Class7ML

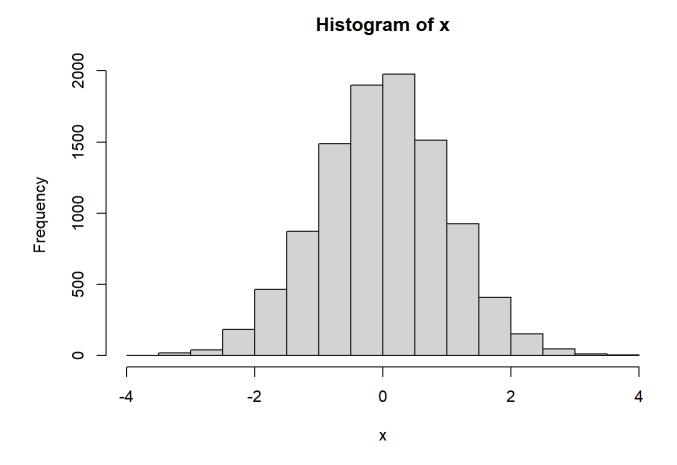
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K-means clustering

First we will test how this works in R with some made up data.

```
#RNORM() Random generation of number

x <- rnorm(10000)
hist(x)</pre>
```

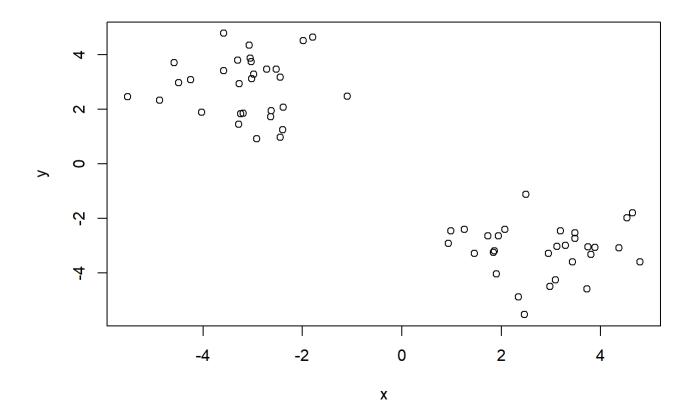


Let's make some numbers center on -3

```
rev(c("a","b"))
[1] "b" "a"
```

```
tmp <- c(rnorm(30, mean=-3), rnorm(30, mean=+3))</pre>
```

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



NOw let's see how 'kmeans' works with this data...

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

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

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

Q. What component of your result object details -cluster assignment/ membership -cluster center

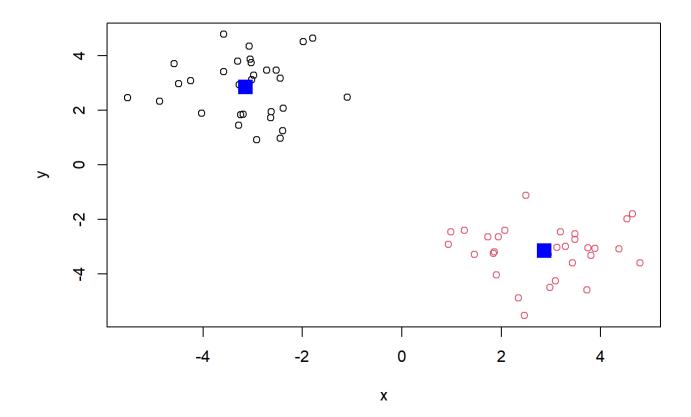
km\$centers

x y 1 -3.145454 2.859793 2 2.859793 -3.145454

km\$cluster

Q. Plot x colored by the kmeans cluster assignment and add cluster centers as blue points

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



Hierarchical Clustering

The 'hclust()' function in R performs hierarchical clustering.

The 'hclust()' function requires an input distance matrix, which i can get from the 'dist()' function.

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

Call: hclust(d = dist(x))

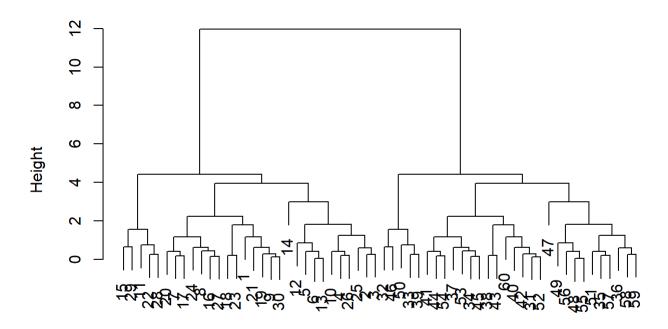
Cluster method : complete
Distance : euclidean

Number of objects: 60

There is a plot()method for hclust objects...

```
plot(hc)
```

Cluster Dendrogram



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

Now to get my cluster membership vector I need to cut the tree to yield separate "branches" with the leaves on each branch being our clusters. To do this we us tge 'cutree()' function.

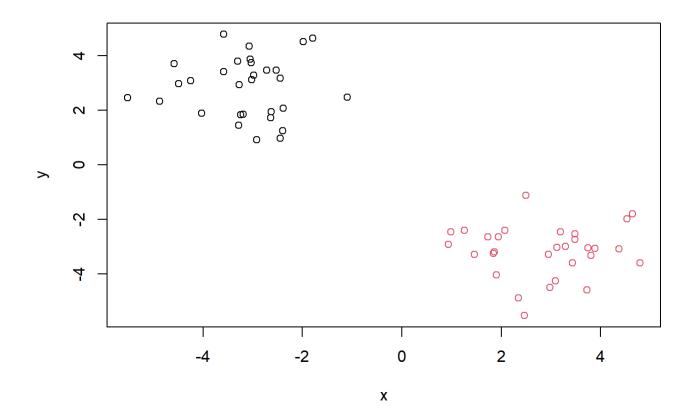
```
cutree(hc,h=8)
```

Use 'cutree()' with a k=2 — Find the height for you

```
grps <- cutree(hc, k=2)</pre>
```

A plot of our data colored by our hclut grps:

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



Principal Component Analysis (PCA)

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

Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?

```
data.frame(x)
```

	England	Wales	${\sf Scotland}$	${\tt N.Ireland}$
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
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

There are 17 rows and 5 columns.

Q2. FUnction view

```
## Preview the first 6 rows
head(x)
```

England Wales Scotland N.Ireland Cheese Carcass_meat Other_meat Fish Fats_and_oils Sugars

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

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

Check dim:

```
dim(x)
```

[1] 17 3

alt approach:

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

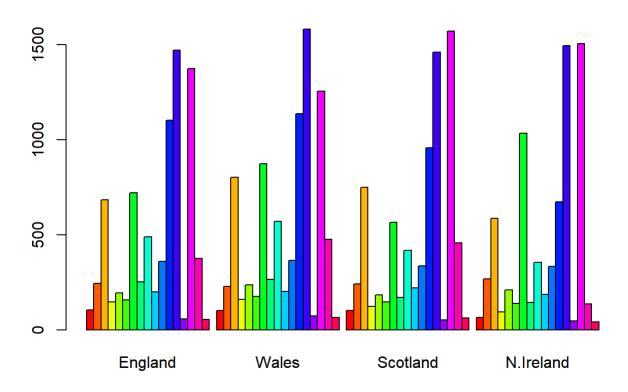
	England	Wales	${\sf Scotland}$	${\tt N.Ireland}$
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139

Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

The second approach is better since it will not delete columns every time we run the function.

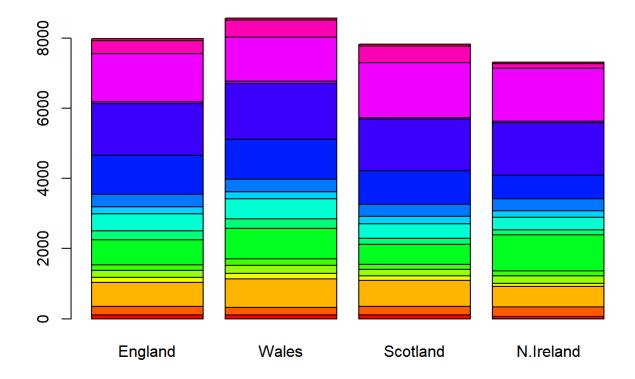
Let's make some not useful plot:

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



Q3: Changing what optional argument in the above barplot() function results in the following plot?

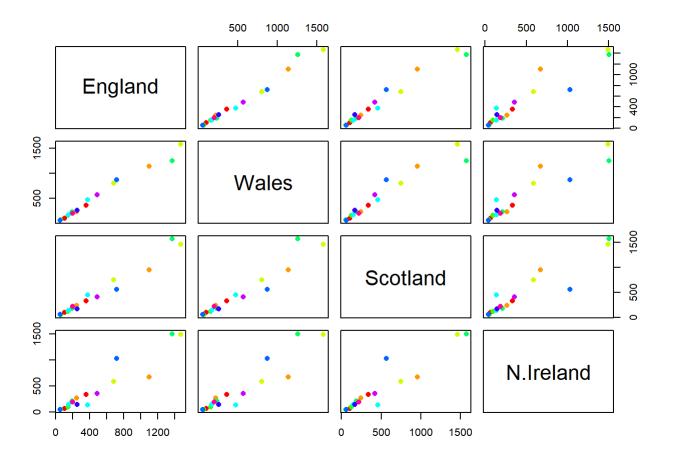
```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



Q5: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

We compare two countires at the same time. If a given point lies on the diagonal, it means the two countries eat the same amount for the type of food.

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



$\log 2 x>y=1 x<y=-1$ below: more of it on x

While this is kind of useful, it takes work to dig into the details here to find out what is different in the countries.

Q6. What is the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

The blue point.

PCA to the rescue

Principal Component Analysis can help where we have a lot of dimension being measure in the data set.

The main PCA function in base R is called 'prcomp()'.

The 'prcomp' function wants us input the transpose of out foodmatrix frame.

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

Importance of components:

```
        PC1
        PC2
        PC3
        PC4

        Standard deviation
        324.1502
        212.7478
        73.87622
        4.189e-14

        Proportion of Variance
        0.6744
        0.2905
        0.03503
        0.000e+00

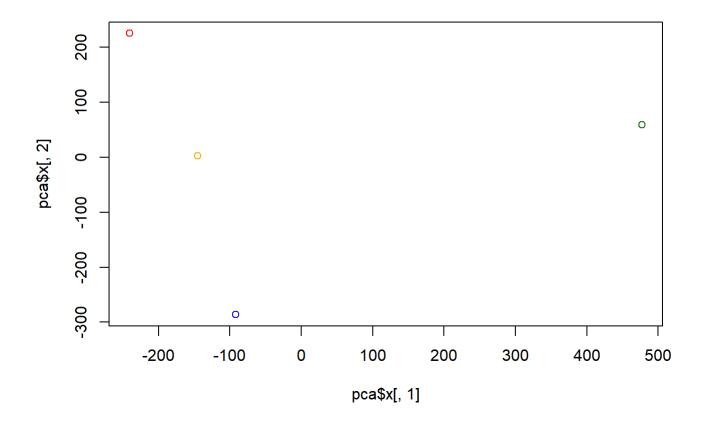
        Cumulative Proportion
        0.6744
        0.9650
        1.00000
        1.000e+00
```

The above result shows PCA captures 67 % of the total variance in the original data in one PC and 96.5% in two PCs.

```
PC1
                            PC2
                                        PC3
                                                      PC4
England
          -144.99315
                       2.532999 -105.768945 2.842865e-14
Wales
          -240.52915 224.646925
                                  56.475555 7.804382e-13
Scotland
           -91.86934 -286.081786
                                  44.415495 -9.614462e-13
N.Ireland 477.39164
                      58.901862
                                   4.877895 1.448078e-13
```

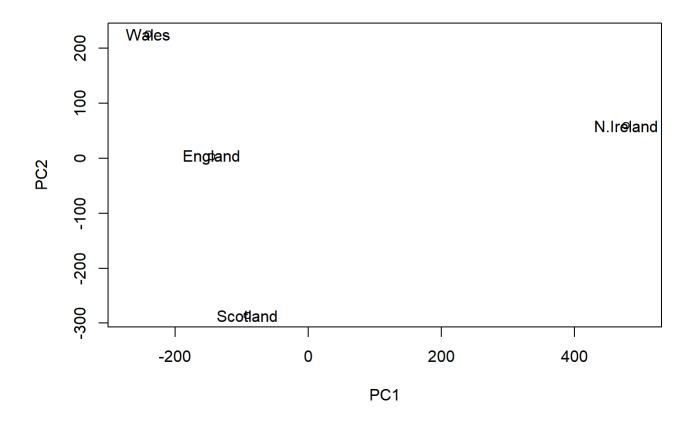
Let's plot our main result: >Q8. Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

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



Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

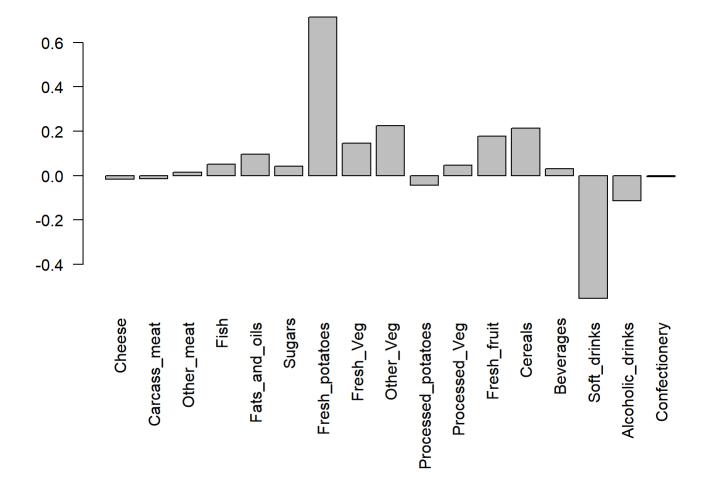
```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x))
```



New axis basically

Q9: Generate a similar 'loadings plot' for PC2. What two food groups feature prominantely and what does PC2 maninly tell us about?

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



Fresh potatoes and soft_drinks features predominately and PC2 mainly tell us the information about the second dimension (2nd axis).

Part 2:

```
url2 <- "https://tinyurl.com/expression-CSV"</pre>
rna.data <- read.csv(url2, row.names=1)</pre>
head(rna.data)
       wt1 wt2 wt3 wt4 wt5 ko1 ko2 ko3 ko4 ko5
      439 458
                     429 420
                              90 88 86
                                              93
gene1
                408
                                          90
gene2
      219 200
                204
                     210 187 427 423 434 433 426
gene3 1006 989 1030 1017 973 252 237 238 226 210
       783 792
                829
                     856 760 849 856 835 885 894
gene4
gene5
       181 249
                204
                     244 225 277 305 272 270 279
       460 502
                491
                     491 493 612 594 577 618 638
gene6
pca <- prcomp(t(rna.data), scale=TRUE)</pre>
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
```

