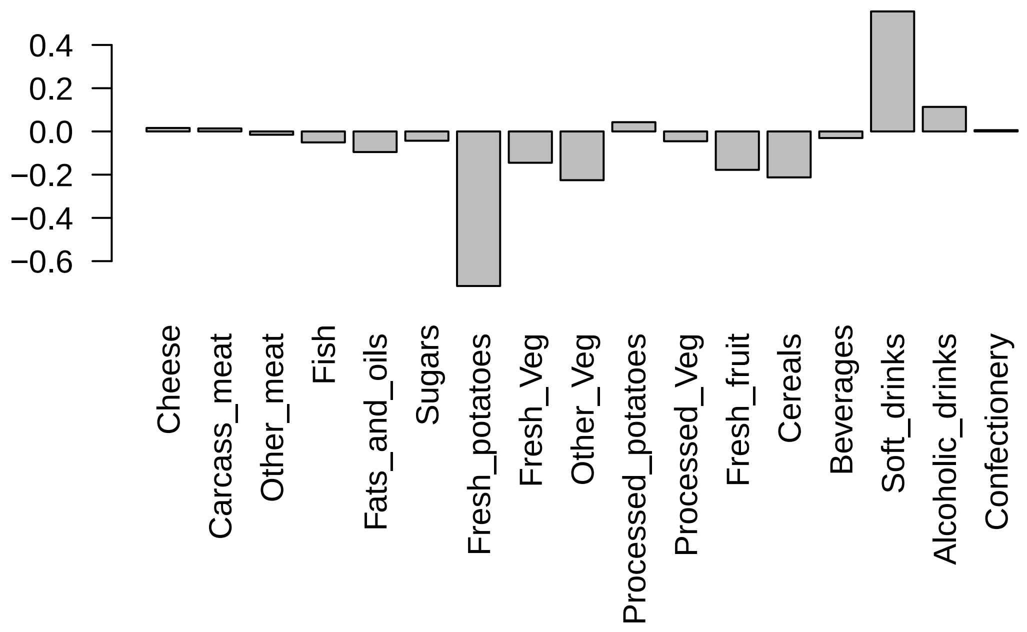


Here we see observations (foods) with the largest positive loading scores that effectively "push" N. Ireland to right positive side of the plot (including Fresh_potatoes and Soft_drinks).

We can also see the observations/foods with high negative scores that push the other countries to the left side of the plot (including Fresh_fruit and Alcoholic_drinks).

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

```
## Lets focus on PC2
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```



This plot predominantly features "Fresh_potatoes" and "Soft_drinks". This tells us that Wales consumes more fresh potatoes while Scotland consumes more soft drinks.