Class 7: Machine Learning 1

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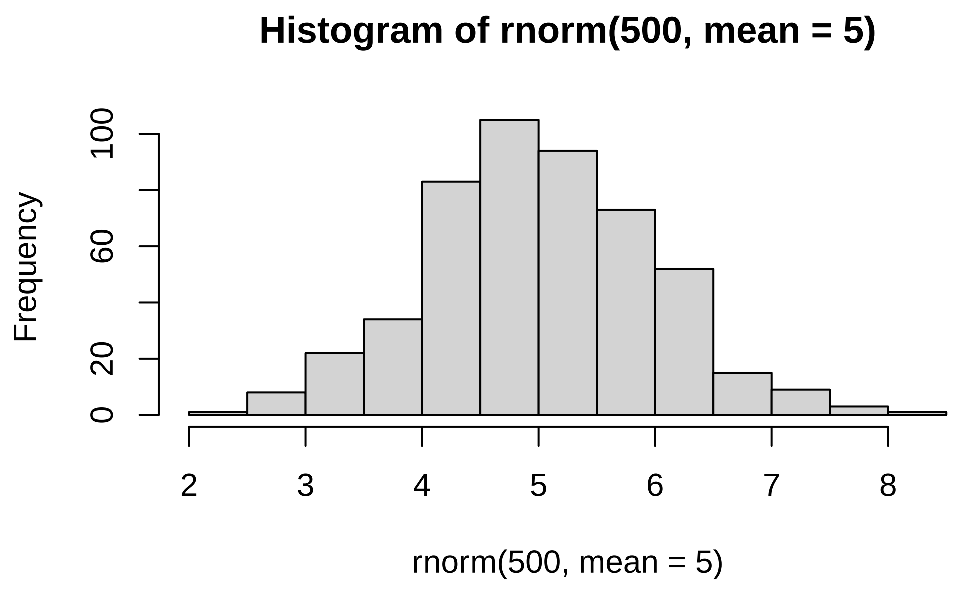
Today we will explore some fundamental machine learning methods including clustering and dimensionality reduction.

K-means clustering

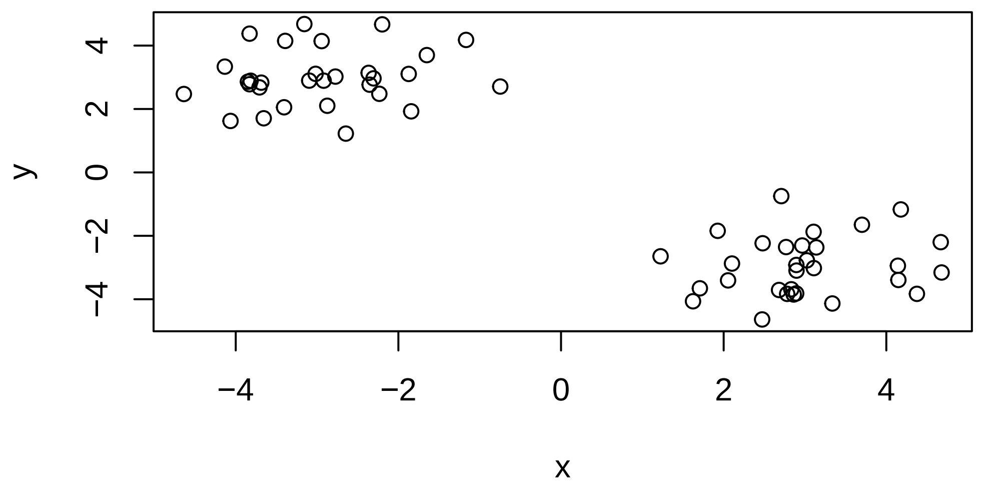
To see how this works let's first makeup some data to cluster where we know that the answer should be. We can use the `rnorm()` function to help here:

```r
hist( rnorm(500, mean=5) )
```



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

```r
x <- cbind(x, y)
plot(x)
```



The function for K-means clustering in “base” R is `kmeans()`

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

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

Cluster means:
          x         y
1 -2.939360  2.982592
2  2.982592 -2.939360

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] 47.75703 47.75703
 (between_SS / total_SS =  91.7 %)

Available components:

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

To get at the results of the returned list object we can use the dollar $ syntax

> Q. How many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

> Q. What 'component' of your result object details - cluster assignment/membership?
> - cluster center?

```
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
```

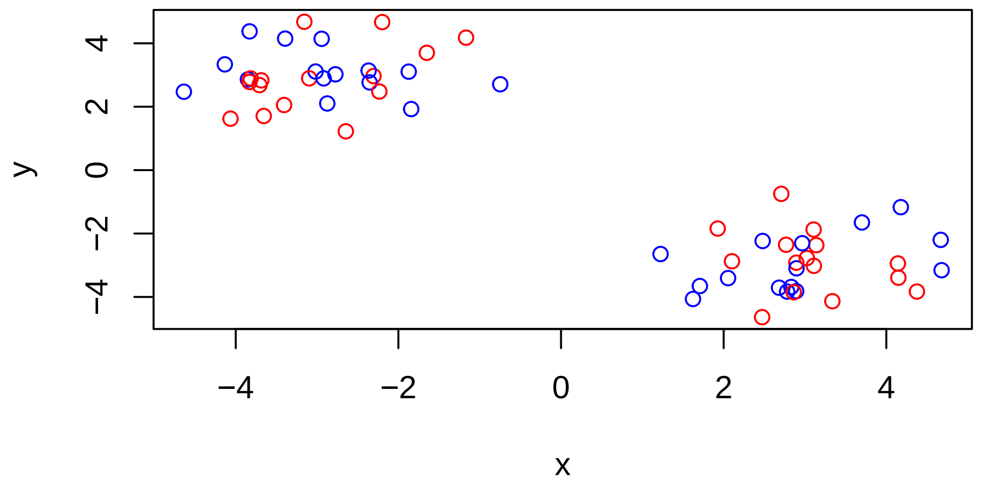
> Q. What a clustering results figer of the data colores by cluster membership?

```
k$centers
```

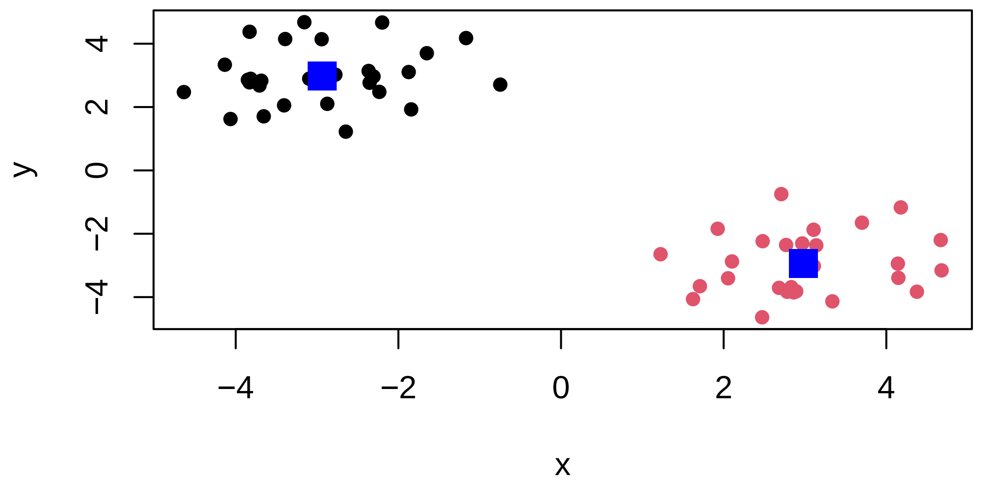
```
          x         y
1 -2.939360  2.982592
2  2.982592 -2.939360
```

> Q. Make a clustering results figure of the data colored by cluster membership and
> show cluster centers.

```
plot(x, col = c("red", "blue") )
```



```r
plot(x, col = k$cluster, pch = 16)
points(k$centers, col = "blue", pch = 15, cex = 2)
```

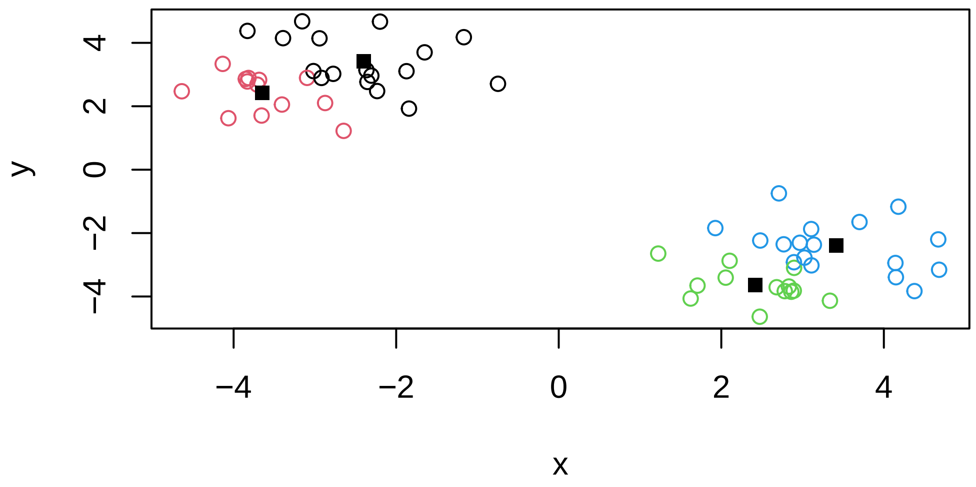


K-means clustering is very popular as it is very fast and relatively straight forward: it takes numeric data as input and returns the clusterm membership vector etc.

The "issue" is we tell `kmeans()` how many clusters we want!

> Q. Run kmeans again and cluster into 4 graphs/clusters and plot the results like we did above?

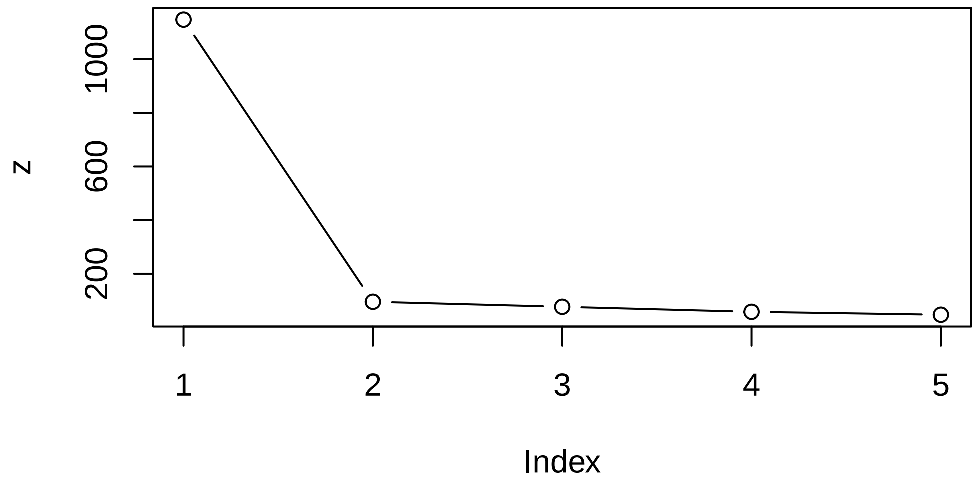
```r
k4 <- kmeans(x, centers = 4)
plot(x, col = k4$cluster)
points(k4$centers, pch = 15)
```



```r
k1 <- kmeans(x, centers = 1)
k2 <- kmeans(x, centers = 2)
k3 <- kmeans(x, centers = 3)
k4 <- kmeans(x ,centers = 4)
k5 <- kmeans(x, centers = 5)
```

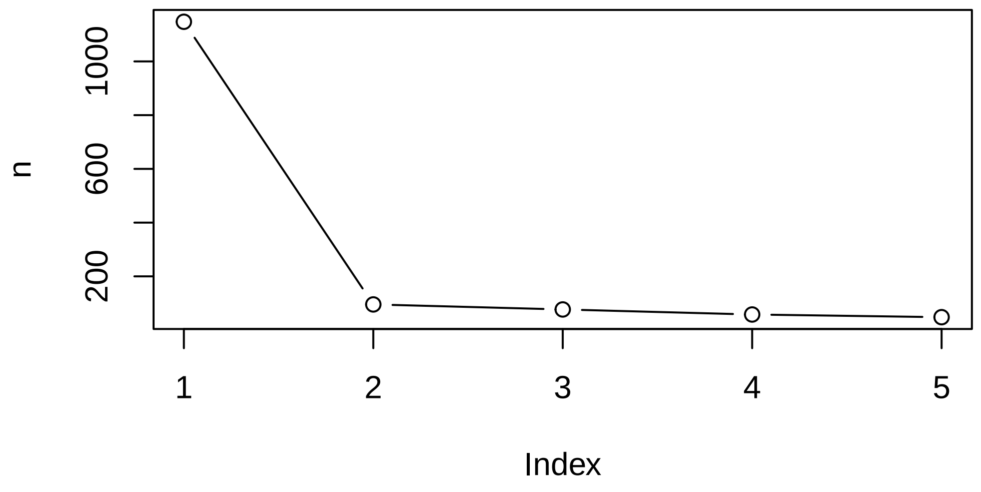
```r
z <- c(k1$tot.withinss,
       k2$tot.withinss,
       k3$tot.withinss,
       k4$tot.withinss,
       k5$tot.withinss)
```

```r
plot(z, type = "b")
```



```r
n <- NULL
for(i in 1:5){
  n <- c(n, kmeans(x, centers = i)$tot.withinss)
}

plot(n, type = "b")
```



Hierarchical Clustering

The main "base" R function for Hierarchical Clustering is classed `hclust()`. Here we can't just input out data we need to first calculate a distance matrix (e.g. `dist()`) for our data and use this as input to `hclust()`.

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

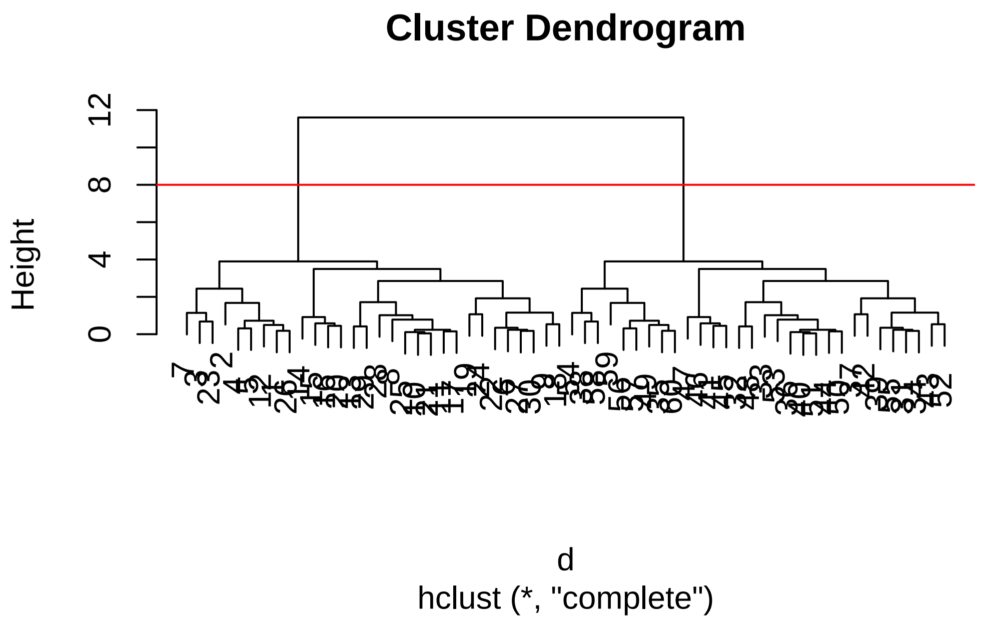
```

Call:
hclust(d = d)

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

There is a plot method for hclust results lets try it

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



To get our cluster "membership" vector (i.e. our main clustering result) we can "cut" the tree at a given height or at a height that yields a given "k" groups.

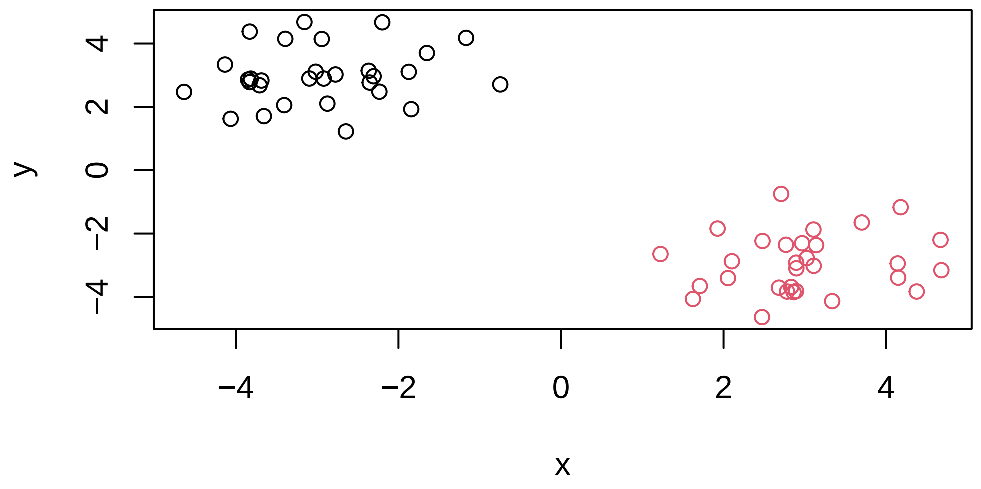
```r
cutree(hc, h=8)
```

```
 [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
```

```r
grps <- cutree(hc, k=2)
```

Q. Plot the data with our hclust result coloring

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



Principal Component Analysis (PCA)

PCA of UK food data

Import food data from an online CSV file:

```r
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
head(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
```

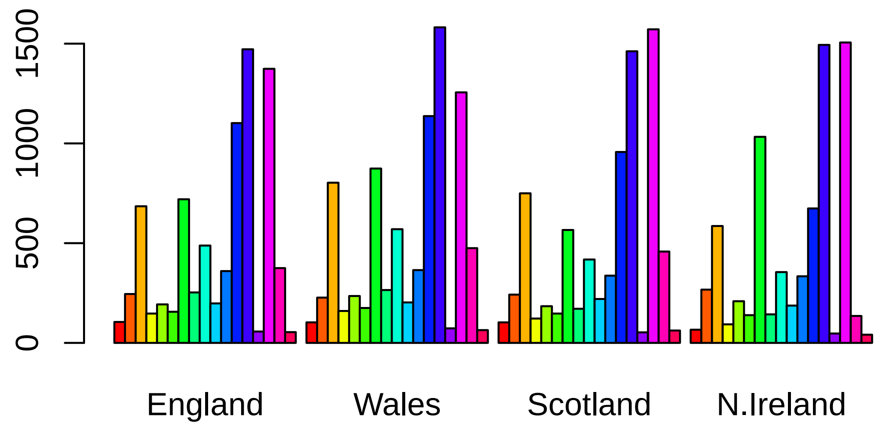
```r
rownames(x) <- x[,1]
x <- x[,-1]
head(x)
```

```
               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
```

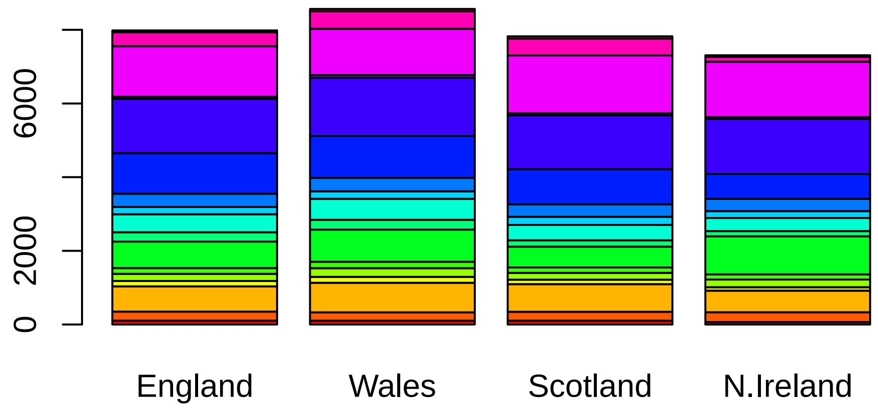
```r
x <- read.csv(url, row.names = 1)
head(x)
```

```
               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
```

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

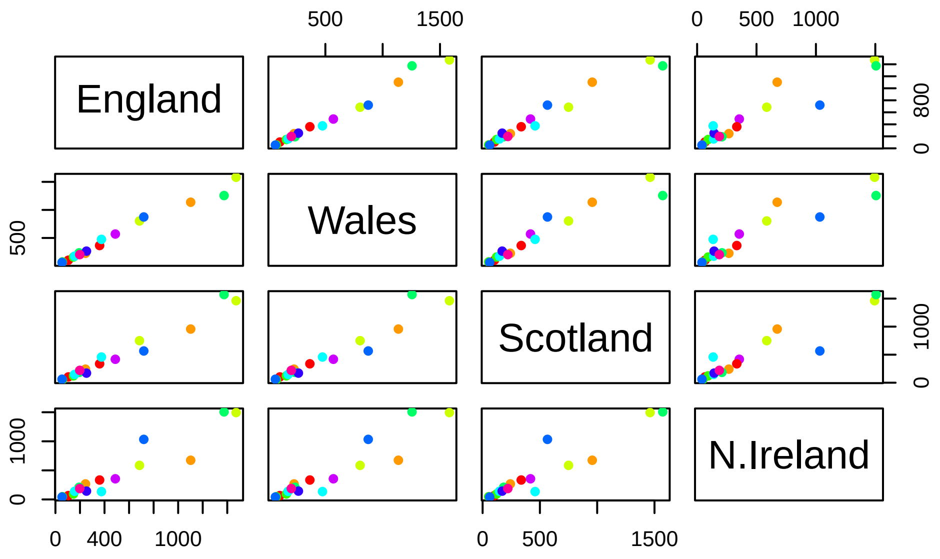


```
barplot(as.matrix(x), beside=FALSE, col=rainbow(nrow(x)))
```



There is one plot that can be useful for small datasets:

```
pairs(x, col=rainbow(10), pch=16)
```



Main point: It can be dificult to spot major trends and patterns even in relatively small multivariate datasets (here we only have 17 dimensions, typically we have 1000s).

PCA to the rescue

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

I will take the transpose of our data so the "foods" are in the columns:

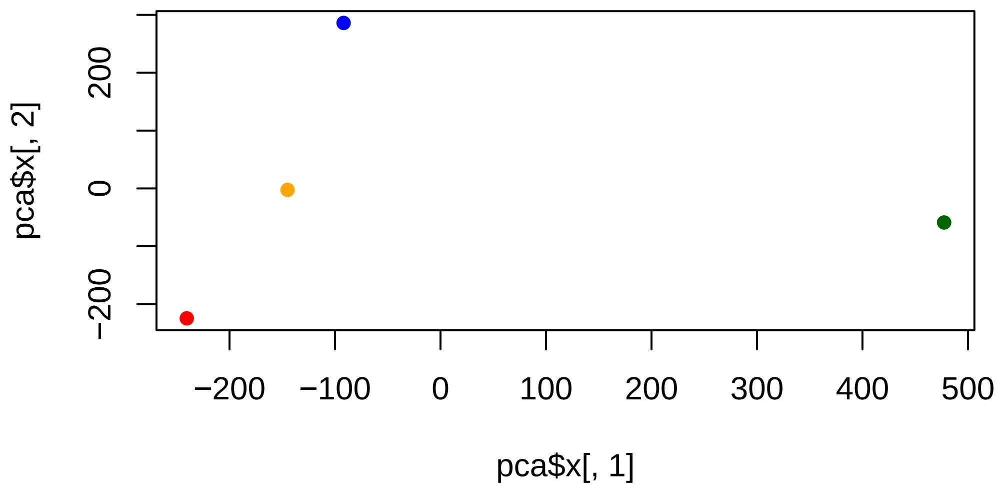
```r
pca <- prcomp( t(x) )
summary(pca)
```

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 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
```

```r
pca$x
```

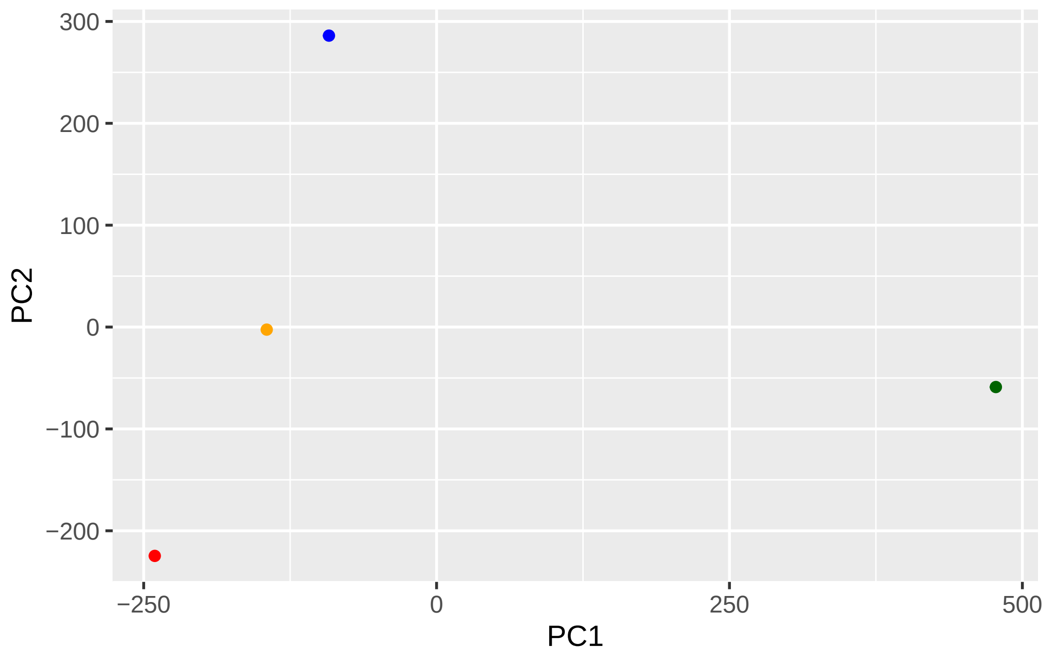
```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -4.894696e-14
Wales     -240.52915 -224.646925 -56.475555  5.700024e-13
Scotland   -91.86934  286.081786 -44.415495 -7.460785e-13
N.Ireland  477.39164  -58.901862  -4.877895  2.321303e-13
```

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

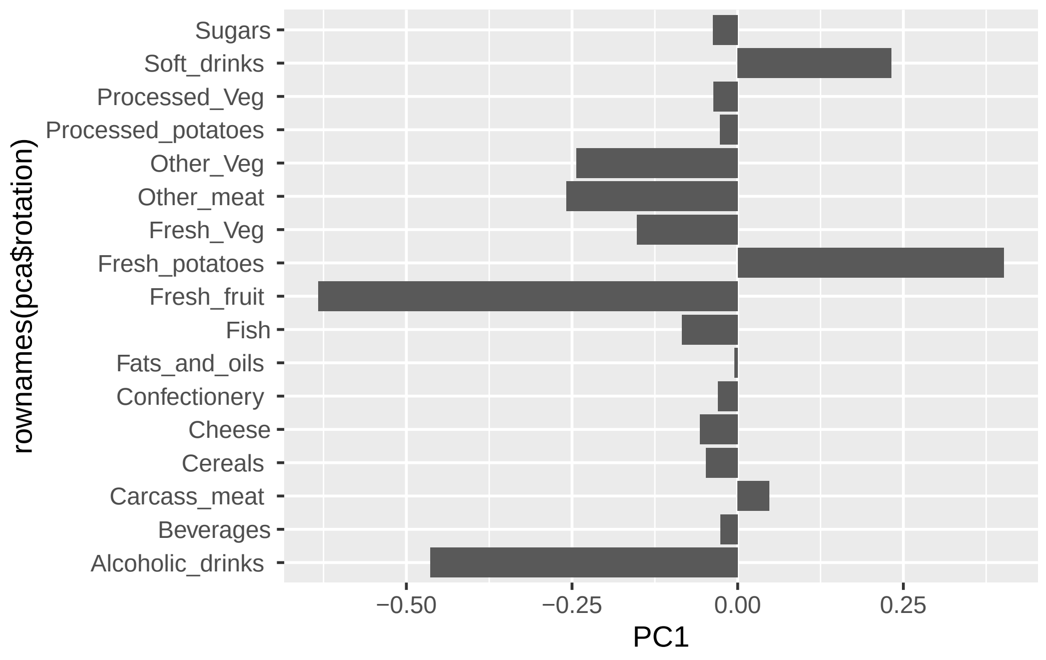


```
library(ggplot2)
```

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



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



PCA looks super useful and we will come back to describe this further next day :)