# Class 7: Machine Learning 1

Gavin Ambrose PID: A18548522

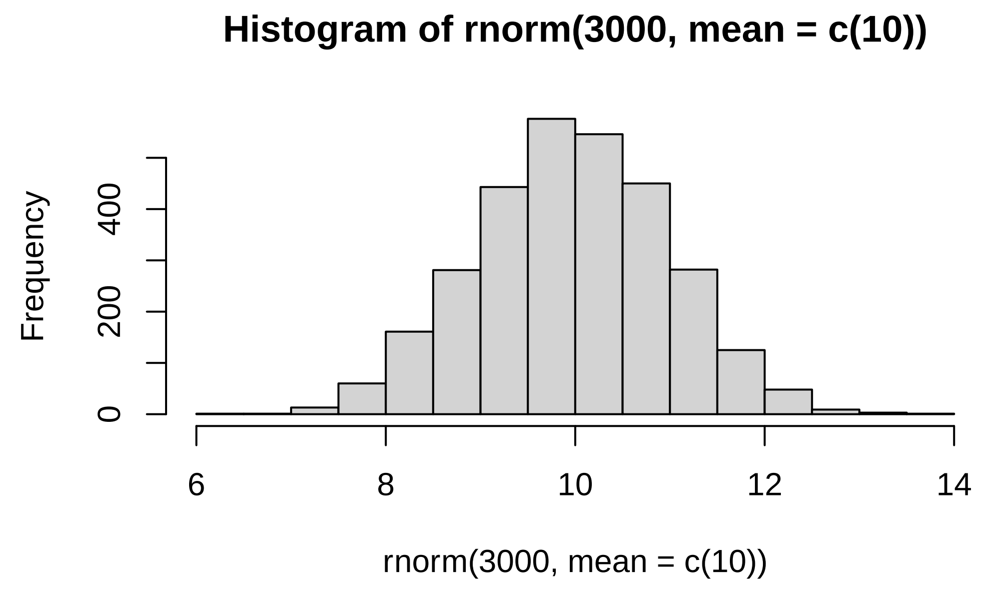
## Table of contents

### Background

Today we will begin our exploration of important machine learning methods with a focus on **clustering** and **dimensionality reduction**.

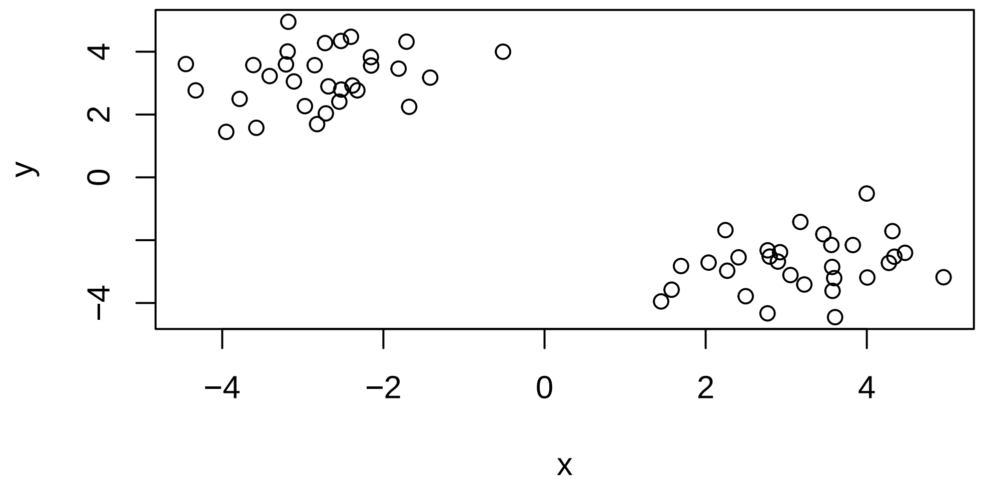
To start testing these methods, let's make up some sample data to cluster, where we know what the answer should be.

```
hist( rnorm(3000, mean = c(10)) )
```



Q. Can you generate 30 numbers centered at +3 and 30 numbers at -3 taken at random from a normal distribution

```
tmp <- c(rnorm(n = 30, mean = 3 ), rnorm(n=30, mean = -3))

x <- cbind(x=tmp, y=rev(tmp))

plot(x)
```



## K-means clustering

The mainn function in "base R" for K-Means clustering is called **`kmeans()`**, let's try it out.

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

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

Cluster means:
          x         y
1  3.178106 -2.757514
2 -2.757514  3.178106

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] 45.54526 45.54526
 (between_SS / total_SS =  92.1 %)
```

```
Available components:

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

Q. What component of your kmeans result object has the cluster centers?

```r
k$centers
```

```
          x         y
1  3.178106 -2.757514
2 -2.757514  3.178106
```

Q. What component of your kmeans result object has the cluster size? (i.e. how many points are in each cluster)?

```r
k$size
```

```
[1] 30 30
```

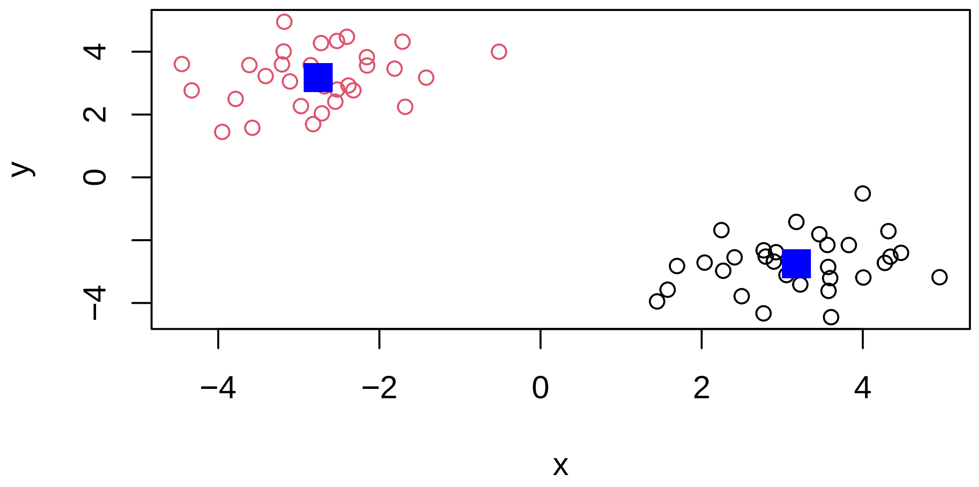
Q. What component of your kmeans result object has the cluster membership vector (i.e. the main clustering result: which points are in which cluster)?

```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
```

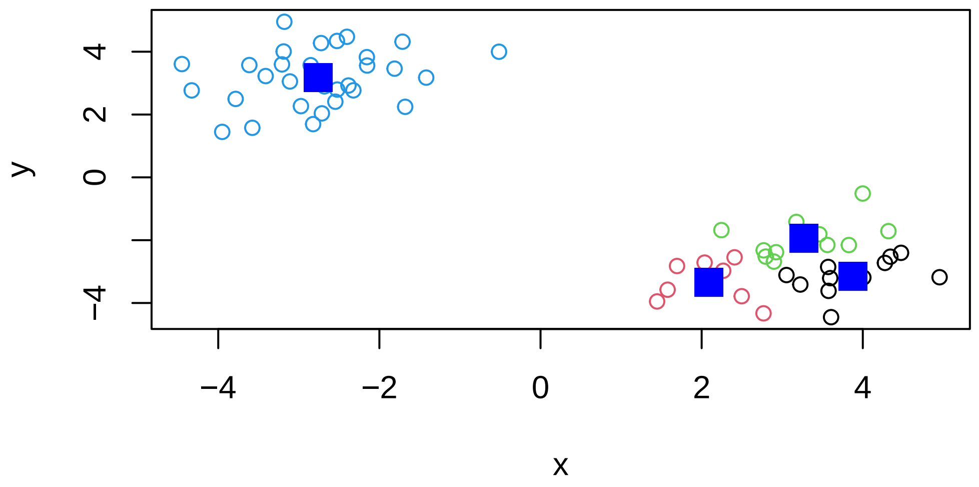
Q. Plot the results of clustering (i.e. our data colored by the clustering result) along with the cluster centers.

```r
plot(x, col = k$cluster)
points(x = k$centers, col = "blue", pch = 15, cex = 2)
```



Q. Can you run `kmeans()` and cluster into 4 clusters and plot the results just like we did with coloring by cluster and the cluster centers shown in blue

```r
k2 <- kmeans(x, centers = 4)

plot(x, col = k2$cluster)
points(x = k2$centers, col = "blue", pch = 15, cex = 2)
```



**Key Points** Kmeans will always return the clustering that we ask for (this is the "K" or "centers" in K-means). It does not find a structure in the data, but imposes a structure on the data!

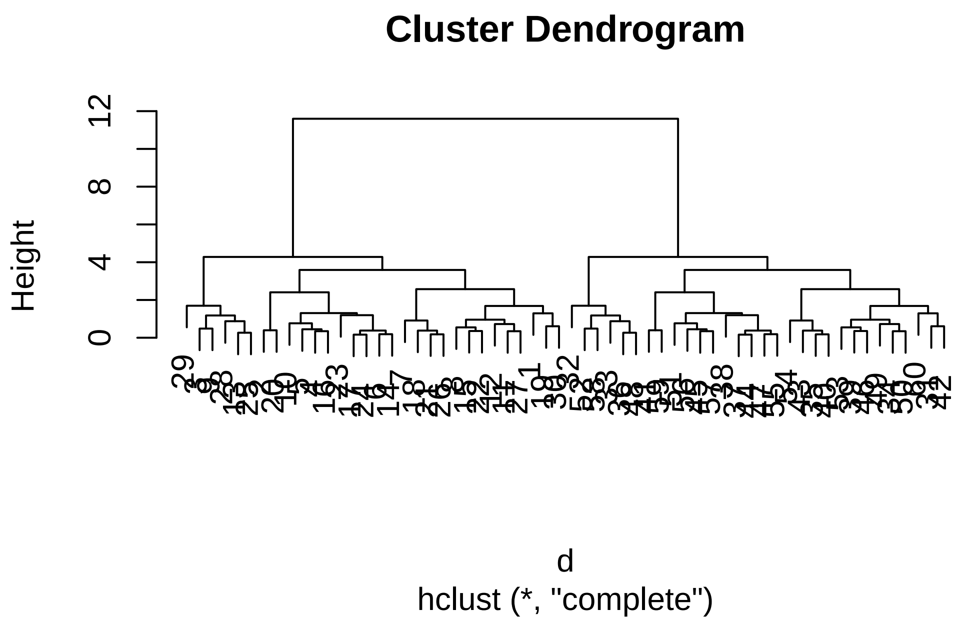
```
k$tot.withinss
```

```
[1] 91.09051
```

## Hierarchical clustering

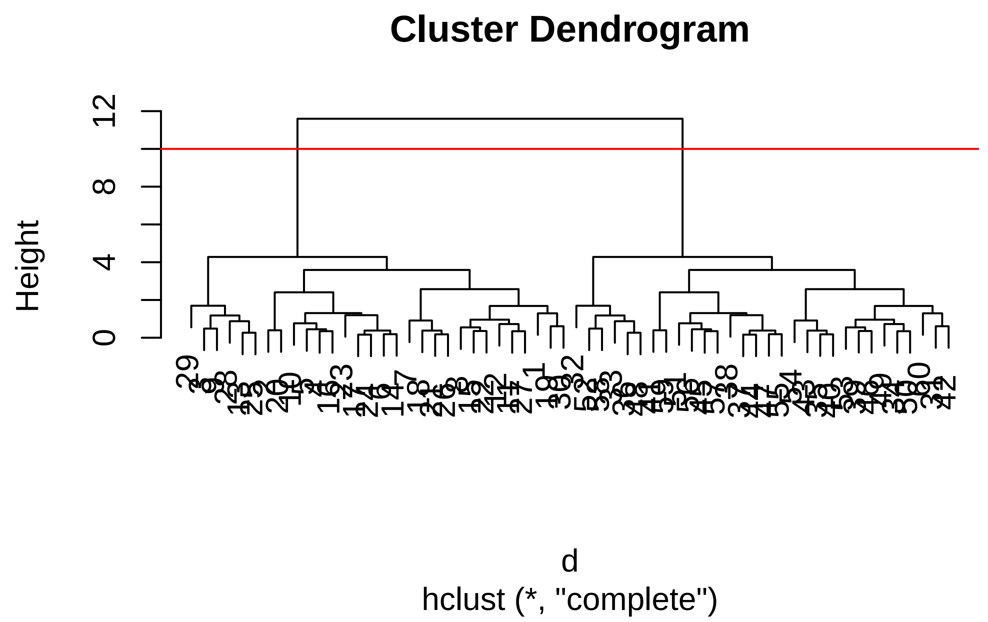
The main function for Hierarchical clustering in base R is called `hclust()`. One of the main differences with respect to the `kmeans()` function is that you cannot just pass your inout data directly into `hclust()`. It needs a "distance matrix" as input. We can get this from lots of places including the `dist()` function.

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



We can "cut the dendrogram or"tree at a given height to yeild our "clusters. For this we use the function `cutree()`.

```r
plot(hc)
abline(h=10, col = "red")
```

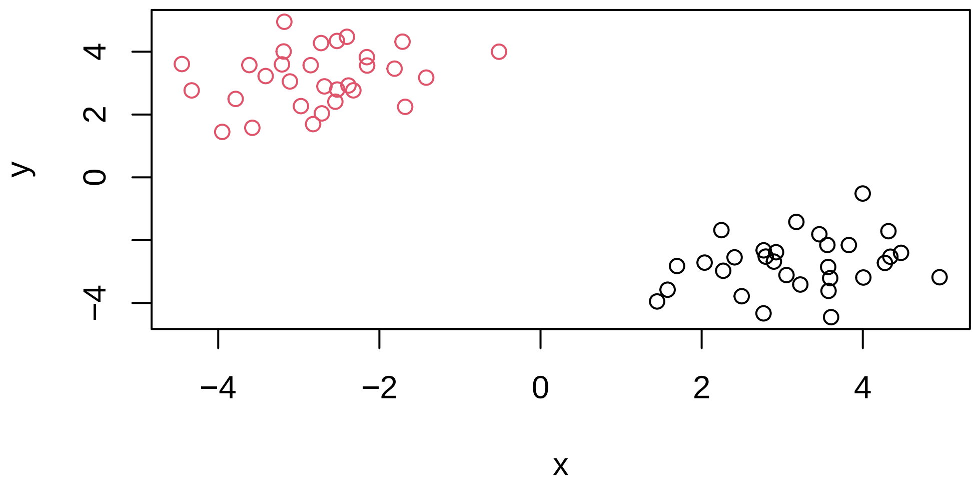


```r
grps <- cutree(hc, h = 10)
grps
```

```
 [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
```

Q. Plot our data `x` colored by the clustering fesults from `hclust()` and `cutree()`

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



## Principal Componet Analysis (PCA)

PCA is a popular dimensionality reduction technique that is widely used in bioinformatics.

### Lab assignment

Let's read the data into R:

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

```
[1] 17  5
```

> Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?
>
> A1. 17 rows and 5 columns

It looks like the row names are not set properly. We can fix this

```r
head(fooddf)
```

```
               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
```

```r
#rownames(fooddf) <- x[,1]
#fooddf2 <- fooddf[,-1]
#head(fooddf2)
#dim(fooddf2)
```

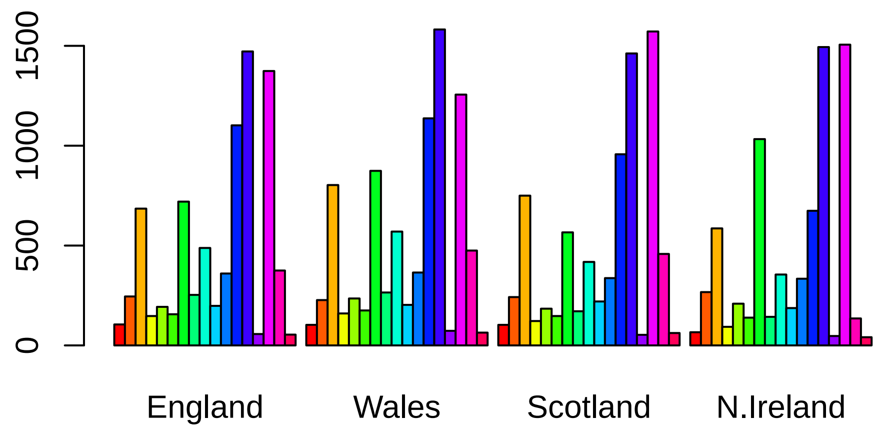
A better way to do this is fix the row names assignment at import time:

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

```
               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
```

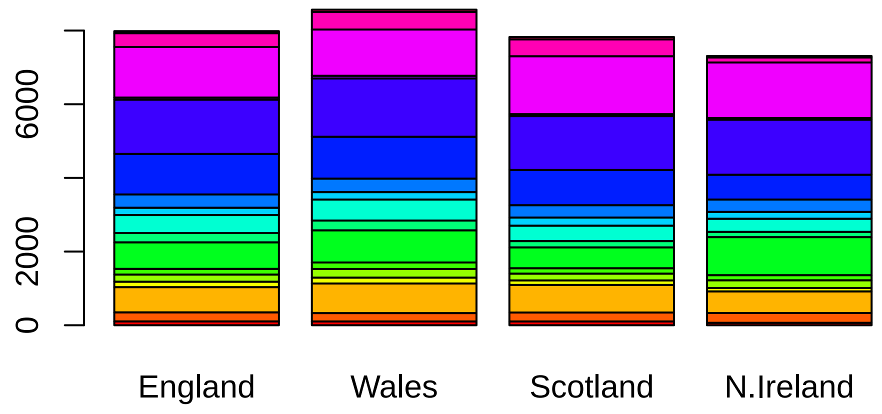
> Q2. Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?
>
> A1. I prefer the `row.names` method because it is less code and preforms the same function in a manner that makes more sense to me. However, the second method is more robust because it allows for repeated use without the unintentional changing of the data frame in a manner that is not beneficial.

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



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

```
barplot(as.matrix(y), col=rainbow(nrow(y)))
```



A3. The `beside=T` is the optional argument results in the above graph.

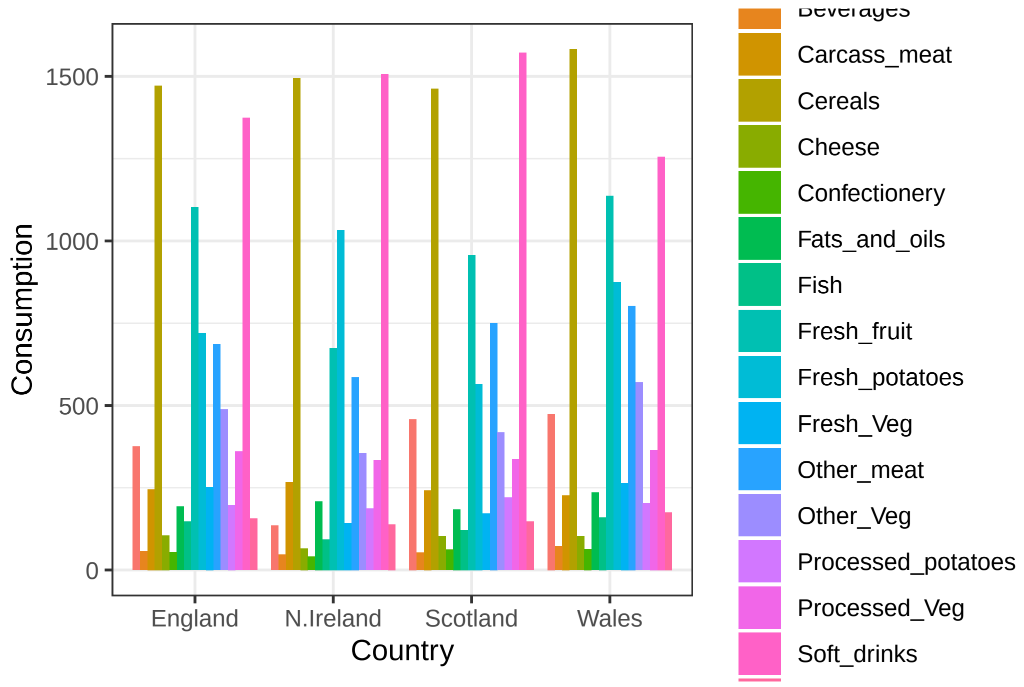
```
library(tidyr)

y_long <- y |>
          tibble::rownames_to_column("Food") |>
          pivot_longer(cols = -Food,
                       names_to = "Country",
                       values_to = "Consumption")

dim(y_long)
```

```
[1] 68  3
```

```
library(ggplot2)
```

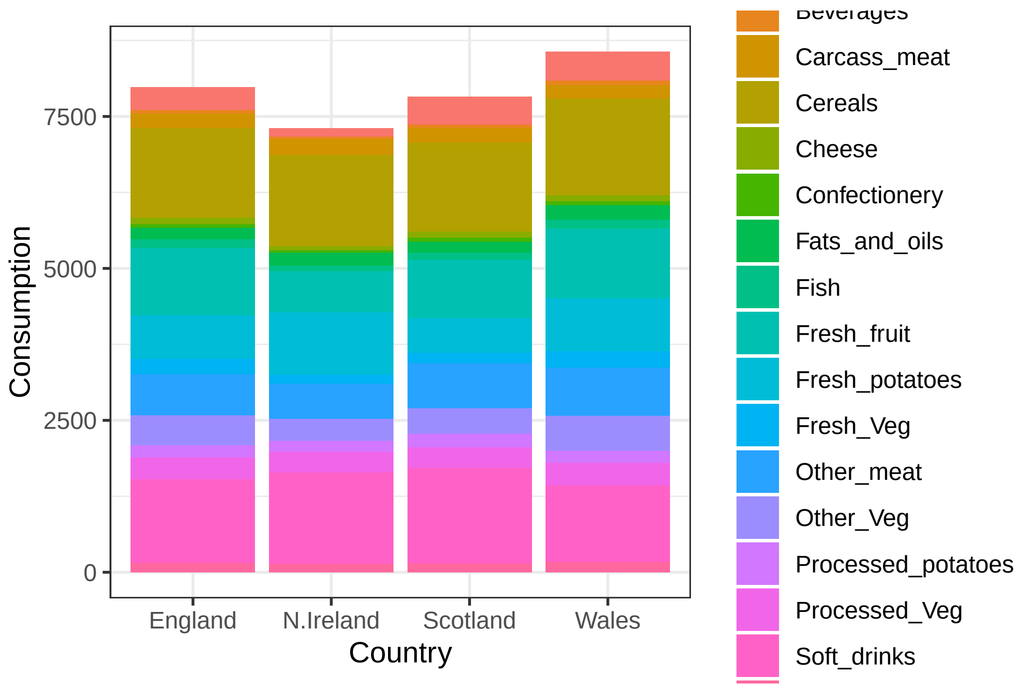
```
Warning: package 'ggplot2' was built under R version 4.4.3
```

```
ggplot(y_long) +
  aes(x = Country, y = Consumption, fill = Food) +
  geom_col(position = "dodge") +
  theme_bw()
```



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

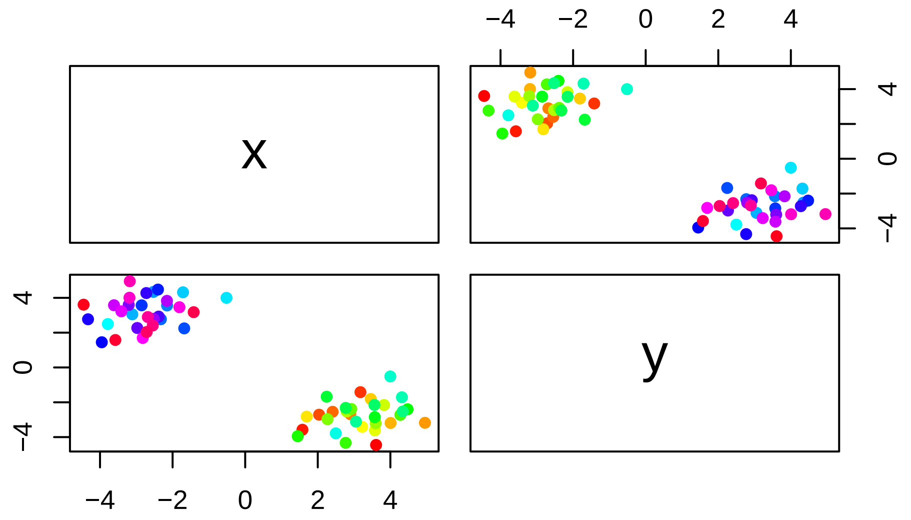
```r
ggplot(y_long) +
  aes(x = Country, y = Consumption, fill = Food) +
  geom_col() +
  theme_bw()
```



A4. Removing the `position = "dodge"` optional argument results in the above graph.

Q5. 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?

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



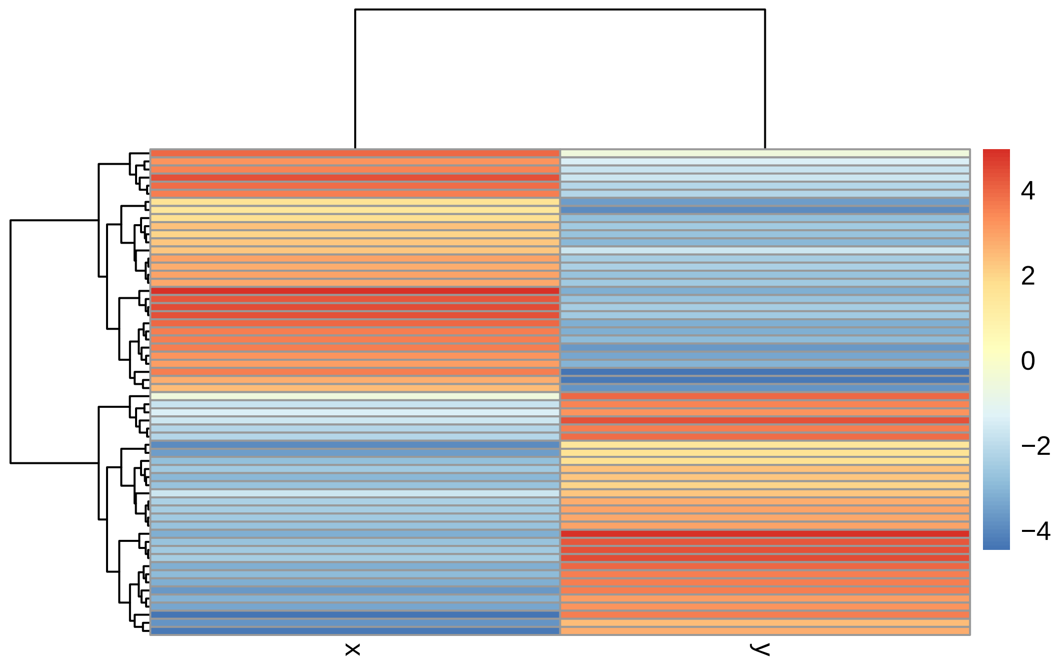
A5. The horizontal axis represent the country that is present within that row. Each plot compares one country to another. The points are the categories that we are comparing across the countrie (i.e. cheese, alcohol, etc.). A perfect diagnol would signal the same consumption as the other country. A value above/below the diagnol would signal greater consumption for the associated country (in row/in column respectively).

## Heatmap

```
#install.packages("pheatmap")
library(pheatmap)
```

```
Warning: package 'pheatmap' was built under R version 4.4.3
```

```
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?

A6. It is possible to tell relative consumption to other countries based on the legend, but it does not easily show differences in specific consumption.

Of all these plot really only the `pairs()` plot was useful. This however, took a vit of work to interpret and will at scale when I am looking at much bigger datasets

## PCA to the rescue

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

```
pca <- prcomp( t(y) )
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
```

> Q. How much variance is captured in the first variance?

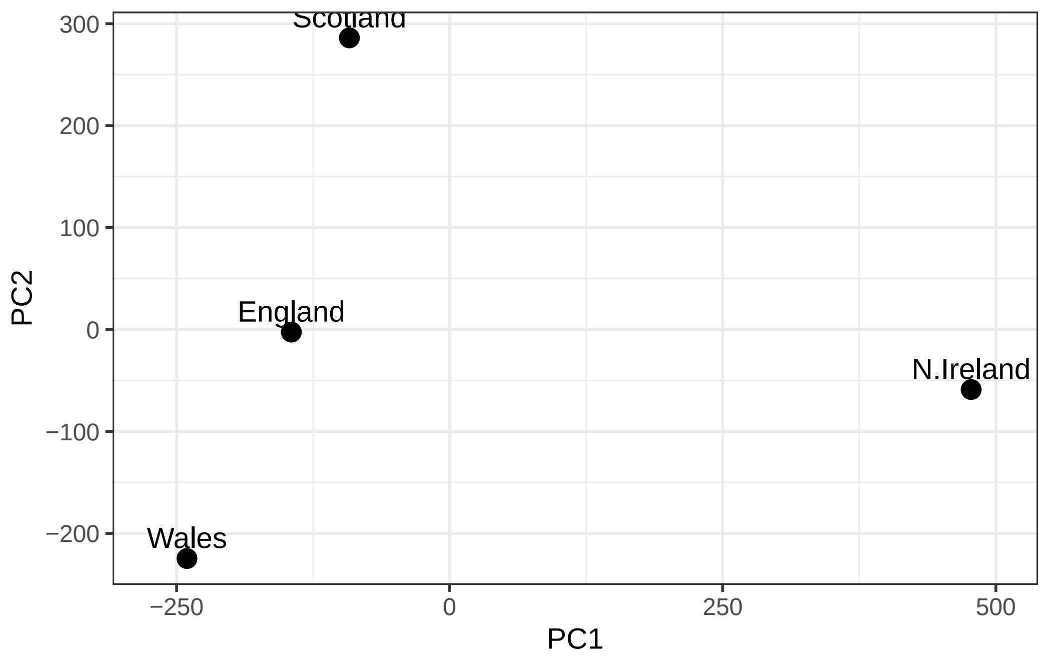
67.44%

> Q. How many PC's do I need to capture at least 90% of the total variance in the data set?

2 PC's are needed for capturing of 90% variance

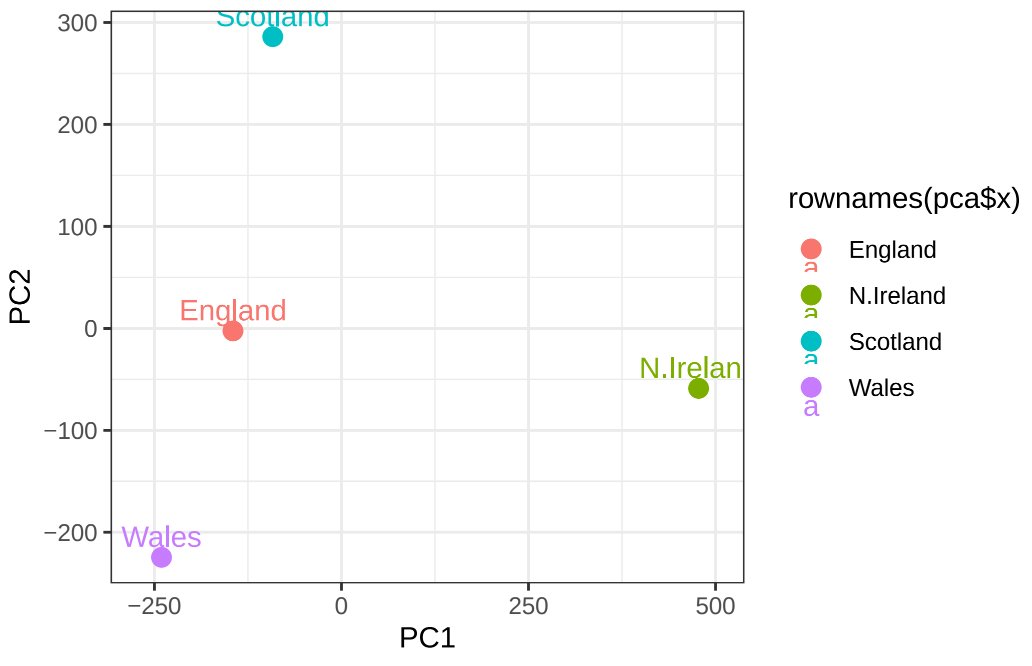
> Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
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) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



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.

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

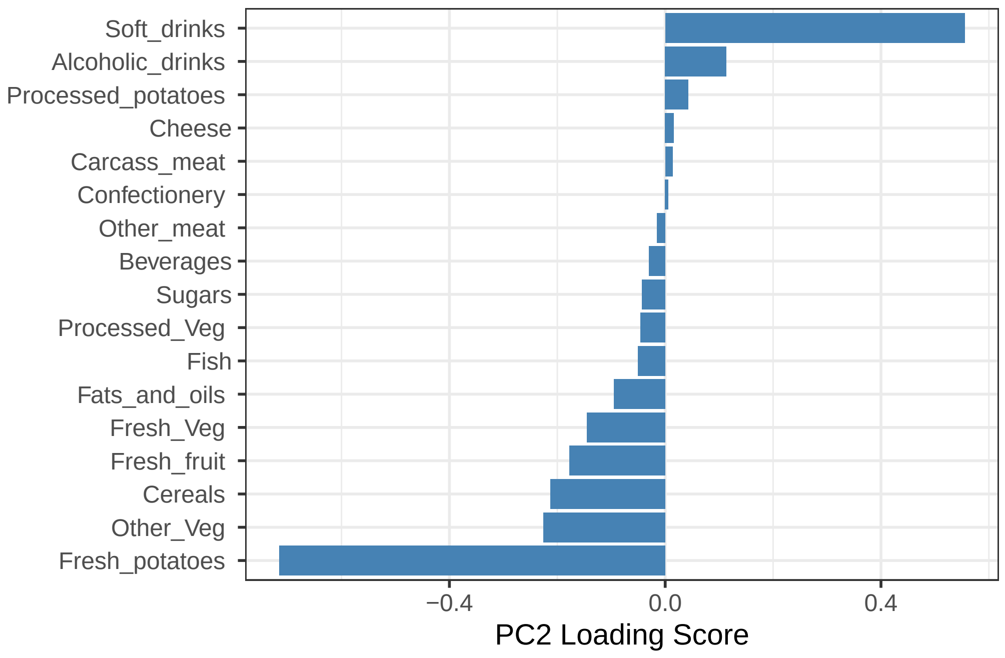


## Diggin deeper (variable loadings)

How do the original variables (i.e. the 17 different foods) contribute to our new PC's?

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

```r
ggplot(pca$rotation) +
  aes(x = PC2,
      y = reorder(rownames(pca$rotation), PC2)) +
  geom_col(fill = "steelblue") +
  xlab("PC2 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```


Soft_drinks
Alcoholic_drinks
Processed_potatoes
Cheese
Carcass_meat
Confectionery
Other_meat
Beverages
Sugars
Processed_Veg
Fish
Fats_and_oils
Fresh_Veg
Fresh_fruit
Cereals
Other_Veg
Fresh_potatoes
PC2 Loading Score