Class 7: Machine Learning 1

Yu (Ericsson) Cao (PID: A16421048)

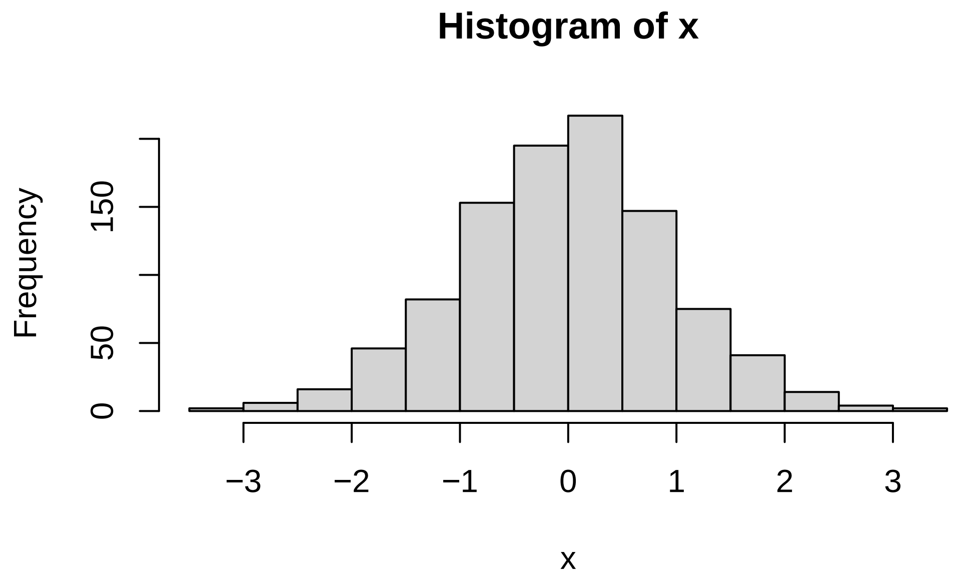
#Clustering Methods

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)
```



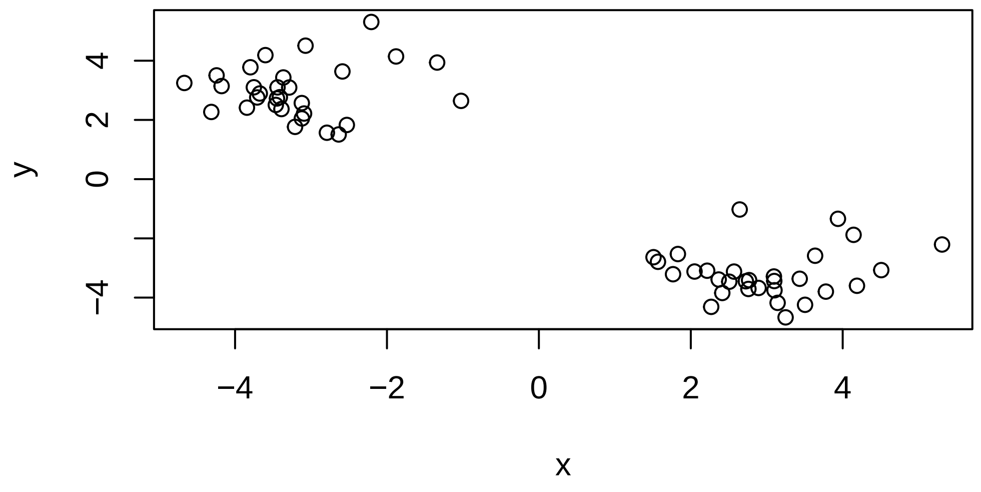
Make a vector of length 60 with 30 points centered at -3 and 30 points centered at +3

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

```
 [1] -3.287247 -2.586324 -2.206540 -3.463605 -3.410626 -3.441128 -1.339530
 [8] -3.708213 -3.448137 -3.389156 -4.668121 -1.880439 -3.091712 -3.752532
[15] -4.243483 -3.364603 -2.791006 -2.528414 -3.121589 -3.798048 -4.177534
[22] -4.312539 -1.024811 -3.600514 -3.210222 -3.120242 -3.072386 -2.635961
[29] -3.674701 -3.843721  2.414547  2.892438  1.509369  4.507604  2.049495
[36]  1.766157  4.187772  2.643593  2.268707  3.143261  3.778334  2.569274
[43]  1.830291  1.567639  3.434061  3.504261  3.102103  2.215567  4.143188
[50]  3.248103  2.367188  2.724765  2.758572  3.937583  3.099056  2.767694
[57]  2.506343  5.308139  3.636785  3.094533
```

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

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



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

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

Cluster means:
          x         y
1  2.965881 -3.206436
2 -3.206436  2.965881

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] 43.18066 43.18066
 (between_SS / total_SS =  93.0 %)

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?

```r
k$size
```

```
[1] 30 30
```

> Q. What "component" of your result object details the cluster membership?

```r
k$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
```

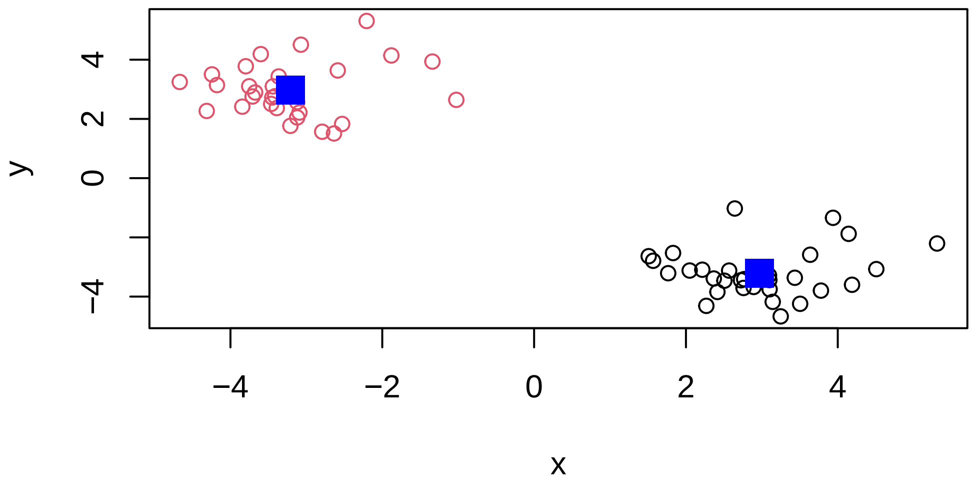
> Q. Cluster centers?

```r
k$centers
```

```
          x         y
1  2.965881 -3.206436
2 -3.206436  2.965881
```

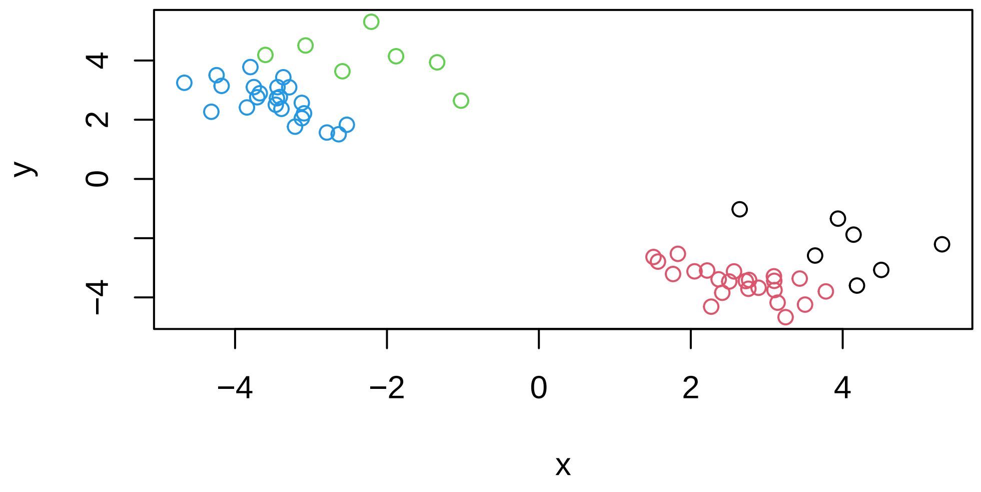
Q. Plot of our clustering results.

```
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

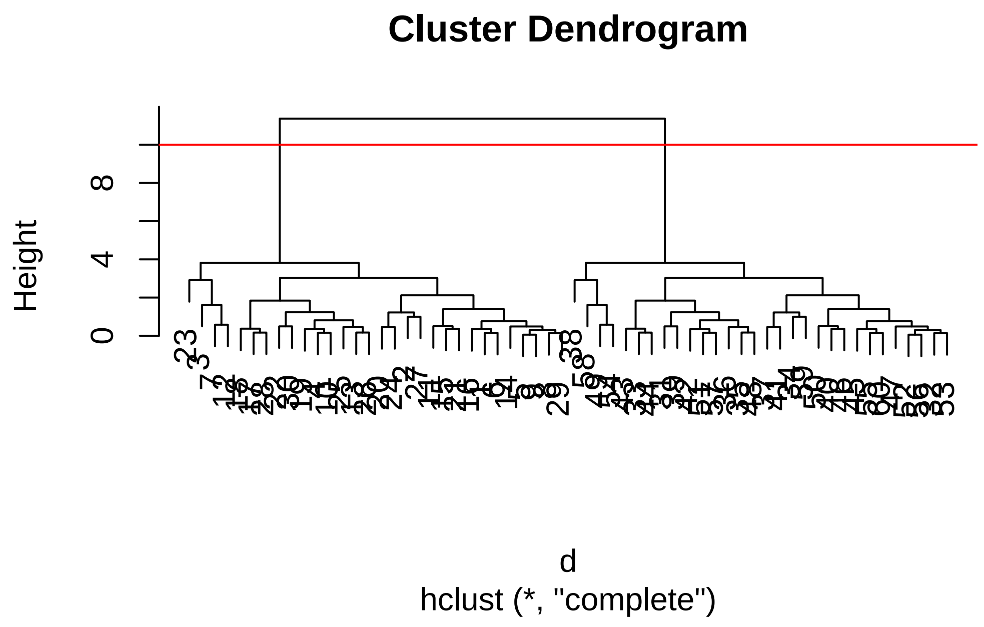
The main base R function for Hierarchial Clustering is `hclust()`. Unlike `kmeans()` you can not just pass it your data as input. You first need to calculate a distance matrix.

```
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

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



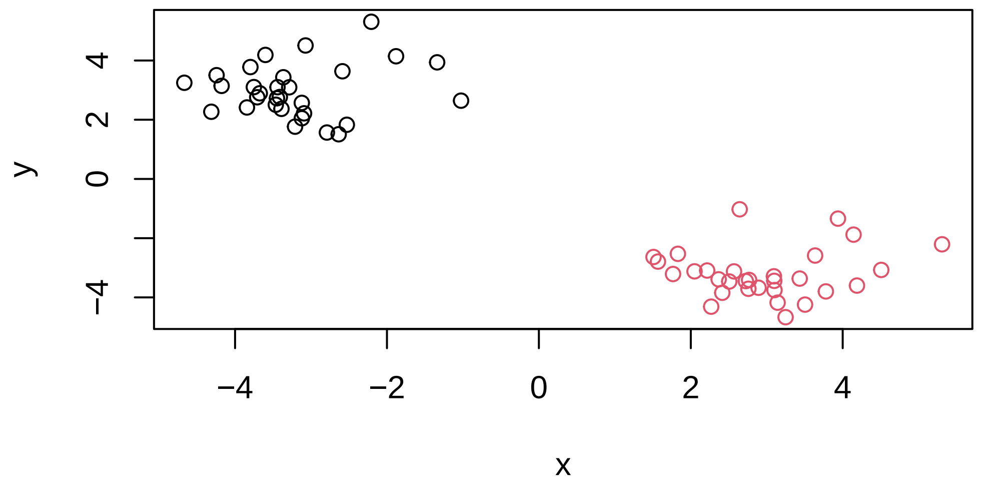
To make the "cut" and get our cluster membership vector we can use the `cutree()` function.

```r
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 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
```

Make a plot of our data colored by hclust results

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



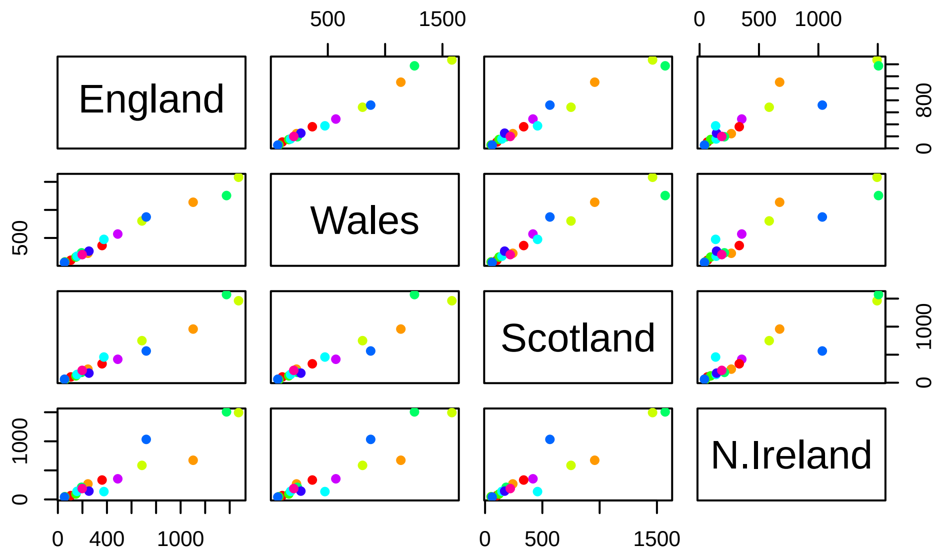
Principal Component Analysis (PCA)

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

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

```
#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 as we want the countries in the rows and food as the column.

```
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 2 PCs

96.5%

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

```
attributes(pca)
```

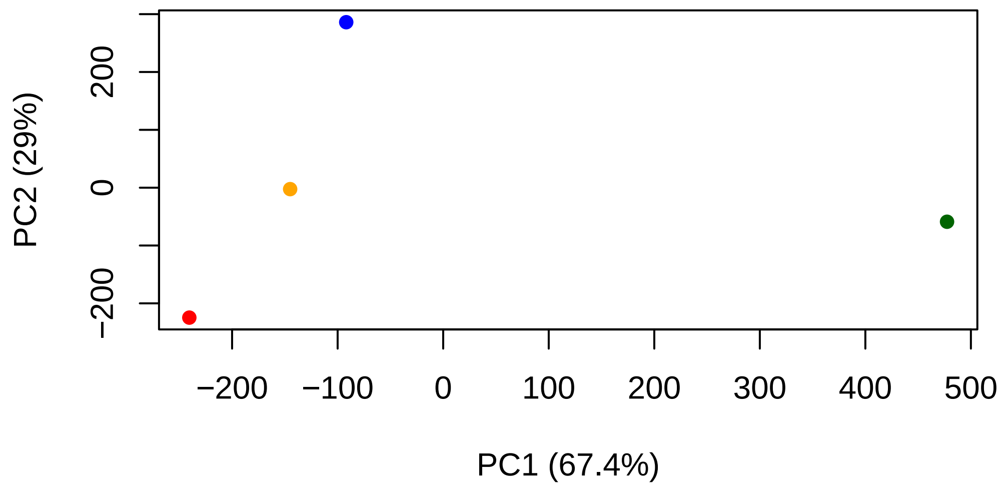
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$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.

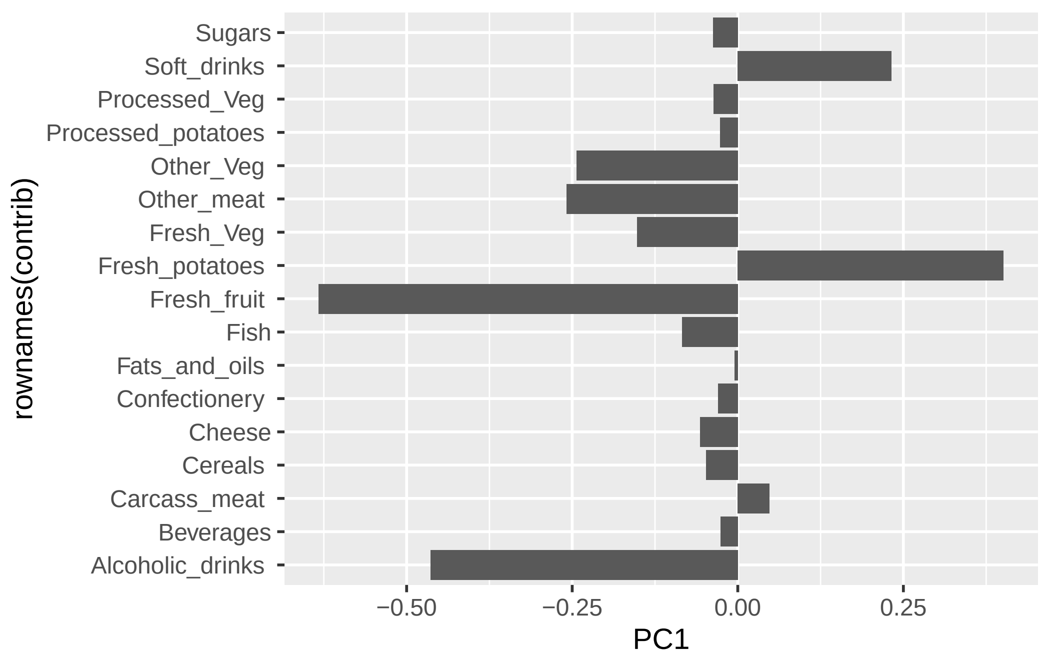
This is contained in the `pca$rotation` object - folks often call this the “loadings” or “contributions” to the PCs

```
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
```

We can make a plot along PC1.

```
library(ggplot2)

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

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



Sugars
Soft_drinks
Processed_Veg
Processed_potatoes
Other_Veg
Other_meat
Fresh_Veg
Fresh_potatoes
Fresh_fruit
Fish
Fats_and_oils
Confectionery
Cheese
Cereals
Carcass_meat
Beverages
Alcoholic_drinks
rownames(contrib)
−0.50
−0.25
0.00
0.25
PC1