Class 07: Machine Learning 1

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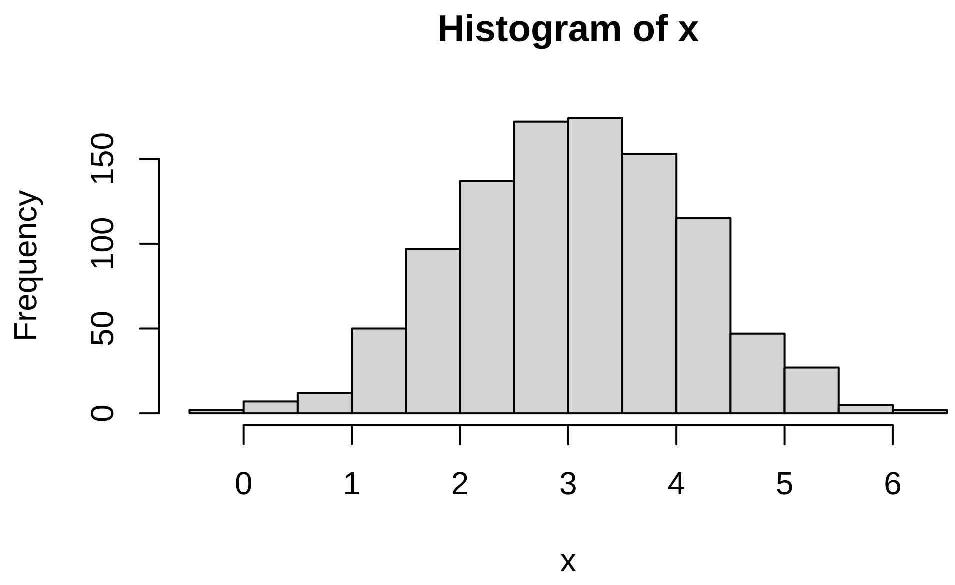
Clustering

We will start today's lab with 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 the answer.

```r
# rnorm function draws random points from a normal distribution
# rnorm(number of points, mean, sd). default: z.
x <- rnorm(1000, mean = 3)
hist(x)
```

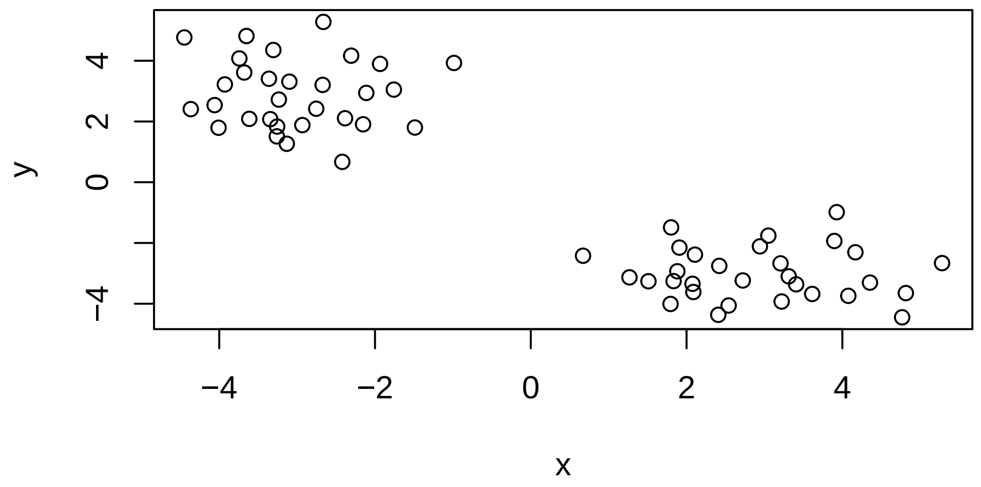


make 60 points

```
# points from two distributions
tmp <- c(rnorm(30, mean = 3), rnorm(30, mean = -3))
# create a y axis as the reversed list of tmp, build matrix by cbind
tdtmp <- cbind(x=tmp, y=rev(tmp))
#check the data
head (tdtmp)
```

```
             x          y
[1,] 3.407357 -3.3618319
[2,] 2.076548 -3.3447115
[3,] 1.801669 -1.4879422
[4,] 3.927693 -0.9860571
[5,] 0.670952 -2.4202559
[6,] 3.312089 -3.0992685
```

```
#plot the data
plot (tdtmp)
```



K-means clustering of two sets of points of size 30, 30.

```
# identify the two clusters by kmeans(). Iteration = 20 times.
k <- kmeans (tdtmp, centers = 2, nstart = 20)
k
```

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

Cluster means:
          x         y
1  2.902282 -3.001785
2 -3.001785  2.902282

Clustering vector:
 [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

Within cluster sum of squares by cluster:
[1] 60.22932 60.22932
 (between_SS / total_SS =  89.7 %)

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
```

```
 [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
```

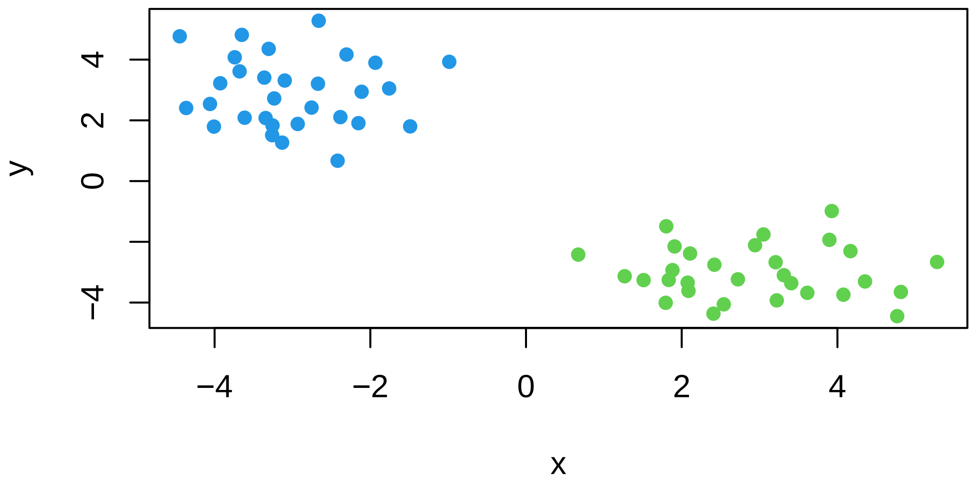
Q3. Cluster centers?

```
k$centers
```

```
          x         y
1  2.902282 -3.001785
2 -3.001785  2.902282
```

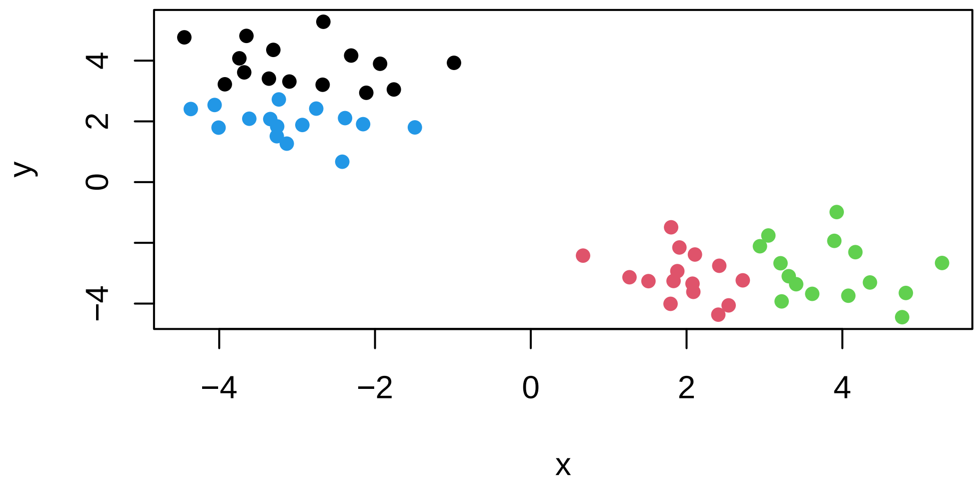
Q4. Plot my clustering results?

```
plot(tdtmp, col = k$cluster+2, pch = 16)
```



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

```
kf <- kmeans(tdtmp, centers = 4, nstart = 20)
plot(tdtmp, col = kf$cluster, pch = 16)
```



K-means is very popular mostly because it is fast and relatively straightforward to run and understand. But it has a big limitation in that you need to tell it how many groups (k, or centers) you want. If we don't know k beforehand, we need trial and error to obtain the optimal result with minimal SS and cluster number.

Hierachical clustering

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

We can generate a distance matrix with the `dist()` function.

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

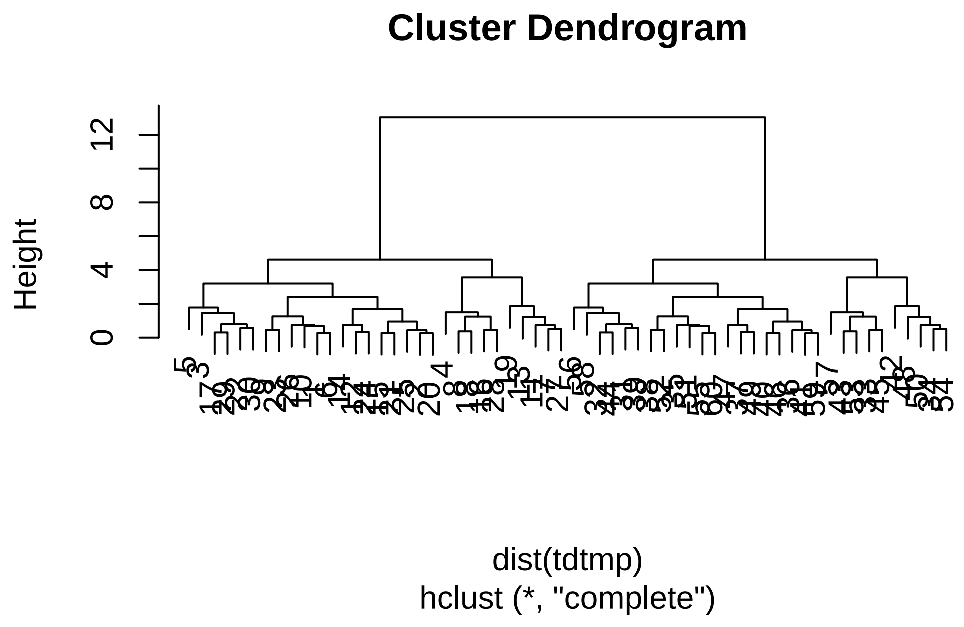
```

Call:
hclust(d = dist(tdtmp))

Cluster method   : complete 
Distance         : euclidean 
```

```
Number of objects: 60
```

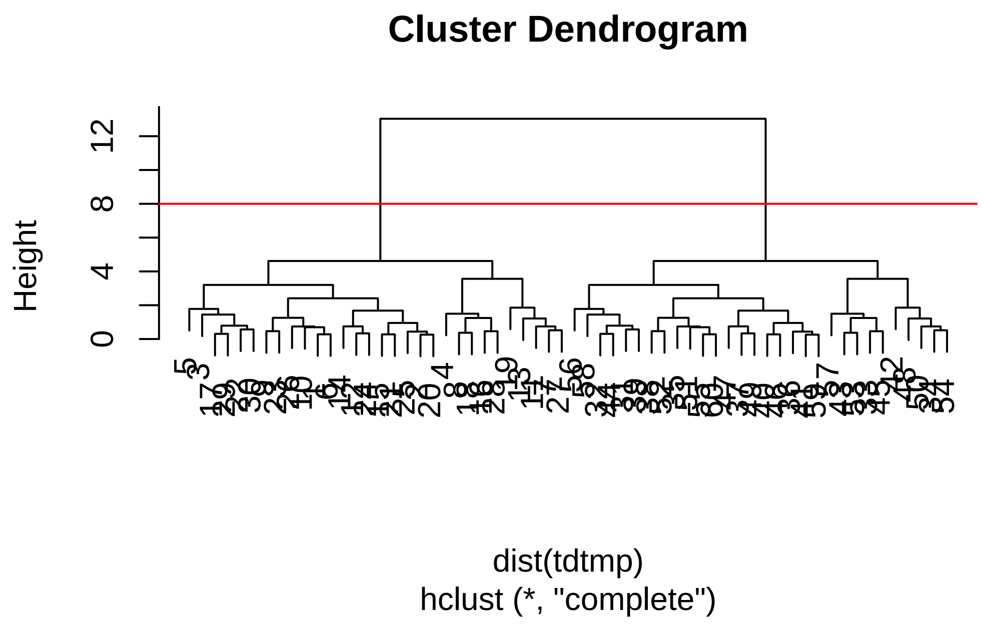
```
plot(hc)
```



Interpretation: - It grouped the numbers into two groups: <=30(left) and >30(right). - Height of bars = distance of points. - Determine number of clusters by observing the number of highest bars.

To find clusters (cluster membership vector) from a 'hclust()' result, we can "cut" the tree at a certain height that we like

```
# cut the tree on plot
plot(hc)
abline(h=8, col = "red")
```

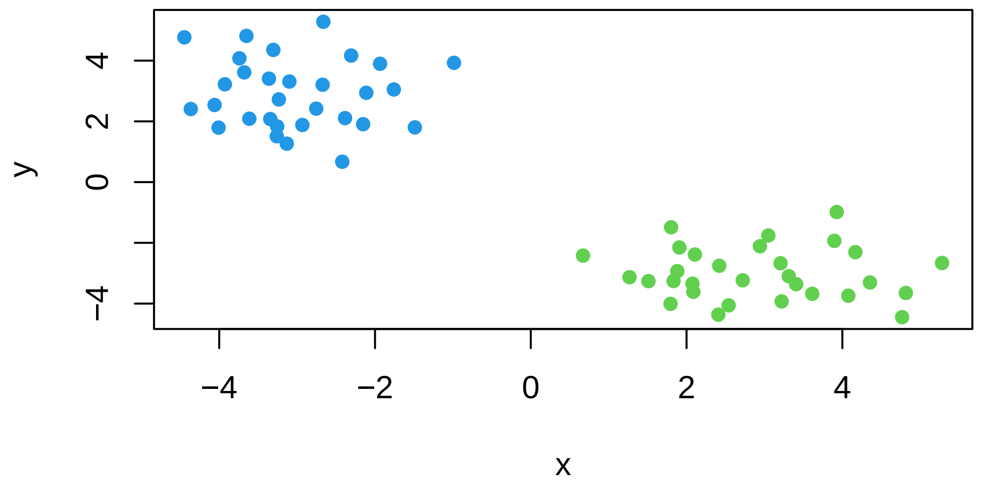


```
#get membership vector
grps <- cutree(hc, h=8)
table(grps)
```

```
grps
 1  2 
30 30 
```

Plot the result

```
plot(tdtmp, col=grps+2, pch = 16)
```



PCA: Principal Component Analysis

Read the data 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.

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

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] 5
```

```r
#or
dim(x)
```

```
[1] 17  5
```

```r
# Checking data
head(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
```

It looks like the row-names here were not set properly as we were expecting 4 columns (one for each of the 4 countries of the UK - not 5 as reported from the dim() function)

```r
rownames(x) <- x[,1]
food <- x[,-1]
head(x)
```

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

It is dangerous way of processing data as it deletes the first column every time we run this code, until all columns removed.

Instead, we can read the data properly

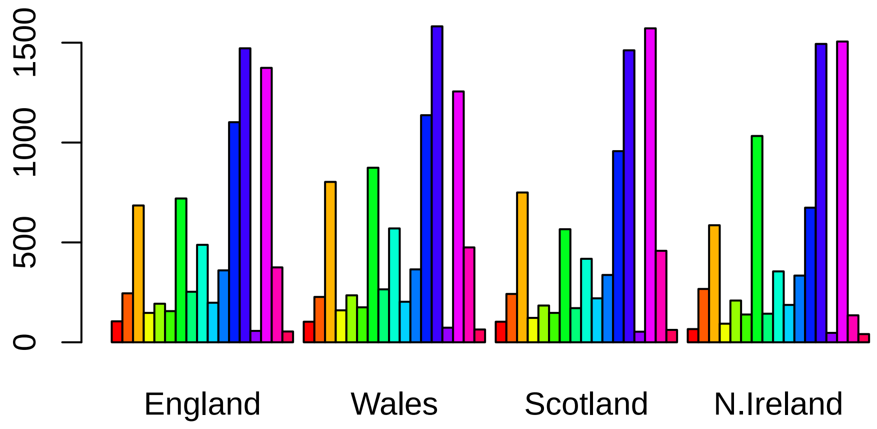
```r
x <- read.csv("https://tinyurl.com/UK-foods", row.names = 1)
head(x)
```

```
               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
```

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?

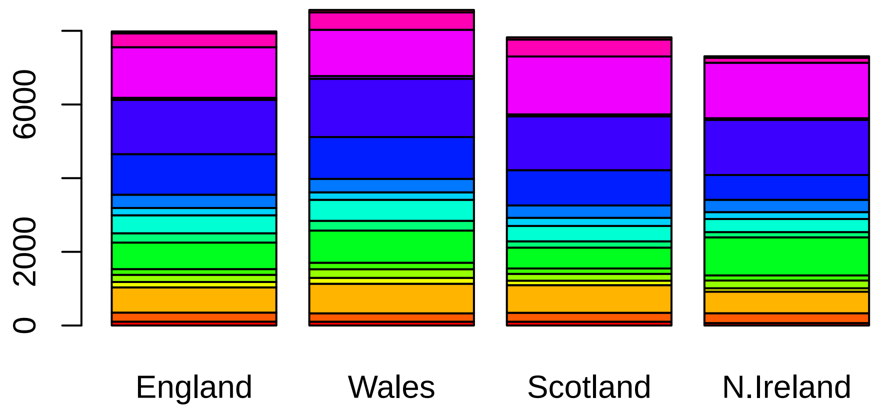
We can do bar plots

```
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?

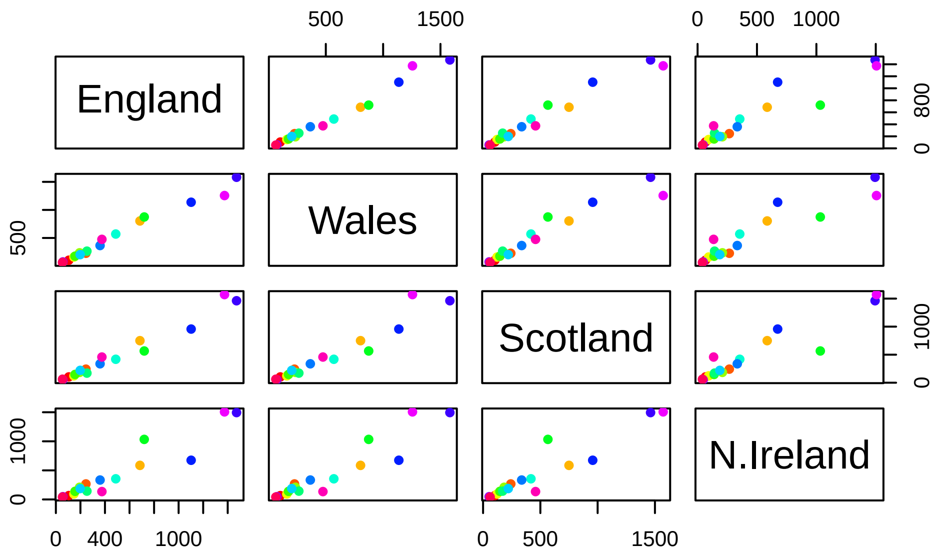
```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



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?

A pairs plot can be useful, if we don't have much dimensions

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



Interpretation: X and Y axis represent data from corresponding country, color of dot represent food category. Deviation from diagonal represent difference in data. Drawback: time-consuming and confusing to interpret.

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

PCA of UK Food Data (17 dimensions)

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 `prcomp()`. It needs matrix column to be the dimensions of analysis (in this case food type), and row to be group (in this case countries).

```
#transpose x by `t()` function
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        143        355                 187
          Processed_Veg  Fresh_fruit  Cereals  Beverages Soft_drinks
England             360         1102     1472         57        1374
Wales               365         1137     1582         73        1256
Scotland            337          957     1462         53        1572
N.Ireland           334          674     1494         47        1506
          Alcoholic_drinks  Confectionery
England                375             54
Wales                  475             64
Scotland               458             62
N.Ireland              135             41
```

```
pca <- prcomp(t(x))
summary(pca)
```

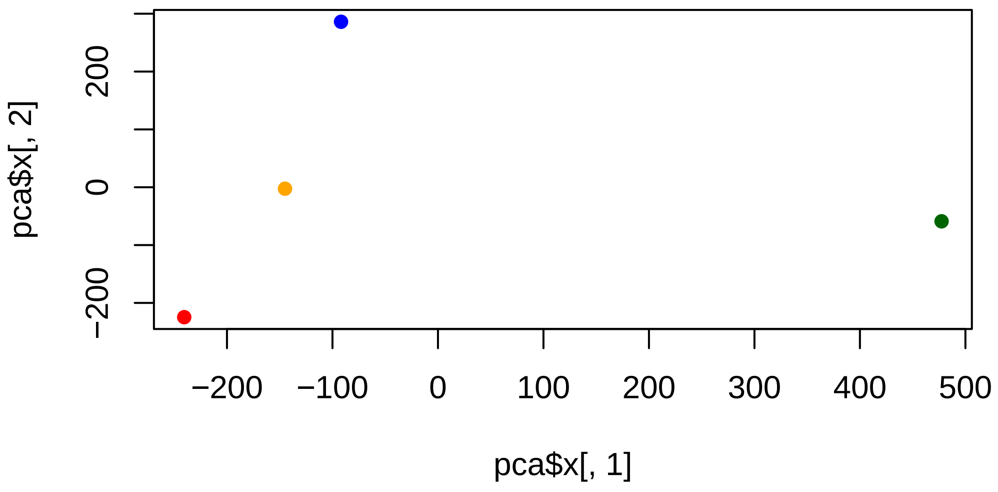
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 3.176e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

Interpretation: PC1 captures 67.44% of variance, and PC2 captures 96.5% variance in data.

```
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)
```



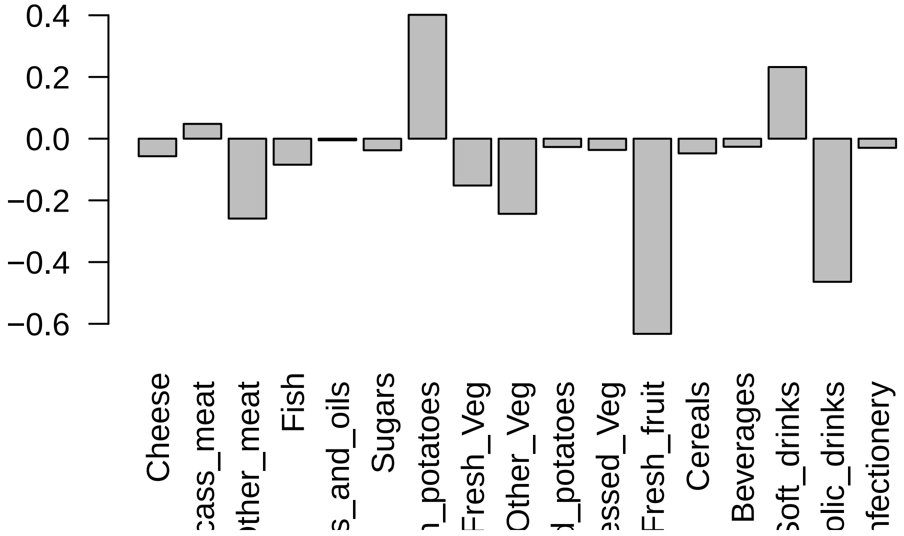
The "loadings" tell us how much the original variables (in our case, food) contribute to the new variable (PC).

```
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
```

```
#plot PC1, with graph margin of 2
barplot(pca$rotation[,1], las = 2)
```


Cheese
cass_meat
ther_meat
Fish
s_and_oils
Sugars
_potatoes
Fresh_Veg
Other_Veg
_potatoes
essed_Veg
Fresh_fruit
Cereals
Beverages
Soft_drinks
olic_drinks
nfectionery