Class 7: Machine Learning

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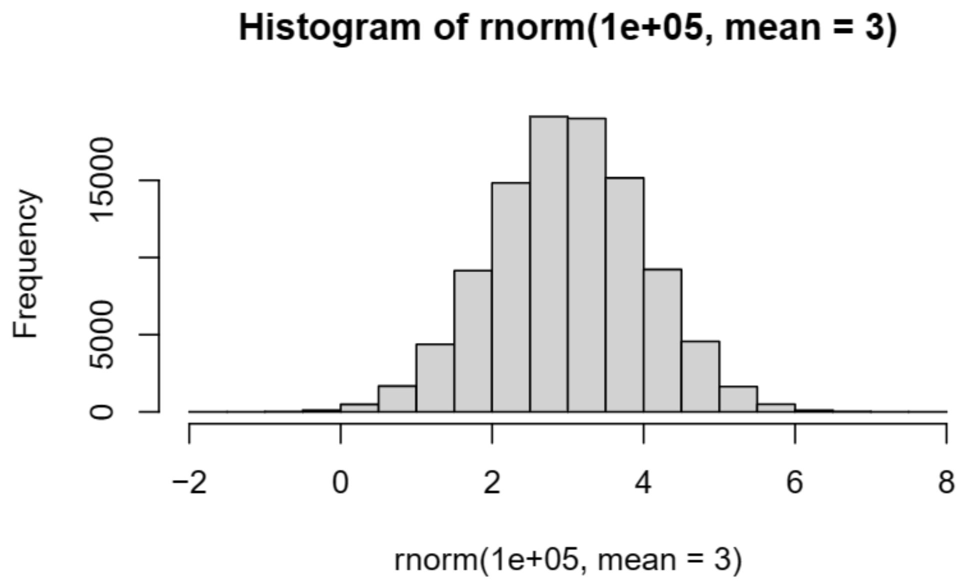
Today we will begin our multi-part exploration of some key machine learning methods. We will begin with clustering - finding groupings in data, and then dimensionallity reduction.

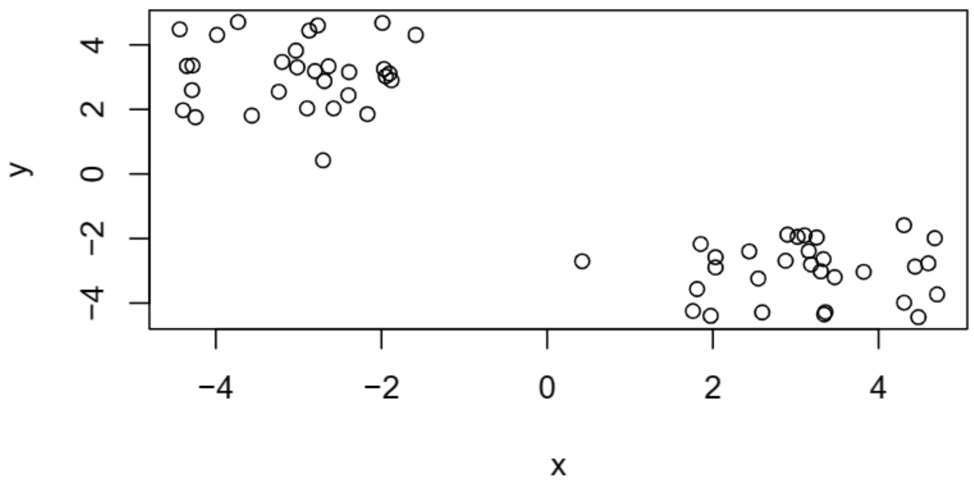
Clustering

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

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



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



Now let's try out `kmeans()`

```r
km <- kmeans(x, center = 2)
km
```

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

Cluster means:
          x         y
1  3.103932 -2.998233
2 -2.998233  3.103932

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] 53.95715 53.95715
 (between_SS / total_SS =  91.2 %)

Available components:

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

```
attributes(km)
```

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

$class
[1] "kmeans"
```

Q. How many points in each cluster?

```
km$size
```

```
[1] 30 30
```

Q. What components of your result object details 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 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
```

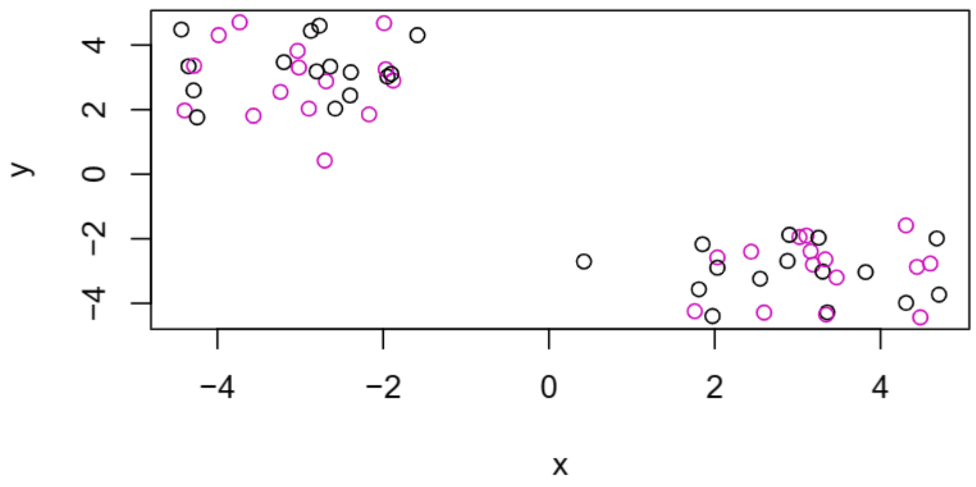
Q. What are centers/mean values of each cluster?

```
km$centers
```

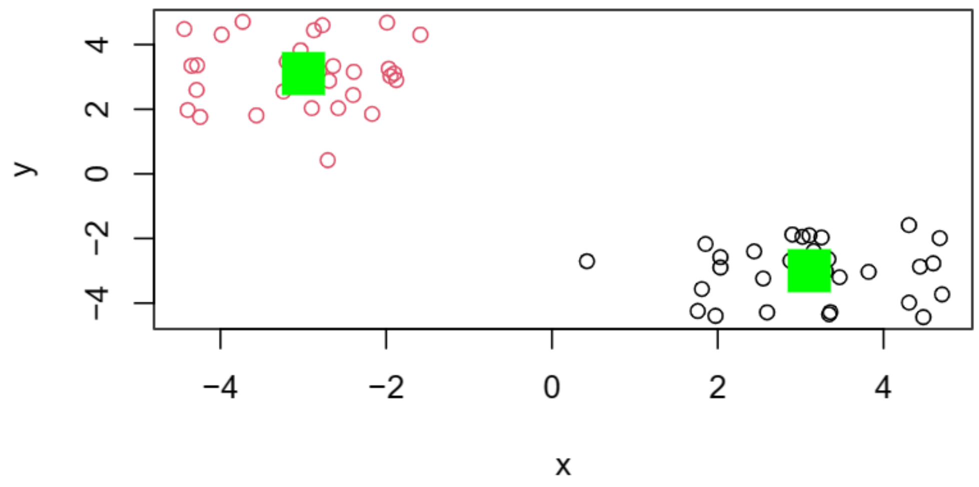
```
          x         y
1  3.103932 -2.998233
2 -2.998233  3.103932
```

Q. Make a plot of your data showing your clustering results

```
plot(x, col= c(1,6))
```

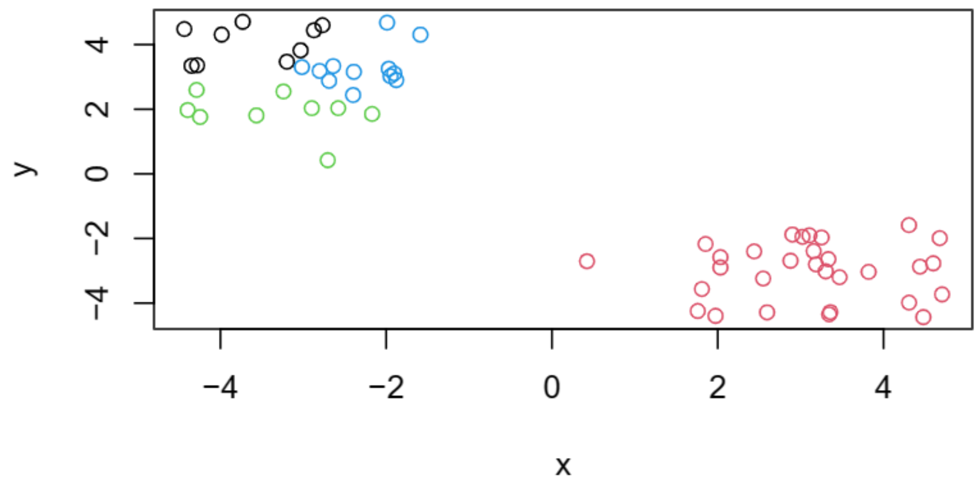


```
plot(x, col = km$cluster)
points(km$centers, col = "green", pch=15, cex=3)
```



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

```
km2 <- kmeans(x, center = 4)
plot(x, col= km2$cluster)
```



Hierchical Clustering

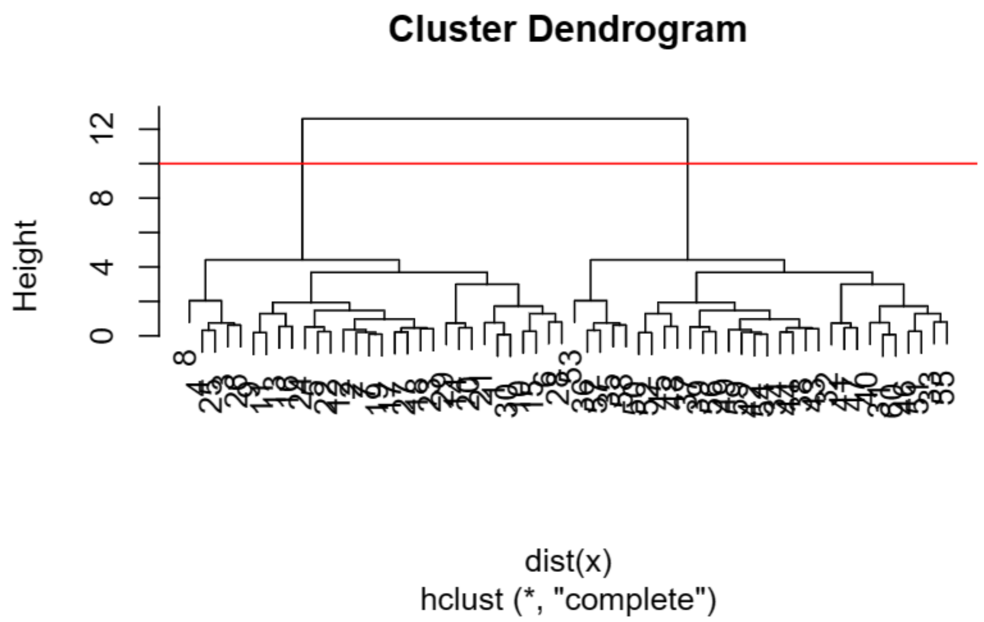
This form of clustering aims to reveal the structure of the data by progressively grouping points into a even smaller number of clusters.

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

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

The print out of hc is not very useful (unlike that from k means) but there is a useful `plot()` method

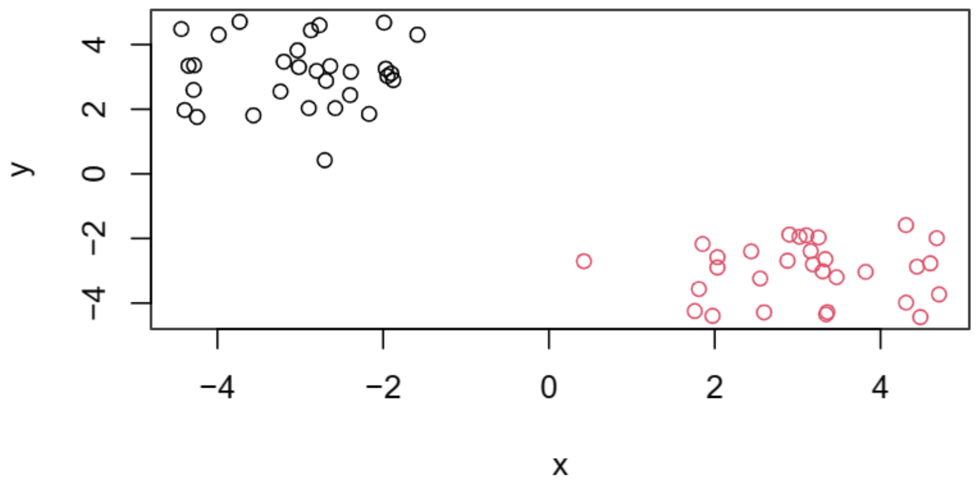
```
plot(hc)
abline(h=10, col="red")
```



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

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

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



Principle Component Analysis (PCA)

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

Lets do a PCA of UK food data

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
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
7      Fresh_potatoes      720   874      566      1033
```

```
8            Fresh_Veg     253  265    171     143
9            Other_Veg     488  570    418     355
10 Processed_potatoes     198  203    220     187
11       Processed_Veg     360  365    337     334
12         Fresh_fruit    1102 1137    957     674
13             Cereals    1472 1582   1462    1494
14           Beverages      57   73     53      47
15         Soft_drinks    1374 1256   1572    1506
16     Alcoholic_drinks    375  475    458     135
17       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?

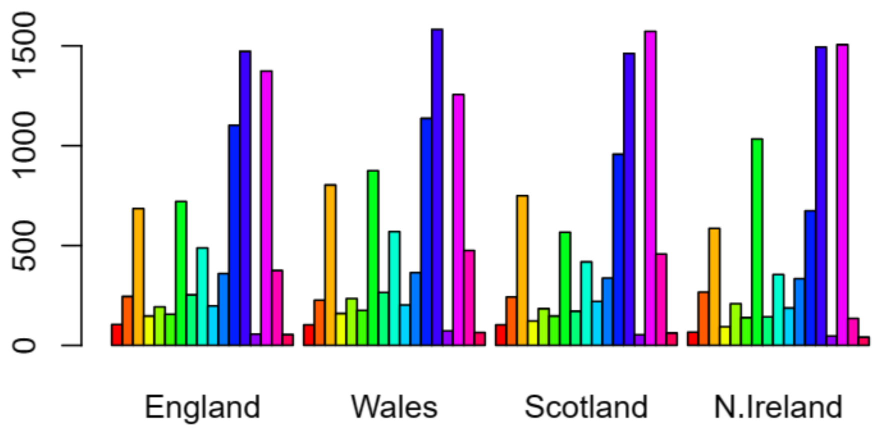
```r
c(nrow(x), ncol(x))
```

```
[1] 17  5
```

```r
x <- read.csv(url, row.names=1)
head(x)
```

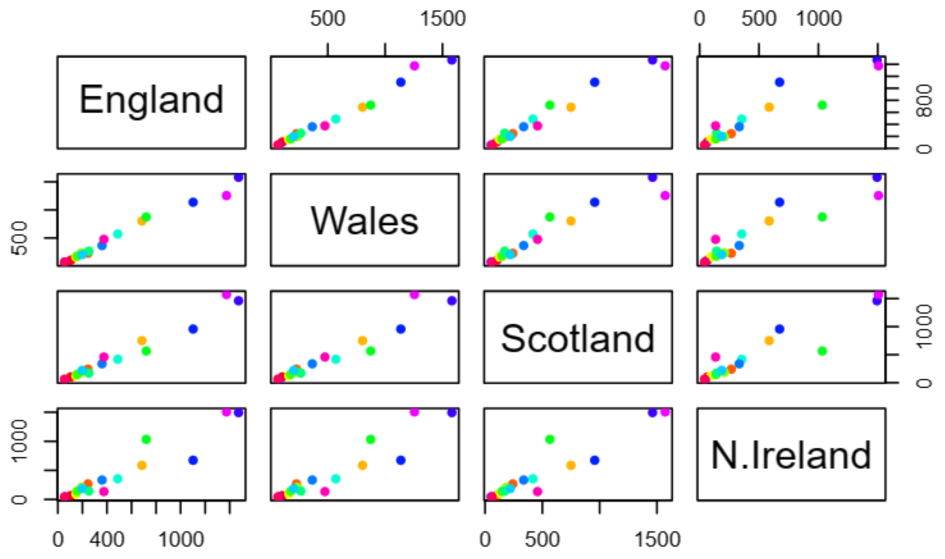
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
Fats_and_oils      193   235      184       209
Sugars             156   175      147       139
```

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



The so-called “pairs” plot can be useful for small datasets

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



This plot is useful for small datasets but it can be lots of work to interpret and gets untraceable for larger datasets.

So PCA to the rescue!

The main function to fo PCA in base R is called `prcomp()`

```
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
```

```
attributes(pca)
```

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

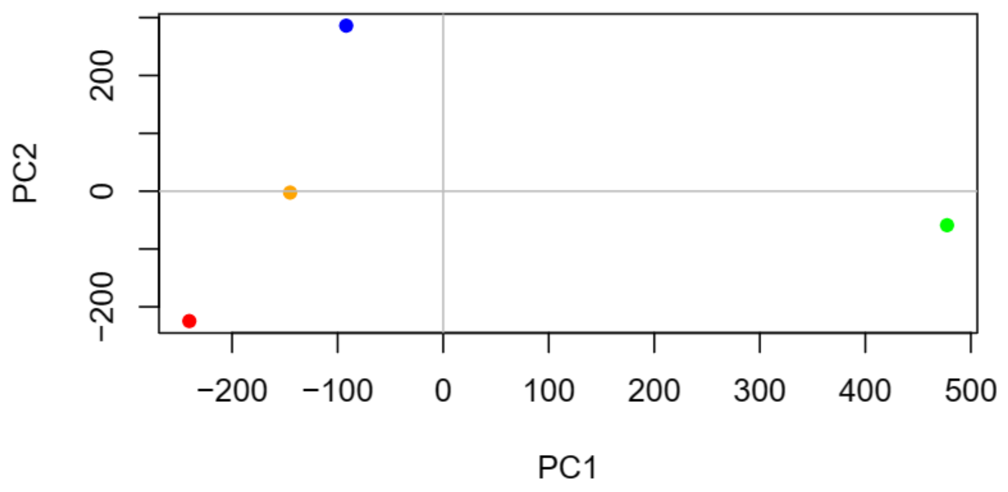
```
$class
[1] "prcomp"
```

```
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" (aka a score plot, biplot, PC1 vs PC2 plot, ordination plot)

```
mycols <- c("orange", "red", "blue", "green")
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")
```



Another important ouput 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 loos to be a super useful method for gaining some insight into high dimensional data that is difficult to examine in other ways.