Class 7: Machine Learning 1

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

Sample data generation

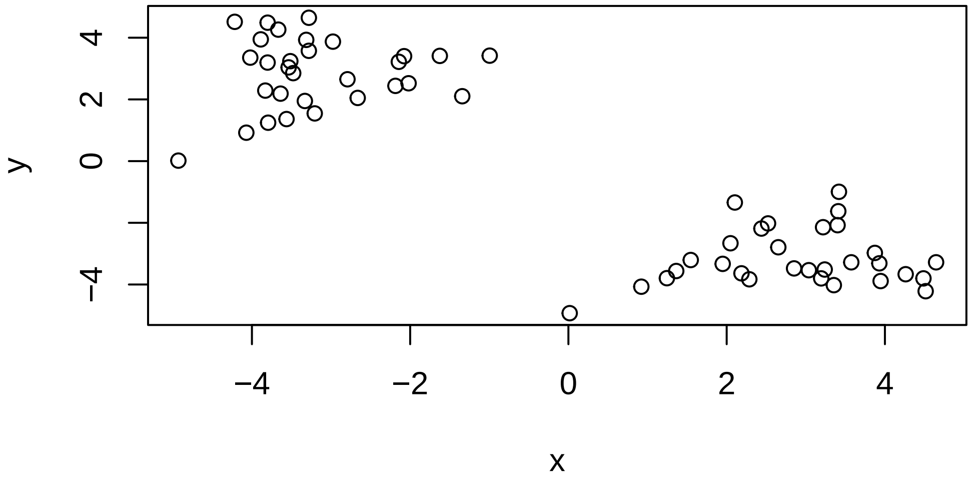
Let's first make up some data to cluster where we know what the answer should be.

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

x <- cbind(x, y)
head(x)
```

```
             x        y
[1,] -3.830939 2.286281
[2,] -3.478330 2.851858
[3,] -3.667056 4.262290
[4,] -2.143311 3.218542
[5,] -3.206095 1.546025
[6,] -3.562809 1.362479
```

A wee peak at x with `plot()`

```
plot(x)
```



K-means clustering

Then, main function in "base" R for K-means clustering is called `kmeans()`.

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

> Q. How big are the clusters?

```
k$size
```

```
[1] 30 30
```

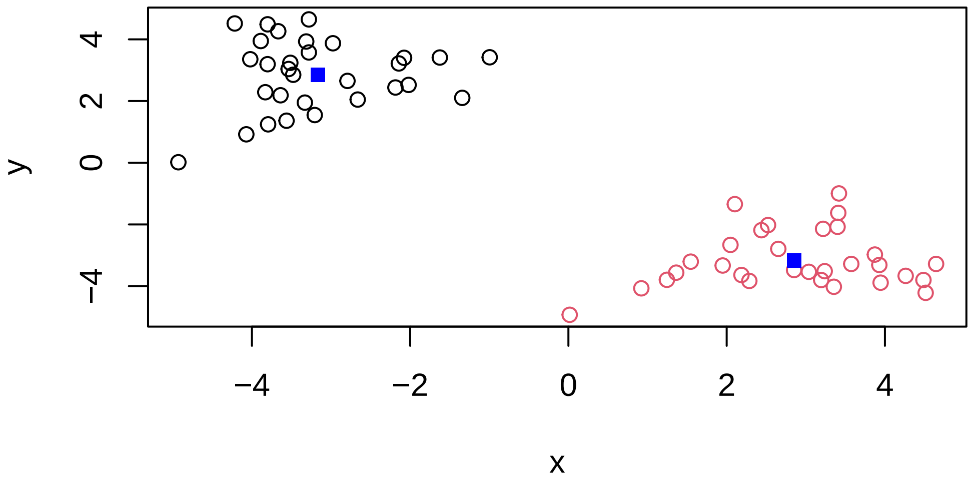
> Q. What clusters do my data points reside in?

```
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 colored by cluster assignment - i.e. Make a result figure

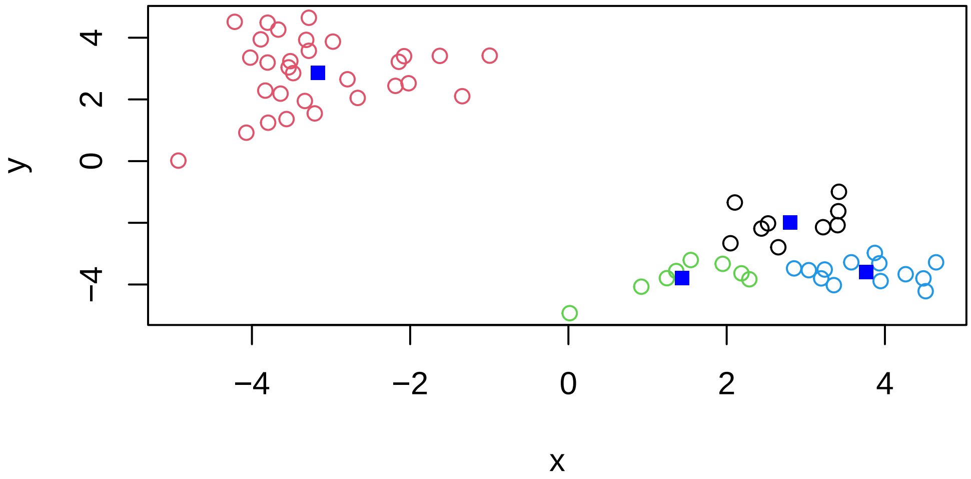
```
plot(x, col = k$cluster) +
points(k$centers, col="blue", pch=15)
```



```
integer(0)
```

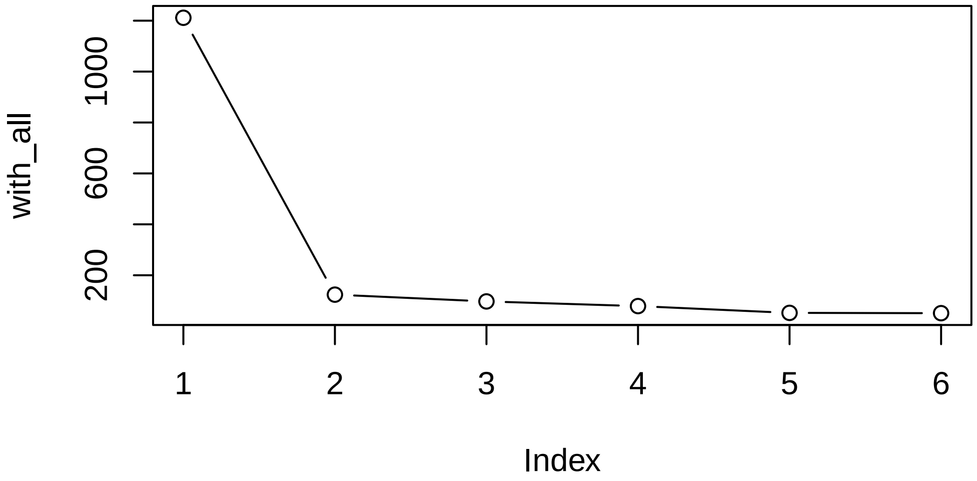
Q. Cluster with k-means into 4 clusters and plot your results as above.

```
k2 <- kmeans(x, centers = 4)
plot(x, col = k2$cluster)
points(k2$centers, col="blue", pch=15)
```



Q. Run k-means with center (i.e., values of k) equal 1 to 6

```
k_all <- 1:6
with_all <- rep(0, length(k_all))

for (k in k_all) {
  km <- kmeans(x, centers = k)
  with_all[k] <- km$tot.withinss
}

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



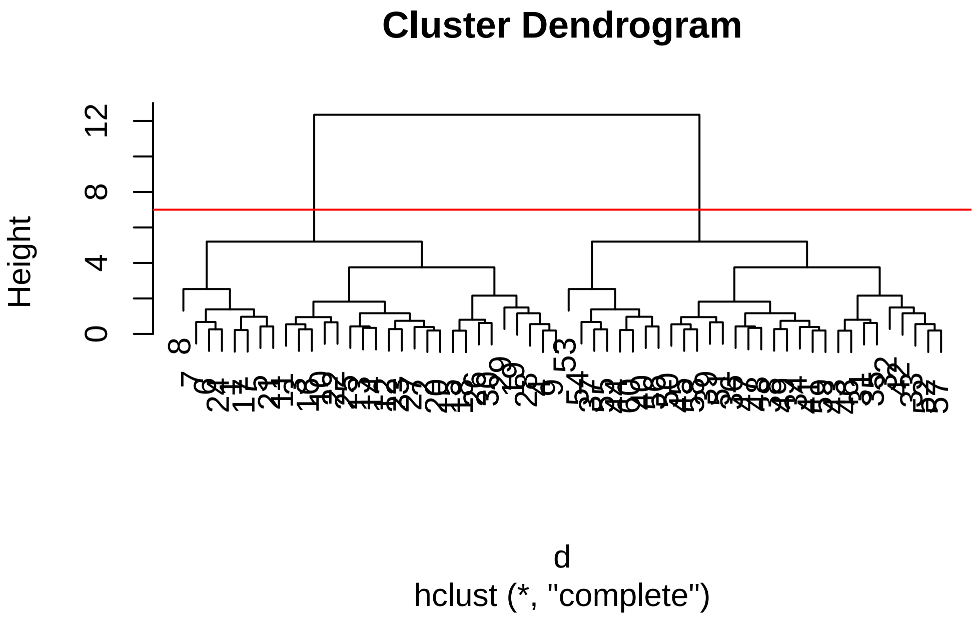
Hierarchical clustering

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

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

```

Call:
hclust(d = d)

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

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

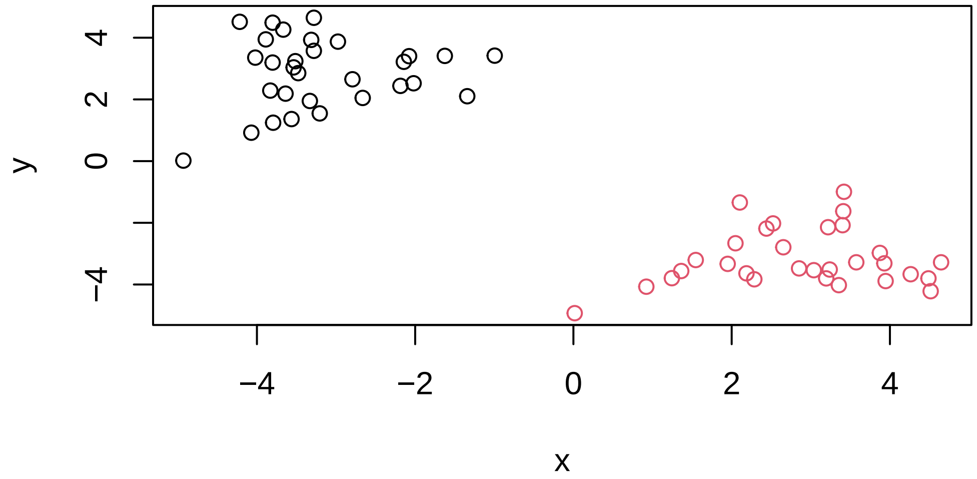


To obtain clusters from our `hiclust` result object **hc** we "cut" the tree to yield different sub branches. For this we use the `cutree()` function

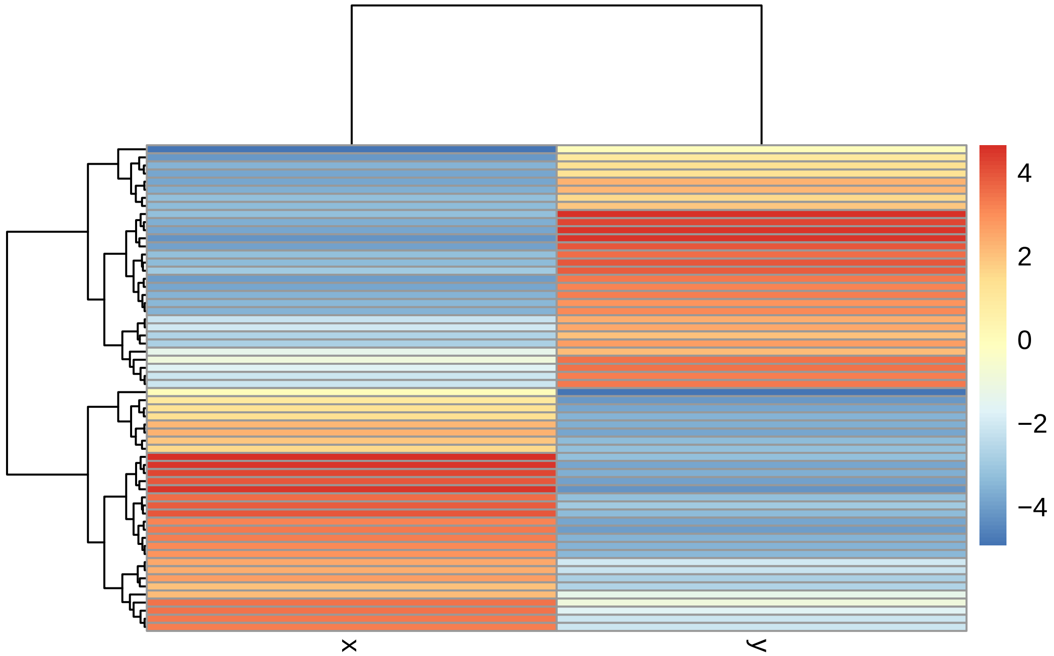
```
grps <- cutree(hc, h=7)
grps
```

```
 [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
```

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



```
library(pheatmap)
pheatmap(x)
```



Principal Component Analysis (PCA)

```
url <- "https://tinyurl.com/UK-foods"
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
```

> 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)
```

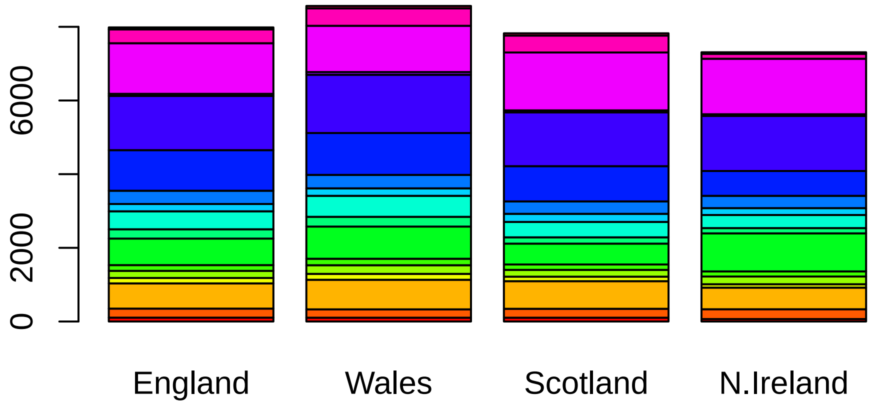
```
[1] 17  4
```

> 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 method (using `read.csv(url, row.names=1)`) would be more robust since if we accidently apply multiple times for the `x <- x[,-1]` code in the first method, it would delete the important row.

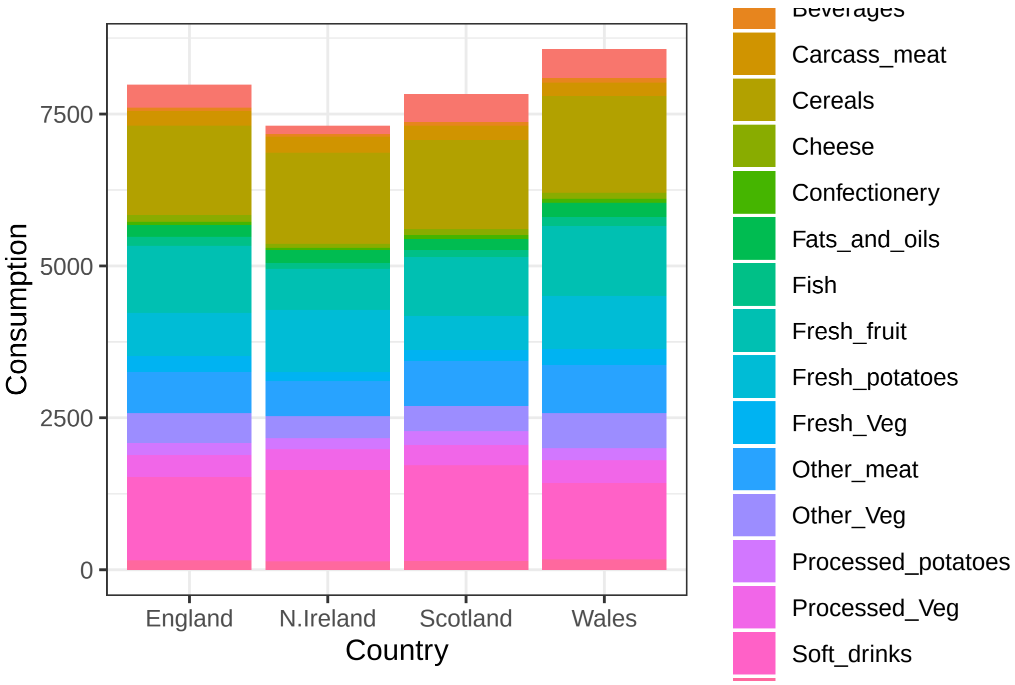
> Q3: Changing what optional argument in the above barplot() function results in the following plot?

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



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

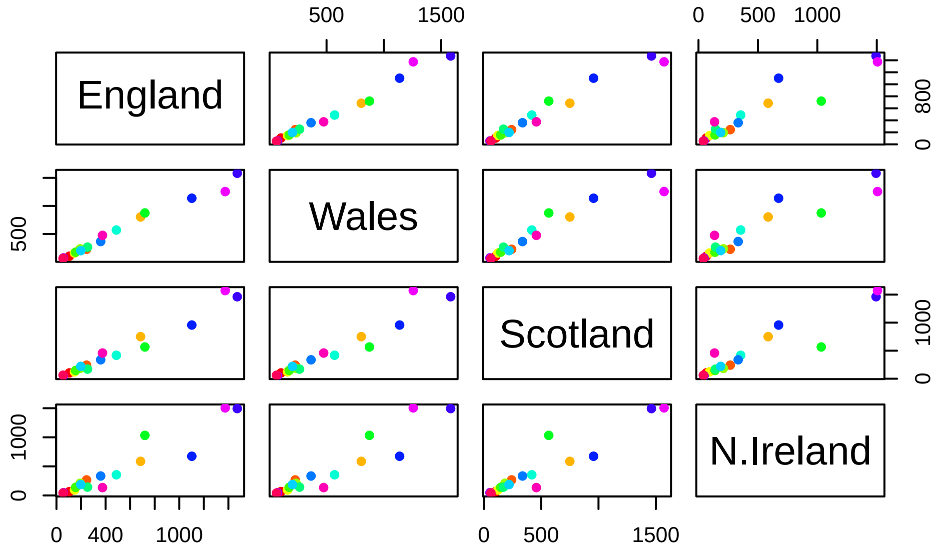
```r
# Create grouped bar plot
library(ggplot2)
library(tidyr)

# Convert data to long format for ggplot with `pivot_longer()`
x_long <- x |>
          tibble::rownames_to_column("Food") |>
          pivot_longer(cols = -Food,
                       names_to = "Country",
                       values_to = "Consumption")
ggplot(x_long) +
  aes(x = Country, y = Consumption, fill = Food) +
  geom_col(position = "stack") +
  theme_bw()
```



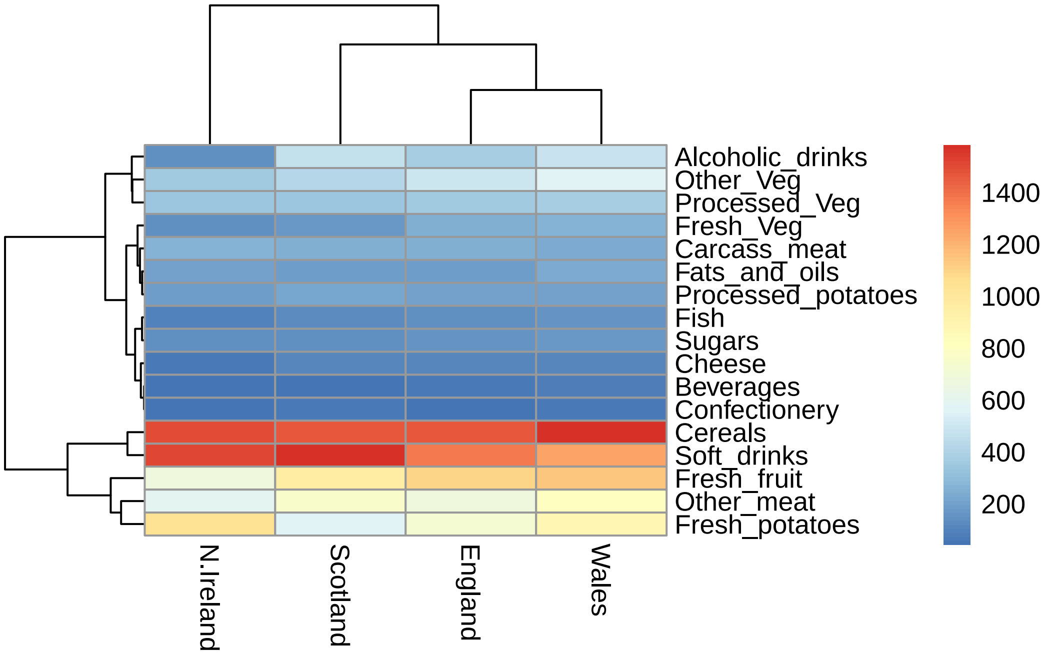
> Q5: We can use the pairs() function to generate all pairwise plots for our countries. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

Scatterplot matrices can be useful for relatively small datasets like this one. Let's have a look (below). It's basically generating all pairwise scatter plots between each country If points lie on the diagonal, it means two countries have similar features (food consumption).

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



```r
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?

Wales, England look quite similar in their consumption of these foods. However, it remains difficult to see how N.Ireland would be different from the other countries due to the high dimensionality.

PCA to the rescue

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

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

```
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
```

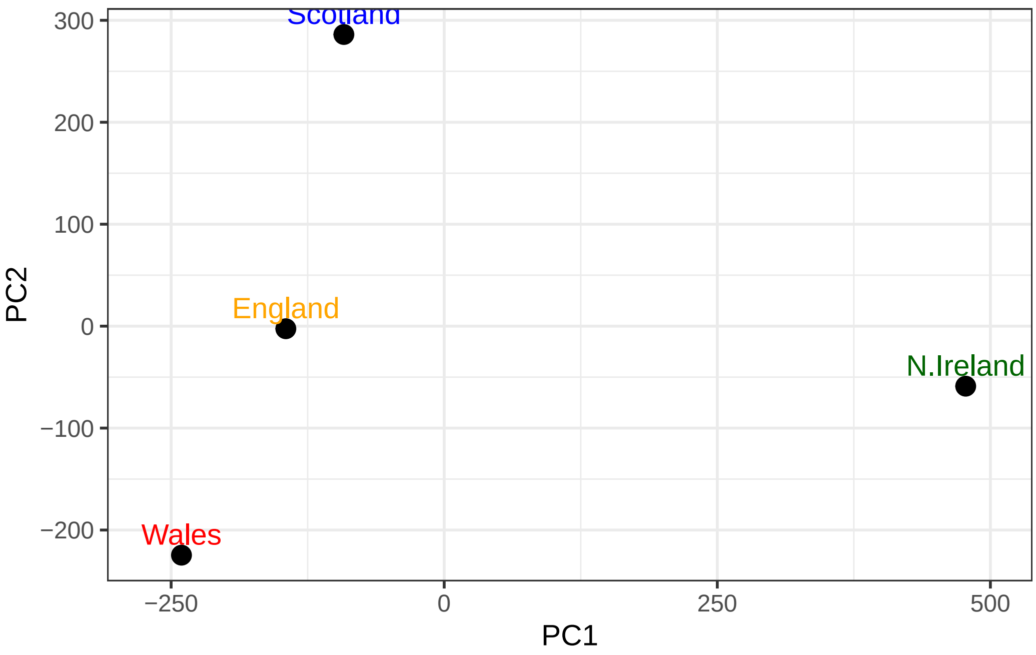
```
pca$x
```

```
                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")

# Create a data frame for plotting
```

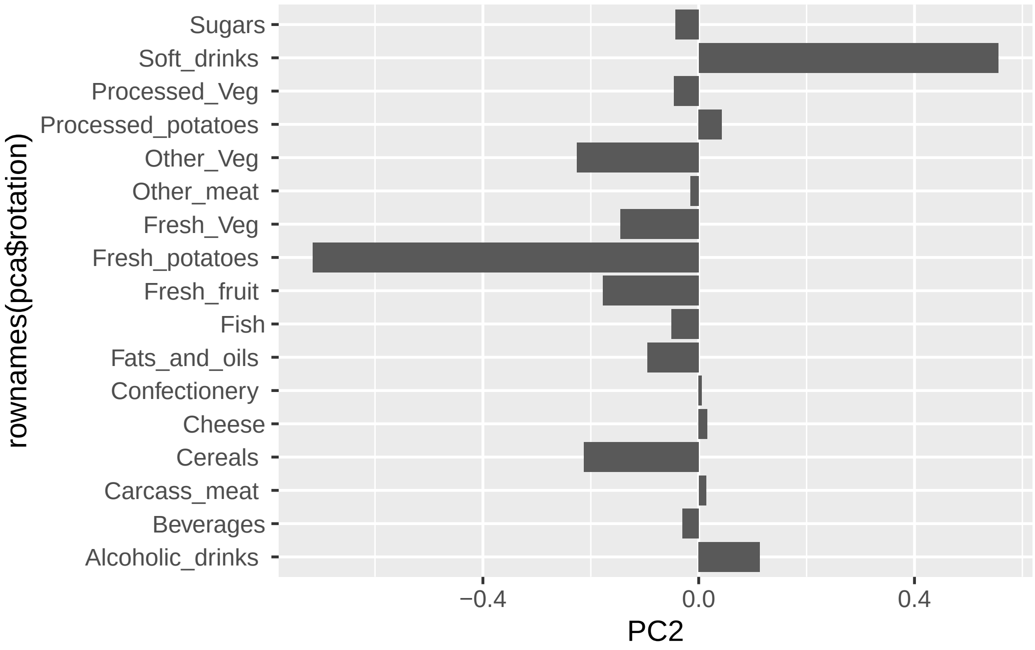
```r
df <- as.data.frame(pca$x)
df$Country <- rownames(df)

# Plot PC1 vs PC2 with ggplot
ggplot(pca$x) +
  aes(x = PC1, y = PC2, label = rownames(pca$x)) +
  geom_point(size = 3) +
  geom_text(vjust = -0.5, col = cols) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



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

Another major result out of PCA is the so-called "variable loadings" or `$rotation` that tells us how the original variables contribute to the new axis. The reuslts show that Soft_drinks have a large and positive contribute to the PC2, and Fresh_potatoes have a large yet negative contribution to the PC2.

```
ggplot(pca$rotation) +
  aes(PC2, rownames(pca$rotation)) +
  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(pca$rotation)
PC2