Class 7: Machine Learning

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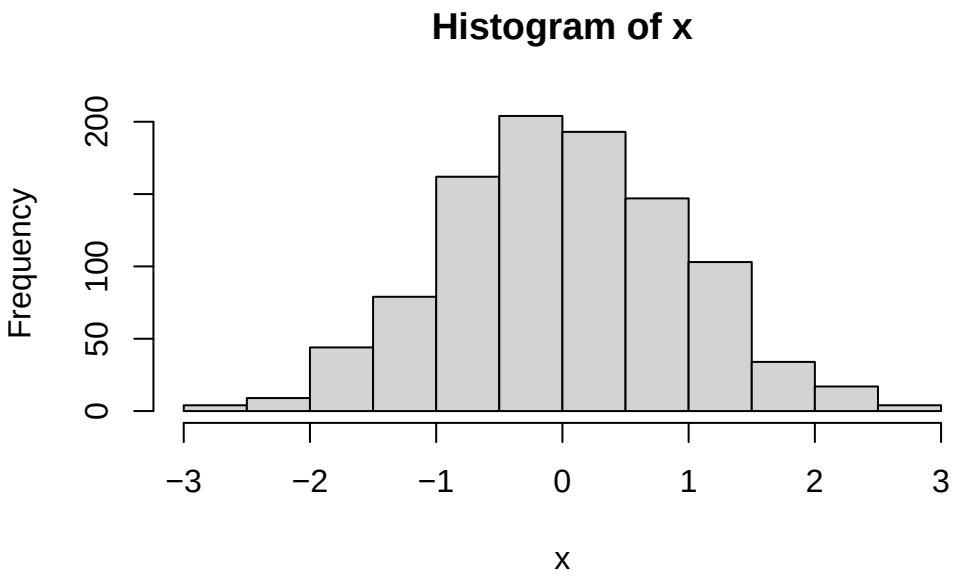
#Clustering Methods

The broad goal here is to find groupings (clusters) in your input data.

##Kmeans

First, let's make up some data to cluster.

```
x <- rnorm(1000)
hist(x)
```



Make a vector of length 60 with 30 points centered at -3 and 30 points centered at +3

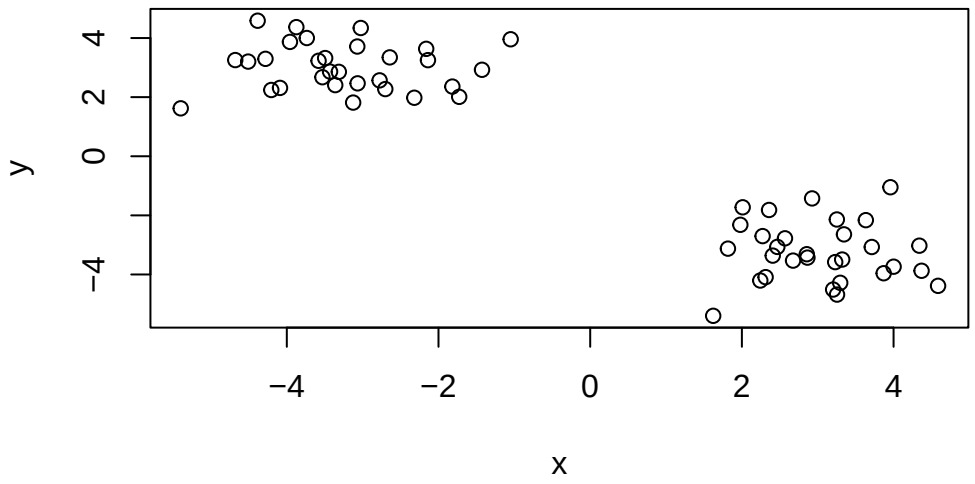
```
tmp <- c(rnorm(30, mean = -3), rnorm(30, mean = 3))
```

I will now make a wee x and y dataset with 2 groups of points.

```
rev( c(1:5) )
```

```
[1] 5 4 3 2 1
```

```
x <- cbind(x=tmp, y=rev(tmp))
plot(x)
```




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

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

Cluster means:
          x         y
1 -3.229090  3.025082
```

```
2  3.025082 -3.229090

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

Within cluster sum of squares by cluster:
[1] 49.04853 49.04853
 (between_SS / total_SS =  92.3 %)

Available components:

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

Q. From your result object `k` how many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q. what "component" of your result ov=bject details the cluster membership?

```
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 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
```

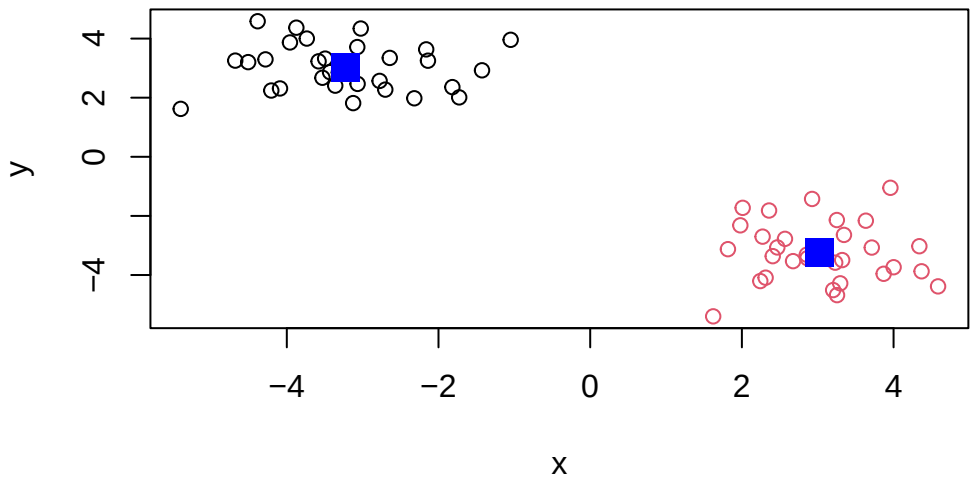
Q. Cluster centers?

```
k$centers
```

```
          x         y
1 -3.229090  3.025082
2  3.025082 -3.229090
```

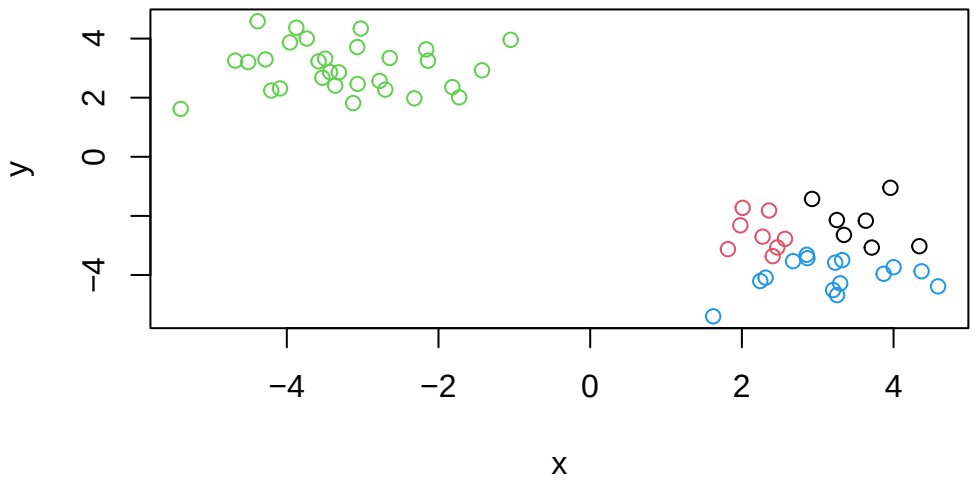
Q. Plot of our clustering results

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



We can cluster into 4 groups

```
# kmeans
k4 <- kmeans(x, centers= 4)
# plot results
plot(x, col = k4$cluster)
```



A big limitation of kmeans is that it does what you ask even if you ask for silly clusters.

Hierarchial Clustering

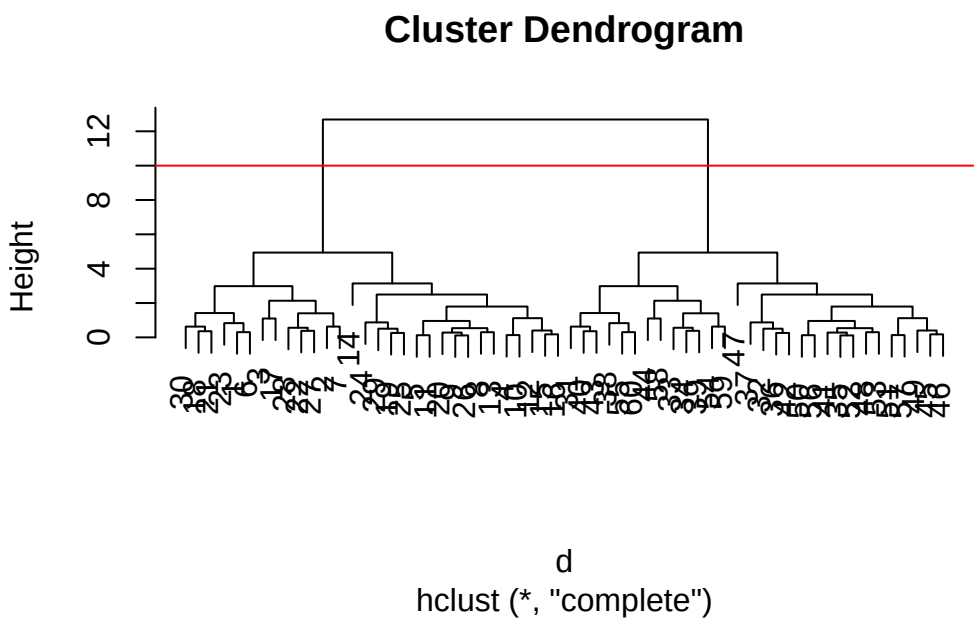
The main base R function for Hierarchial Clustering is `hclust()`. unlike `kmeans()`. you can not just pass it your data as input. you first need to calculate a distance matrix.

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

```
Call:
hclust(d = d)

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

Use `plot()` to view results

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



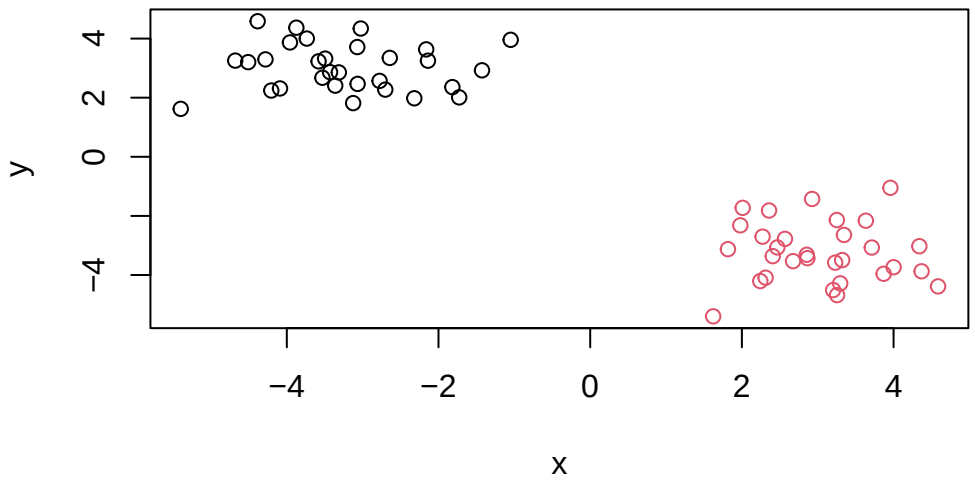
To make the "cut" and get our cluster membership vector we can use `cutree()` function.

```
grps <- cutree(hc, h=10)
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 2 2
```

Make a plot of our data colored by hclust results.

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



Pricipal Componet Analysis (PCA)

Here we will do Principal Component Analysis (PCA) on some food data from UK.

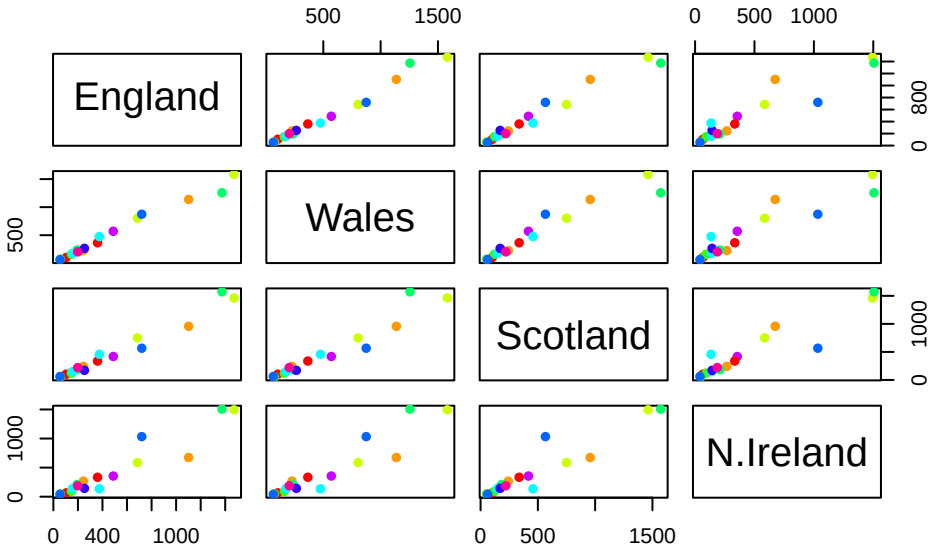
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
x
```

	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

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

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



PCA to the rescue

The main "base" R function for PCA is called `prcomp()`. Here we need to take the transpose of our input

```
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
```

Q. How much variance is captured in 2PCs?

96.5%

To make our main "PC Score Plot" or "PC1 vs. PC2 plot", (a.k.a "PC plot", or "ordination plot".)

```
attributes(pca)
```

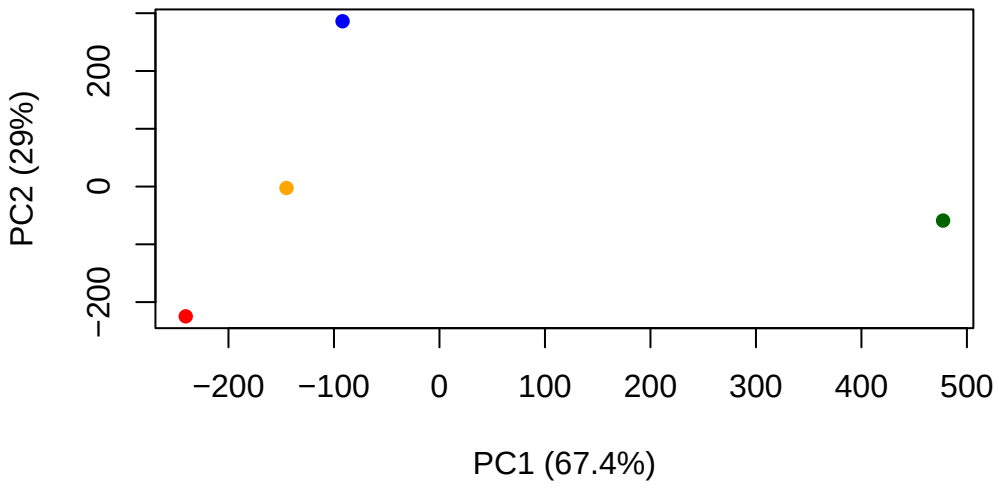
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

We are after the `pca$x` result component to make our main PCA plot.

```
pca$x
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -9.152022e-15
Wales     -240.52915 -224.646925 -56.475555  5.560040e-13
Scotland   -91.86934  286.081786 -44.415495 -6.638419e-13
N.Ireland  477.39164  -58.901862  -4.877895  1.329771e-13
```

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



Another important result from PCA is how the original variables (in this case the foods) contribute to the PCs.

This is contained i the `pca$rotation` object - folks often call this the "loading" or "contributions" to the PCs.

```
pca$rotation
```

	PC1	PC2	PC3	PC4
Cheese	-0.056955380	0.016012850	0.02394295	-0.409382587
Carcass_meat	0.047927628	0.013915823	0.06367111	0.729481922
Other_meat	-0.258916658	-0.015331138	-0.55384854	0.331001134
Fish	-0.084414983	-0.050754947	0.03906481	0.022375878
Fats_and_oils	-0.005193623	-0.095388656	-0.12522257	0.034512161
Sugars	-0.037620983	-0.043021699	-0.03605745	0.024943337
Fresh_potatoes	0.401402060	-0.715017078	-0.20668248	0.021396007
Fresh_Veg	-0.151849942	-0.144900268	0.21382237	0.001606882
Other_Veg	-0.243593729	-0.225450923	-0.05332841	0.031153231
Processed_potatoes	-0.026886233	0.042850761	-0.07364902	-0.017379680
Processed_Veg	-0.036488269	-0.045451802	0.05289191	0.021250980
Fresh_fruit	-0.632640898	-0.177740743	0.40012865	0.227657348
Cereals	-0.047702858	-0.212599678	-0.35884921	0.100043319

```
Beverages           -0.026187756 -0.030560542 -0.04135860 -0.018382072
Soft_drinks          0.232244140  0.555124311 -0.16942648  0.222319484
Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.273126013
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001890737
```

```
#higher values mean more contributions
```

We can make a plot along PC1.

```
library(ggplot2)

contrib <- as.data.frame(pca$rotation)

ggplot(contrib) +
  aes(PC1, rownames(contrib))+
  geom_col()
```