Class 7: Machine Learning 1

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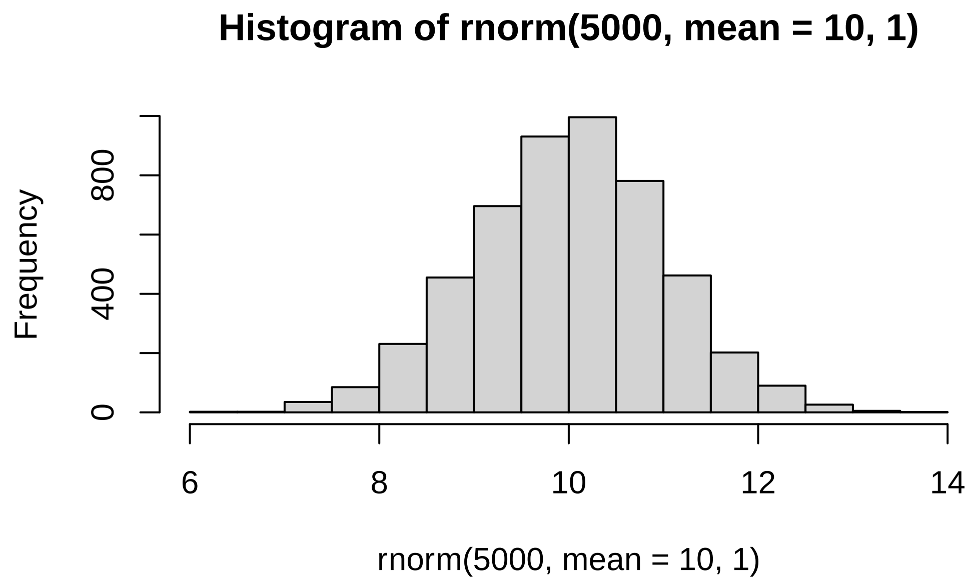
Background

Today we will begin our exploration of some important machine learning methods, namely **clustering** and **dimensionality reduction**

Let's make up some input data for clustering where we know what the natural "clusters" are.

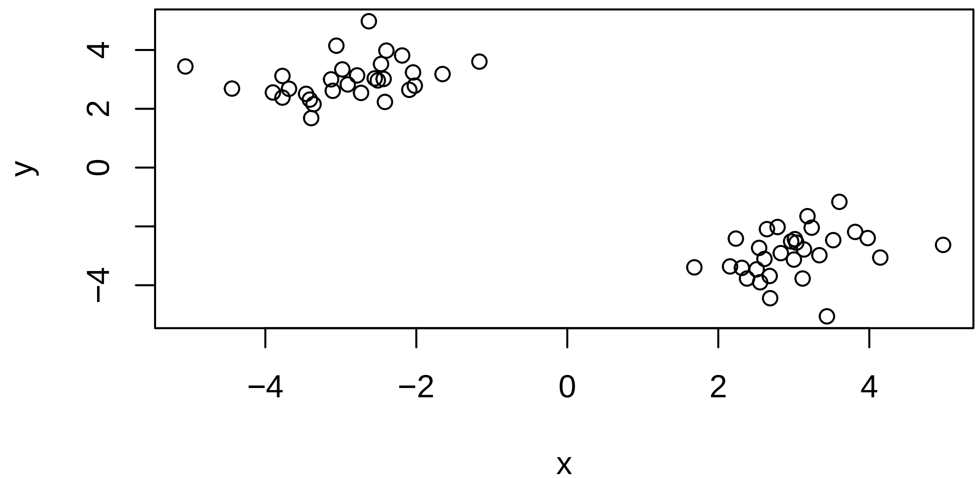
The function `rnorm()` can be useful here.

```
hist(rnorm(5000, mean=10, 1))
```



Q. Generate 30 random numbers centered at +3 and another 30 centered at -3

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



K-means cluster

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

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

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

Cluster means:
          x         y
1 -2.917336  3.003647
2  3.003647 -2.917336

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 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] 32.85627 32.85627
 (between_SS / total_SS =  94.1 %)
```

```
Available components:

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

Q. What component of the results object details the cluster sizes?

```r
km$size
```

```
[1] 30 30
```

Q. What component of the results object details the cluster centers?

```r
km$centers
```

```
          x         y
1 -2.917336  3.003647
2  3.003647 -2.917336
```

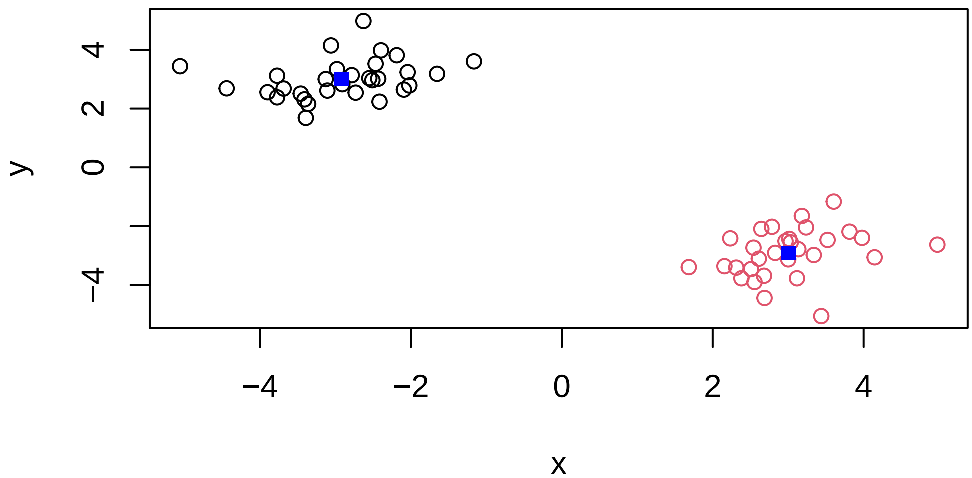
Q. What component of the results object details the cluster membership vector (i.e. our main result of which points lie in which cluster)?

```r
km$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 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
```

Q. Plot our clustering results with points colored by cluster and also add the cluster centers as new points colored blue?

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



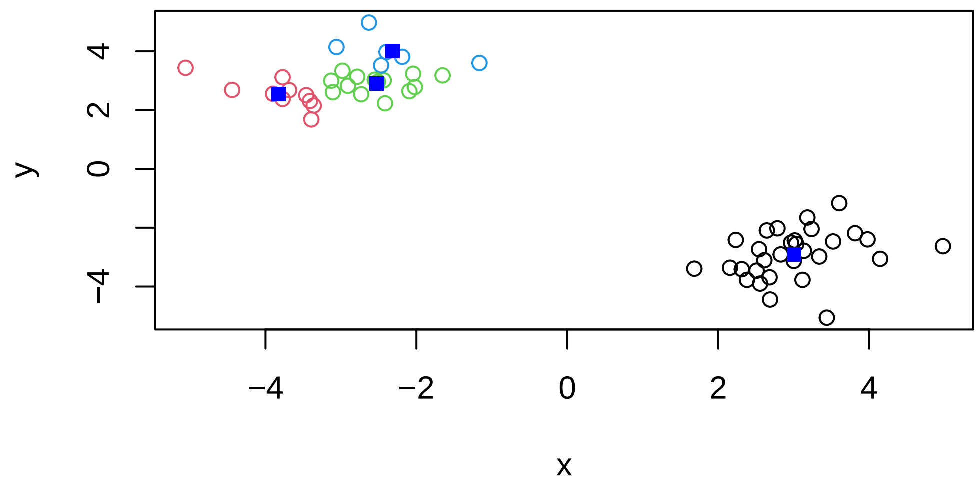
Q. run `kmeans` again and this time produce 4 clusters 9and call your result object `k4`) and make a results figure like above?

```
k4 <- kmeans(x,centers=4)
k4
```

```
K-means clustering with 4 clusters of sizes 30, 10, 14, 6

Cluster means:
          x         y
1  3.003647 -2.917336
2 -3.825754  2.551697
3 -2.525601  2.896446
4 -2.317357  4.007030

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 3 3 3 4 3 3 2 3
[39] 4 2 2 4 2 4 2 3 2 4 3 2 3 3 4 2 3 2 2 3 3 3

Within cluster sum of squares by cluster:
[1] 32.856272  4.782111  3.849807  3.419740
 (between_SS / total_SS =  96.0 %)
```

```
Available components:

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

```
plot(x, col=k4$cluster)
points(k4$centers, col="blue", pch=15)
```



The metric

```
km$tot.withinss
```

```
[1] 65.71254
```

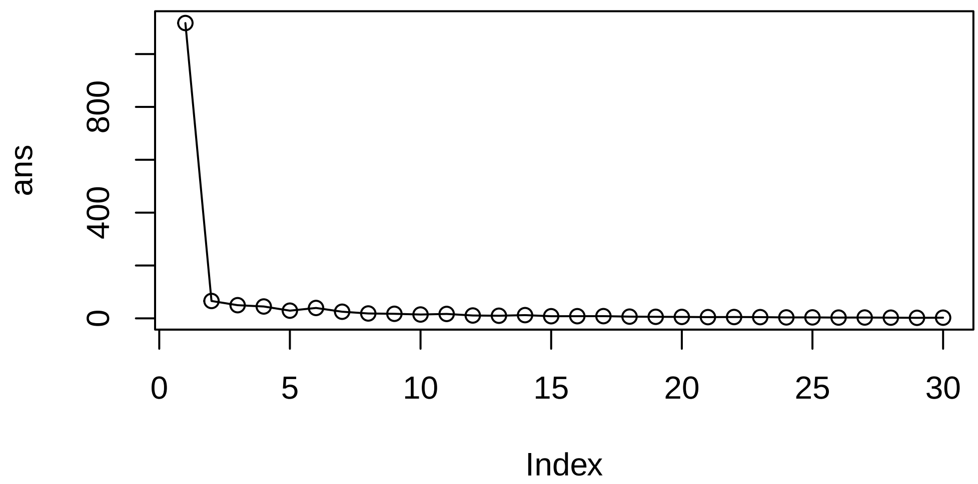
```
k4$tot.withinss
```

```
[1] 44.90793
```

> Q. Let's try different number of K (centers) from 1 to 30 and see what the best result is?

```r
ans <- NULL
for(i in 1:30){
ans <- c(ans, kmeans(x, centers=i)$tot.withinss)
}
```

```r
plot(ans, type="o")
```



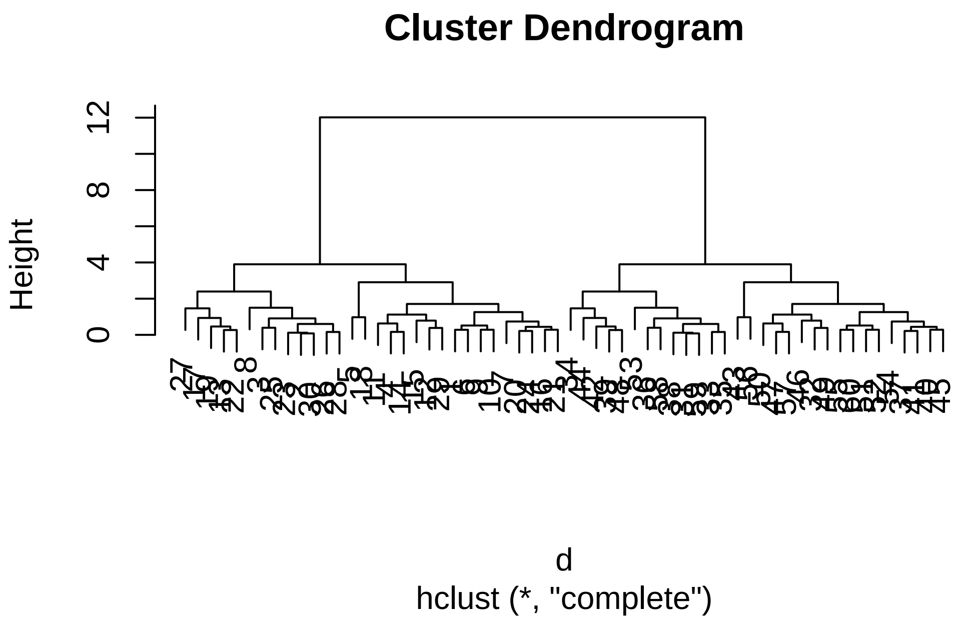
Key-pont: K-means will impose a clustering structure on your data even if it is not there - it will always give you the answer you asked for even if that answer is silly. With `tot.withinss` you are able to see that the higher your centers amount there are are the lower your value will be which means the spreads will be and the tighter the clusters will be.

Hierarchical Clustering

The main function for Hierarchical Clustering is called `hclust()`.

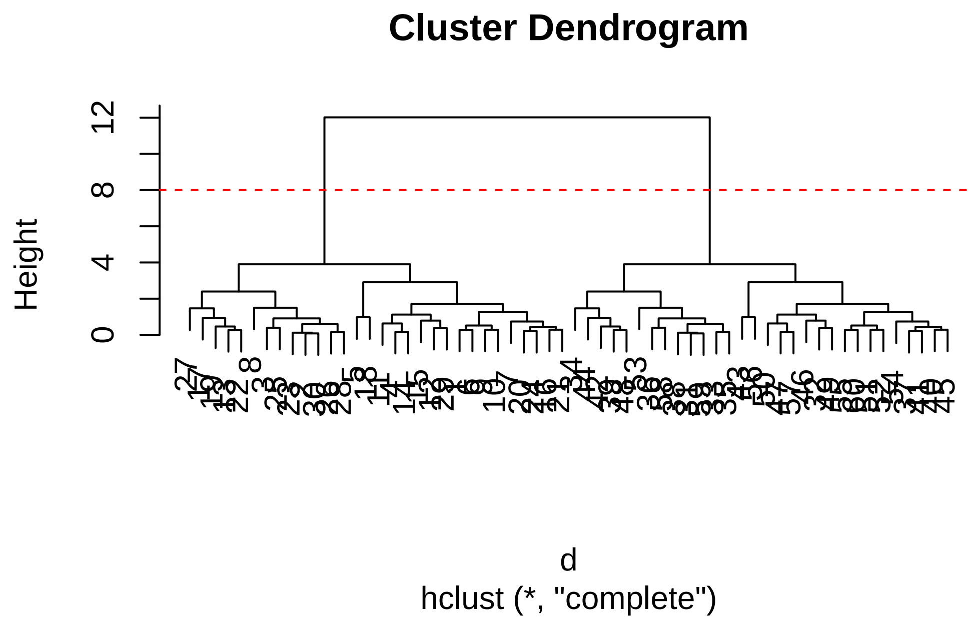
Unlike `kmeans()` (which does all of the work for you) you can't just pass `hclust()` our raw data input. It needs a "distance matrix" like the one returned from the `dist()` function.

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



To extract our cluster membership vector from a `hclust()` result object we have to "cut" our tree at a given height to yield seperate "groups"/"branches".

```
plot(hc)
abline(h=8, col="red", lty=2)
```



To do this we use the `cutree()` function on our `hclust()` object:

```
grps <- cutree(hc, h=8)
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 2 2
```

```
table(grps,
km$cluster)
```

```
grps  1  2
   1  0 30
   2 30  0
```

PCA of UK food data

Import the dataset of 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
```

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

```r
nrow(x)
```

```
[1] 17
```

```r
ncol(x)
```

```
[1] 5
```

```r
#or
dim(x)
```

```
[1] 17  5
```

One solution to set the row names is to do it by hand…

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

```
                                      X England Wales Scotland N.Ireland
Cheese                           Cheese     105   103      103        66
Carcass_meat               Carcass_meat     245   227      242       267
Other_meat                   Other_meat     685   803      750       586
Fish                               Fish     147   160      122        93
Fats_and_oils             Fats_and_oils     193   235      184       209
Sugars                           Sugars     156   175      147       139
Fresh_potatoes           Fresh_potatoes     720   874      566      1033
Fresh_Veg                     Fresh_Veg     253   265      171       143
Other_Veg                     Other_Veg     488   570      418       355
Processed_potatoes   Processed_potatoes     198   203      220       187
Processed_Veg             Processed_Veg     360   365      337       334
Fresh_fruit                 Fresh_fruit    1102  1137      957       674
Cereals                         Cereals    1472  1582     1462      1494
Beverages                     Beverages      57    73       53        47
Soft_drinks                 Soft_drinks    1374  1256     1572      1506
Alcoholic_drinks       Alcoholic_drinks     375   475      458       135
Confectionery             Confectionery      54    64       62        41
```

To remove the first column I can use the minus index trick

```r
x <- x[,-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
```

A better way to do this is to set the row names of the first column with `read.csv()`

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

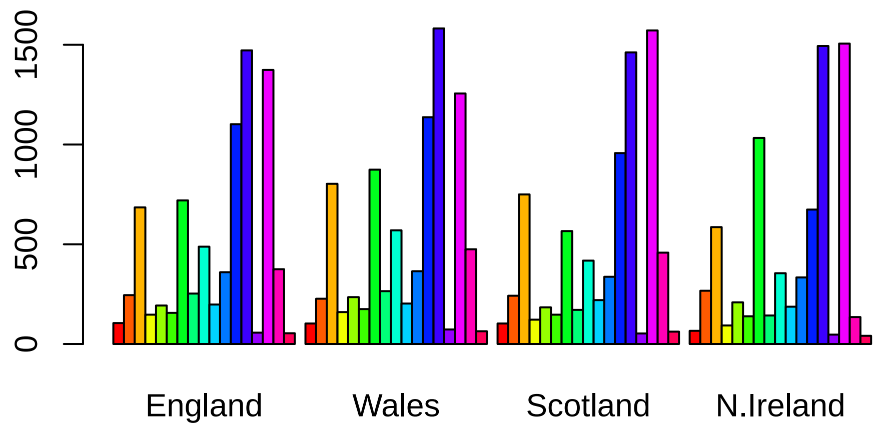
```
                    England Wales Scotland N.Ireland
Cheese                  105   103      103        66
Carcass_meat            245   227      242       267
Other_meat              685   803      750       586
Fish                    147   160      122        93
Fats_and_oils           193   235      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?

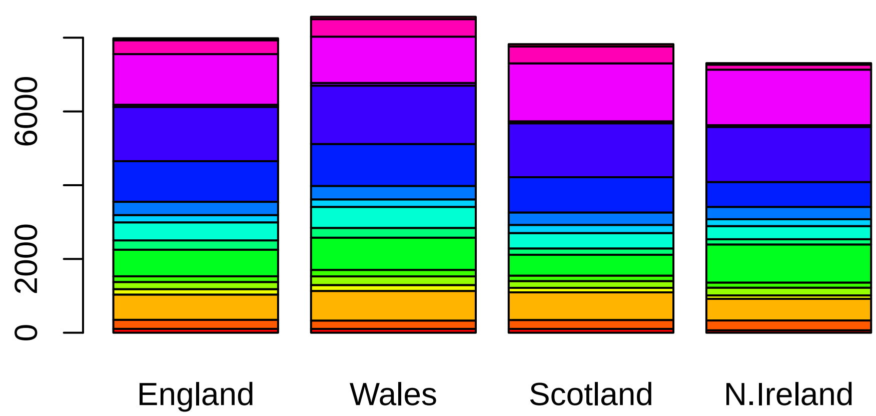
Spotting major differences and trends

Is difficult even in this wee 17D dataset…

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

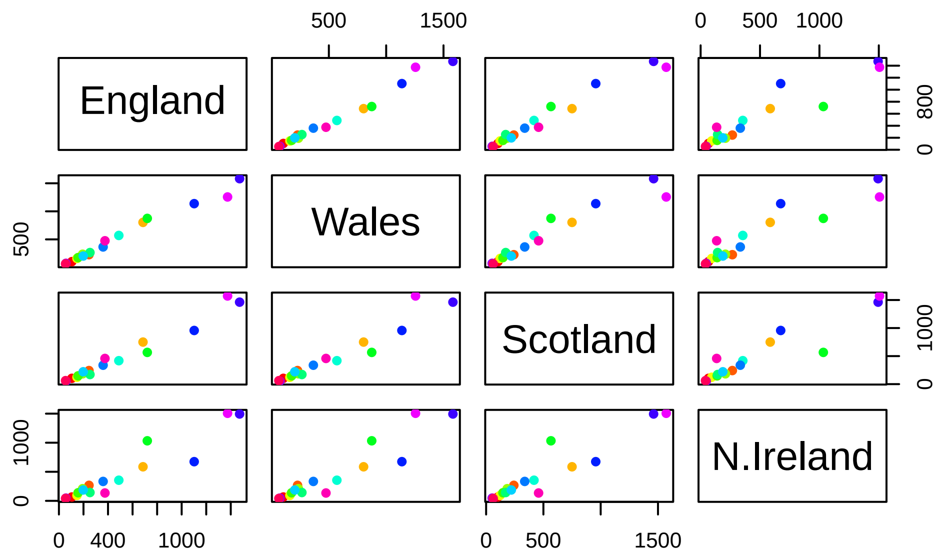



```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```

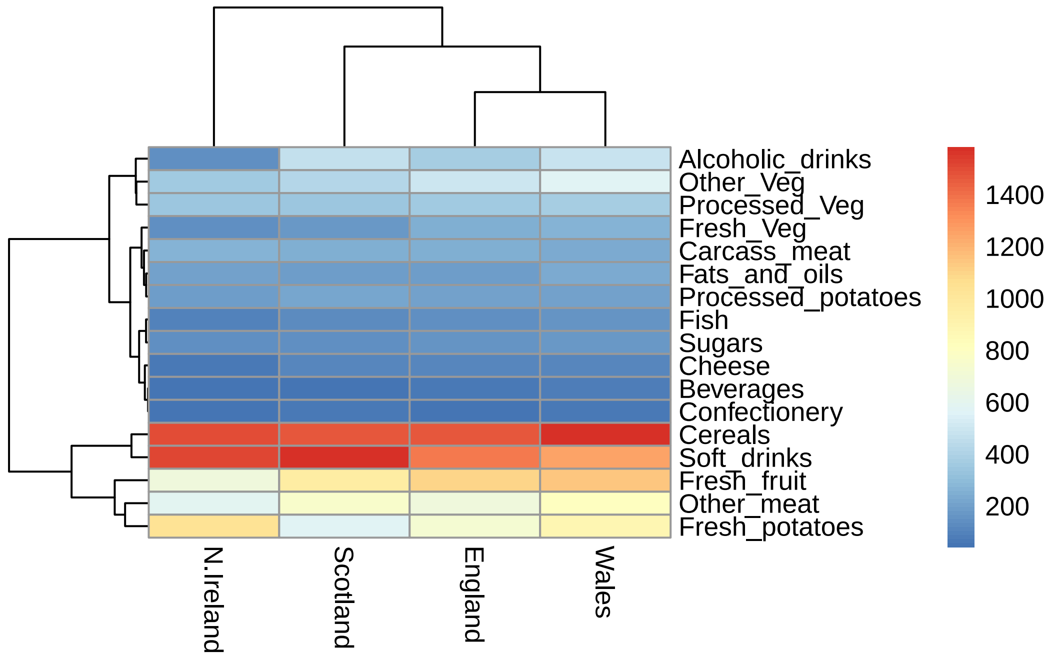


Pairs plot and heatmaps

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




```
library(pheatmap)

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



PCA to the rescue

The main PCA function in "base R" is called `prcomp()`. This function wants the transpose of our food data as input (i.e. the foods as columns and the countries as rows).

```
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
```

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

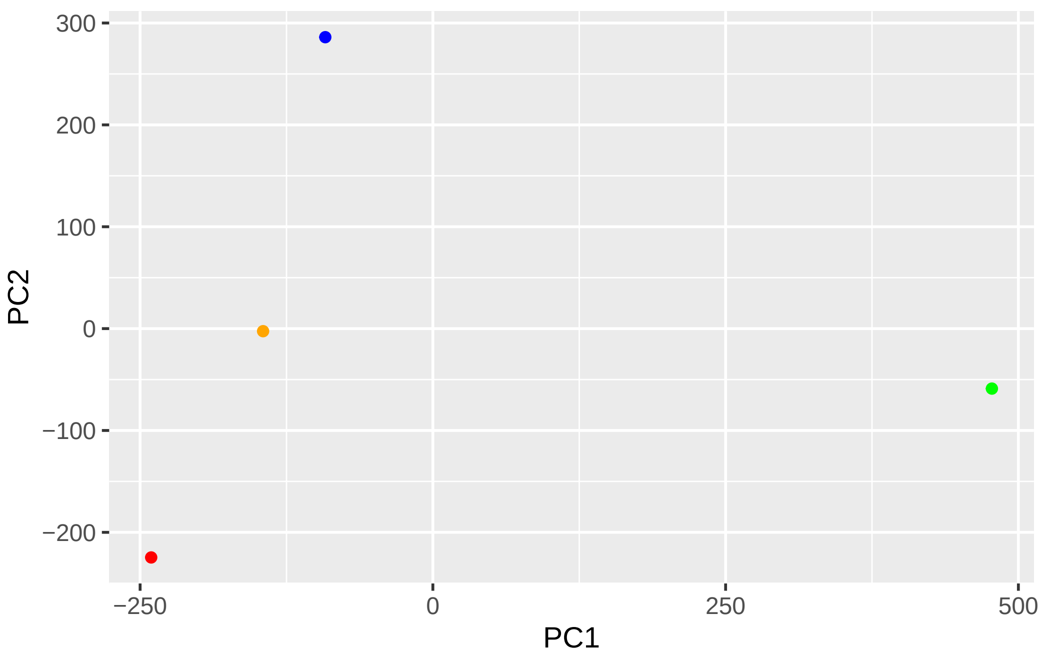
To make one of the main PCA results figures we turn to `pca$x` the scores along our new PCs. This is called "PC plot" or "score plot: or"ordination plot" ...

```
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
```

```
my_cols <- c("orange","red","blue","green")
```

```
library(ggplot2)

ggplot(pca$x)+
  aes(PC1,PC2)+
  geom_point(col=my_cols)
```



The second major resuly figure is called a "loadings plot" or "variable contributions plot" or "weight plot".

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