Class 07: Machine Learning 1

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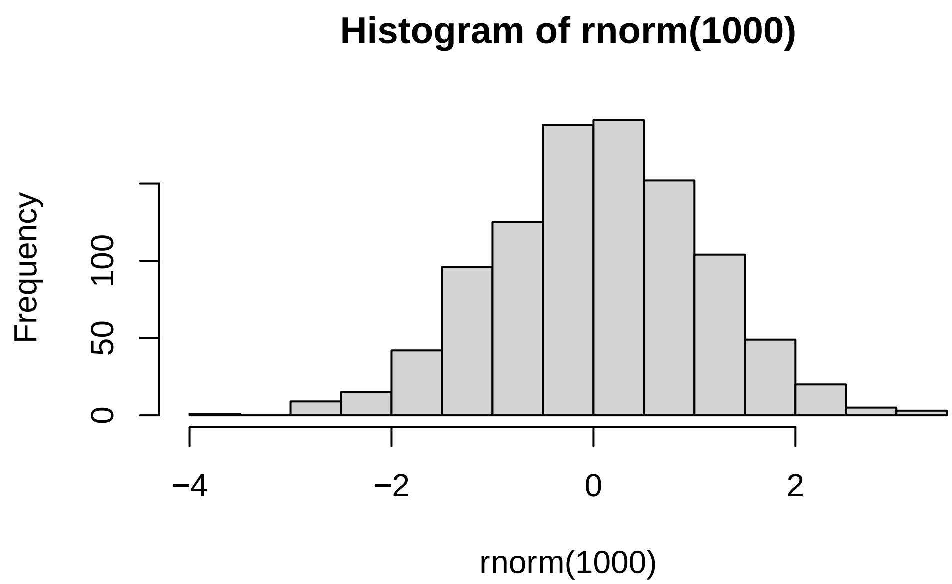
Today we wll begin our exploration of some "classical" machine learning approaches. We'll start with clustering:

Let's first make up some data cluster where we know what the answer should be

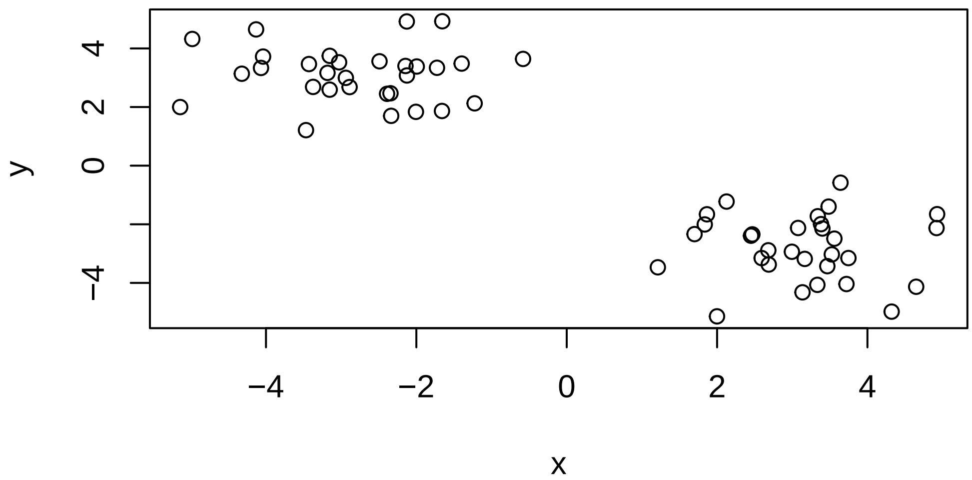
```
hist(rnorm(1000))
```




```
x <- c(rnorm(30, -3), rnorm(30, 3))
y <- rev(x)
z <- cbind(x,y)
```

Let's plot z using `plot()`

```r
plot(z)
```



The main function in "base" R for k-means clustering is called `kmeans()`

```r
k <- kmeans(z,centers = 2)
k
```

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

Cluster means:
          x         y
1 -2.782877  3.113843
2  3.113843 -2.782877

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] 60.3723 60.3723
 (between_SS / total_SS =  89.6 %)
```

```
Available components:

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

Q. How big are the clusters (i.e. their size)?

```r
k$size
```

```
[1] 30 30
```

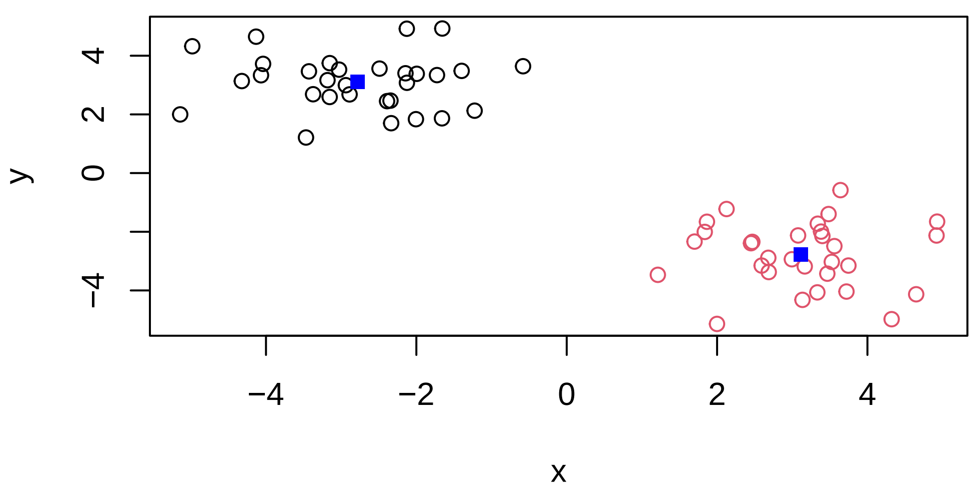
Q. What clusteres do my data points reside in?

```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
```

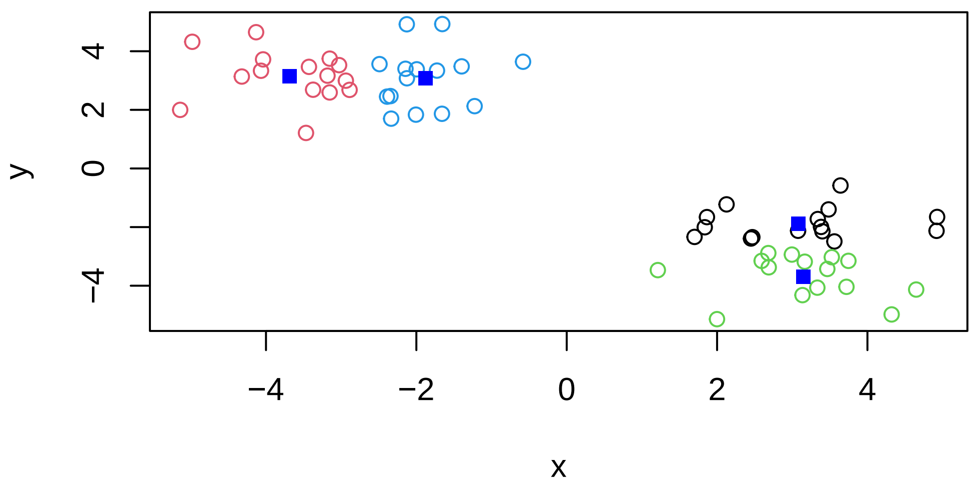
Q. Make a plot of our data of colored by cluster assignment - make a result figure

```r
plot(z, col = k$cluster)
points(k$centers, col = "blue", pch = 15)
```



Q. Clustering with k-means into 4 clusters and plot your results as above

```
k4 <- kmeans(z, centers = 4)
plot(z, col = k4$cluster)
points(k4$centers, col = "blue", pch = 15)
```

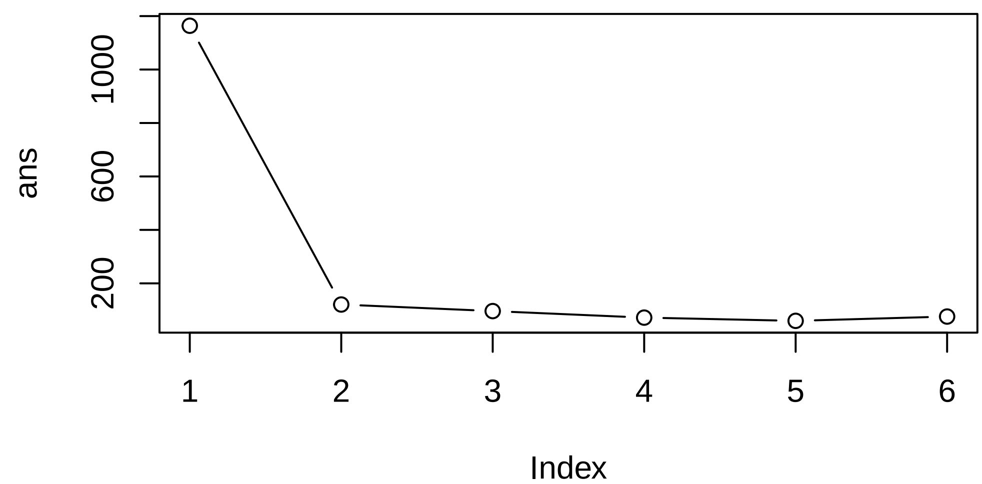


Run K-means with centers (values of k) equal to 1 to 6

```
ans <- NULL
for(i in 1:6){
  ans <- c(ans, kmeans(z, centers = i)$tot.withinss)
}
ans
```

```
[1] 1163.88386  120.74459   96.24586   71.74712   59.64421   75.72588
```

```
plot(ans, typ = "b")
```



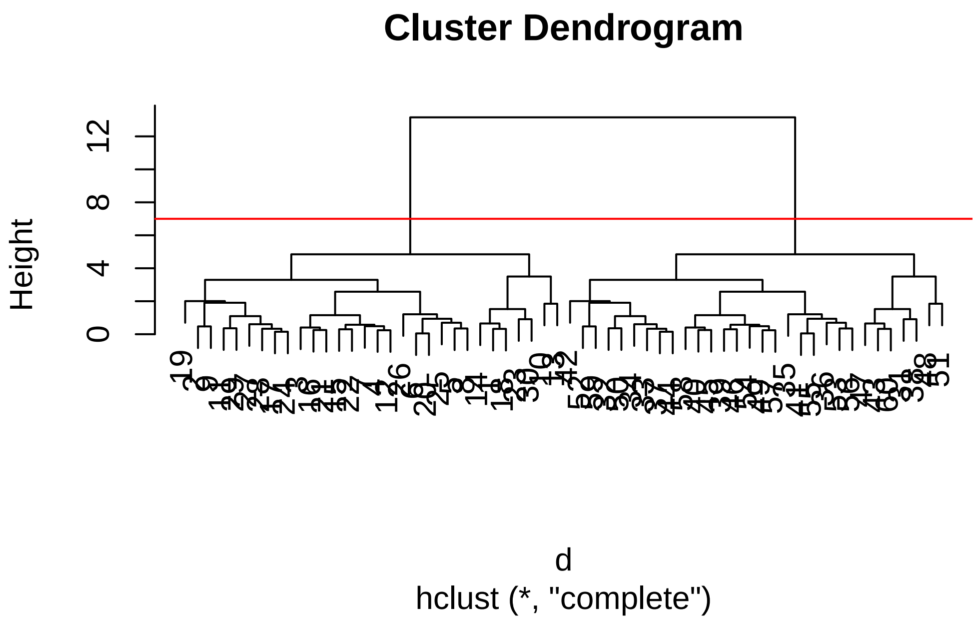
Hierarchial clustering

The main function in "base" R for this in called `hclust()`

```
d <- dist(z)
hc <- hclust(d)
hc
```

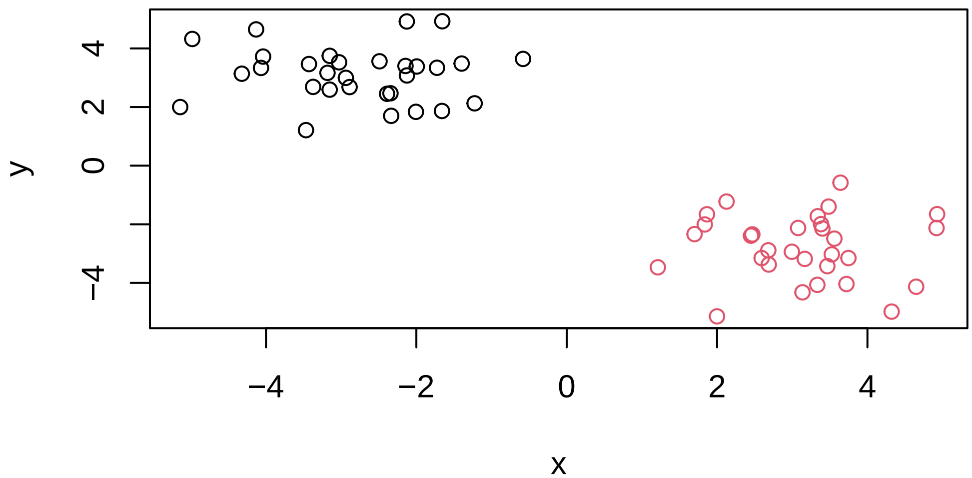
```
Call:
hclust(d = d)

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

```
plot(hc)
abline(h=7, col = "red")
```



To obtain clusters from hour `hclust` result object **hc** we "cut the tree to yield different sub branches. For this we use the `cutree()` function

```
grps <- cutree(hc, h=7)
plot(z, col= grps)
```



Principal component Analysis (PCA)

```
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
```

There are 17 rows and 5 columns

> 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?

```
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
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
```

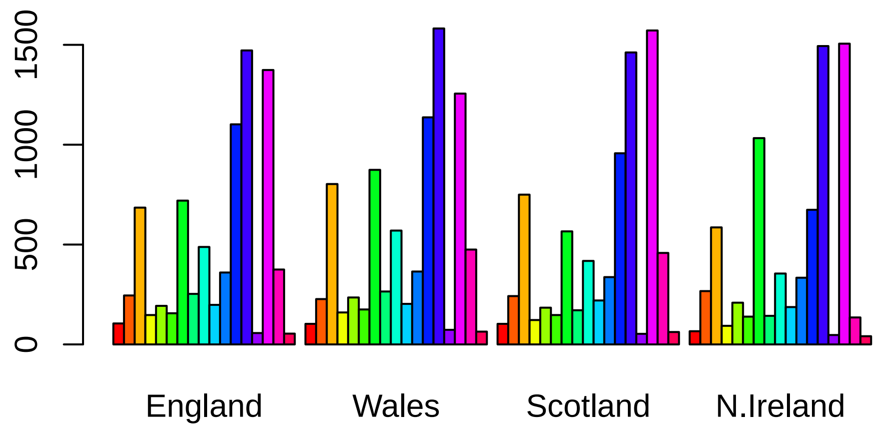
The second method with `read.csv()` is more robust. When you run the first method, i.e. indexing, the index changes everytime and we lose one column until it run out of the dimension of the df.

Spotting major differences and trends

```r
rainbow(nrow(x))
```

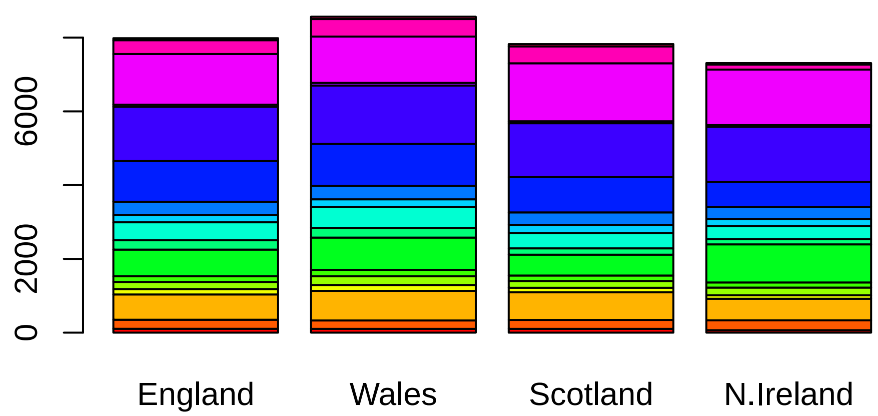
```
 [1] "#FF0000" "#FF5A00" "#FFB400" "#F0FF00" "#96FF00" "#3CFF00" "#00FF1E"
 [8] "#00FF78" "#00FFD2" "#00D2FF" "#0078FF" "#001EFF" "#3C00FF" "#9600FF"
[15] "#F000FF" "#FF00B4" "#FF005A"
```

```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=FALSE, col=rainbow(nrow(x)))
```



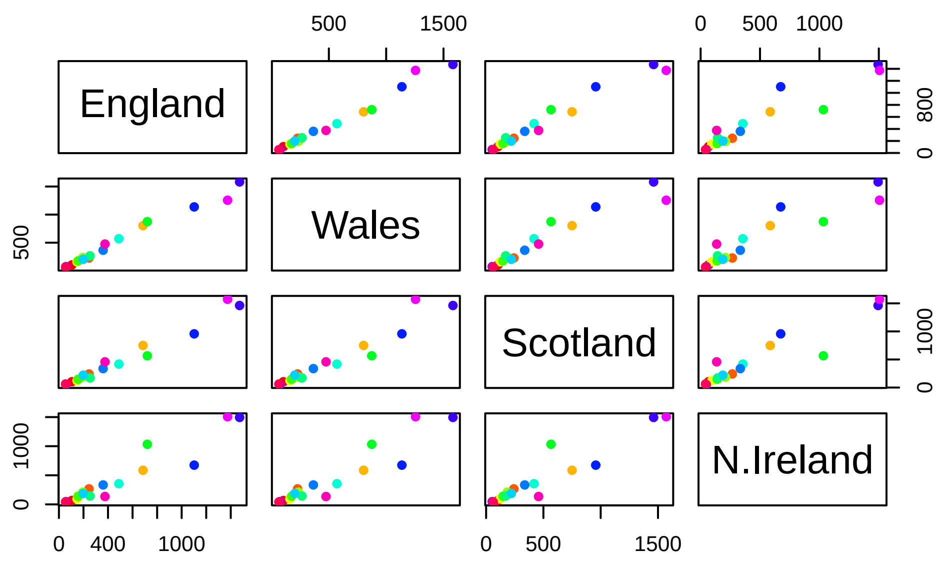
By setting the `beside = FALSE` we can make the stacked barplot

> Q4: Changing what optional argument in the above ggplot() code results in a stacked barplot figure?

Paris plots and heatmaps

Scatterplot matrices (aka "paris plots") can be useful for the relatively small datasets like this one.

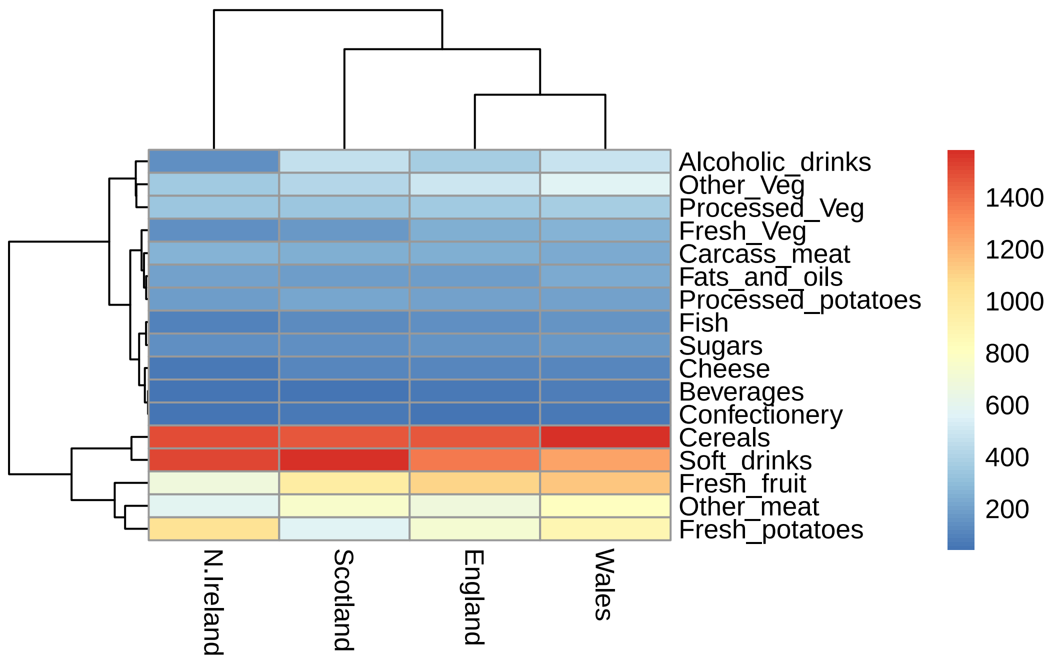
```
pairs(x, col=rainbow(nrow(x)), pch=16)
```



> Q5: We can use the pairs() function to generate all pairwise plots for our countries. 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 x and y axes are different countries. For example, England on x axis and Wales on y axis. The points represent different food. So the plots are showing the amount of food consumed in one country vs in another country. If a point lies on the diagnal then it means the quantity of this food consumed in both countries is the same.

```r
library(pheatmap)
pheatmap( as.matrix(x) )
```



> Q6. Based on the pairs and heatmap figures, which countries cluster together and what does this suggest about their food consumption patterns? Can you easily tell what the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

It looks like Wales and England are quite similar in their consumption of these foods, It is still quite difficult to tell what is going on in the dataset

PCA to the rescue

The main funciton in "base" R for PCA is called `prcomp()`

As we want to do PCA on the food data for the different countries we wil want the foods in the columns

```r
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
```

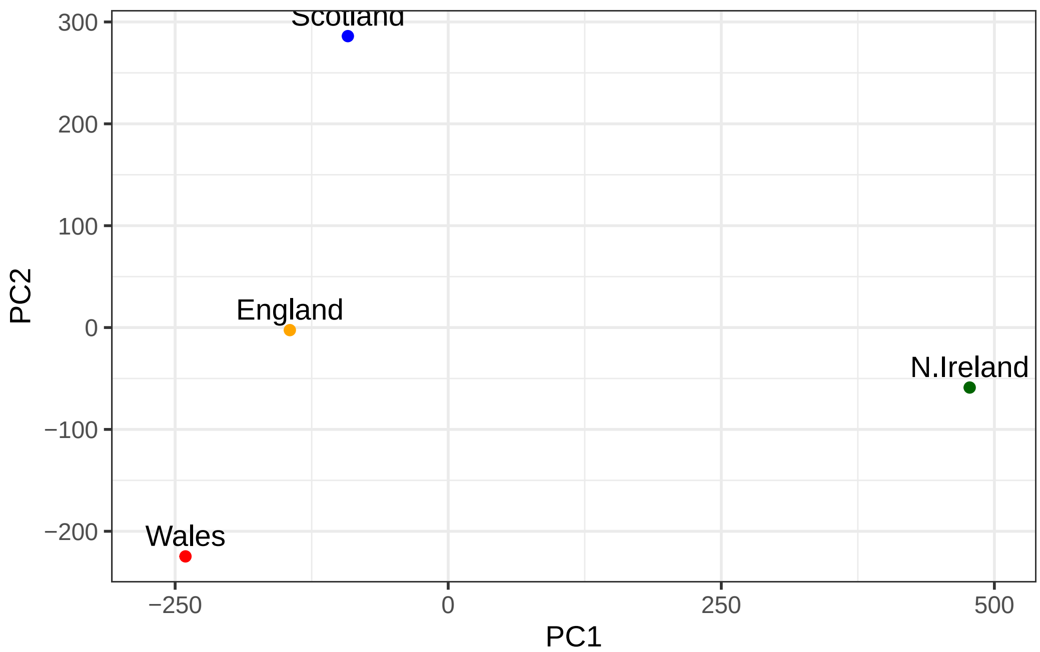
our result object is called `pca` and it has a `$x` component that we will look at first

```
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
```

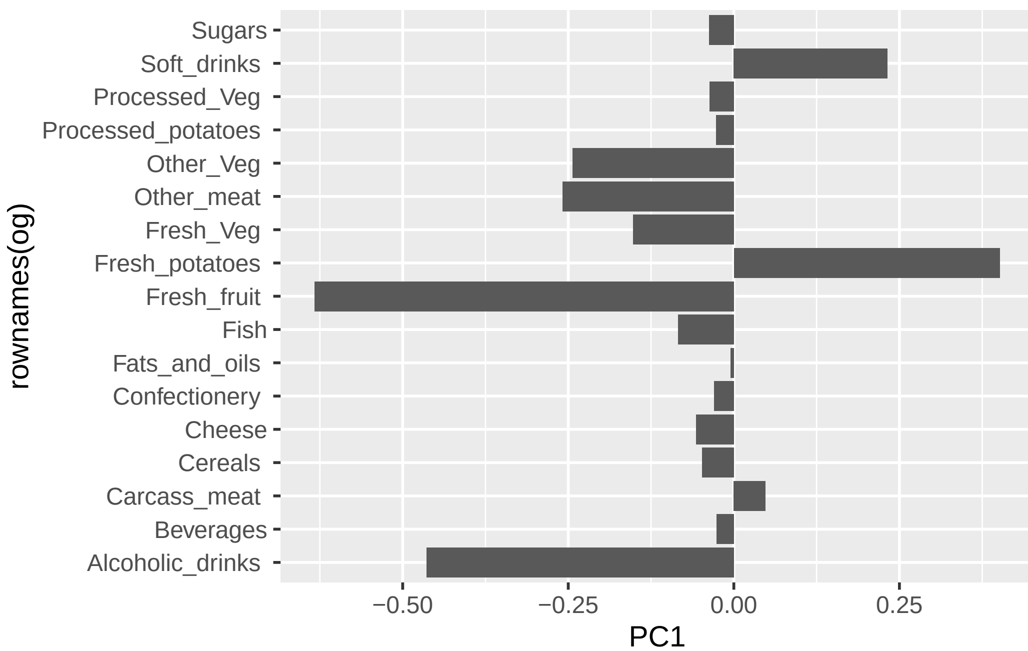
> Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points. Q8. Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

```
library(ggplot2)
cols <- c("orange", "red", "blue", "darkgreen")

ggplot(pca$x) +
  aes(PC1, PC2, label = rownames(pca$x)) +
  geom_point(col = cols) +
  geom_text(vjust = -0.5) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



Another major result out of PCA is the "variable loadings" or `$rotation` that tells us how the original variables (foods) contribute contribute to the PCs (our new axes)

```
og <- pca$rotation
ggplot(og) +
  aes(PC1, rownames (og)) +
  geom_col()
```


Sugars
Soft_drinks
Processed_Veg
Processed_potatoes
Other_Veg
Other_meat
Fresh_Veg
Fresh_potatoes
Fresh_fruit
Fish
Fats_and_oils
Confectionery
Cheese
Cereals
Carcass_meat
Beverages
Alcoholic_drinks
rownames(og)
−0.50
−0.25
0.00
0.25
PC1