Class 07: Machine Learning 1

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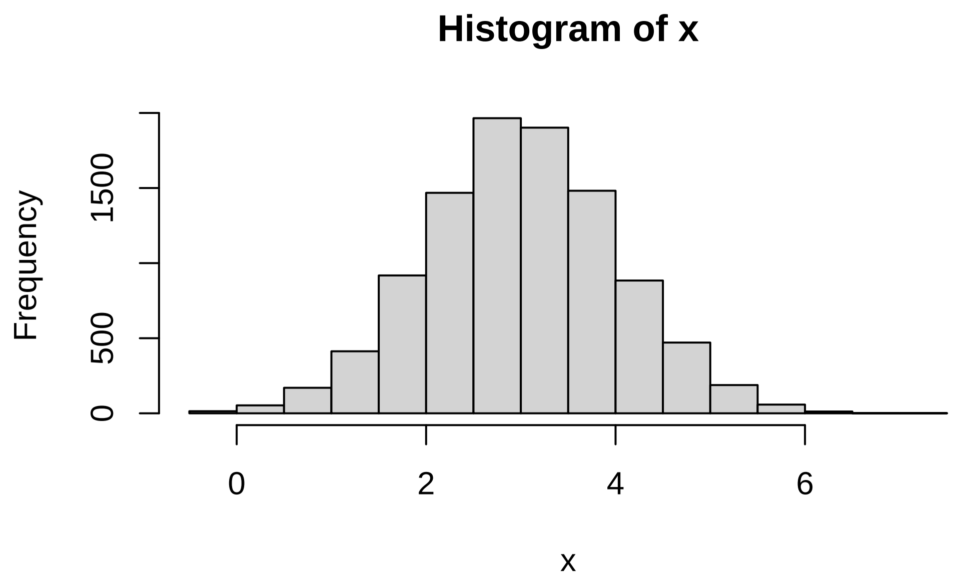
#Clustering We will start today's lab with clustering methods, in particular so-called K-means. The main functions for this in R is `kmeans()`

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)
```



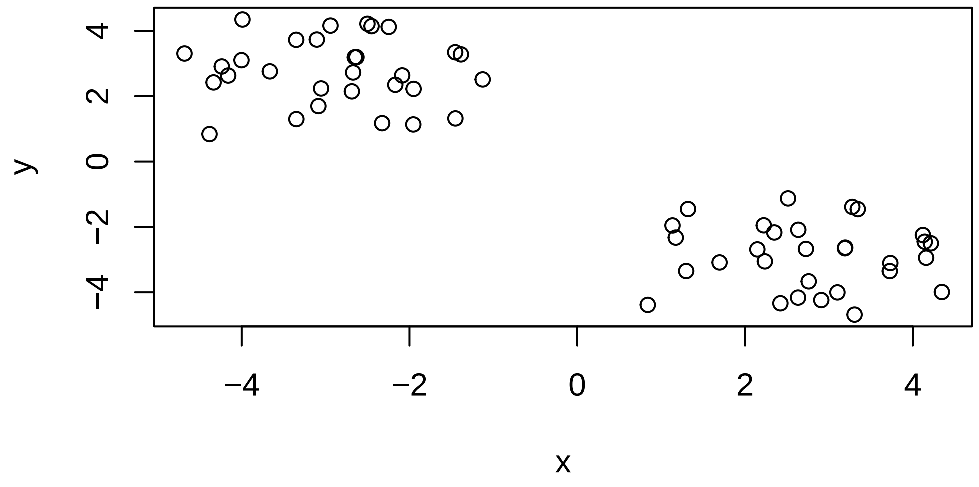
60 points

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

```
            x         y
[1,] 4.120075 -2.247609
[2,] 4.215088 -2.501098
[3,] 2.908802 -4.237551
[4,] 3.305526 -4.682018
[5,] 2.236210 -3.053769
[6,] 2.223211 -1.950865
```

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  2.762319 -2.869839
2 -2.869839  2.762319

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] 57.3778 57.3778
 (between_SS / total_SS =  89.2 %)

Available components:

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

Q.1 How many points are in each cluster

```
k$size
```

```
[1] 30 30
```

Q.2 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
```

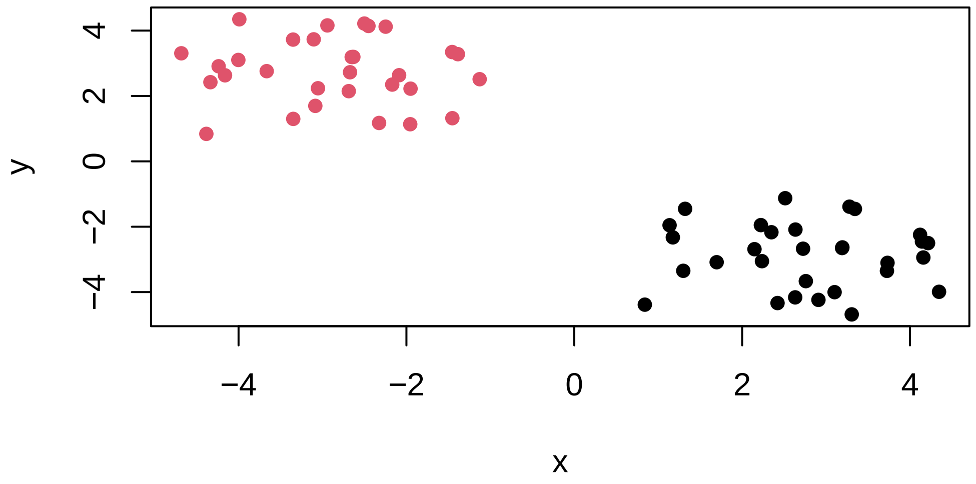
Q3. Cluster centers?

```
k$centers
```

```
          x         y
1  2.762319 -2.869839
2 -2.869839  2.762319
```

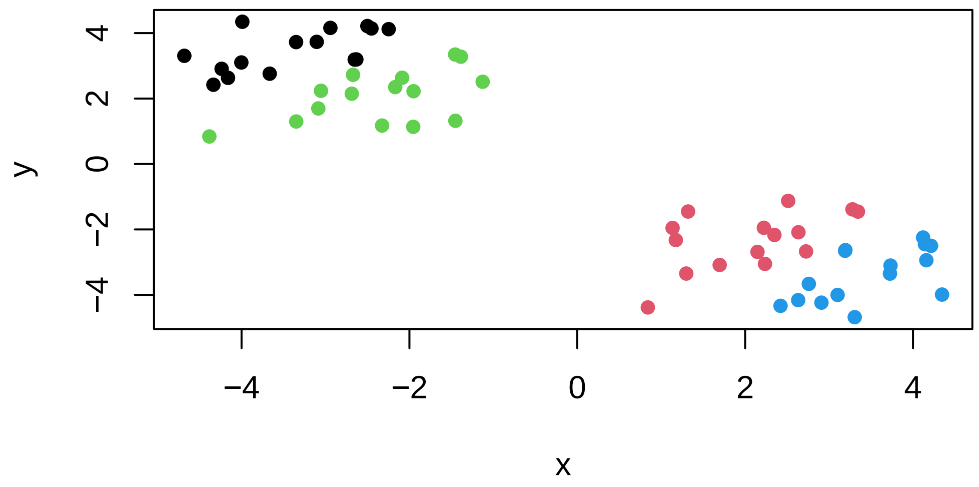
Q4. Plot my clustering results

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



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

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



K-means is very popular mostly because its fast and relatively straightforward 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

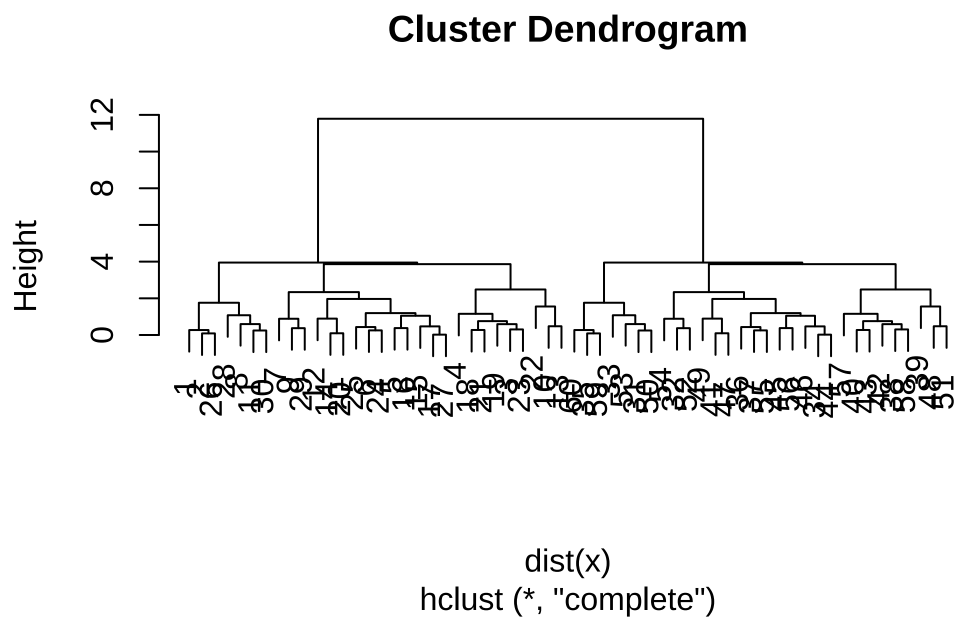
The main function in base R is called `hclust()`. You have to pass it in a "distance matrix" not just your input data. (won't work with just the data itself, need to pass it into the distance matrix)

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

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

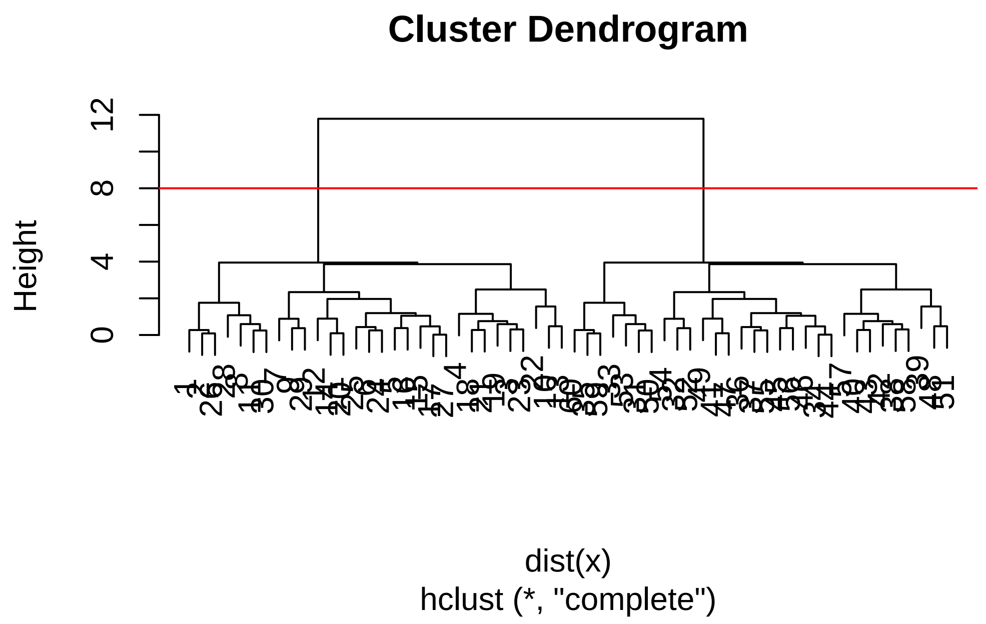
```
Call:
hclust(d = dist(x))

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")
```



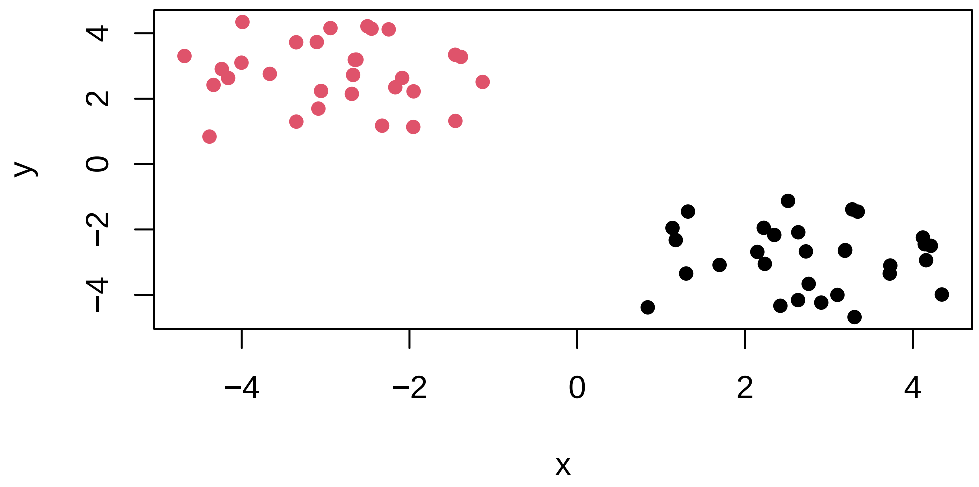
```
groups <- cutree(hc, h=8)
```

```
table(groups)
```

```
groups
 1  2 
30 30 
```

Q6. Plot our hclust results

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



#Principal Component Analysis

##PCA of UK food data

Read data 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

Let's see how PCA can help us but first we can try conventional analysis

```r
url <- "https://tinyurl.com/UK-foods"
rownames(x) <- x[,1]
x <- x[,-1]
head(x)
```

```
4.12007538325253 4.21508848293159 2.90880238997983 3.30552623758085
       -2.247609        -2.501098        -4.237551        -4.682018
2.23620979966985 2.22321067565731
       -3.053769        -1.950865
```

> 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)
```

```
NULL
```

Preview the first 6 rows

```r
head(x)
```

```
4.12007538325253 4.21508848293159 2.90880238997983 3.30552623758085
       -2.247609        -2.501098        -4.237551        -4.682018
2.23620979966985 2.22321067565731
       -3.053769        -1.950865
```

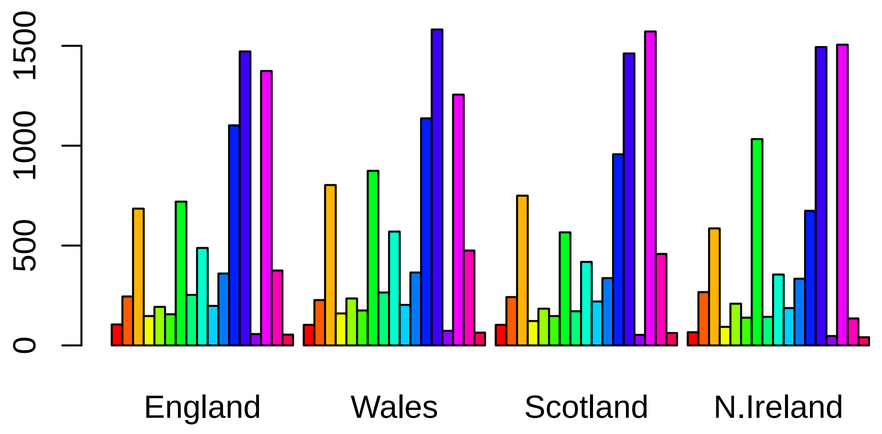
```r
x <- read.csv(url, row.names=1)
head(x)
```

```
               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?

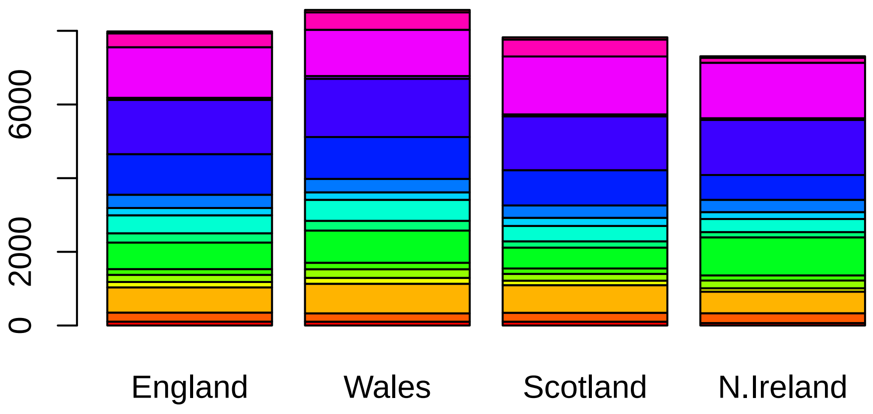
I prefer the row.names=1' code. This approach is stronger than the x[,-1] approach because the code over writes the same object each time and it keeps getting rid of rows ever time that I run it.

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

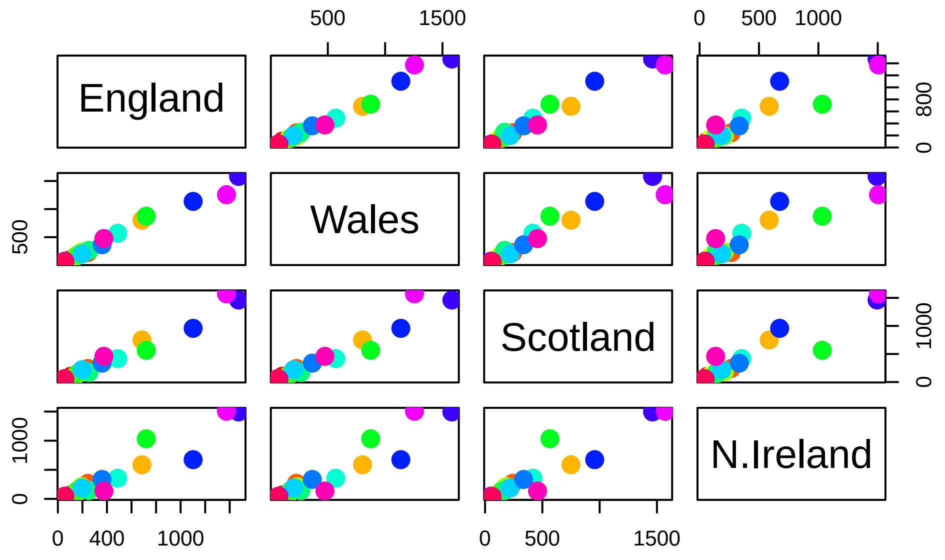


Q3: Changing what optional argument in the above barplot() function results in the following plot?

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



```
pairs(x, col=rainbow(17), pch=16, cex=2)
```



> 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?

If a given point lies along the diagonal for a given plot means that the each country's consumption is about the same similarity, whereas if certain plots lie below the diagonal line this means dissimilarity and lower type of consumption.

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

In this data set, the main differences between N. Ireland and the other countries in the UK is a bit more difficult to see.However, compared to the other countries in the UK and their graphs, each plot of N. Ireland vs the other UK countries has less of of a straight diagonal line indicating that it's properly more dissimilar.

##Principal Compoenent analysis (PCA)

PCA can help us make sense of these types of data sets. 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 counties 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
```

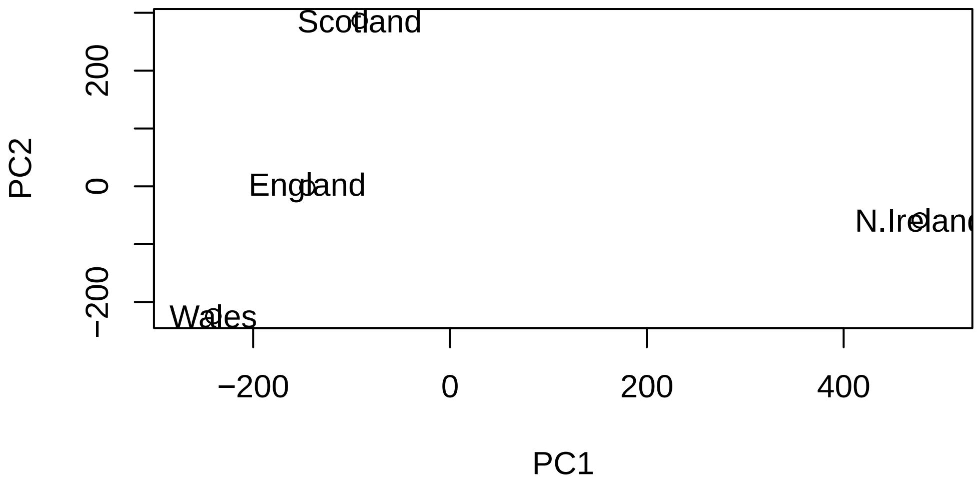
```
Scotland                458             62
N.Ireland               135             41
```

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

```
Importance of components:
                             PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 2.921e-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.

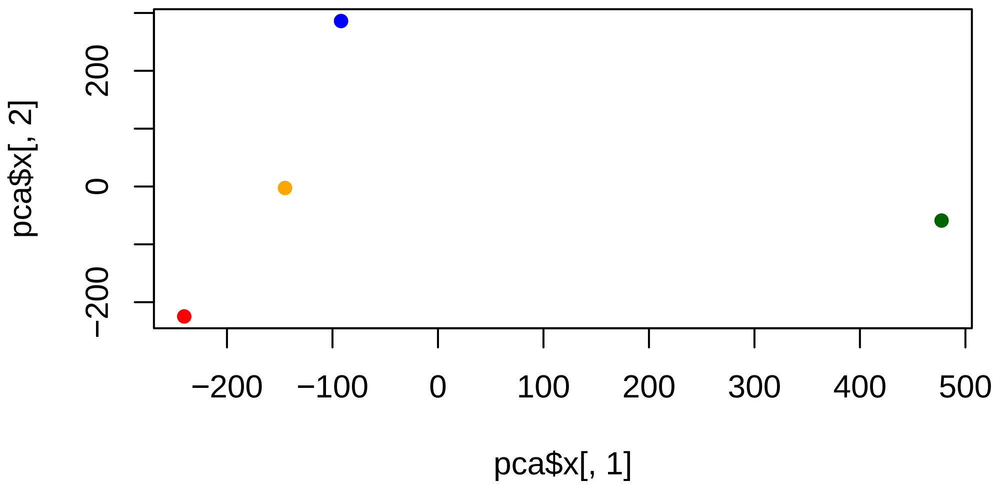
```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x))
```



```
pca$x
```

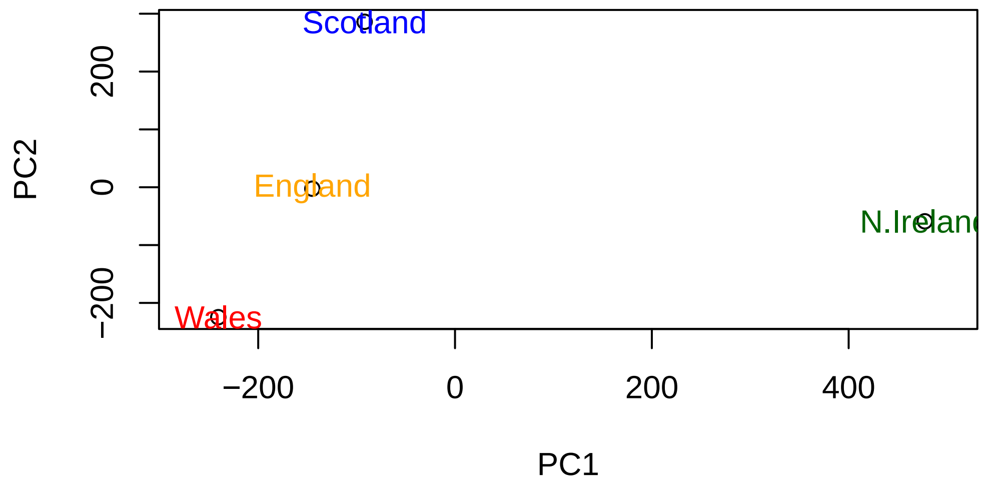
```
                 PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -9.152022e-15
Wales     -240.52915 -224.646925 -56.475555  5.560040e-13
Scotland   -91.86934  286.081786 -44.415495 -6.638419e-13
N.Ireland  477.39164  -58.901862  -4.877895  1.329771e-13
```

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



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], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x), col=c("orange", "red", "blue","darkgreen"))
```



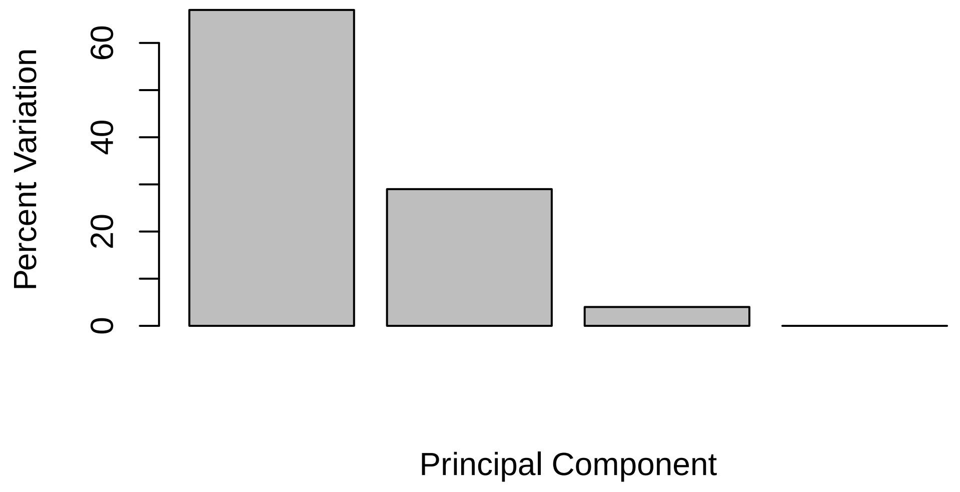
```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

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

```
z <- summary(pca)
z$importance
```

```
                             PC1       PC2      PC3          PC4
Standard deviation     324.15019 212.74780 73.87622 2.921348e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

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



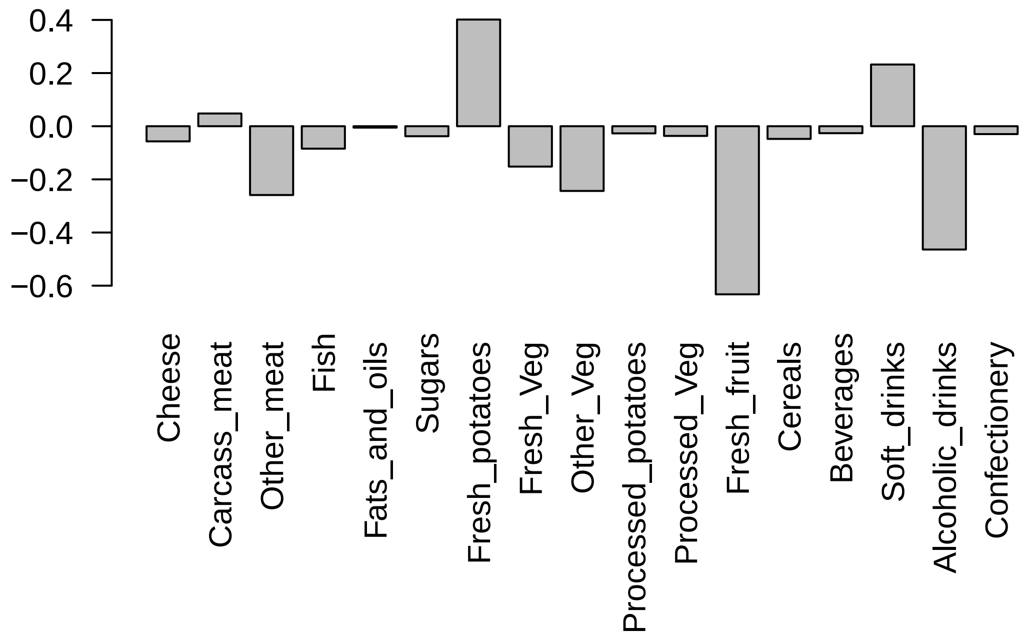
The "loadings" tell us how much of the original variables (in our cause the foods, contribute) to the new variables i.e. PCs

```
pca$rotation
```

```
                            PC1          PC2         PC3          PC4
Cheese             -0.056955380  0.016012850  0.02394295 -0.409382587
Carcass_meat        0.047927628  0.013915823  0.06367111  0.729481922
Other_meat         -0.258916658 -0.015331138 -0.55384854  0.331001134
Fish               -0.084414983 -0.050754947  0.03906481  0.022375878
Fats_and_oils      -0.005193623 -0.095388656 -0.12522257  0.034512161
Sugars             -0.037620983 -0.043021699 -0.03605745  0.024943337
Fresh_potatoes      0.401402060 -0.715017078 -0.20668248  0.021396007
Fresh_Veg          -0.151849942 -0.144900268  0.21382237  0.001606882
Other_Veg          -0.243593729 -0.225450923 -0.05332841  0.031153231
Processed_potatoes -0.026886233  0.042850761 -0.07364902 -0.017379680
Processed_Veg      -0.036488269 -0.045451802  0.05289191  0.021250980
Fresh_fruit        -0.632640898 -0.177740743  0.40012865  0.227657348
Cereals            -0.047702858 -0.212599678 -0.35884921  0.100043319
Beverages          -0.026187756 -0.030560542 -0.04135860 -0.018382072
Soft_drinks         0.232244140  0.555124311 -0.16942648  0.222319484
Alcoholic_drinks   -0.463968168  0.113536523 -0.49858320 -0.273126013
```

```
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001890737
```

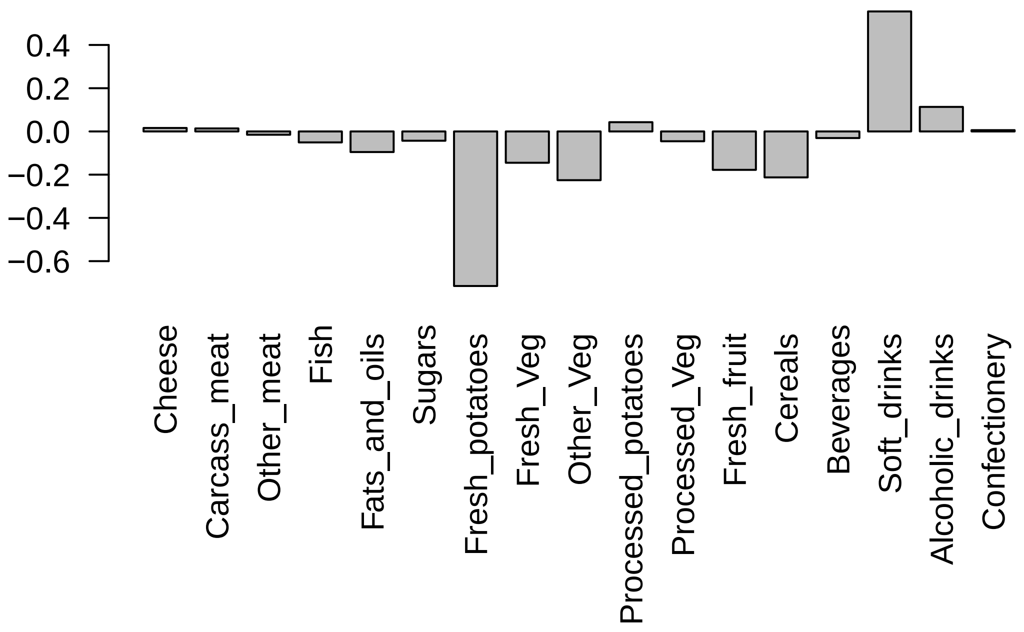
```
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```



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

The two food group features that are most prominent are fresh potatoes and soft drinks. PC1 captures the most variance through a certain point, but PC2 will capture the second most variance in comparison to PC1. In other words, PC2 will be able to capture the rest of the variance that PC1 wasn't able to capture.

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


0.4
0.2
0.0
−0.2
−0.4
−0.6
Cheese
Carcass_meat
Other_meat
Fish
Fats_and_oils
Sugars
Fresh_potatoes
Fresh_Veg
Other_Veg
Processed_potatoes
Processed_Veg
Fresh_fruit
Cereals
Beverages
Soft_drinks
Alcoholic_drinks
Confectionery