Class 7: Machine Learning 1

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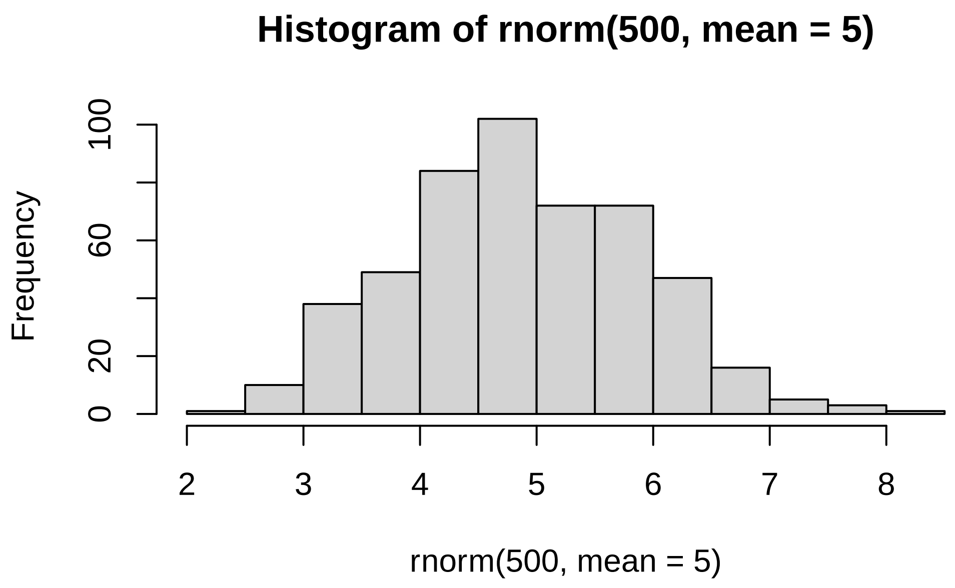
Today we will be exploring some fundamental machine learning methods including clustering and dimensionality reduction

K-means clustering

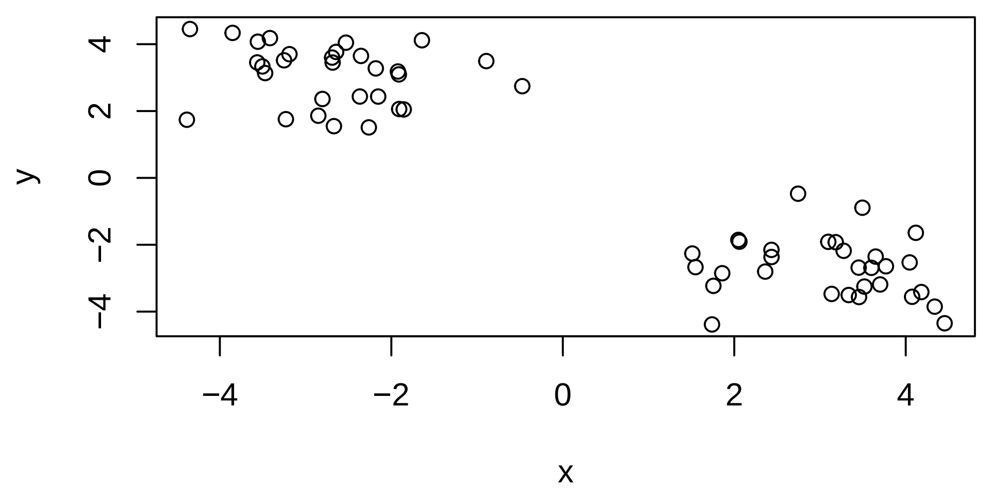
To see how this works let's first makeup some data to cluster where we know what the answer should be. We can use the `rnorm()` function to help here:

```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  3.079132 -2.685518
2 -2.685518  3.079132

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] 47.21263 47.21263
 (between_SS / total_SS =  91.3 %)

Available components:

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

To get 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
```

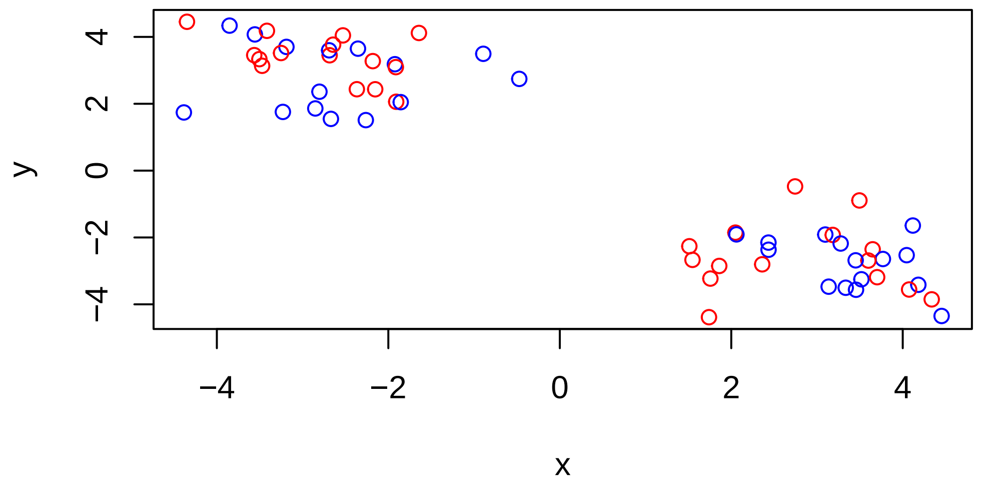
```
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

```
k$centers
```

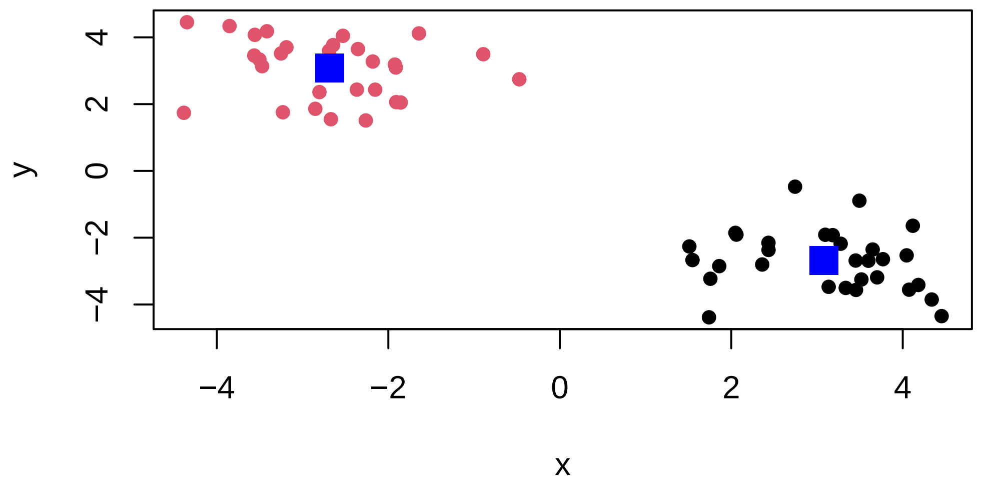
```
          x         y
1  3.079132 -2.685518
2 -2.685518  3.079132
```

> 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)
```

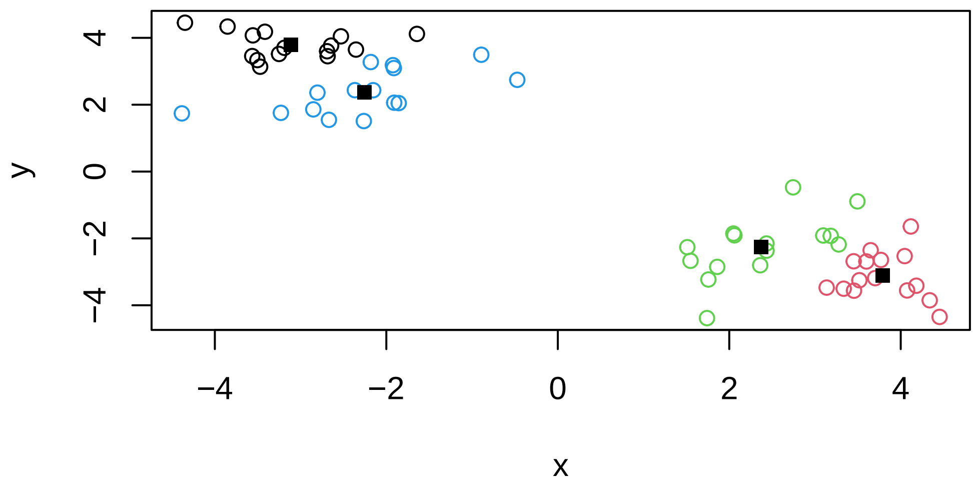


K-means clustering is very popular as it is very fast and relatively straight forward: it takes numeric data as input and returns the clusters membership vector etc.

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

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

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

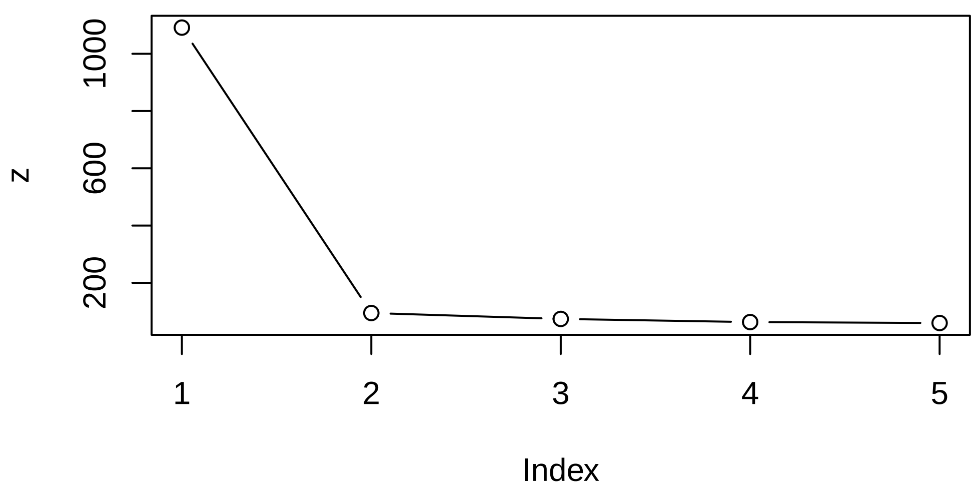


Scree plot to pick k `centers` value

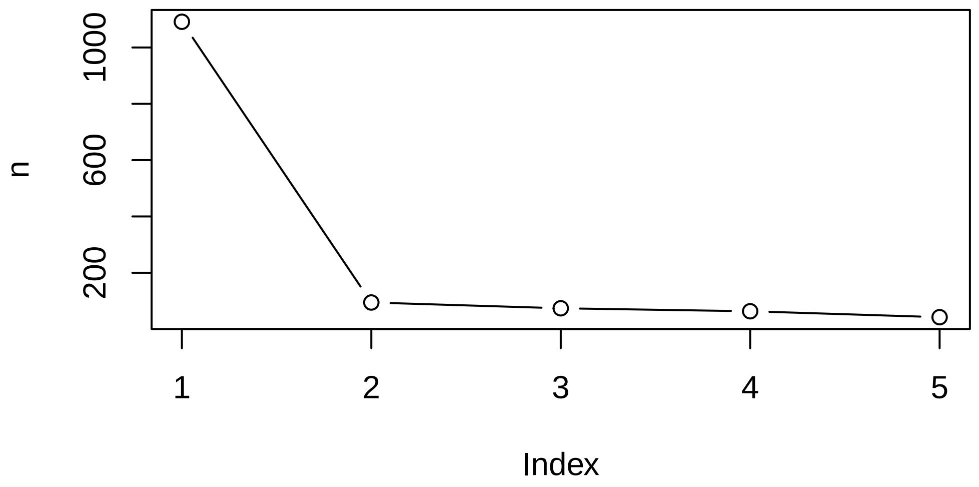
brute-force

```
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)
```

```
z <- c( k1$tot.withinss,
        k2$tot.withinss,
        k3$tot.withinss,
        k4$tot.withinss,
        k5$tot.withinss)
plot(z,type="b")
```



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



Hierarchical Clustering

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

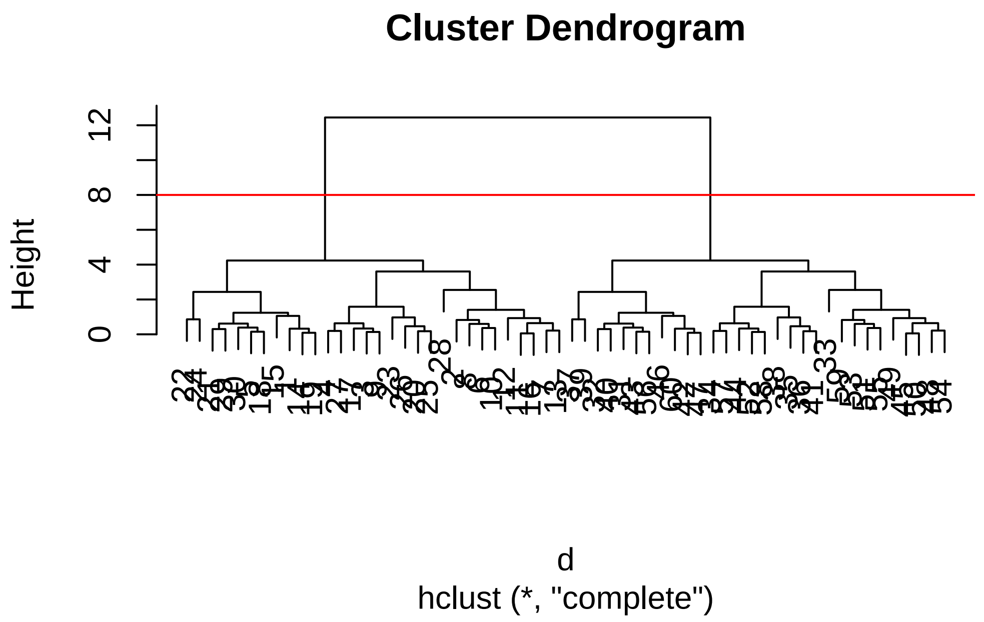
```
d <- dist(x)
hc <-hclust(d)
hc
```

```
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 results) we can "cut" the tree at any given height or at a height that yields a given "k" groups.

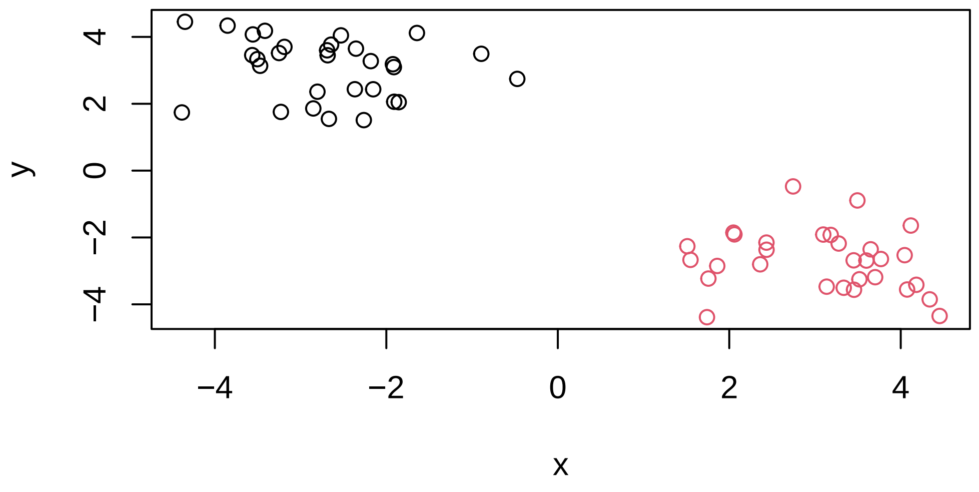
```r
cutree(hc, h=8)
```

```
 [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 out hclust result coloring

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



Principle Component Analysis (PCA)

PCA of UK food data

Import food data from an online CSV file:

```
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
```

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

```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
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Soft_drinks            1374  1256     1572      1506
Alcoholic_drinks        375   475      458       135
Confectionery            54    64       62        41
```
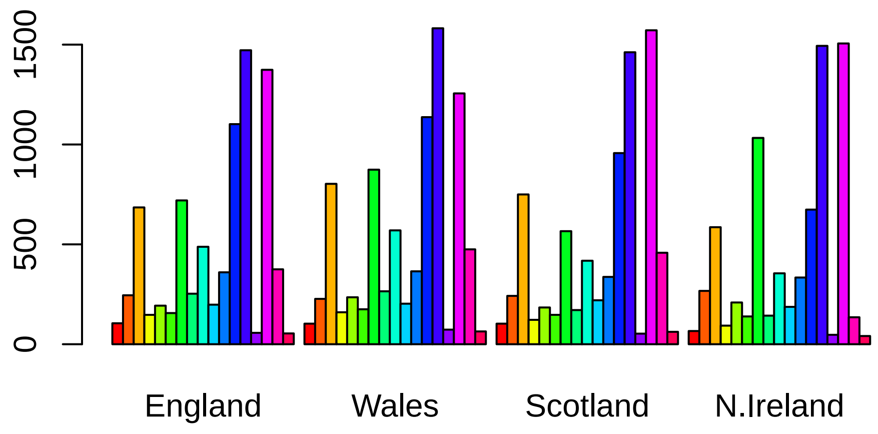
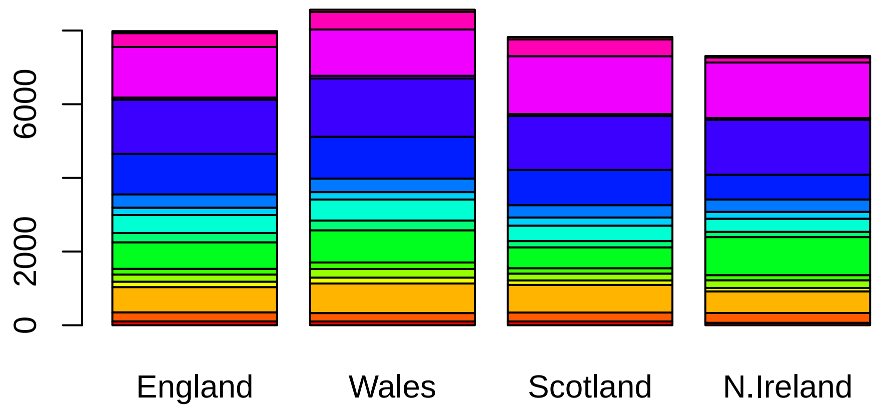

Some base figures

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

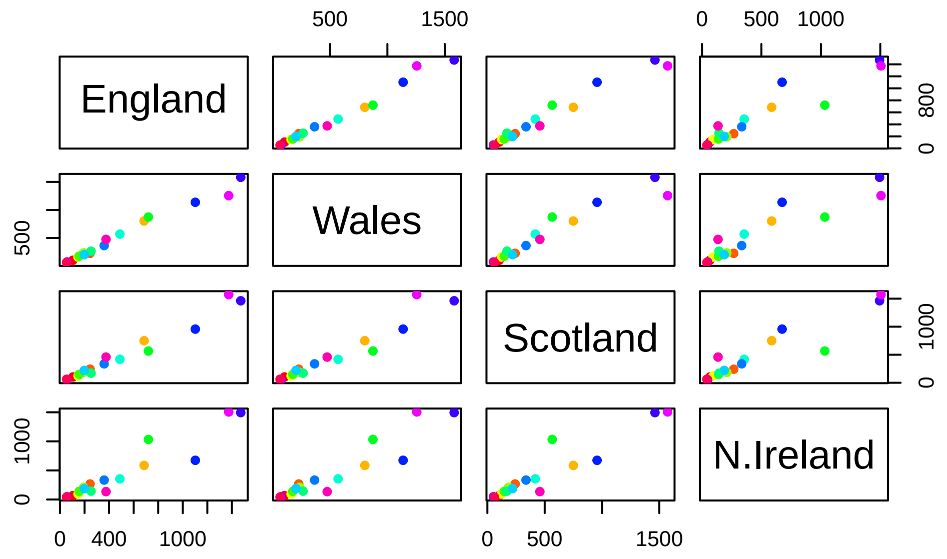


```r
barplot(as.matrix(x), col=rainbow(nrow(x)))
```



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

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



Main point: It can be difficult 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

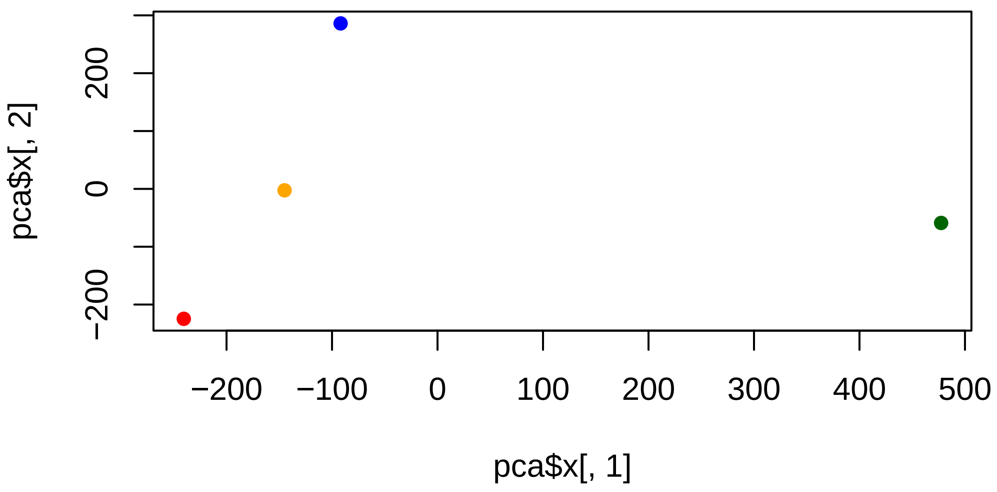
The main function in "base" R for PCA is called `prcomp()`

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

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

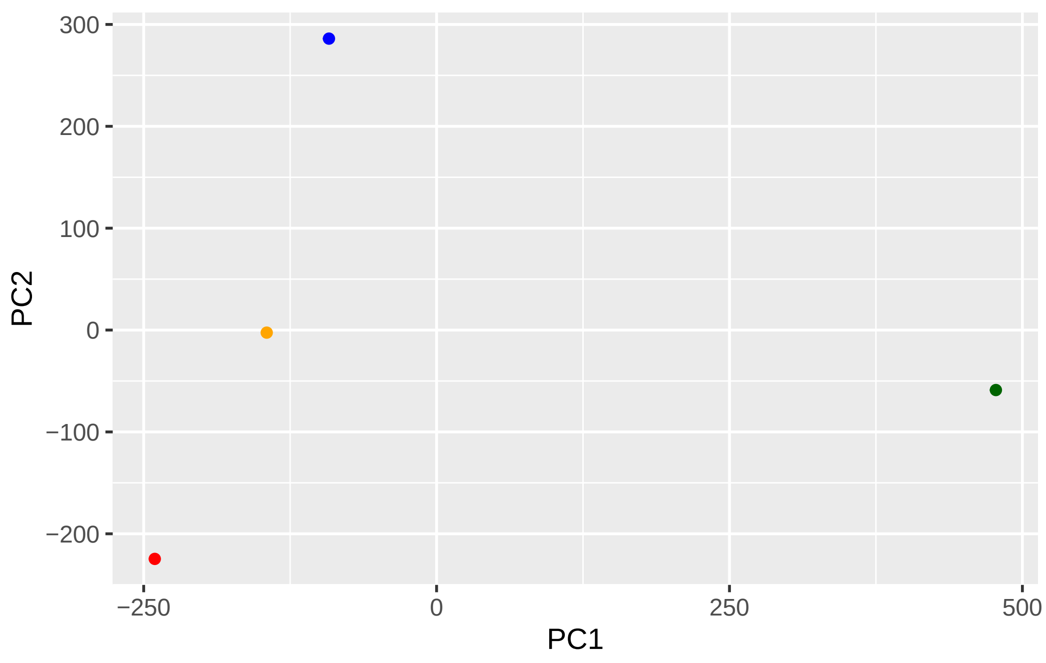
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 2.921e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

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

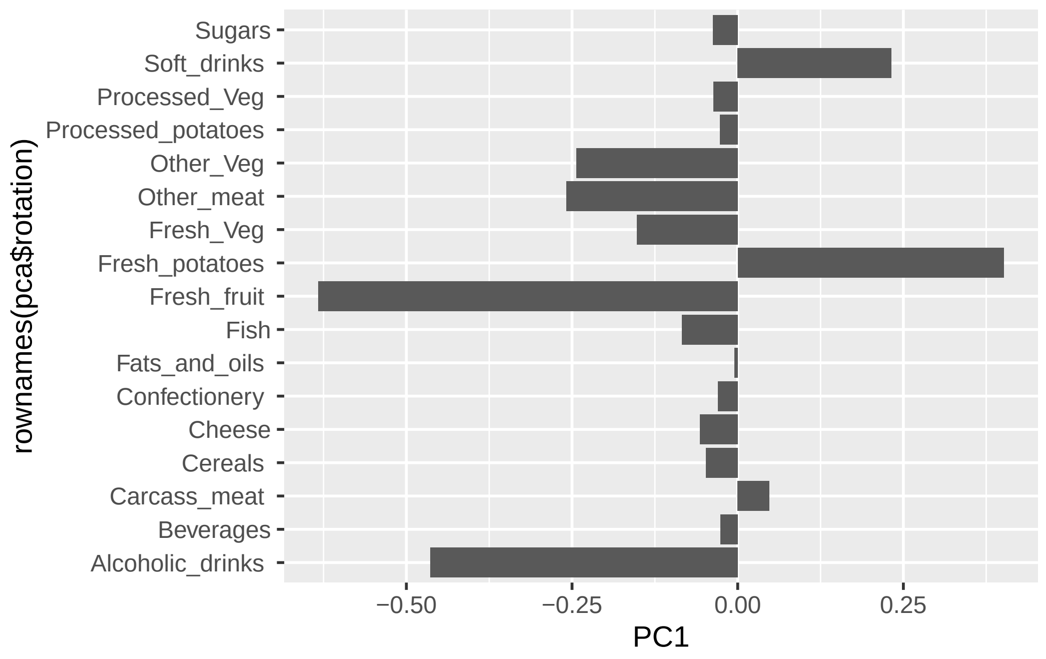


```r
library(ggplot2)
```

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



```r
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 :)