# Class 07: Machine Learning 1

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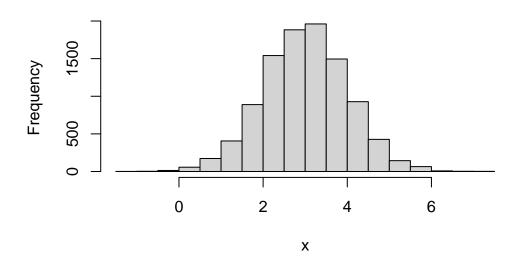
### #Clustering

We will start today's lab eith clustering methods, in particular so-called K-means. The main function for this in R is kmeans().

Let's try it on some made up data where we know what the answer should be.

```
x <- rnorm(10000, mean=3)
hist(x)</pre>
```

## Histogram of x



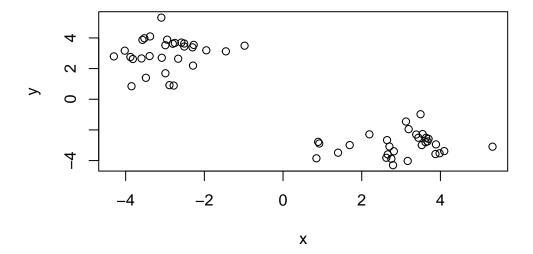
60 points

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

```
x y
[1,] 2.7042652 -3.081993
[2,] 2.7533664 -3.879674
[3,] 2.1948090 -2.288239
[4,] 2.8165253 -3.391509
[5,] 0.8925488 -2.778935
[6,] 3.6212085 -2.801708
```

We can pass this to the base R plot() function for a quick

```
plot(x)
```



```
k <- kmeans(x, centers=2, nstart=20)
k</pre>
```

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

# Cluster means:

1 2.987221 -2.955259

2 -2.955259 2.987221

Clustering vector:

Within cluster sum of squares by cluster:

[1] 47.39761 47.39761

(between\_SS / total\_SS = 91.8 %)

Available components:

- [1] "cluster" "centers" "totss" "withinss" "tot.withinss"
- [6] "betweenss" "size" "iter" "ifault"
  - Q1. How many points are in each cluster?

k\$size

[1] 30 30

Q2. Cluster membership?

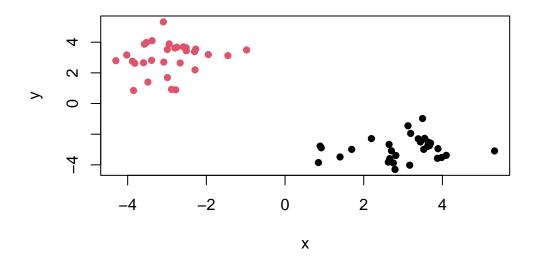
k\$cluster

- - Q3. Cluster Centers?

k\$centers

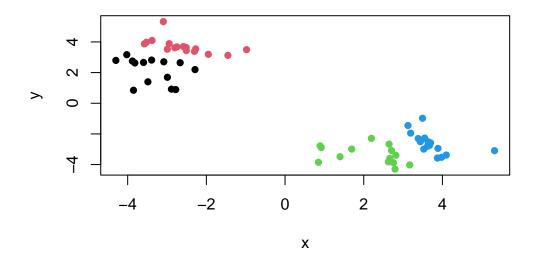
x

- 1 2.987221 -2.955259
- 2 -2.955259 2.987221
  - Q4. Plot my clustering results



Q5. Cluster the data again with kmeans() into 4 groups and plot the results.

```
k4 <- kmeans(x, centers=4, nstart=20)
plot(x, col=k4$cluster, pch=16)</pre>
```



K-mean is very popular mostly because it is fast and relatively straight forward to run and understand. It has a big limitation in that you needs to tell it how many groups (k, or centers) you want.

### #Hierarchical clustering

The main function in base R is called hclust(). You have to pass it in a "distance matrix" not just your input data

You can generate a distance matix with the dist() function.

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

#### Call:

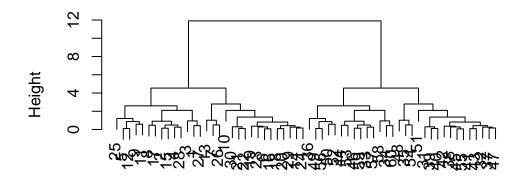
hclust(d = dist(x))

Cluster method : complete
Distance : euclidean

Number of objects: 60

plot(hc)

## **Cluster Dendrogram**

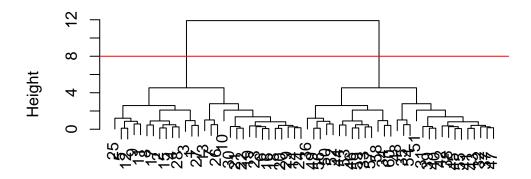


dist(x)
hclust (\*, "complete")

To find the clusters (cluster memebership vector) from a hclust() result we can "cut" the tree at a certain height that we like. For this we use the '

```
plot(hc)
abline(h=8, col="red")
```

# **Cluster Dendrogram**



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

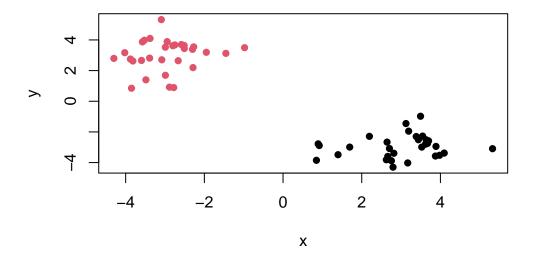
```
grps <- cutree(hc, h=8)

table(grps)

grps
1 2
30 30

Q6. Plot our hclust results

plot(x, col=grps, pch=16)</pre>
```



#Principal Componenet Analysis

### ##PCA of UK food data

Read data showing the consumption in grams (per person, per week) of 17 different types of food-stuff measured and averaged in the four countries of the United Kingdom in 1997

Let's see how PCA can help us but first we can try conventional analysis

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

	Х	England	Wales	${\tt Scotland}$	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 F	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. 5 columns and 17 rows

```
nrow(x)
```

[1] 17

ncol(x)

### [1] 5

```
# Note how the minus indexing works
rownames(x) <- x[,1]
x <- x[,-1]
head(x)</pre>
```

	England	Wales	${\tt Scotland}$	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

dim(x)

[1] 17 4

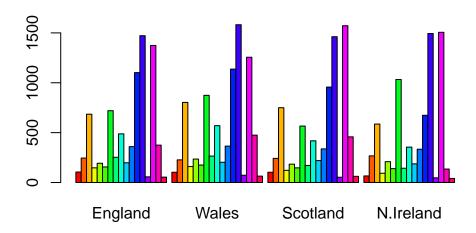
Second approach to correct row names

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

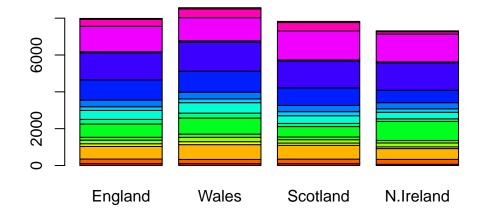
	England	Wales	${\tt Scotland}$	${\tt N.Ireland}$
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139

Q2. I prefer to use the second approach to correct our row-names problem because it is faster and takes less work for me. The second approach is more robust because if you rerun the first approach it will overwrite itself.

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

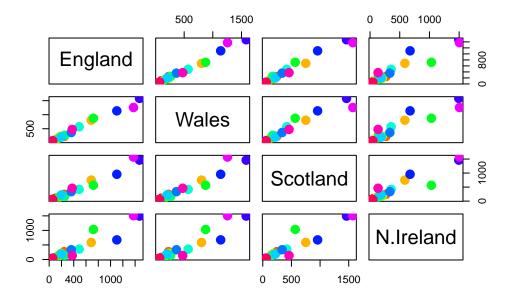


Q3. barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))



A pairs plot can be useful if we dont have 2 dimensions...

```
pairs(x, col=rainbow(17), pch=16, cex=2)
```



Q5. This pairwise plot shows a matrix of scatterplots. Each country has its own respective row and column. The rainbow code give each of the 17 food types its own color. If a point lies within the diagonal line for a given plot, it means that the food type is consumes equally in those countries

Q6. The main difference we can see between N. Irelandis that they have different amount of consumption of food types and this can be seen as the best of fit line is not very diagonal compared to the others.

###Principal Component Analysis

PCA can help us make sense of these types of datasets. Let's see how it works.

The main function in "base" R is called  $\mathtt{prcomp}()$ . In this case we want to first take the transpose  $\mathtt{t}()$  of our input  $\mathtt{x}$  so the columns are the food types and the countries are the rows

### head( t(x) )

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

```
Fresh_potatoes Fresh_Veg Other_Veg Processed_potatoes
England
                       720
                                  253
                                              488
                                                                   198
Wales
                       874
                                  265
                                              570
                                                                   203
Scotland
                       566
                                  171
                                              418
                                                                   220
N.Ireland
                      1033
                                              355
                                  143
                                                                   187
          Processed_Veg Fresh_fruit Cereals Beverages Soft_drinks
England
                      360
                                  1102
                                            1472
                                                        57
Wales
                      365
                                  1137
                                            1582
                                                        73
                                                                    1256
Scotland
                      337
                                   957
                                            1462
                                                        53
                                                                    1572
                                   674
                                            1494
                                                        47
                                                                    1506
N.Ireland
                      334
          Alcoholic_drinks Confectionery
                         375
                                          54
England
Wales
                         475
                                          64
Scotland
                         458
                                          62
N.Ireland
                         135
                                          41
```

```
# Use the prcomp() PCA function
pca <- prcomp( t(x) )
summary(pca)</pre>
```

#### 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

Q7.

pca\$x

```
      PC1
      PC2
      PC3
      PC4

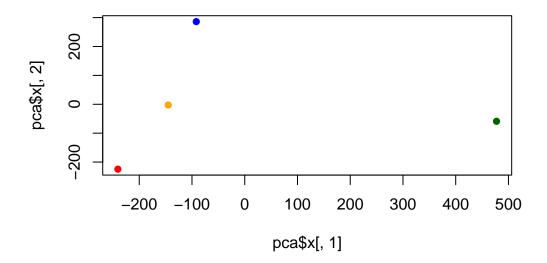
      England
      -144.99315
      -2.532999
      105.768945
      -4.894696e-14

      Wales
      -240.52915
      -224.646925
      -56.475555
      5.700024e-13

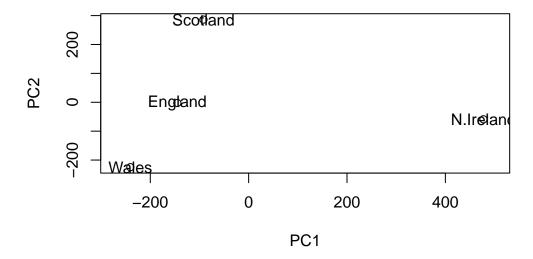
      Scotland
      -91.86934
      286.081786
      -44.415495
      -7.460785e-13

      N.Ireland
      477.39164
      -58.901862
      -4.877895
      2.321303e-13
```

```
plot(pca$x[,1], pca$x[,2], col= c("orange", "red", "blue", "darkgreen"), pch=16 )
```

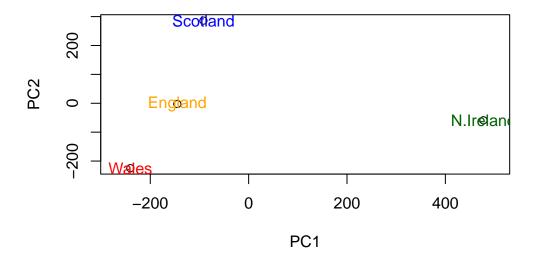


```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x))
```



Q8

```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x), col= c("orange", "red", "blue", "darkgreen"))
```



```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v

[1] 67 29 4 0

## or the second row here...
z <- summary(pca)
z$importance</pre>
```

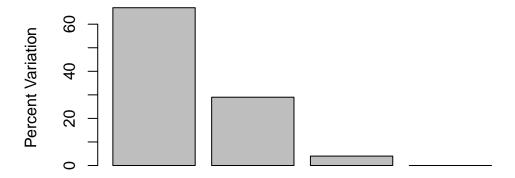
```
        PC1
        PC2
        PC3
        PC4

        Standard deviation
        324.15019
        212.74780
        73.87622
        3.175833e-14

        Proportion of Variance
        0.67444
        0.29052
        0.03503
        0.000000e+00

        Cumulative Proportion
        0.67444
        0.96497
        1.00000
        1.000000e+00
```

```
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```



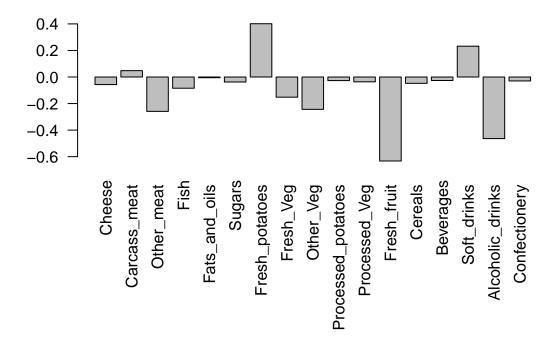
**Principal Component** 

The loadings tell us how much of the original variables (in our case the foods) contribute to the new variables i.e. the PCs

```
## Lets focus on PC1 as it accounts for > 90% of variance ]
head(pca$rotation)
```

```
PC2
                        PC1
                                                 PC3
                                                               PC4
Cheese
               -0.056955380
                             0.01601285
                                          0.02394295 -0.694538519
                0.047927628
                             0.01391582
                                          0.06367111
                                                      0.489884628
Carcass_meat
Other_meat
               -0.258916658 -0.01533114 -0.55384854
                                                      0.279023718
Fish
               -0.084414983 -0.05075495
                                          0.03906481 -0.008483145
Fats_and_oils
               -0.005193623 -0.09538866 -0.12522257
                                                      0.076097502
Sugars
               -0.037620983 -0.04302170 -0.03605745
                                                      0.034101334
```

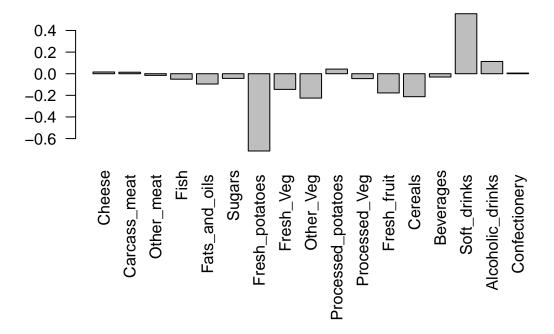
```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```



### head(pca\$rotation)

```
PC1
                                     PC2
                                                 PC3
                                                              PC4
                             0.01601285
                                         0.02394295 -0.694538519
Cheese
               -0.056955380
                             0.01391582
                                          0.06367111
Carcass_meat
                0.047927628
                                                      0.489884628
Other_meat
               -0.258916658 -0.01533114 -0.55384854
                                                      0.279023718
Fish
               -0.084414983 -0.05075495
                                          0.03906481 -0.008483145
Fats_and_oils
               -0.005193623 -0.09538866 -0.12522257
                                                      0.076097502
Sugars
               -0.037620983 -0.04302170 -0.03605745
                                                      0.034101334
```

```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```



Q9. The two prominent good groups are fresh potatoes and soft drinks. PC2 mainly tells us about the more prominent food groups because of the lesser amount of variance with PC2