# Class 7: Machine Learning 1

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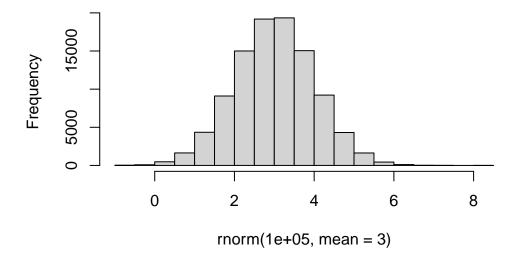
Today we will start our multi-part exploration of some key machine learning methods. We will begin with clustering - finding groupings in data, and then dimensionality reduction.

### Clustering

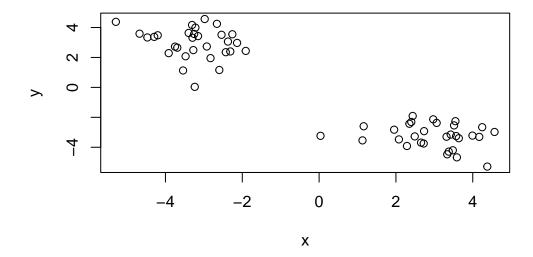
Let's start with "k-means" clustering. The main function in base R for this is kmeans().

```
# Make up some data
hist( rnorm(100000, mean=3))
```

## Histogram of rnorm(1e+05, mean = 3)



```
tmp <- c(rnorm(30, -3), rnorm(30, +3))
x <- cbind(x=tmp, y=rev(tmp))
plot(x)</pre>
```



Now let's try kmeans()

```
km <- kmeans(x, centers=2)
km</pre>
```

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

Cluster means:

```
x y
1 2.953548 -3.246112
2 -3.246112 2.953548
```

Clustering vector:

Within cluster sum of squares by cluster:

[1] 49.06963 49.06963 (between\_SS / total\_SS = 92.2 %)

Available components:

- [1] "cluster" "centers" "totss" "withinss" "tot.withinss"
- [6] "betweenss" "size" "iter" "ifault"
  - Q. How many points are in each cluster?

km\$size

[1] 30 30

Q2. What component of your result object details cluster assignment/ member-ship?

km\$cluster

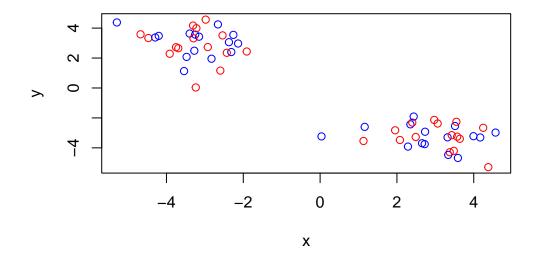
- - Q3. What are centers/mean values of each cluster?

km\$centers

x y 1 2.953548 -3.246112 2 -3.246112 2.953548

Q4. Make a plot of your data showing your clustering results (groupings/clusters and cluster centers).

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

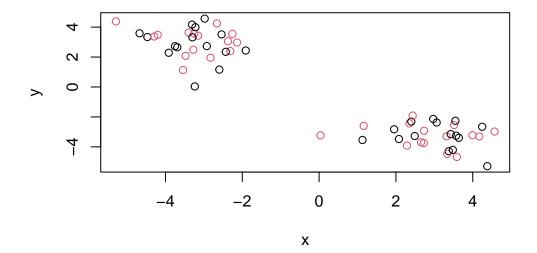


```
c(1:5) + c(100, 1)
```

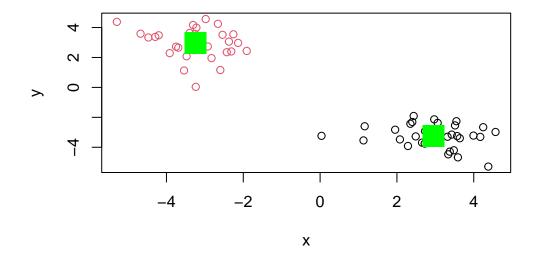
Warning in c(1:5) + c(100, 1): longer object length is not a multiple of shorter object length

[1] 101 3 103 5 105

plot(x, col= c(1,2))

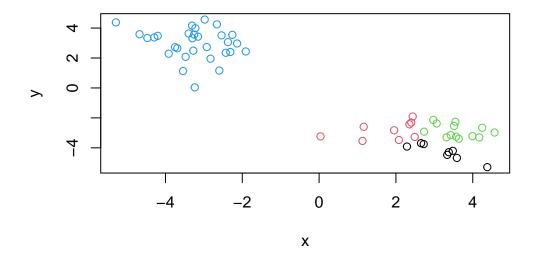


plot(x, col=km\$cluster)
points(km\$centers, col= "green", pch=15, cex=3)



Q5. Run kmeans() again and cluster in 4 groups and plot the results.

```
km4 <- kmeans(x, centers = 4)
plot(x, col=km4$cluster)</pre>
```



#### **Hierarchal Clustering**

This form of clustering aims to reveal the structure in your data by progressively grouping points into an ever smaller number of clusters.

The main function in base R for this is called hclust(). This function does not take our input data directly but wants a "distance matrix" that details how (dis)similar all our input points are to each other.

```
hc <- hclust( dist(x) )
hc</pre>
```

```
Call:
hclust(d = dist(x))
```

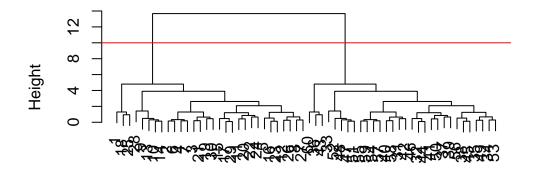
Cluster method : complete
Distance : euclidean

Number of objects: 60

The print out above is not very useful (unlike that from kmeans) but there is a useful plot() method.

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

## **Cluster Dendrogram**

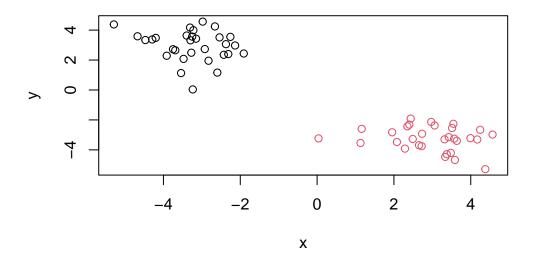


dist(x)
hclust (\*, "complete")

To get my main result (my cluster membership vector) I need to "cut" my tree using the fucntion cutree()

```
grps <- cutree(hc, h=10)
grps</pre>
```

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



## Principal Component Analysis (PCA)

The goal of PCA is to reduce the dimensionality of a dataset down to some smaller subset of new variables (called PCs) that are a useful basis for further analysis, like visualization, clustering, etc.

## **Data Entry**

Read data about crazy eating trends in the UK and N. Ireland

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

|               | 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 you use to answer this questions?

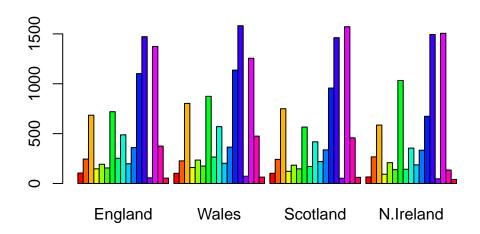
```
nrow(x)

[1] 17

ncol(x)

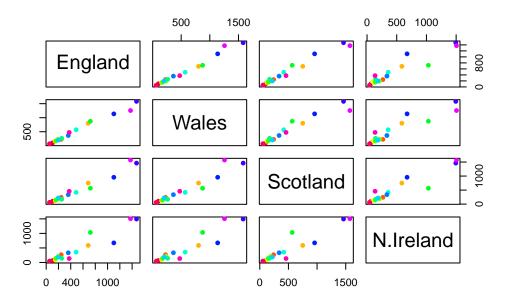
[1] 4

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



The so-called "pairs" plot can be useful for small datasets:

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



So the pairs plot is useful for small datasets but it can be lots of work to interpret and gets intractable for larger datasets.

#### So PCA tot he rescue...

The main function to do PCA in base R is called prcomp(). This function wants the transpose of our data in this case.

```
pca <- prcomp(t(x))
summary(pca)</pre>
```

#### Importance of components:

```
attributes(pca)
```

#### \$names

[1] "sdev" "rotation" "center" "scale" "x"

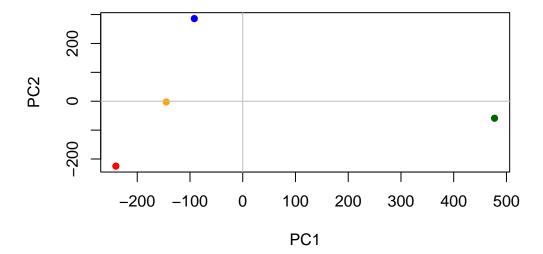
```
$class
[1] "prcomp"
```

```
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
```

A major PCA result viz is called a "PCA plot" (a.k.a. a score plot, biplot, PC1 vs PC2 plot, ordination plot)

```
mycols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=mycols, pch=16, xlab="PC1", ylab="PC2")
abline(h=0, col="gray")
abline(v=0, col="gray")</pre>
```



Another important output from PCA is called the "loadings" vector or the "rotation" component - this tells us how much the original variables (the foods in this case) contribute to the new PCs.

## pca\$rotation

|                    | PC1          | PC2          | PC3         | PC4          |
|--------------------|--------------|--------------|-------------|--------------|
| Cheese             | -0.056955380 | 0.016012850  | 0.02394295  | -0.694538519 |
| Carcass_meat       | 0.047927628  | 0.013915823  | 0.06367111  | 0.489884628  |
| Other_meat         | -0.258916658 | -0.015331138 | -0.55384854 | 0.279023718  |
| Fish               | -0.084414983 | -0.050754947 | 0.03906481  | -0.008483145 |
| Fats_and_oils      | -0.005193623 | -0.095388656 | -0.12522257 | 0.076097502  |
| Sugars             | -0.037620983 | -0.043021699 | -0.03605745 | 0.034101334  |
| Fresh_potatoes     | 0.401402060  | -0.715017078 | -0.20668248 | -0.090972715 |
| Fresh_Veg          | -0.151849942 | -0.144900268 | 0.21382237  | -0.039901917 |
| Other_Veg          | -0.243593729 | -0.225450923 | -0.05332841 | 0.016719075  |
| Processed_potatoes | -0.026886233 | 0.042850761  | -0.07364902 | 0.030125166  |
| Processed_Veg      | -0.036488269 | -0.045451802 | 0.05289191  | -0.013969507 |
| Fresh_fruit        | -0.632640898 | -0.177740743 | 0.40012865  | 0.184072217  |
| Cereals            | -0.047702858 | -0.212599678 | -0.35884921 | 0.191926714  |
| Beverages          | -0.026187756 | -0.030560542 | -0.04135860 | 0.004831876  |
| Soft_drinks        | 0.232244140  | 0.555124311  | -0.16942648 | 0.103508492  |
| Alcoholic_drinks   | -0.463968168 | 0.113536523  | -0.49858320 | -0.316290619 |
| Confectionery      | -0.029650201 | 0.005949921  | -0.05232164 | 0.001847469  |

PCA looks to be a super useful method for gaining some insight into high dimensional data that is difficult to examine in other ways.