Class 07: Machine Learning

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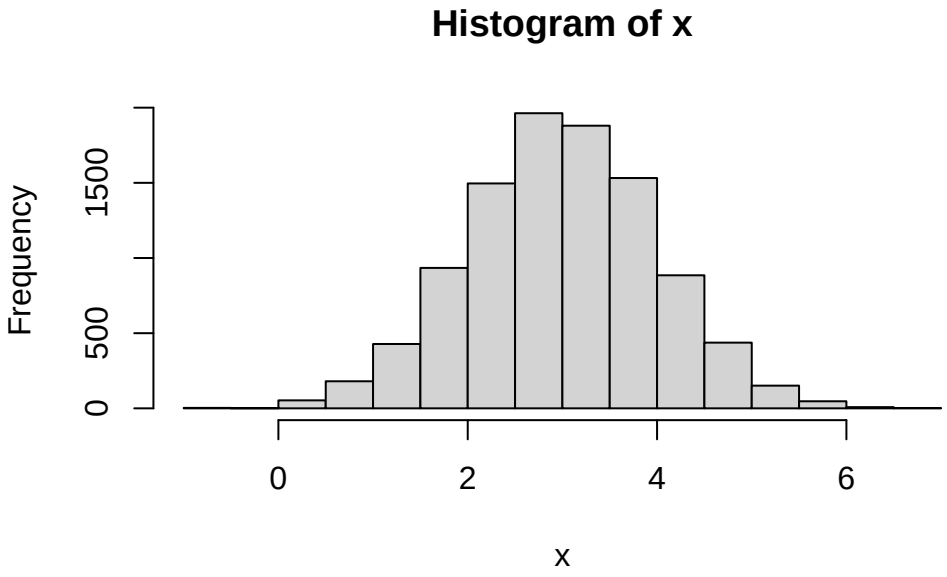
Clustering

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

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



60 points

```
tmp <-c(rnorm(30, mean=3), rnorm(30, -3))
#numbers change each time code runs
tmp
```

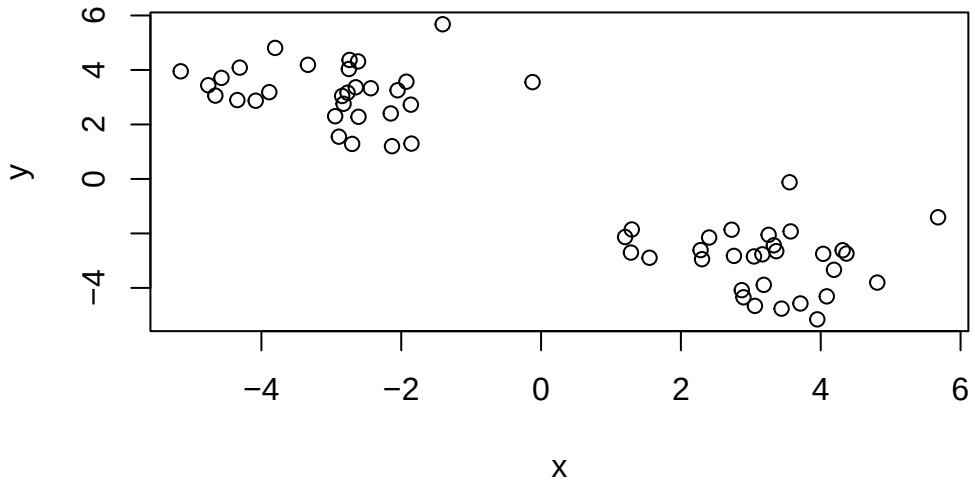
```
 [1]  3.0589206  2.7258080  3.0450541  4.3138325  2.8710780  4.0353594
 [7]  1.2855013  4.1894176  5.6784229  2.2815882  1.2018482  4.3679754
[13]  3.9508892  3.5700212  1.2973875  3.2549886  3.1657508  2.7588144
[19]  3.1854772  3.7094600  2.3022692  4.0861912  2.4041619  3.3639805
[25]  3.4396690  2.8951672  1.5509700  3.5543528  4.8086686  3.3292985
[31] -2.4351174 -3.8037205 -0.1217635 -2.8923754 -4.3444715 -4.7603526
[37] -2.6504771 -2.1498431 -4.3097610 -2.9450982 -4.5711247 -3.8874150
[43] -2.8250410 -2.7677699 -2.0522816 -1.8538929 -1.9265929 -5.1540674
[49] -2.7390719 -2.1320820 -2.6112930 -1.4073633 -3.3349944 -2.7024823
[55] -2.7490729 -4.0814757 -2.6176603 -2.8448669 -1.8626499 -4.6591038
```

```
#flips order of the code
x <- cbind(x=tmp, y=rev(tmp))
head(x)
```

```
            x         y
[1,] 3.058921 -4.659104
[2,] 2.725808 -1.862650
[3,] 3.045054 -2.844867
[4,] 4.313832 -2.617660
[5,] 2.871078 -4.081476
[6,] 4.035359 -2.749073
```

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

```
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 -2.973109  3.189411
2  3.189411 -2.973109

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] 69.14185 69.14185
 (between_SS / total_SS =  89.2 %)

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] 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
```

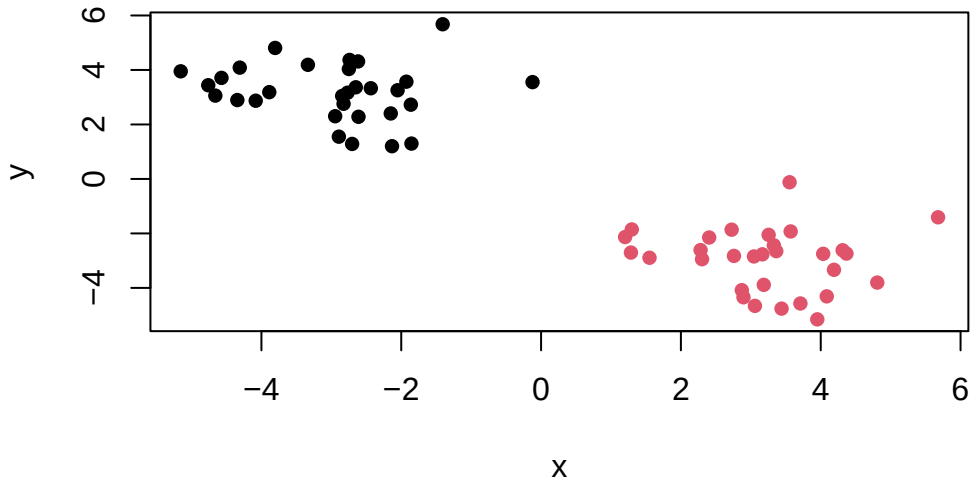
Q3. Cluster centers?

```
k$centers
```

```
          x         y
1 -2.973109  3.189411
2  3.189411 -2.973109
```

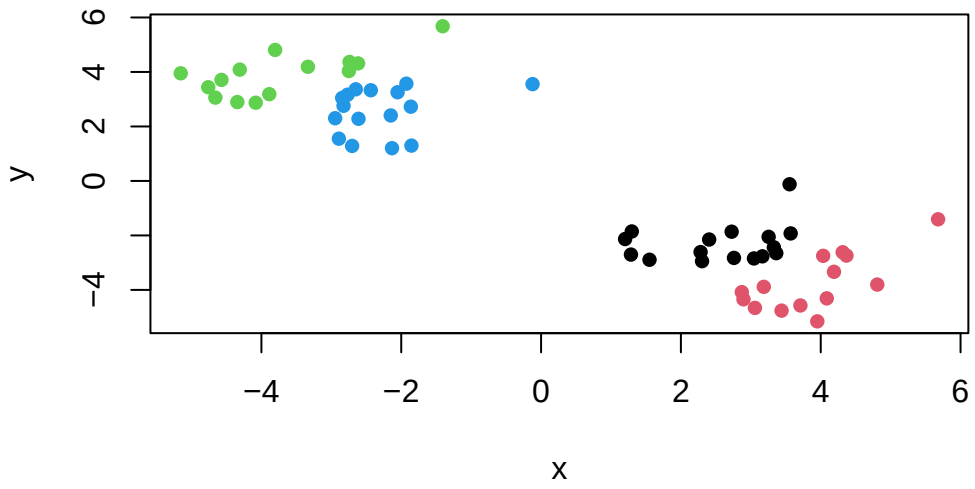
Q4. Plot my clustering results (with base R)

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



Q5. Cluster the data again with kmeans() into 4 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 it is 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

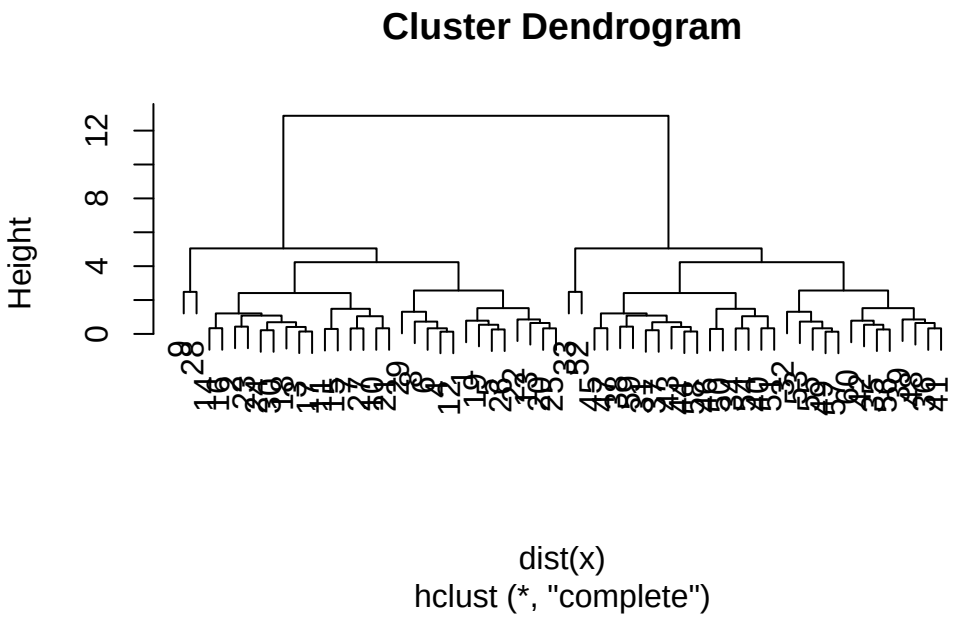
The main function in base R is called `hclust()`. You have to pass it in a "distance matrix" not just your input data

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

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

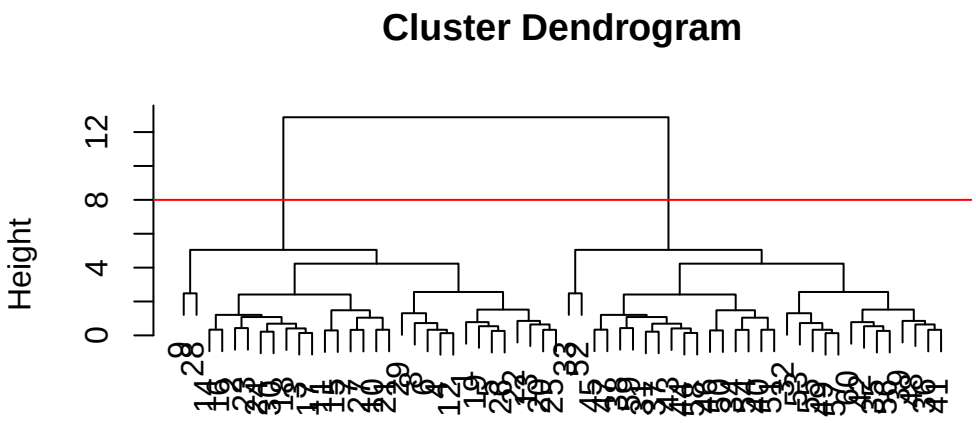
```
Call:
hclust(d = dist(x))

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

```
plot(hc)
```



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

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



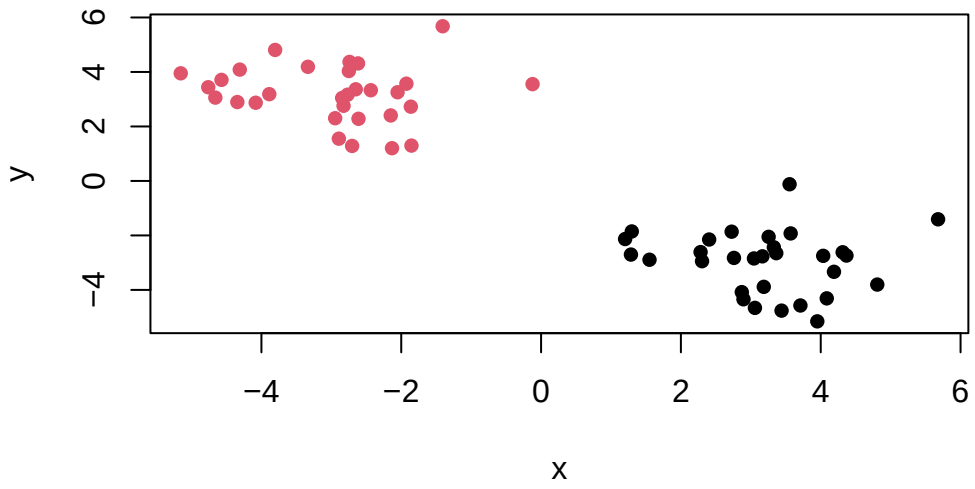

```
grps <- cutree(hc, h=8)
```

```
table(grps)
```

```
grps
 1  2
30 30
```

Q6. Plot our hclust results

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



#Principle 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

```
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?

```
dim(x)
```

```
[1] 17  5
```

```
# 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
```

```
#this removes the first column
```

```
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

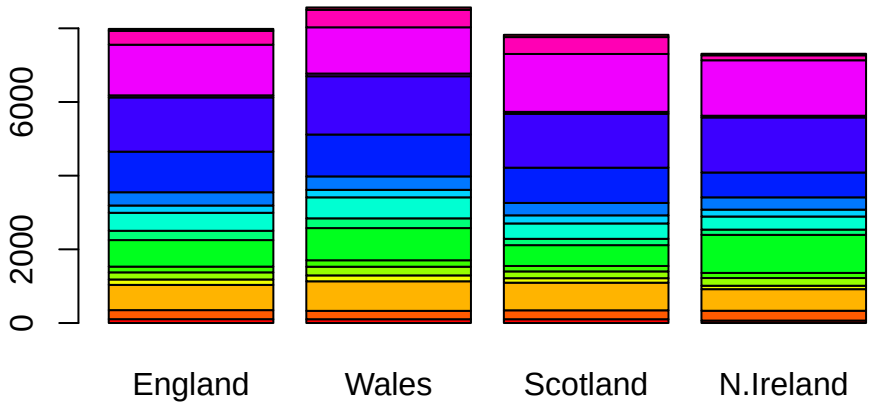
> Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

I prefer the second approach using row.names. It is more simplied and does not affect the code as you run it multiple times.

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

By changing the beside argument to False results in the following plot:

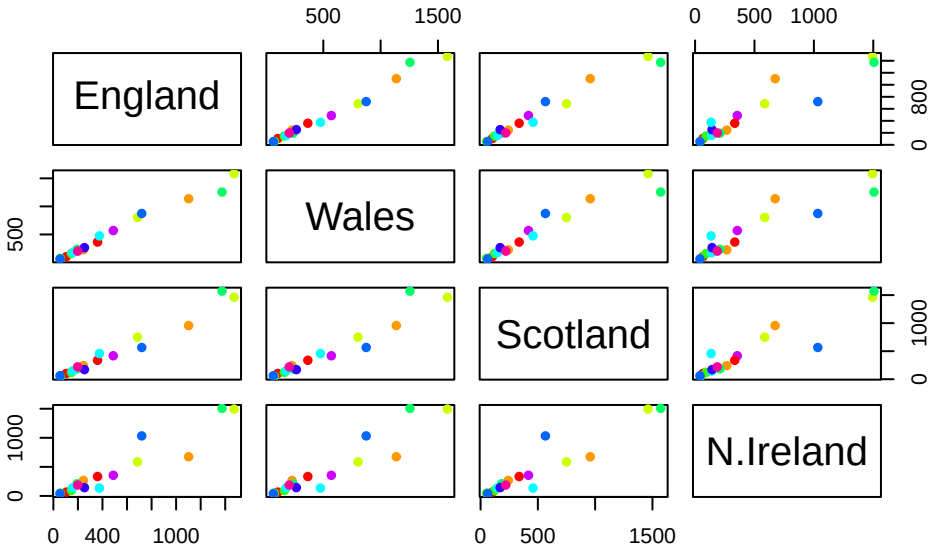
```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



If beside argument is FALSE, the columns of height are portrayed as stacked bars. If it is TRUE, the columns are portrayed as juxtaposed bars.

> 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)
```



A given point that lies on the diagonal for a given plot indicates that consumption of a particular food matches between countries.

##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
```

```
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
```

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

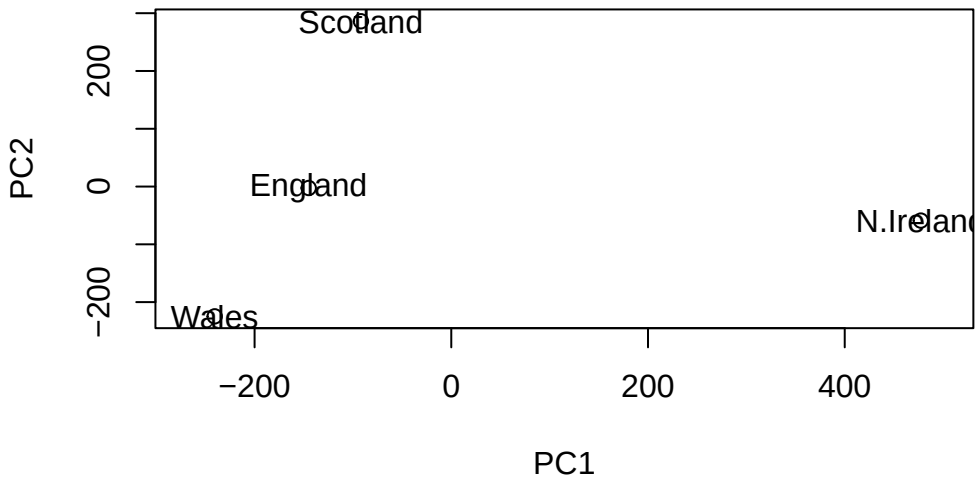
The plots show more off diagonal points when N. Ireland is compared to other countires of the UK

```
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
```

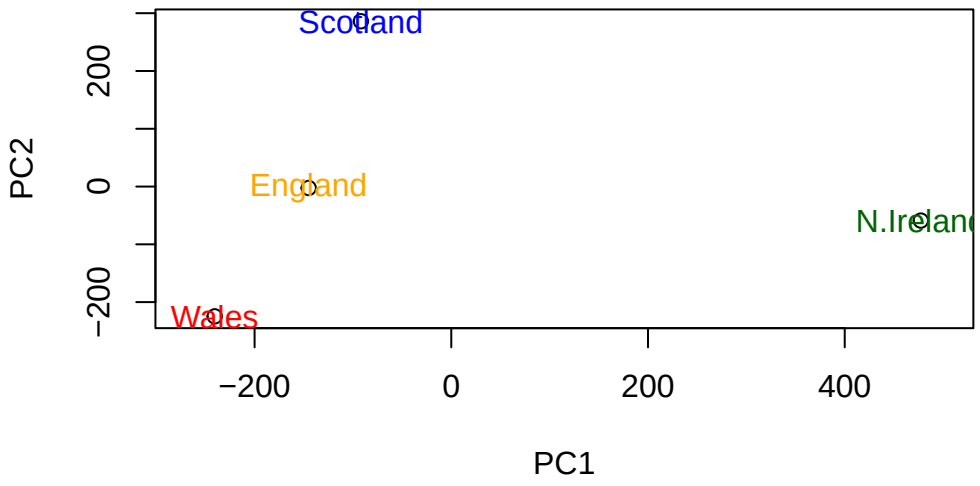
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

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



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

```
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
```

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

PC2 tells us fresh potatoes and soft drinks feature prominently. PC2 mainly tells us the second most variance in the data set and that potatoes and soft drinks varied the second most between the countries.

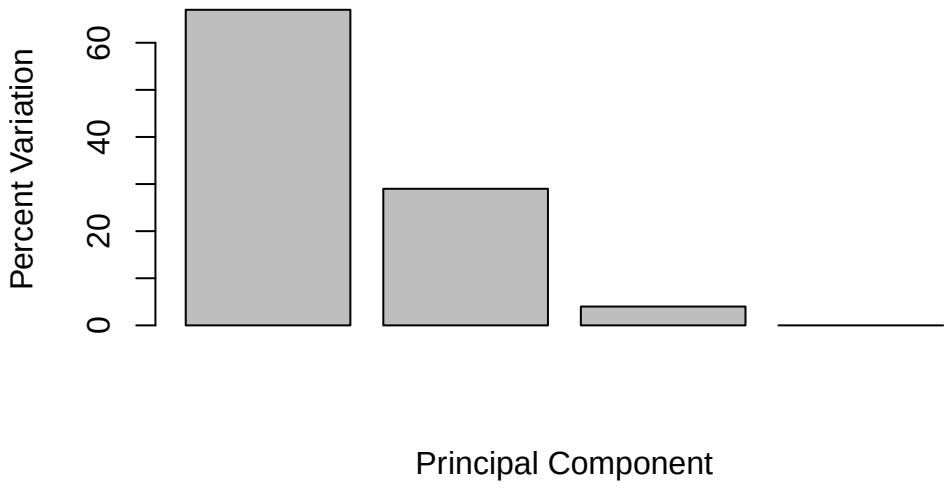
```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

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

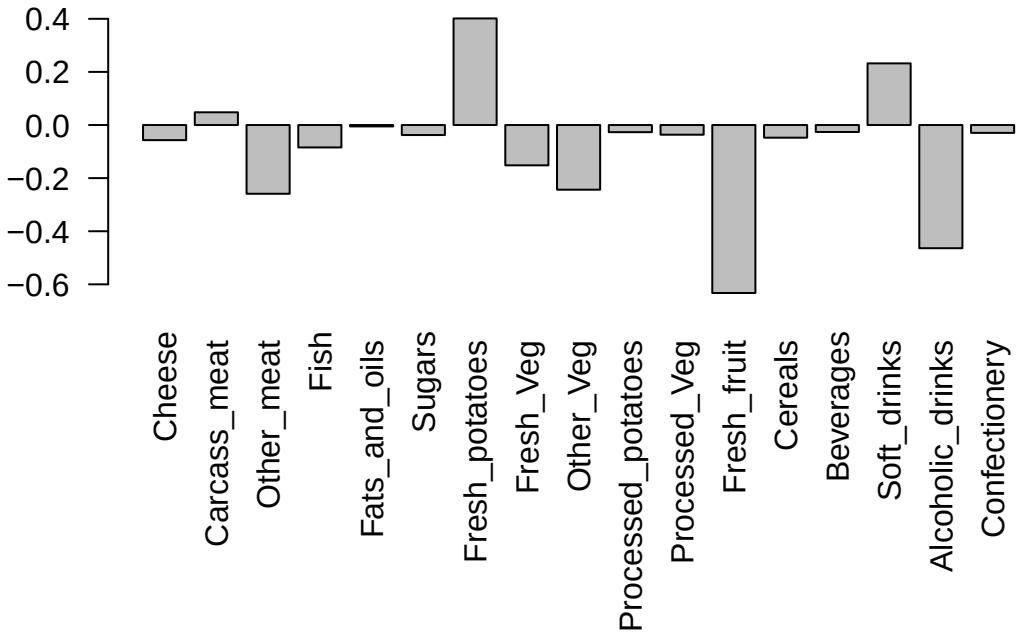
```
## or the second row here...
z <- summary(pca)
z$importance
```

```
                            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
```

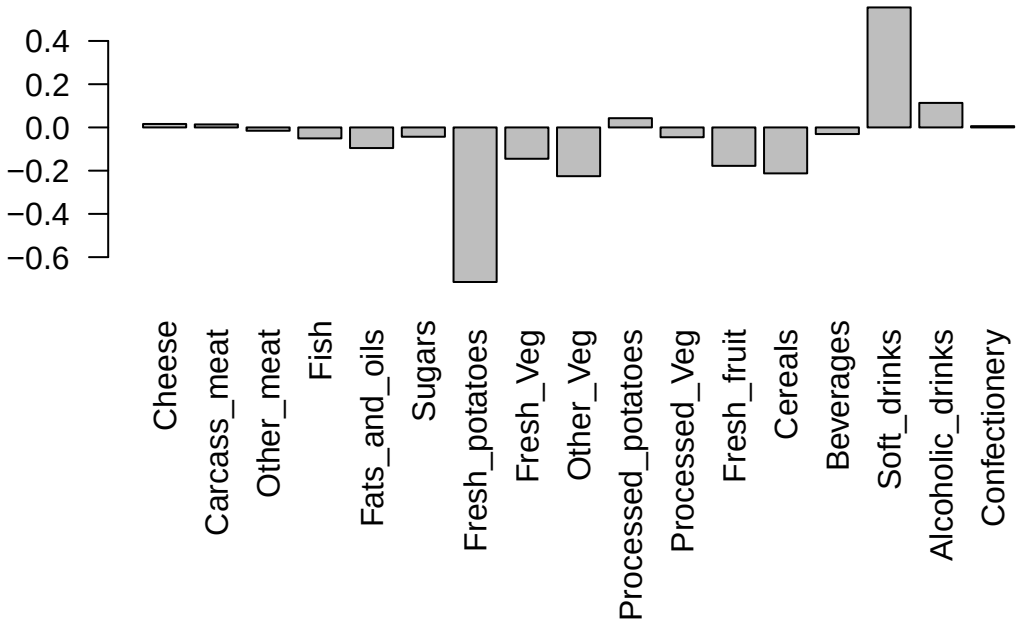
```
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```




```
## 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 )
```




```r
#PC2
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