Class 7: Machine Learning I

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Today we are going learn how to apply different machine learning methods, begining with clustering:

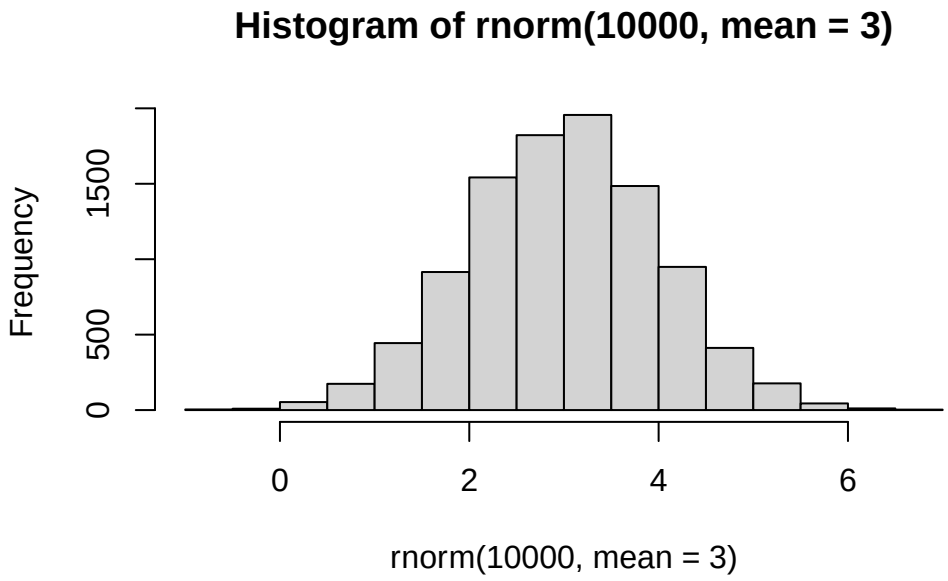
The goal here is to find groups/clusters in your input data.

First I will make up some data with clear groups. For this I will use the `rnorm()` function:

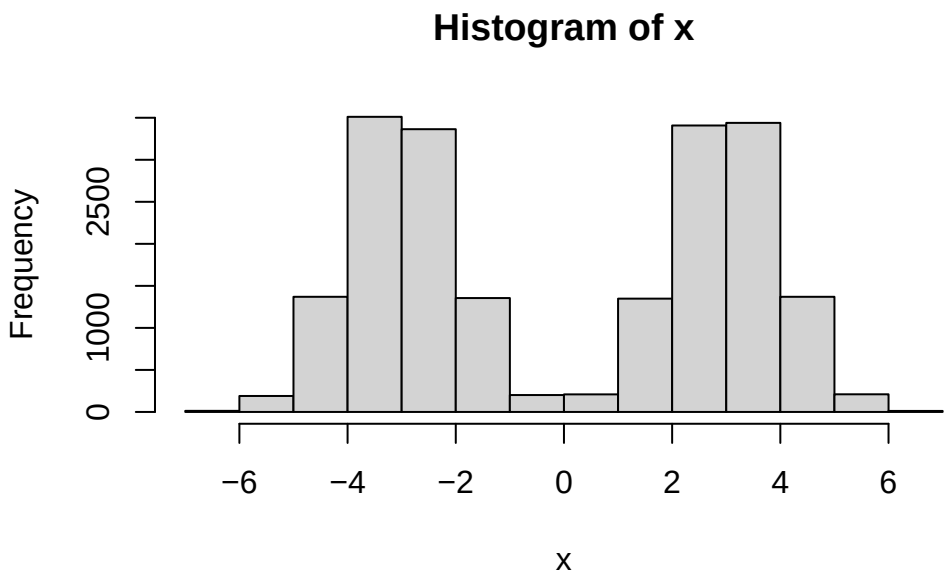
```
rnorm(10)
```

```
 [1] -2.66764641  0.08478972 -0.63371376  0.59045074 -0.16011147 -0.97610539
 [7]  0.27864623 -0.12031448  0.17481372  1.89487970
```

```
hist( rnorm(10000, mean=3) )
```



```r
n <- 10000
x <- c(rnorm(n, -3), rnorm(n, +3))
hist(x)
```

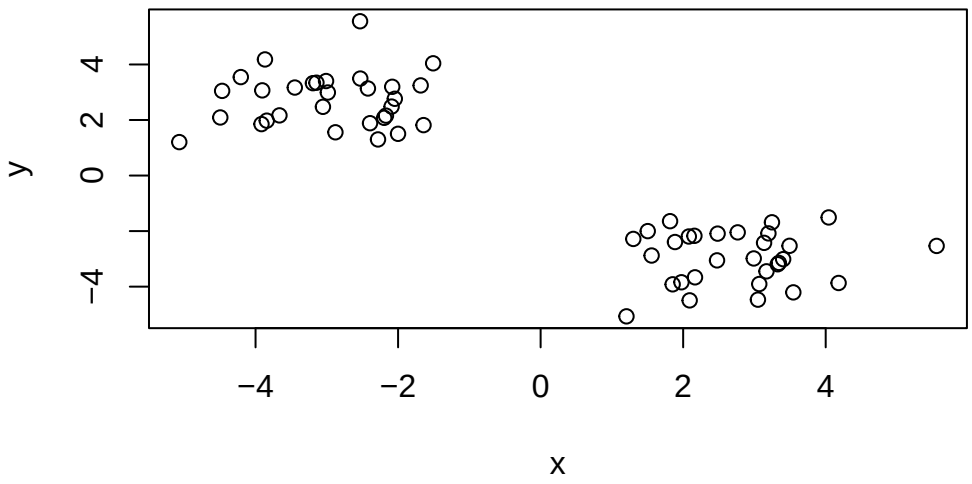



```r
n <- 30
x <- c(rnorm(n, -3), rnorm(n, +3))
y <- rev(x)

z <- cbind(x, y)
head(z)
```

```
             x        y
[1,] -3.842535 1.975916
[2,] -2.879338 1.557367
[3,] -3.449100 3.168791
[4,] -2.533579 5.556358
[5,] -3.010511 3.403109
[6,] -3.905420 3.067628
```

```r
plot(z)
```



Use the `kmeans()` function setting k to 2 and nstart=20

Inspect/print the results

> Q. How many points are in each cluster?
>
> Q. What 'component' of your result object details - cluster size? - cluster assignment/membership? - cluster center?
>
> Q. Plot z colored by the kmeans cluster assignment and add cluster centers as blue points

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

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

Cluster means:
          x         y
1  2.735193 -2.957913
2 -2.957913  2.735193

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 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] 53.40304 53.40304
 (between_SS / total_SS =  90.1 %)

Available components:

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

Results in kmeans object `km`

```
attributes(km)
```

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

$class
[1] "kmeans"
```

cluster size?

```
km$size
```

```
[1] 30 30
```

cluster assignment/membership?

```
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 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
```

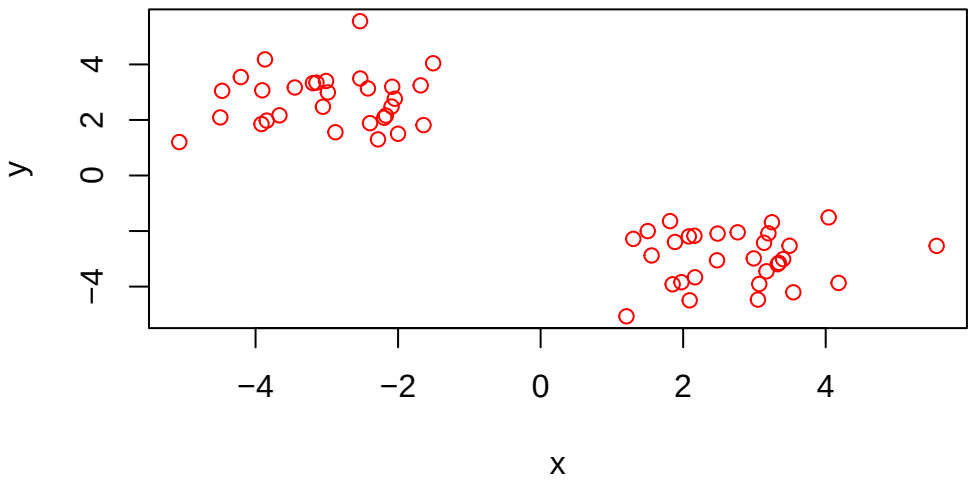
cluster center?

```
km$centers
```

```
          x         y
1  2.735193 -2.957913
2 -2.957913  2.735193
```

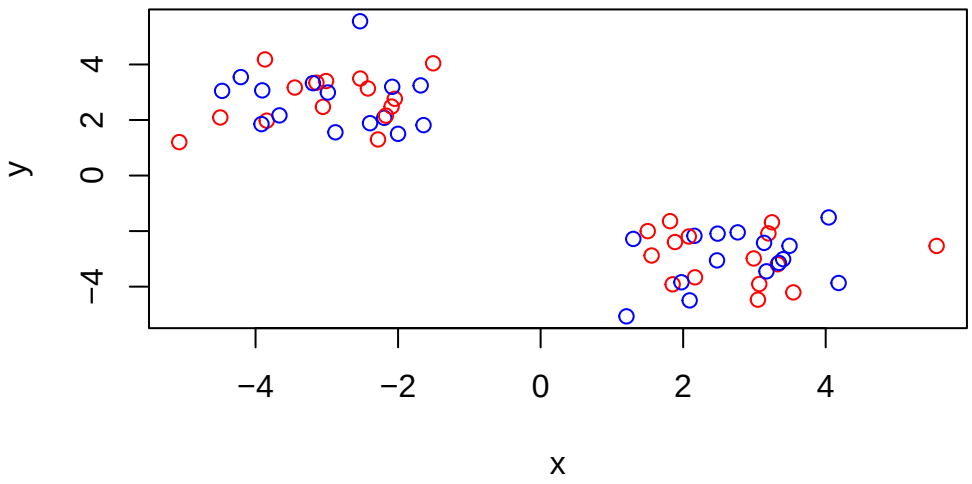
Q. Plot z colored by the kmeans cluster assignment and add cluster centers as blue points

```
plot(z, col="red")
```

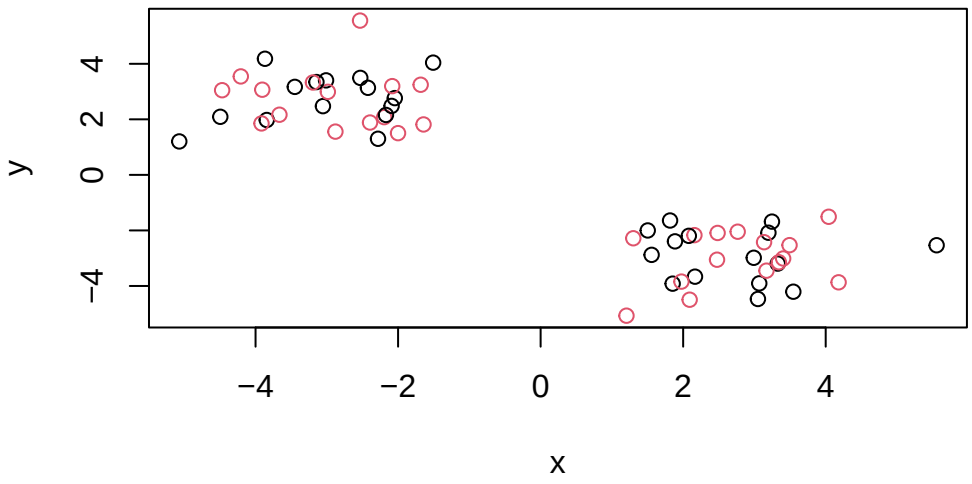


R will re-cycle the shorter color vector to be the same length as the longer (number of data points) in z

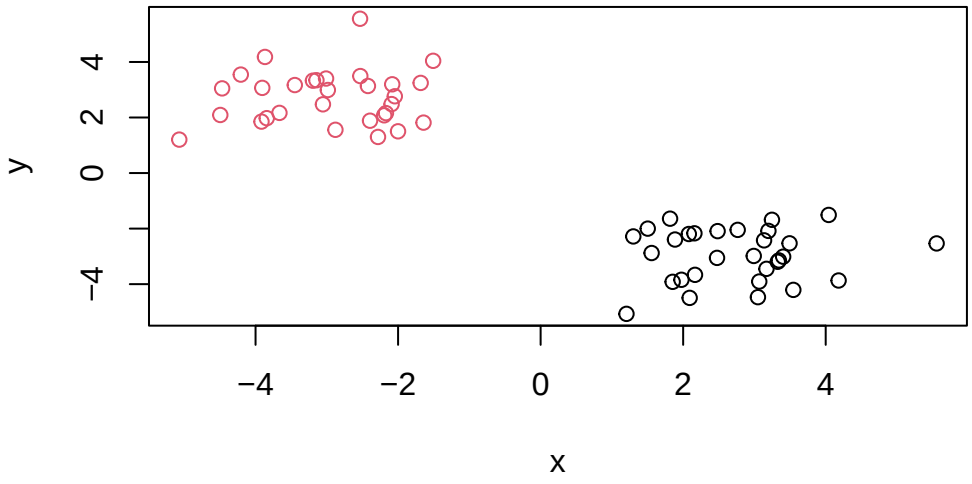
```
plot(z, col=c("red","blue") )
```




```
plot(z, col=c(1,2) )
```

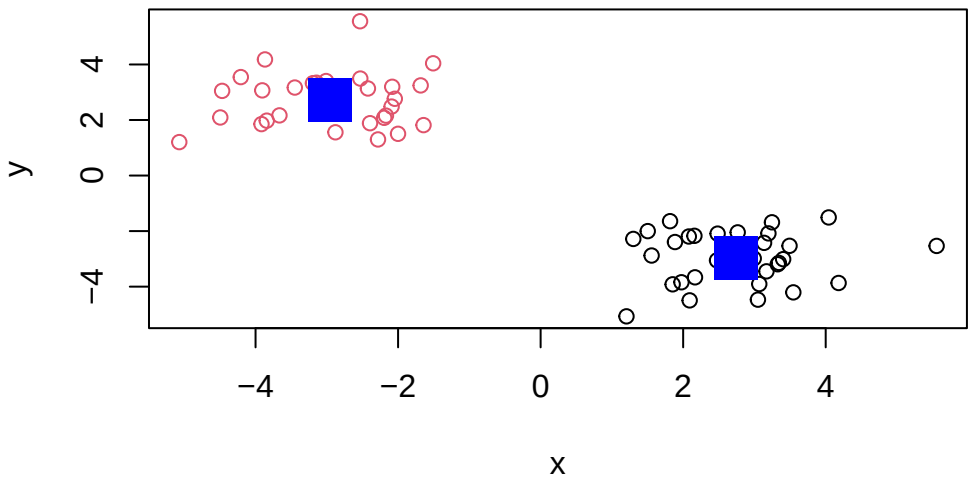


```r
plot(z, col=km$cluster)
```



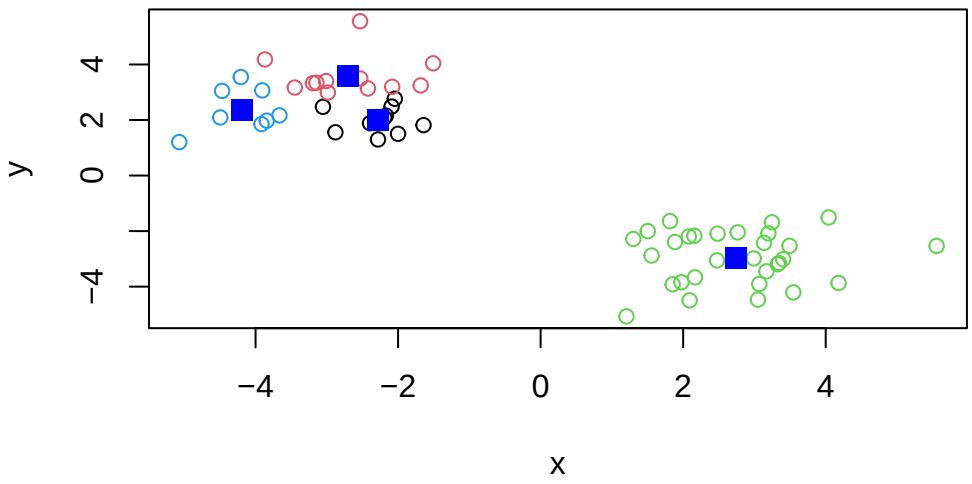
We can use the `points()` function to add new points to an existing plot… like the cluster centers.

```r
plot(z, col=km$cluster)
points(km$centers, col="blue", pch=15, cex=3)
```



Q. Can you run kmeans and ask for 4 clusters please and plot the results like we have done above?

```
km4 <- kmeans(z, centers = 4)
plot(z, col=km4$cluster)
points(km4$centers, col="blue", pch=15, cex=1.5)
```



Hierarchical Clustering

Let's take our same made-up data **z** and see how hclust works.

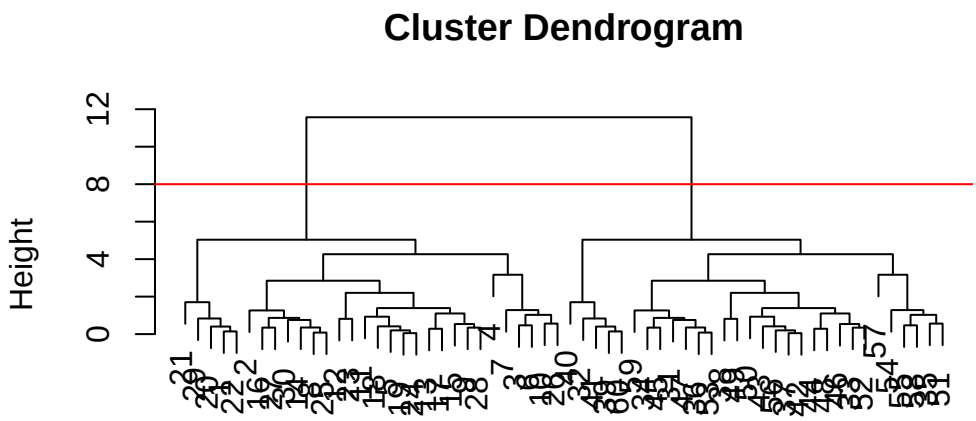
First we need a distance matrix of our data to be clustered.

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

```
Call:
hclust(d = d)

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

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



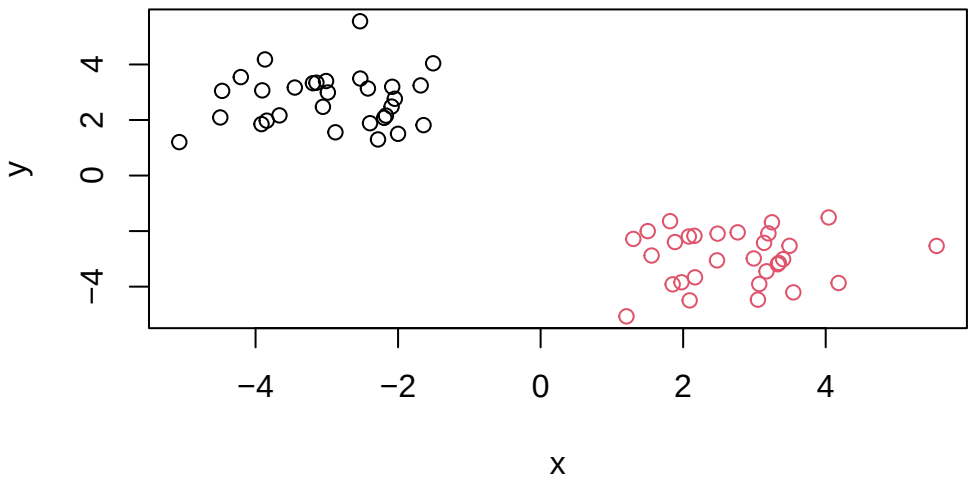
I can get my cluster membership vector by "cutting the tree" with the `cutree()` function like so:

```
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 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
```

Can you plot `z` colored by our hclust results:

```
plot(z, col=grps)
```



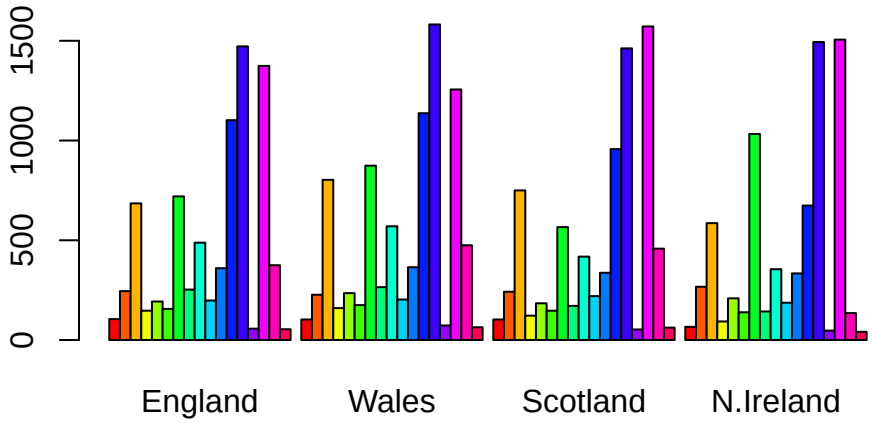
PCA of UK food data

Read data from the UK on food consumption in different parts of the UK

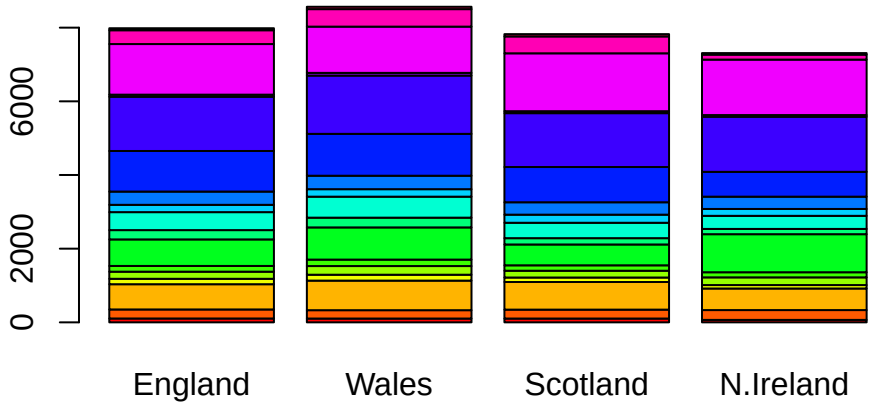
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names=1)
head(x)
```

```
              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
```

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

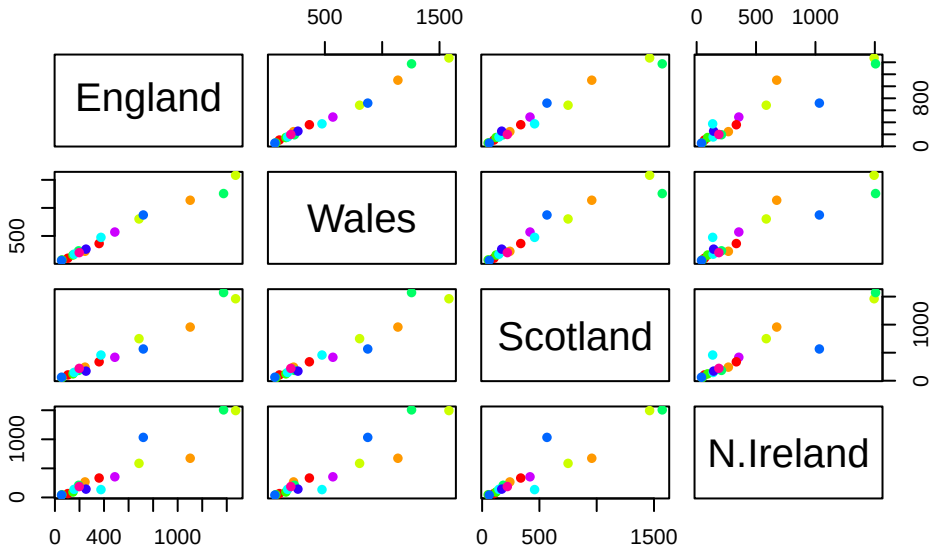



```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



A so-called "Pairs" plot can be useful for small datasets like this one

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



It is hard to see structure and trends in even this small data-set. How will we ever do this when we have big datasets with 1,000s or 10s of thousands of things we are measuring…

PCA to the rescue

Let's see how PCA deals with this dataset. So main function in base R to do PCA is called `prcomp()`

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

```
Importance of components:
                            PC1      PC2      PC3        PC4
Standard deviation     324.1502 212.7478 73.87622 4.189e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

Let's see what is inside this `pca` object that we created from running `prcomp()`

```
attributes(pca)
```

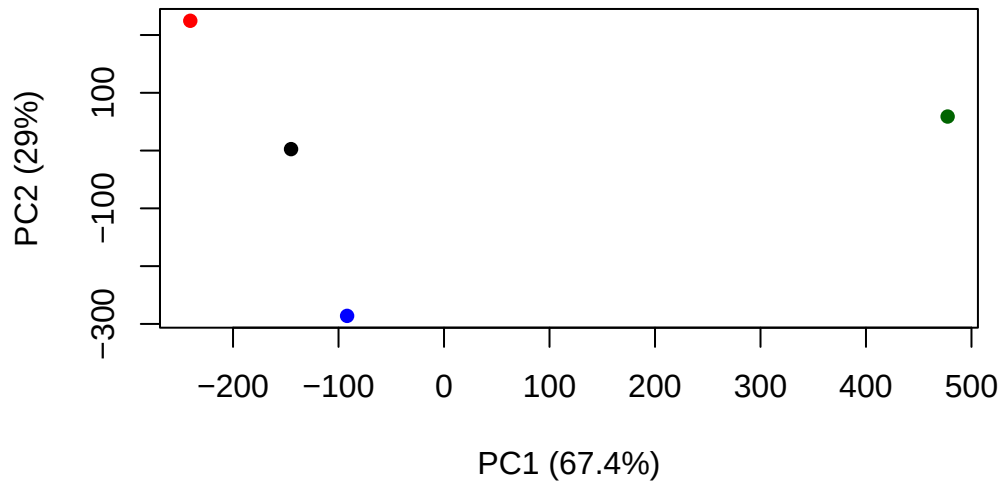
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

```
pca$x
```

```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  2.842865e-14
Wales     -240.52915  224.646925   56.475555  7.804382e-13
Scotland   -91.86934 -286.081786   44.415495 -9.614462e-13
N.Ireland  477.39164   58.901862    4.877895  1.448078e-13
```

```
plot(pca$x[,1], pca$x[,2],
     col=c("black","red","blue","darkgreen"), pch=16,
     xlab="PC1 (67.4%)", ylab="PC2 (29%)")
```



Loadings plot

```r
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```