Class 7: Machine Learning 1

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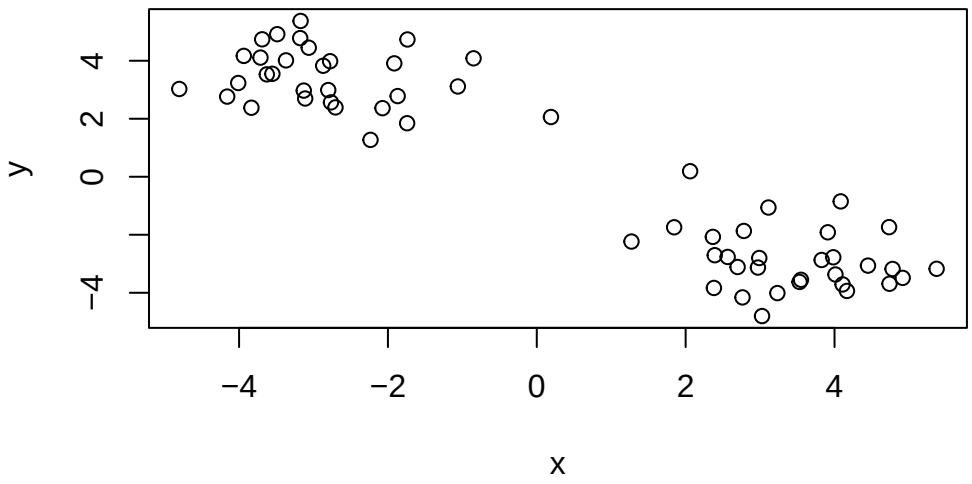
Before we get into clustering methods let's make some sample data to cluster where we know what the answer should be.

To help with this I will use the `rnorm()` function.

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



K-mean clustering

The function in base R for k-means clustering is called `kmeans()`.

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

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

Cluster means:
          x         y
1  3.420498 -2.835073
2 -2.835073  3.420498

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 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

Within cluster sum of squares by cluster:
[1] 64.37361 64.37361
 (between_SS / total_SS =  90.1 %)

Available components:

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

```
km$centers
```

```
          x         y
1  3.420498 -2.835073
2 -2.835073  3.420498
```

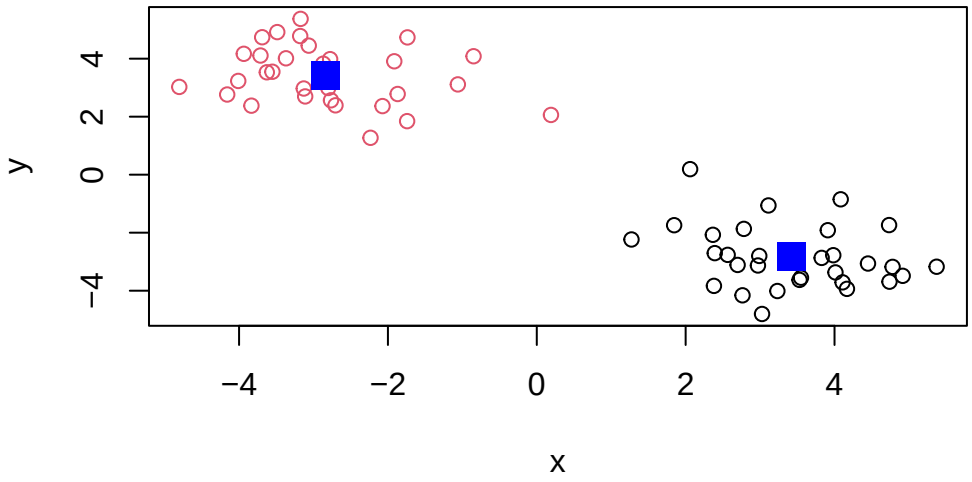
Q. Print out the cluster membership vector (i.e. our main answer)

```
km$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 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
```

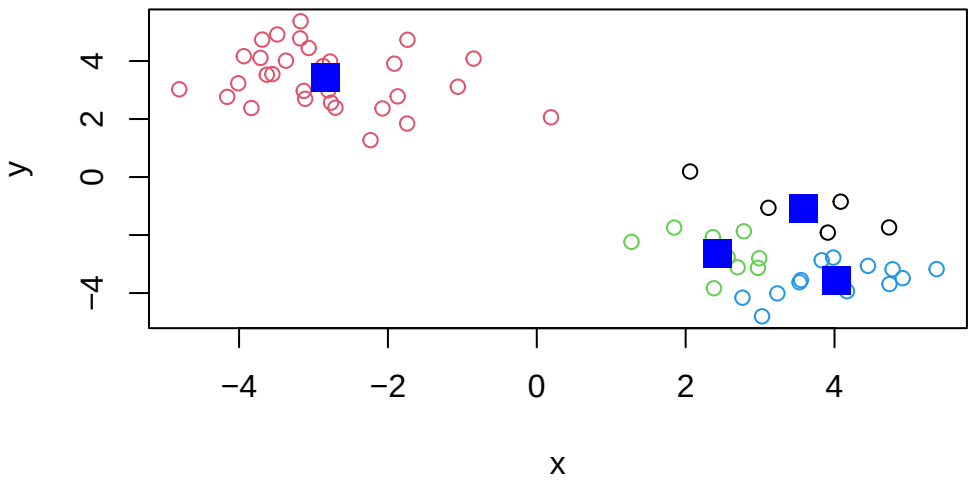
Plot with clustering result and add cluster centers:

```
plot(z, col=km$cluster)
points(km$centers, col="blue", pch=15, cex=2)
```



Q. Can you cluster our data in 'z' into four clusters please?

```
km4 <- kmeans(z, 4)
plot(z, col=km4$cluster)
points(km4$centers, col="blue", pch=15, cex=2)
```



Scree Plot - scree is rubble at the base of a cliff - big drop at the cliff, A way to tell how many clusters you want - looks for inflection point in sum of squares (ss) vs k plot - you want the drop off - where each change in k clusters results in a smaller decrease in ss - it will always decrease as the points will always be closer together with infinitely more clusters, but after a certain point there are diminishing returns Won't always be an inflection point, means there isnt great reason for you to choose that number of clusters kmeans is super quick, works well with large datasets, will do everything for your, but will always give you an answer, whatever you ask it for

Hirarchical Clustering

The main function for hierarchical clustering in base R is called `hclust()`

Unlike `kmeans()` I can not just pass in my data as input I first need a distance matrix from my data.

dist - can feed it anything that is a number describing how far apart points are - in euclidian space, manhattan distance etc

object oriented - means it has methods specific for type of object

height of bar means that those points are more different - more separation means more dissimilarities between data that it separates

cut like a tree where it is easiest to cut, have largest height, and separate so that you have the most leaves attached to the branch below

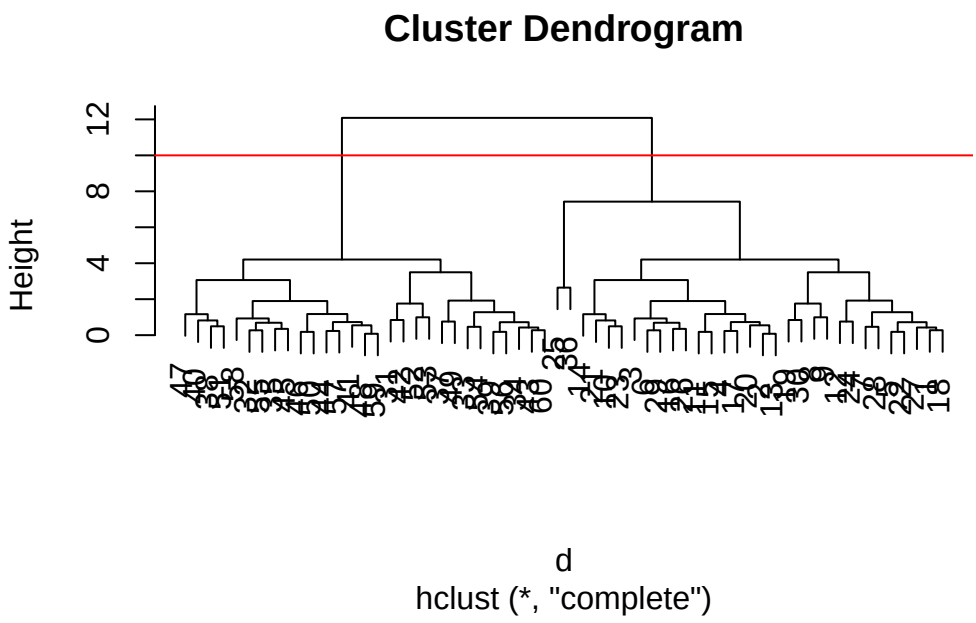
```
?hclust()
```

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

```
Call:
hclust(d = d)

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

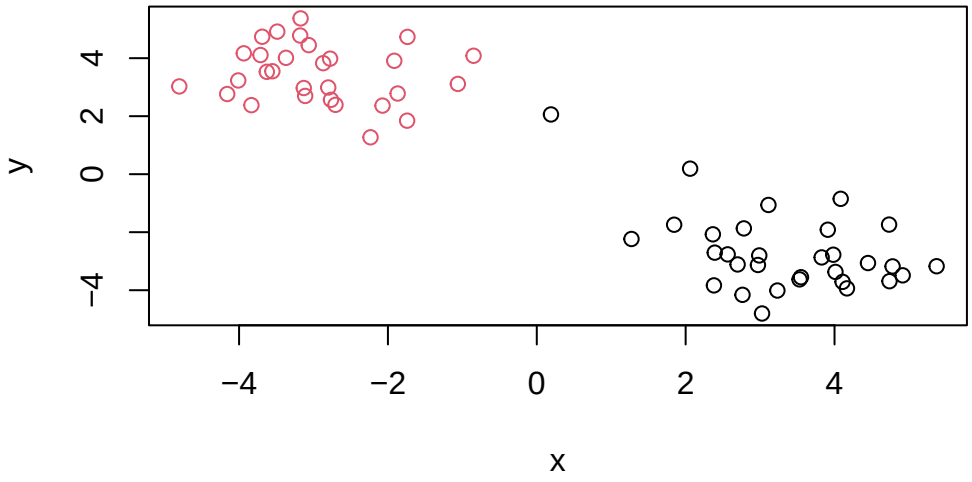
There is a specific hclust plot() method...

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



To get my main clustering result (i.e. the membership vector) I can "cut" my tree at a given height. To do this I will use the 'cutree()' function

```
grps <- cutree(hc, h=10)
# can also use arguement k for specifying how many clusters you want - h specifies height, k
plot(z, col=grps)
```



Principal Component Analysis

Used anywhere there are lots of observations and you want to look for larger patterns Similar to principal coordinate analysis - coordinate is with distance matrix instead of covariance matrix (component)

Sets up new axes that are better - data is more spread along the axis meaning that it captures the most variance in the data

Principal component analysis (PCA) is a well established "multivariate statistical technique" used to reduce the dimensionality of a complex data set to a more manageable number (typically 2D or 3D). This method is particularly useful for highlighting strong paterns and relationships in large datasets (i.e. revealing major similarities and diferences) that are otherwise hard to visualize. As we will see again and again in this course PCA is often used to make all sorts of bioinformatics data easy to explore and visualize.

Axes always has to be perpendicular - how is this accounted for in math? Doesnt just maximize PC1 - it maximizes explaining the total variance in two variables/dimensions - can you run PCA with more than 2 dimensions?

```
url <- "https://tinyurl.com/UK-foods"
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
```

```
## Q1. How many rows and columns are in your new data frame named x? What R functions could
## Complete the following code to find out how many rows and columns are in x?
dim(x)
```

```
[1] 17  4
```

```
head(x)
```

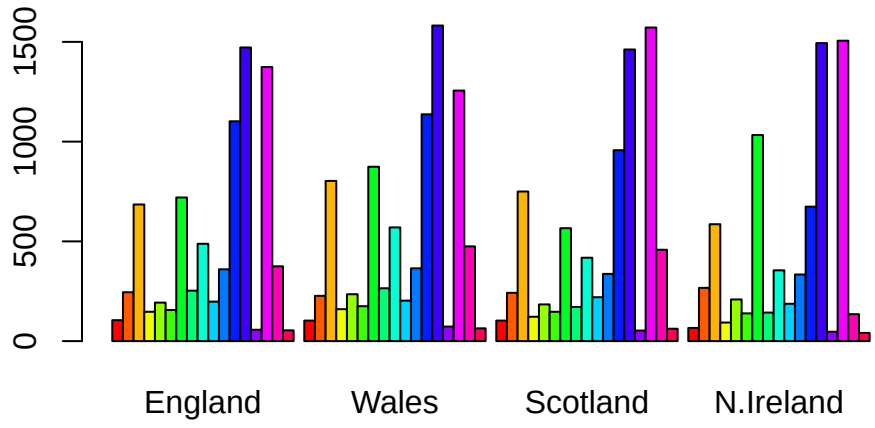
```
              England Wales Scotland N.Ireland
Cheese            105   103      103        66
Carcass_meat      245   227      242       267
Other_meat        685   803      750       586
Fish              147   160      122        93
```

```
Fats_and_oils      193    235       184        209
Sugars             156    175       147        139
```

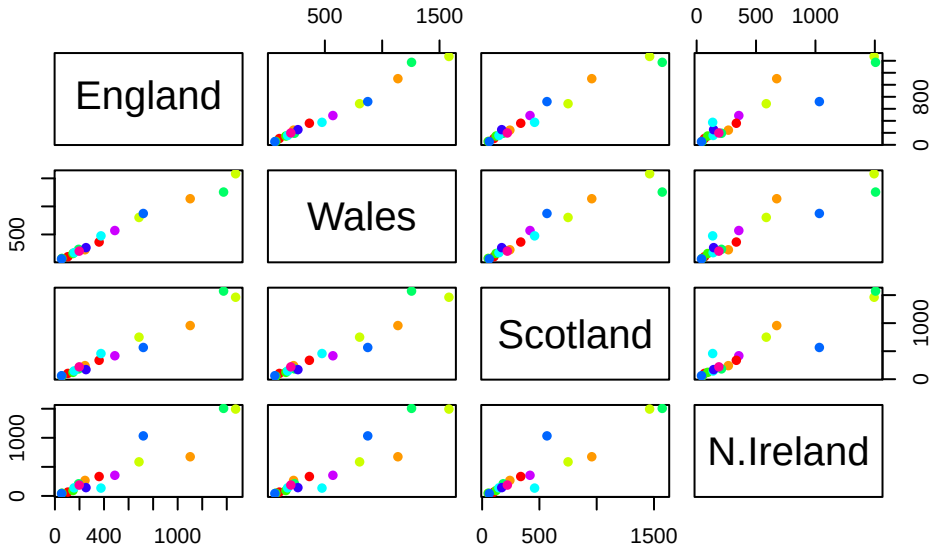
```
tail(x)
```

```
                England Wales Scotland N.Ireland
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
```

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




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



PCA to the rescue

The main function to do PCA in base R is called 'prcomp()'

```
# Use the prcomp() PCA function
# You want the things you care about - like gene expression data - in columns
# Use t to transpose the data
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
```

Let's see what is inside our result object `pca` that we just calculated

```
attributes(pca)
```

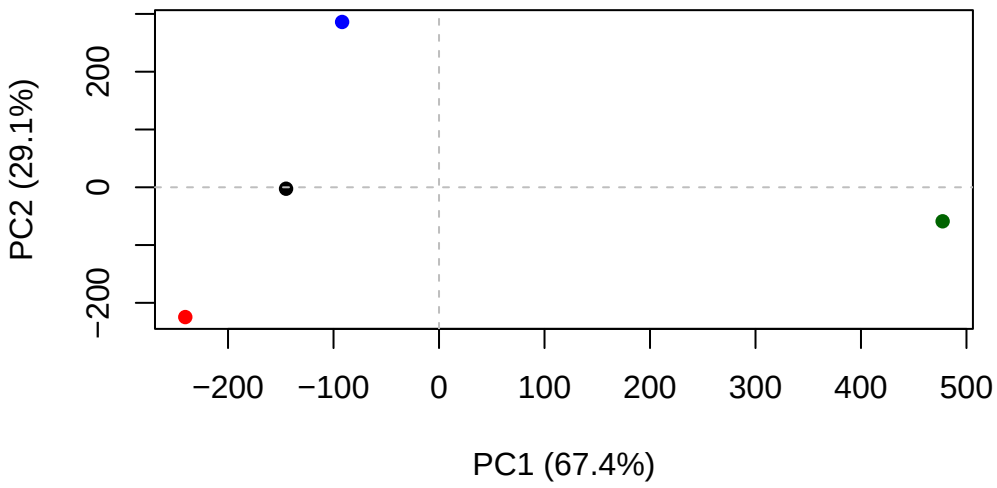
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

```
pca$x
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -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
```

To make our main result figure, called a "PC plot" (or "score plot", "ordination plot or"PC1 vs PC2 plot".)

```
plot(pca$x[,1], pca$x[,2],
     col=c("black", "red", "blue", "darkgreen"),
     pch=16, xlab="PC1 (67.4%)", ylab="PC2 (29.1%)")
abline(h=0, col='gray', lty=2)
abline(v=0, col='gray', lty=2)
```



Variable loadings plot

Can give us insight on how the original variables (in this case the foods) contribute to our new PC axis

```
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```