Class 7: Machine Learning 1

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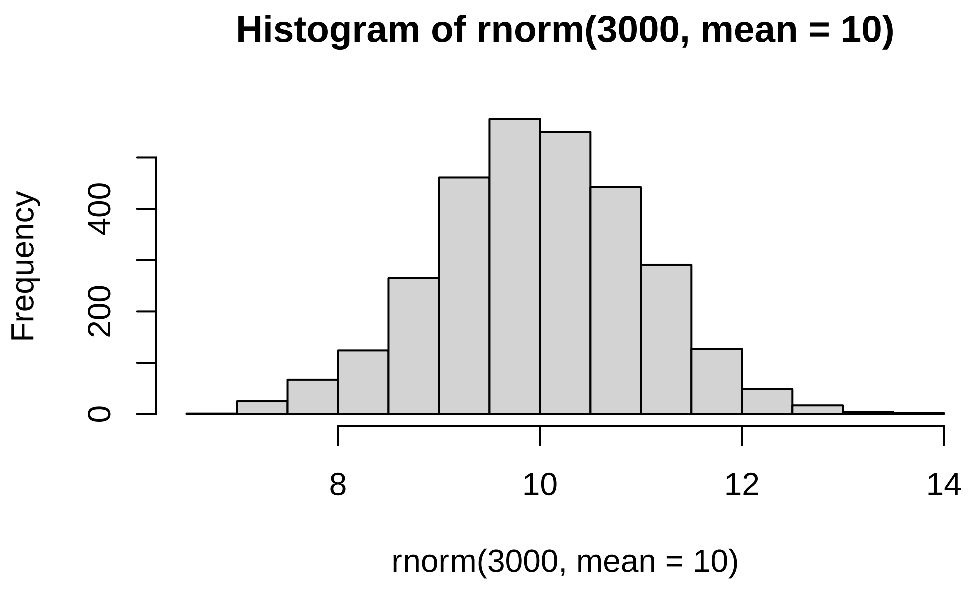
Background

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

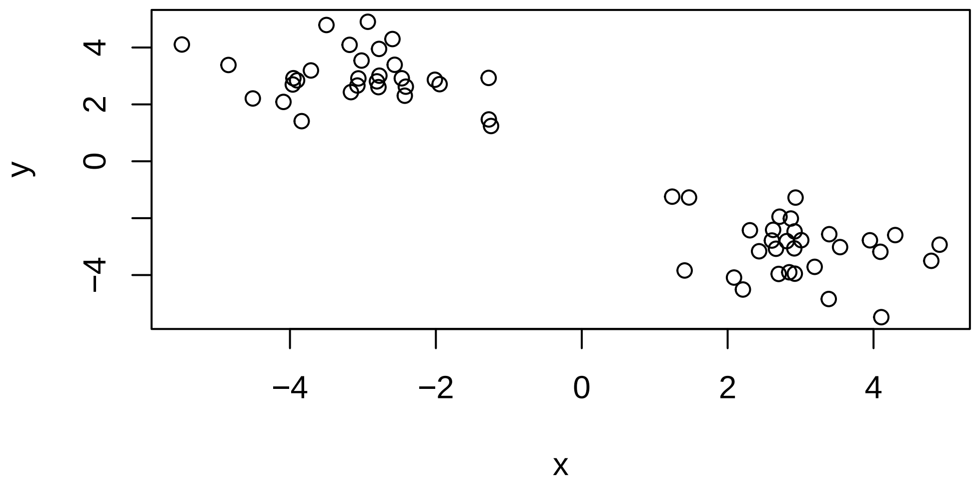
To start testing these methods, let's make some sample data to cluster where we know what the answer should be.

```
hist(rnorm(3000, mean=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(30,3),
rnorm(30,-3))

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

plot(x)
```



K-means clustering

The main function in "base R" for k-means clustering is called `kmeans()`, let's try it out:

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

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

Cluster means:
          x         y
1  2.977595 -3.053180
2 -3.053180  2.977595

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] 53.11144 53.11144
 (between_SS / total_SS =  91.1 %)
```

```
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  2.977595 -3.053180
2 -3.053180  2.977595
```

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

```r
k$size
```

```
[1] 30 30
```

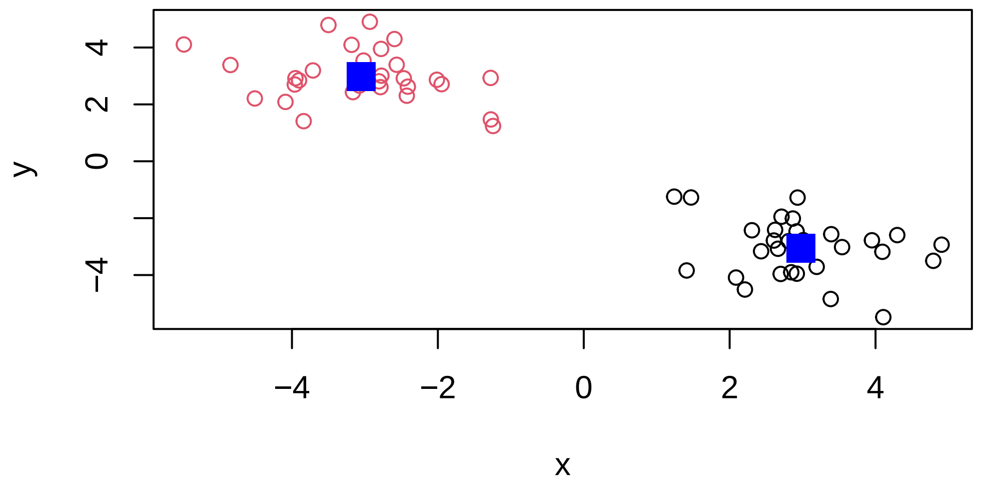
> Q. What component of your kmeans result has the cluster membership vector (i.e the main clustering result: which points are in the which cluster) ?

```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
```

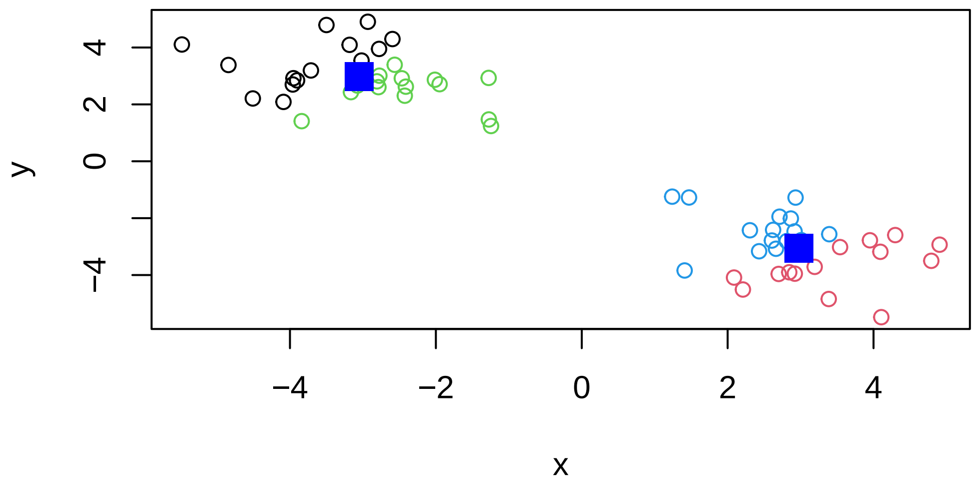
> Q. Plot thr results of clustering (i.e our data colored by the clustering results) along with the cluster centers.

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



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

```r
k4 <- kmeans(x, 4)
plot(x, col=k4$cluster)
points(k$centers, col="blue", pch=15, cex=2)
```



> **Key-point:** Kmeans will always return the clustering that we ask for (this is the "K" or "centers" in K-means)!

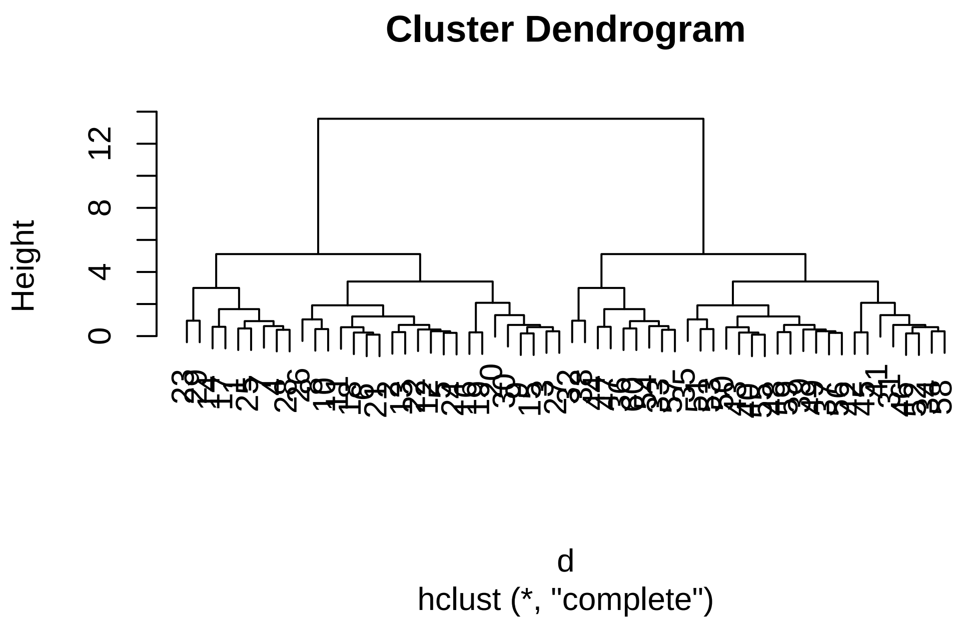
```r
k4$tot.withinss
```

```
[1] 66.50817
```

Hierarchical clustering

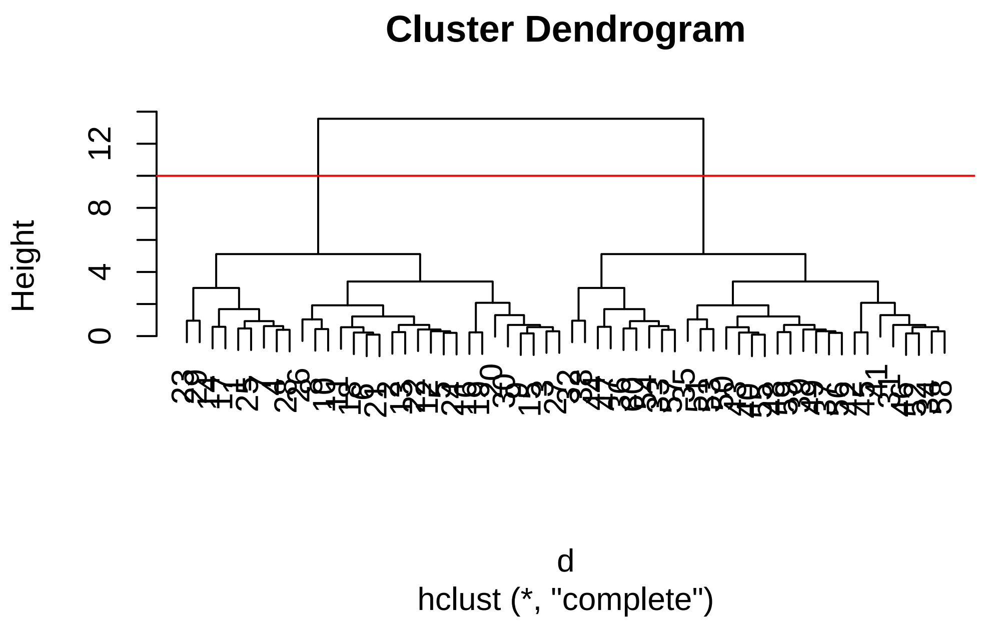
The main function for hierarchical clustering in base R is called `hclust()`. One of the main differences with respect to the K-means function is that you can not just pass your input data directly to `hclust()`- it needs a "distance matrix" as input. We can get this from lot's of places including the `dist()` function.

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



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

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



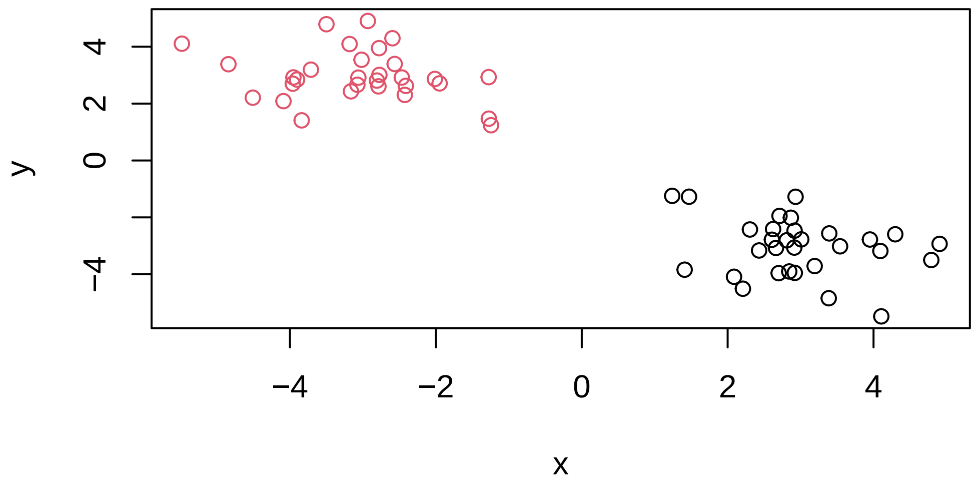
```r
grps <- cutree(hc, h=10)
```

```r
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 result from `hclust()` and `cutree`.

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



Principal Component Analysis (PCA)

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

PCA of UK food data

Read data on food consumption in the UK

```r
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
```

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

```
rownames(x) <- x[,1]
x <- x[,-1]
```

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

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

> Q1. Complete the following code to find out how many rows and columns are in x? _____(x)

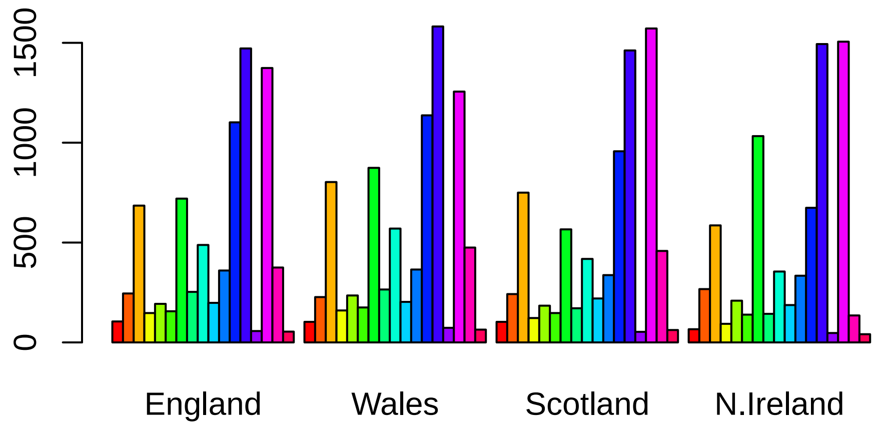
```
dim(x)
```

```
[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?

Approach 2 is better because it fixes the row names problem when reading the data, making it easier and more consistent to work with eventually. The first approach can lead to data deletion if we run more than once so it is dangerous and less recommended.

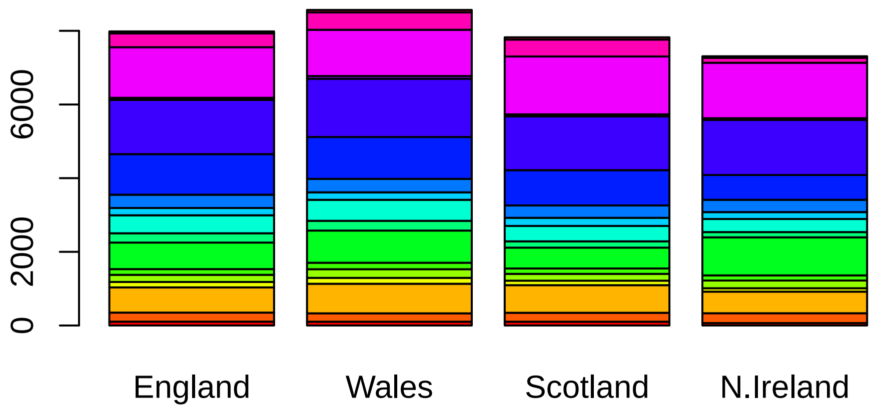
```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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

Changing the `beside` optional argument in the above `barplot()` from T to F results in the change of plot from the one above to the following one.

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



- Tidying up the data

```r
# install.packages("tidyr")
library(tidyr)
x_long <- x |>
          tibble::rownames_to_column("Food") |>
          pivot_longer(cols = -Food,
                       names_to = "Country",
                       values_to = "Consumption")

dim(x_long)
```

```
[1] 68  3
```

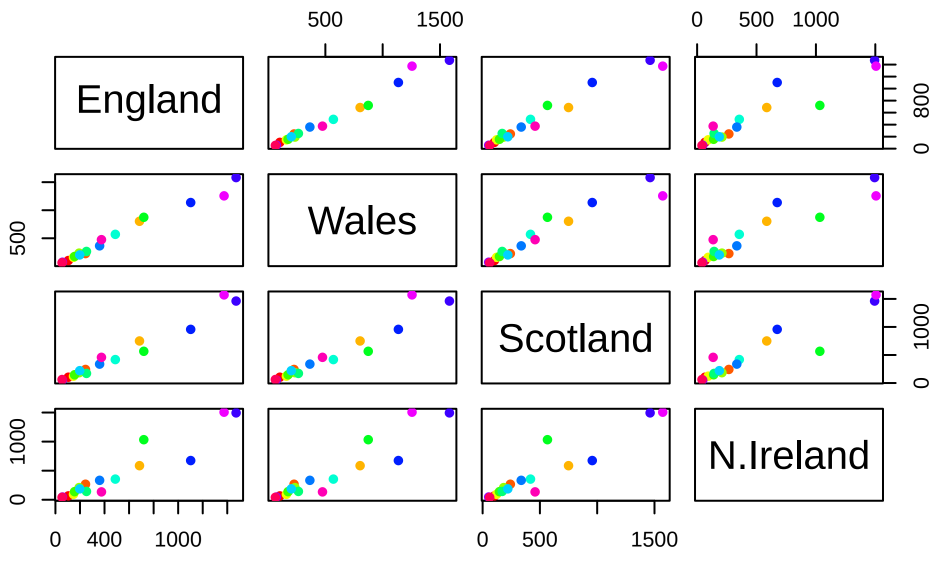
> Q4: Changing what optional argument in the above ggplot() code results in a stacked barplot figure?

Skipping Q4 as instructed by Prof. Grant

Pair plots and heatmaps

> 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)
```

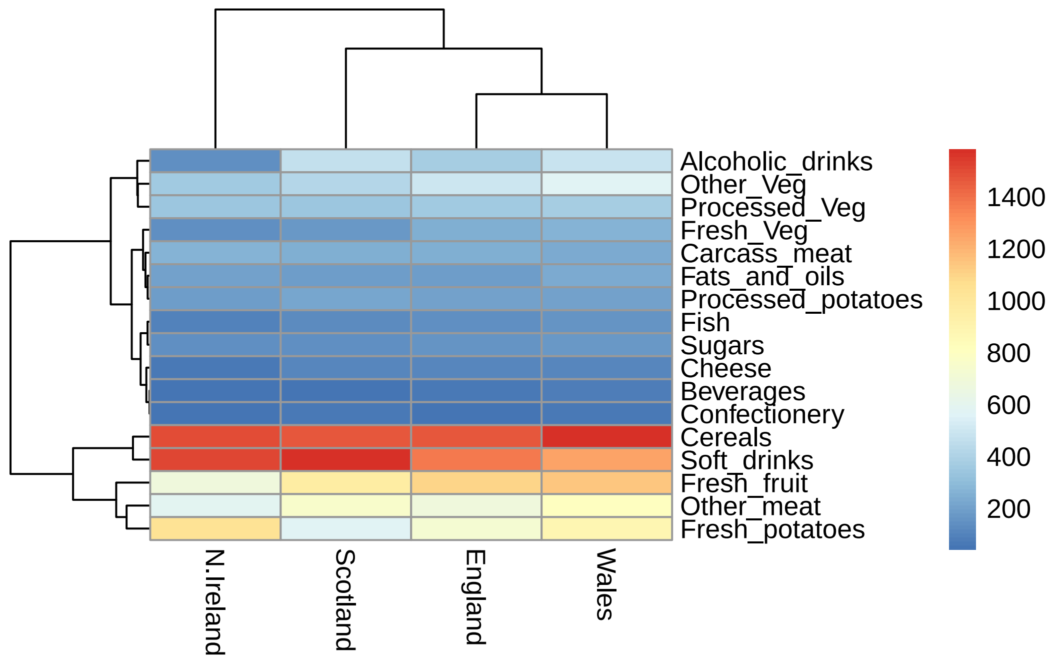


17 different points give the 17 different food categories being studied. If the countries had similar values of the food categories, the points would lie on the diagonal. If the two countries being compared have different value for a particular food category, then the point will not be on the diagonal.

Heatmap

We can install the **pheatmap** package with the `install.packages()` command used previously. Remember that we always run this in the console and not in the code chunk.

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



Of all these plot really the `pairs()` plot was useful. This however took a bit of work to interpret and will it scale when I am looking at much bigger data sets.

> 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?

Based on the pairs and heatmap figures, England and Wales seem to cluster closer together with Scotland clustering nearby while Northern Ireland seems more distant from the other countries. However, it quite difficult to analyze even this small data set from these graphs and therefore, not easy to tell what the main differences between N. Ireland and the other countries of the UK in terms of this data-set.Therefore, we use PCA as a better analytical method.

PCA to the rescue

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

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

```
Importance of components:
                            PC1      PC2      PC3     PC4
Standard deviation     324.1502 212.7478 73.87622 2.7e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.0e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.0e+00
```

> Q. How much variance is captired in the first PC?

From the table, we see for that variance captured for PC1 is 67.4%

> Q. How many PCs do I need to capture atleast 90% of the total variance

From the table, we see that two PCs capture 96.5% of the total variance.

> Q. Plot our main PCA result. Folks can call this different things depending on their field of study e.g. “PC plot”, “ordienation plot”, “score plot” etc.

```r
attributes(pca)
```

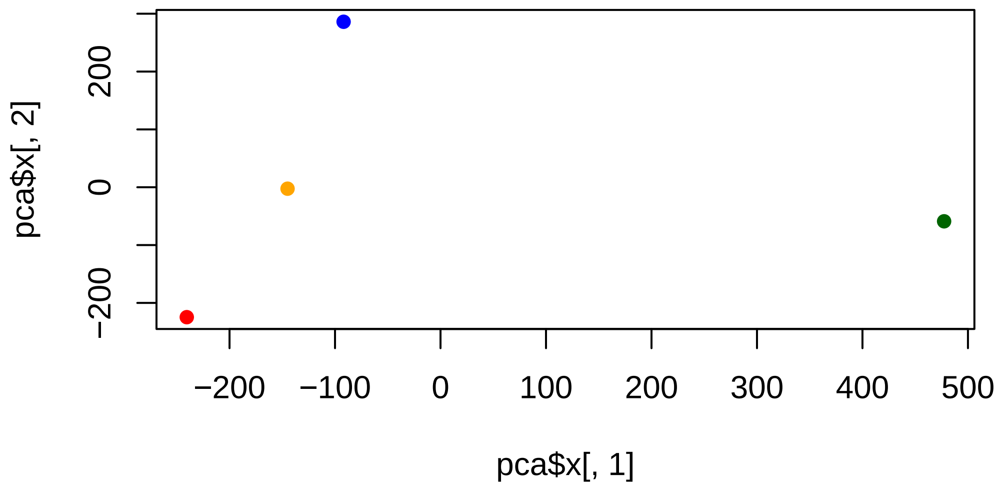
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"       

$class
[1] "prcomp"
```

To generate our PCA score plot we want the `pca$x` component of the result object.

```r
pca$x
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945  1.612425e-14
Wales     -240.52915 -224.646925 -56.475555  4.751043e-13
Scotland   -91.86934  286.081786 -44.415495 -6.044349e-13
N.Ireland  477.39164  -58.901862  -4.877895  1.145386e-13
```

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

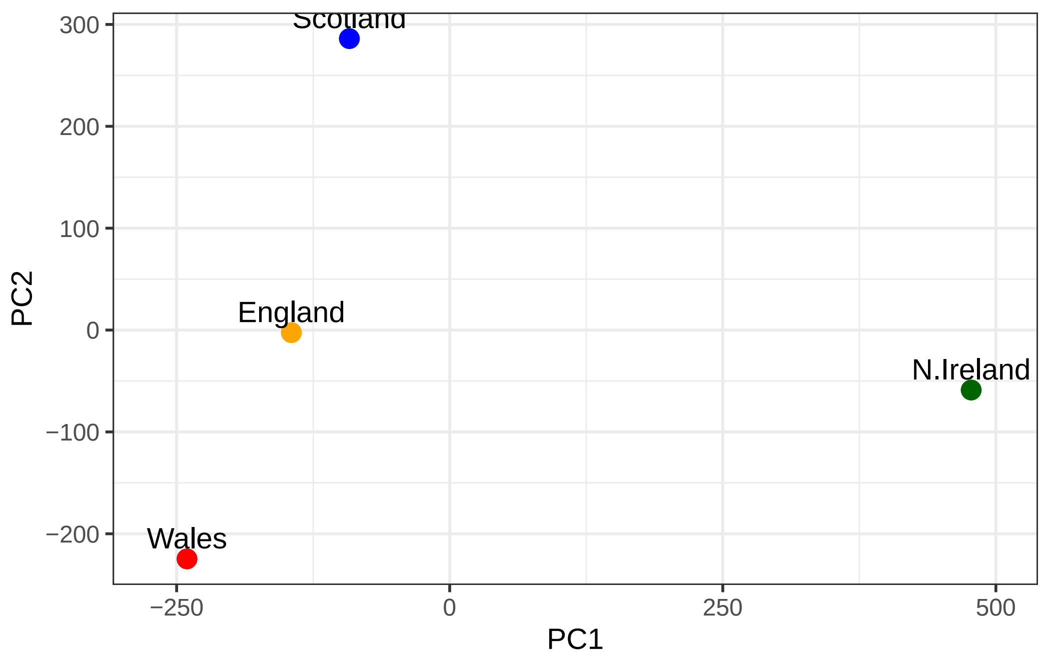


Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
library(ggplot2)
```

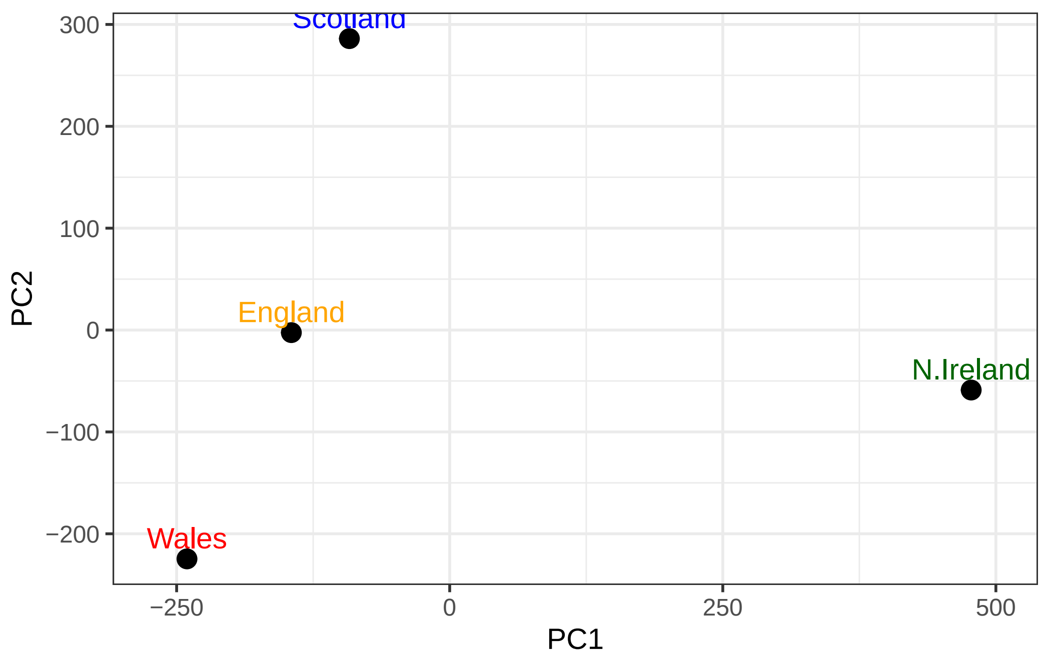
- Plot PC1 vs PC2 with ggplot

```
ggplot(pca$x) +
  aes(x = PC1, y = PC2, label = rownames(pca$x)) +
  geom_point(size = 3,col=my_cols ) +
  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.

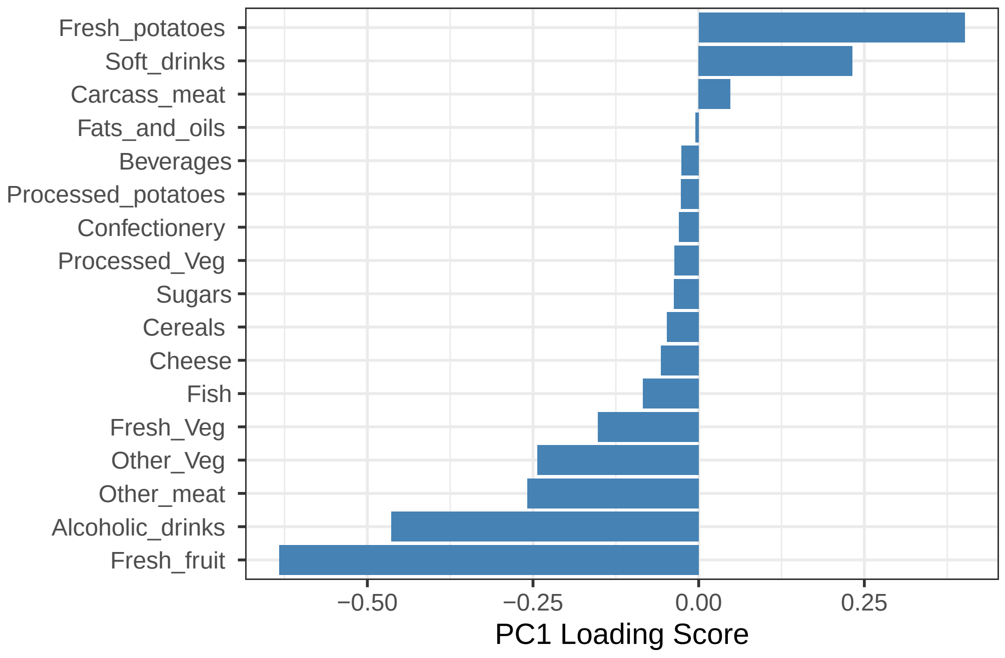
```r
ggplot(pca$x) +
  aes(x = PC1, y = PC2, label = rownames(pca$x)) +
  geom_point(size = 3 ) +
  geom_text(vjust = -0.5, col= my_cols) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



Digging deeper (variable loadings)

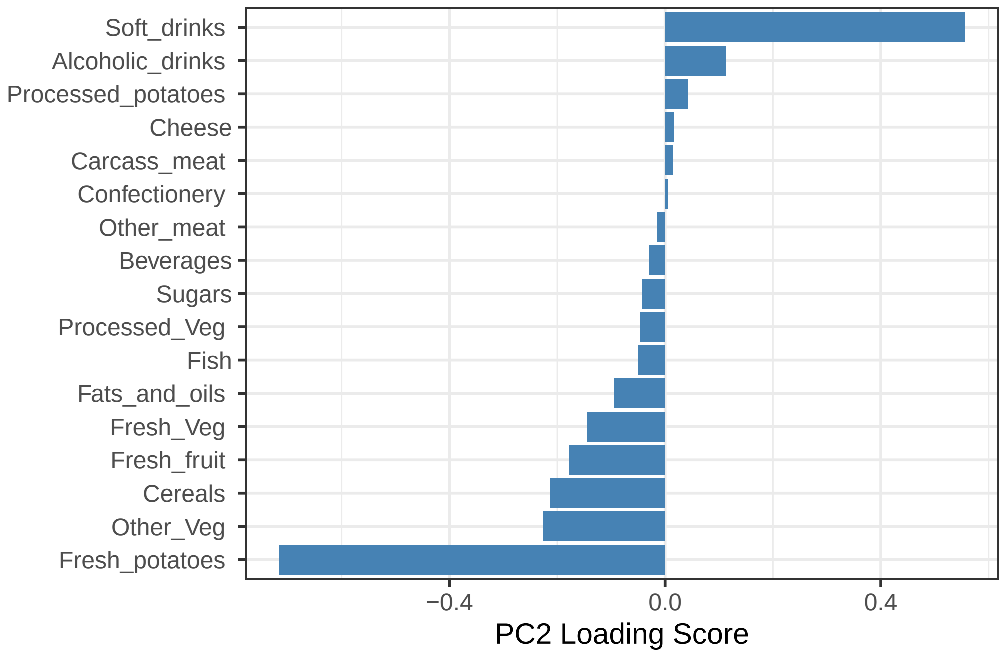
How do the original variables (i.e. the 17 different foods) contribute to our new PCs.

```r
library(ggplot2)
ggplot(pca$rotation) +
  aes(x = PC1,
      y = reorder(rownames(pca$rotation), PC1)) +
  geom_col(fill = "steelblue") +
  xlab("PC1 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```



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))
```



Two groups that feature prominently are "Fresh_potatoes" and "Soft_drinks" on the plot. The observations (foods) with the largest positive loading scores that "push" Scotland upwards positive side of the plot include "Soft_drinks" and "Alcoholic_drinks". Observations/foods with high negative scores that push the other countries downward on the plot include "Fresh_potatoes" and "Other_veg". So, PC2 loading plot helps us to analyze which food categories determine the difference between countries with high PC2 scores from countries with low PC2 scores.