Class 7: Machine Learning 1

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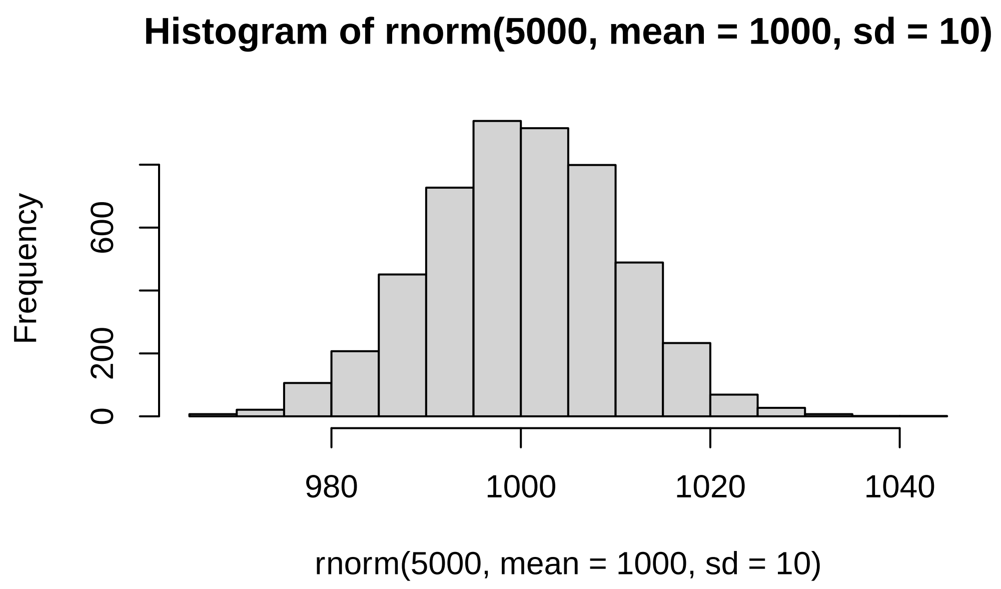
Background

Today we will begin our exploration of some important machine learning methods, namely **clustering** and **dimensionality reduction**

Let's make up some input data where we know what the natural "clusters" are.

The function `rnorm()` can be useful here. ## K-means clustering

```r
hist(rnorm(5000, mean=1000, sd= 10))
```



Q.Generate 30 random numbers centered at +3 and another 30 at -3.

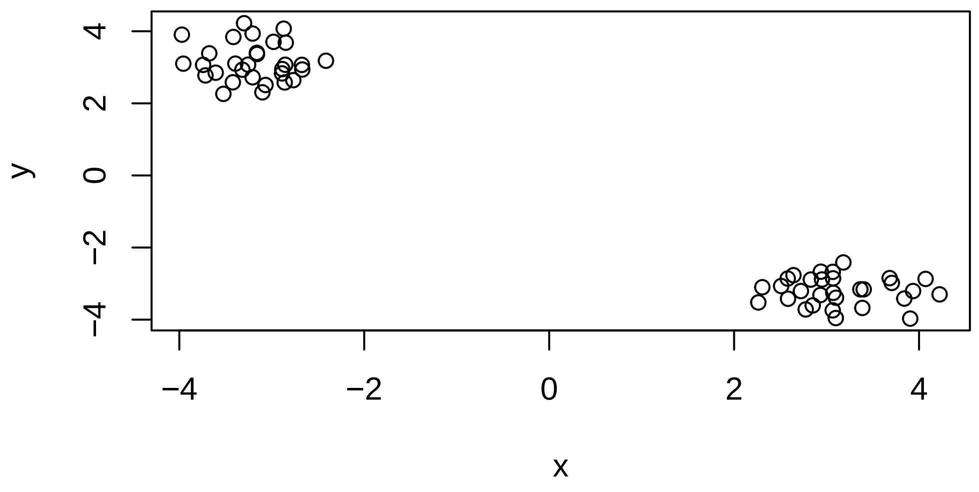
```r
rnorm(30, mean=3,sd=0.5)
```

```
 [1] 3.151270 2.878303 3.522507 3.294686 2.977663 2.484887 2.582619 3.007110
 [9] 3.180163 3.612721 3.690591 2.666465 3.142286 2.516513 2.630786 2.785373
[17] 2.742216 3.469601 3.240985 3.169851 3.378167 2.650891 2.680185 3.005377
[25] 2.841057 3.976550 3.660054 2.302960 3.398023 2.203407
```

```r
rnorm(30, mean=-3,sd=0.5)
```

```
 [1] -2.372569 -2.522981 -2.752637 -2.300521 -2.981157 -1.778568 -3.384532
 [8] -3.315427 -2.860868 -2.035190 -2.630400 -2.852770 -3.043116 -2.963215
[15] -3.672775 -2.484820 -3.235167 -3.199280 -2.744795 -3.667816 -3.093506
[22] -2.394515 -3.201059 -3.714107 -3.300802 -2.805318 -2.115911 -3.755147
[29] -2.421337 -2.785730
```

```r
tmp<- c(rnorm(30, mean=3,sd=0.5),rnorm(30, mean=-3,sd=0.5))

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



K-means clustering

The main function in "base R" for k-means clustering is called surprisingly `kmeans()`:

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

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

Cluster means:
          x         y
1  3.135264 -3.197237
2 -3.197237  3.135264

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] 12.39775 12.39775
 (between_SS / total_SS =  98.0 %)

Available components:

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

> Q. What component of the results object details the cluster sizes?

```r
km$size
```

```
[1] 30 30
```

> Q. What component of the results object details the cluster centers?

```r
km$centers
```

```
          x         y
1  3.135264 -3.197237
2 -3.197237  3.135264
```

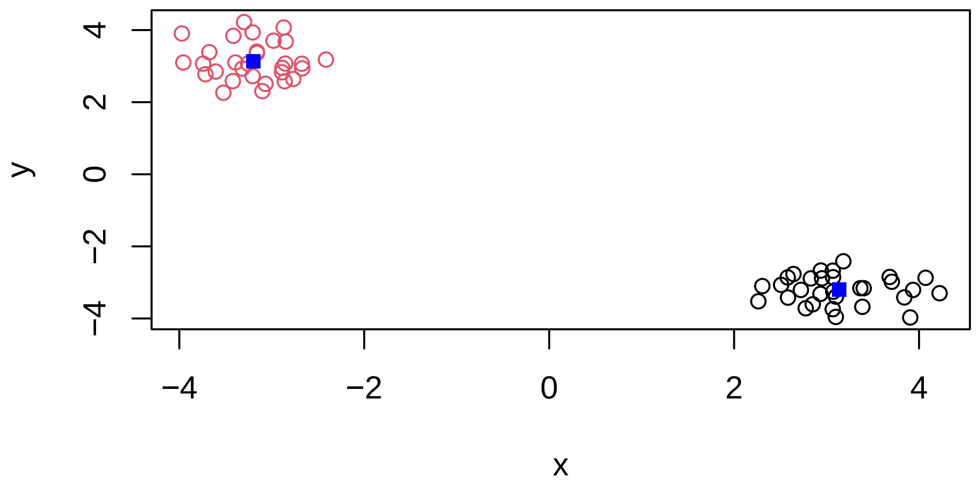
Q. What component of the results object details the cluster membership vector(i.e our main result of which points lie in which cluster)?

```r
km$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 2 2
```

Q. Plot our clustering results with points colored by cluster and also add the cluster centers as new points colored blue.

```r
plot(x, col=km$cluster)
points(km$centers, col="blue",pch=15)
```

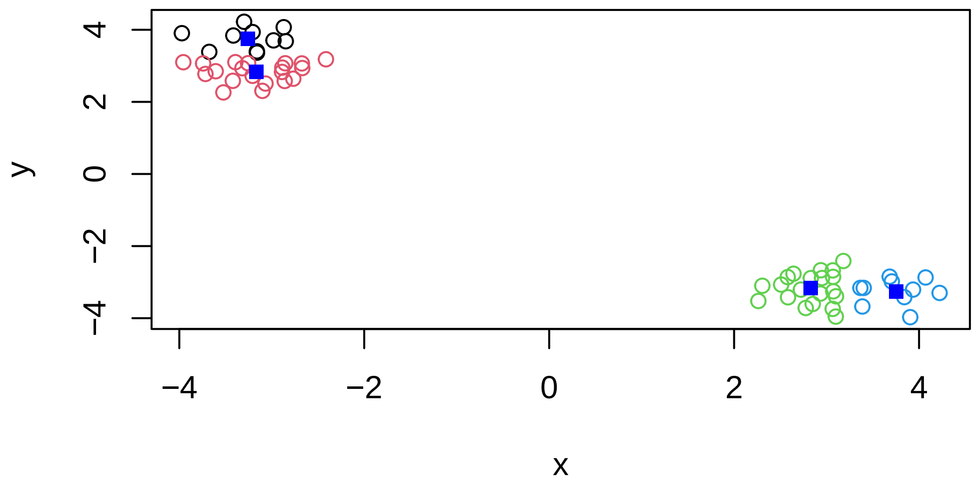


Q. Run`kmeans()` agains but this time produce 4 clusters and call your resulting object `k4` and make a reulsts figure like the one we made above.

```r
k4 <- kmeans(x,4)
k4
```

```
K-means clustering with 4 clusters of sizes 10, 20, 20, 10

Cluster means:
          x         y
1 -3.259139  3.751668
2 -3.166286  2.827062
3  2.827062 -3.166286
4  3.751668 -3.259139

Clustering vector:
 [1] 3 4 3 3 3 3 3 3 3 3 4 4 3 3 4 4 3 4 4 4 3 3 4 3 3 3 3 3 3 4 1 2 2 2 2 2 2 1
[39] 2 2 1 1 1 2 1 1 2 2 1 1 2 2 2 2 2 2 2 2 1 2

Within cluster sum of squares by cluster:
[1] 1.926699 4.714257 4.714257 1.926699
 (between_SS / total_SS =  98.9 %)

Available components:

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

```r
plot(x, col=k4$cluster)
points(k4$centers, col="blue",pch=15)
```



The Metric

```
km$tot.withinss
```

```
[1] 24.7955
```

```
k4$tot.withinss
```

```
[1] 13.28191
```

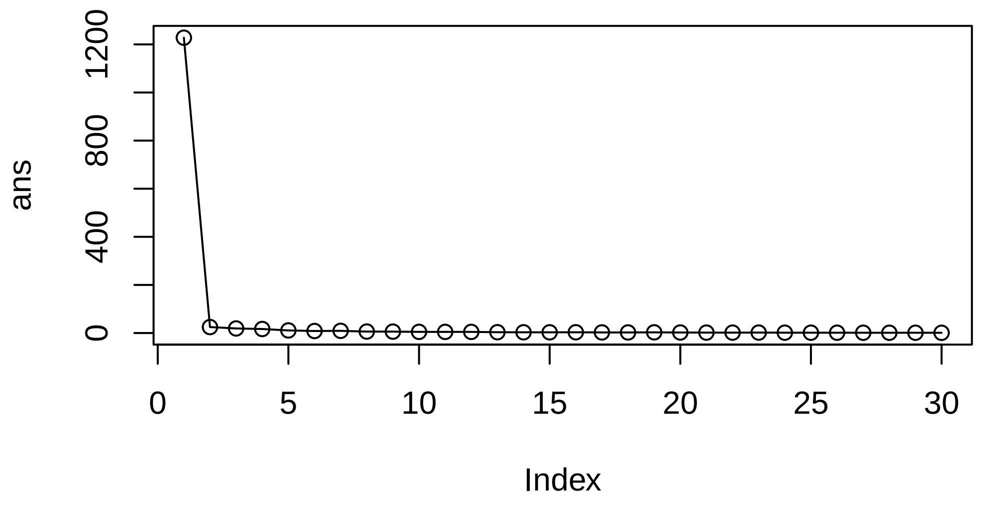
> Q. Let's ty different number of K (centers) from 1-30 and see what the best result is.

```
ans <- NULL
for(i in 1:30){
ans <- c(ans, kmeans(x,centers=i)$tot.withinss)
}
ans
```

```
 [1] 1227.8126552   24.7954977   19.0387051   16.6640108   10.8002881
 [6]    8.4255939    9.1017182    6.0942003    5.8563116    4.8615038
[11]    4.6927577    4.6976621    3.4026164    3.1212455    2.9868517
```

```
[16]    3.2023638    2.5194383    2.4075950    2.8037573    2.2076444
[21]    1.7566220    1.6426979    1.8279377    1.3700086    1.3671189
[26]    1.2906851    1.2009566    1.0615792    1.1961547    0.9312107
```

```
plot(ans, typ="o")
```



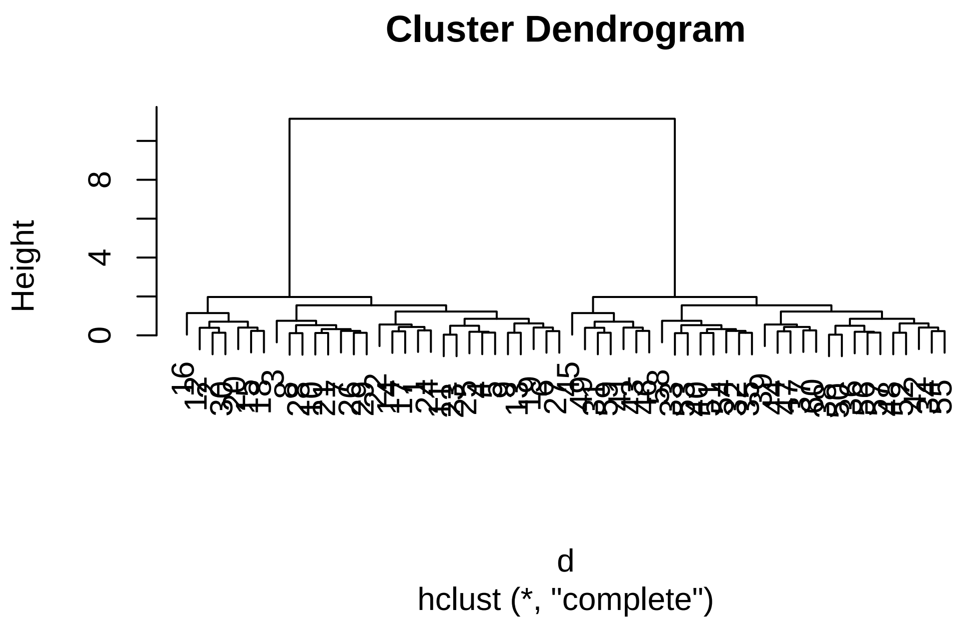
`tot.withinss` shows how tight the clusters are. The lower the value the tighter the clusters.

Key-point: ** K-means will impose a clustering structure on your data even if it is not there- it will always give the answer you asked for

Hierarchical CLustering

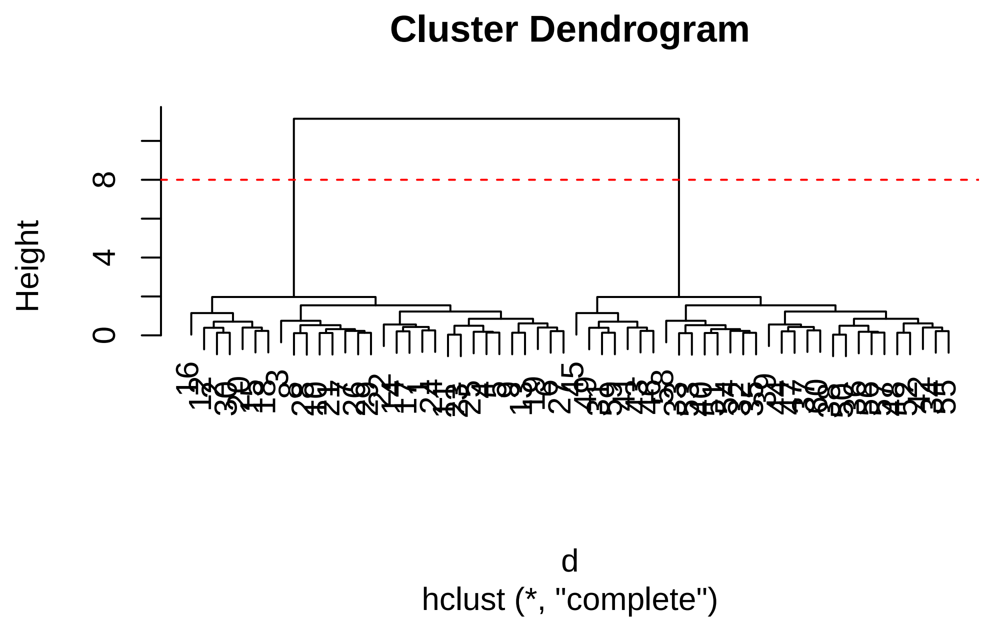
The main function for Hierarchical Clustering is called `hclust()`. Unlike `kmeans()` (which does all the work for us) you can't just pass `hclust()` our raw input data. It needs a "distance matrix" like the one returned frm the `dist()` function.

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



To extract our cluster membership vector from a `hclus` result object we have to "cut" our tree at a given height to yield seperate "groups"/"branches".

```
plot(hc)
abline(h=8, col="red",lty=2)
```



To do this we use the `cutree()` function o our `hclust()` object:

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

```r
table(grps, km$cluster)
```

```
grps  1  2
   1 30  0
   2  0 30
```

PCA of UK food data

Import the data set of food consumption in the UK:

```r
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
dim(x)
```

```
[1] 17  5
```

One solution to set the row names is to do it by hand.

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

```
 [1] "Cheese"               "Carcass_meat "        "Other_meat "
 [4] "Fish"                 "Fats_and_oils "       "Sugars"
 [7] "Fresh_potatoes "      "Fresh_Veg "           "Other_Veg "
[10] "Processed_potatoes "  "Processed_Veg "       "Fresh_fruit "
[13] "Cereals "             "Beverages"            "Soft_drinks "
[16] "Alcoholic_drinks "    "Confectionery "
```

```r
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
Fresh_potatoes             Fresh_potatoes     720   874      566      1033
Fresh_Veg                       Fresh_Veg     253   265      171       143
Other_Veg                       Other_Veg     488   570      418       355
Processed_potatoes Processed_potatoes     198   203      220       187
Processed_Veg               Processed_Veg     360   365      337       334
Fresh_fruit                   Fresh_fruit    1102  1137      957       674
Cereals                           Cereals    1472  1582     1462      1494
Beverages                       Beverages      57    73       53        47
Soft_drinks                   Soft_drinks    1374  1256     1572      1506
Alcoholic_drinks         Alcoholic_drinks     375   475      458       135
Confectionery               Confectionery      54    64       62        41
```

To remove the first column I can use the minus index trick.

```
x <- x[,-1]
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
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
```

A better way to do this is to set the row names to the first column by arguing with `read.csv()`.

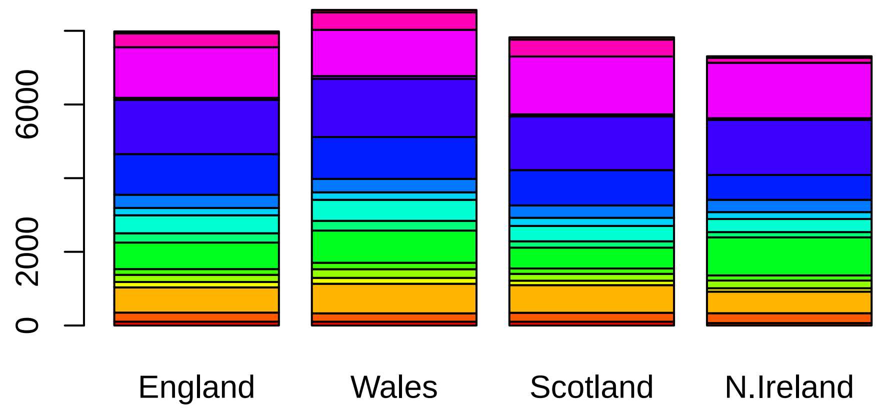
```
x <- read.csv(url,row.names=1)
x
```

```
                    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
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
```

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?

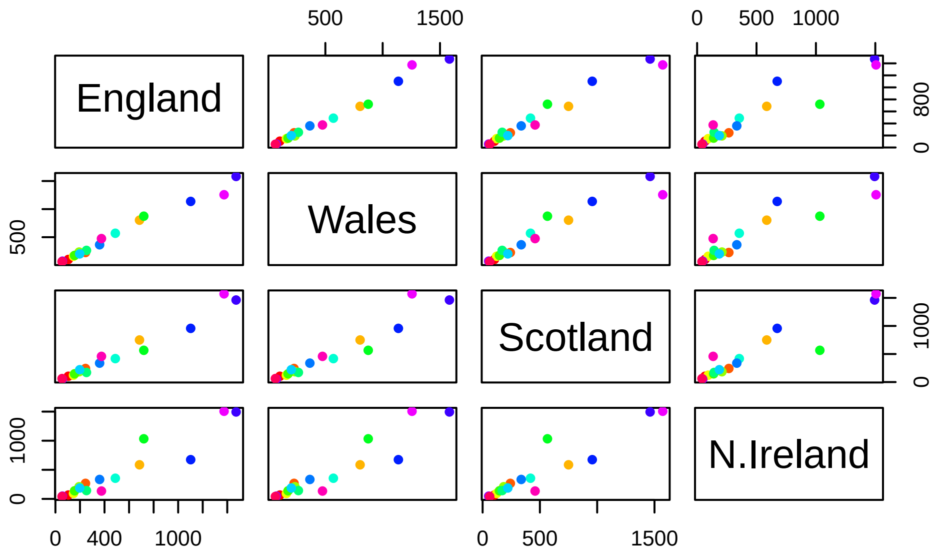
Spotting major differences and trends

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

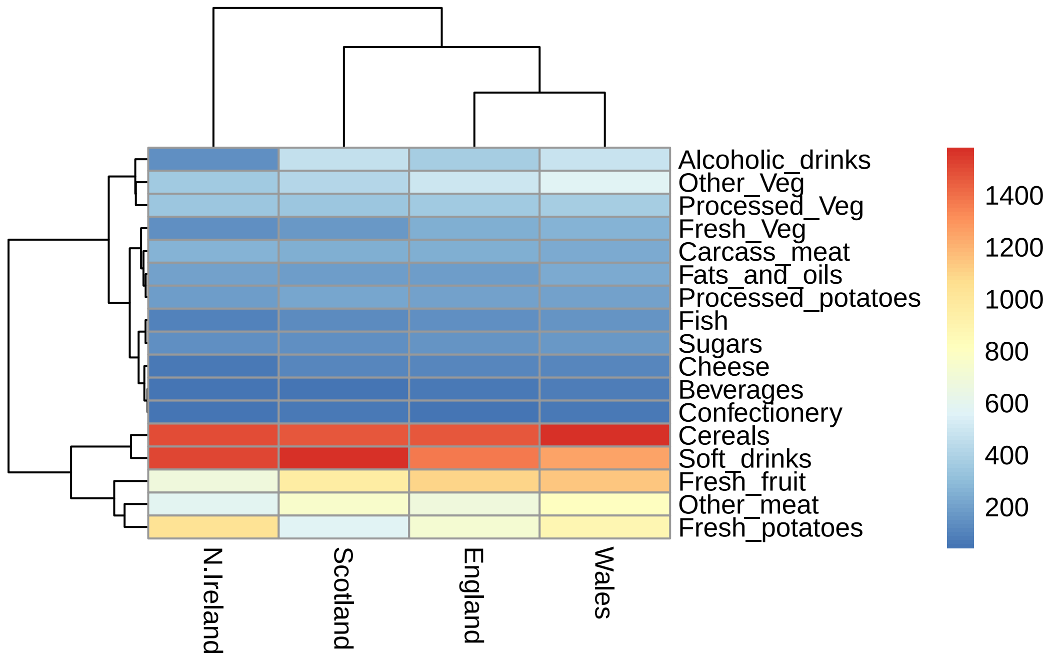


Pairs plots and heatmaps

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



```r
library(pheatmap)

pheatmap( as.matrix(x) )
```



PCA to the rescue

The main PCA in "base R" is called `prcomp()`. This function wants the transpose of our food data as input(i.e the food as columns and the countries as rows).

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

```
Standard deviations (1, .., p=4):
[1] 3.241502e+02 2.127478e+02 7.387622e+01 3.175833e-14

Rotation (n x k) = (17 x 4):
                            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
```

```r
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
```

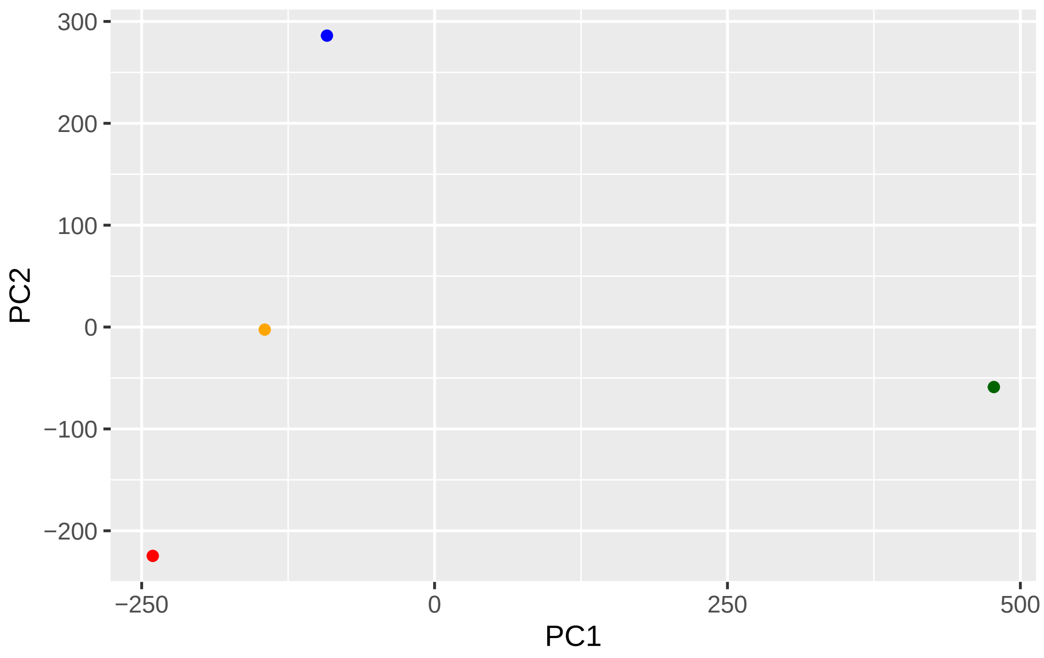
```r
attributes(pca)
```

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

$class
[1] "prcomp"
```

To make one of our main PCA result figures we turn to `pca$x` the scores along our new PCs. This is called "PC plot" or "score plot" or "Ordination plot" etc.

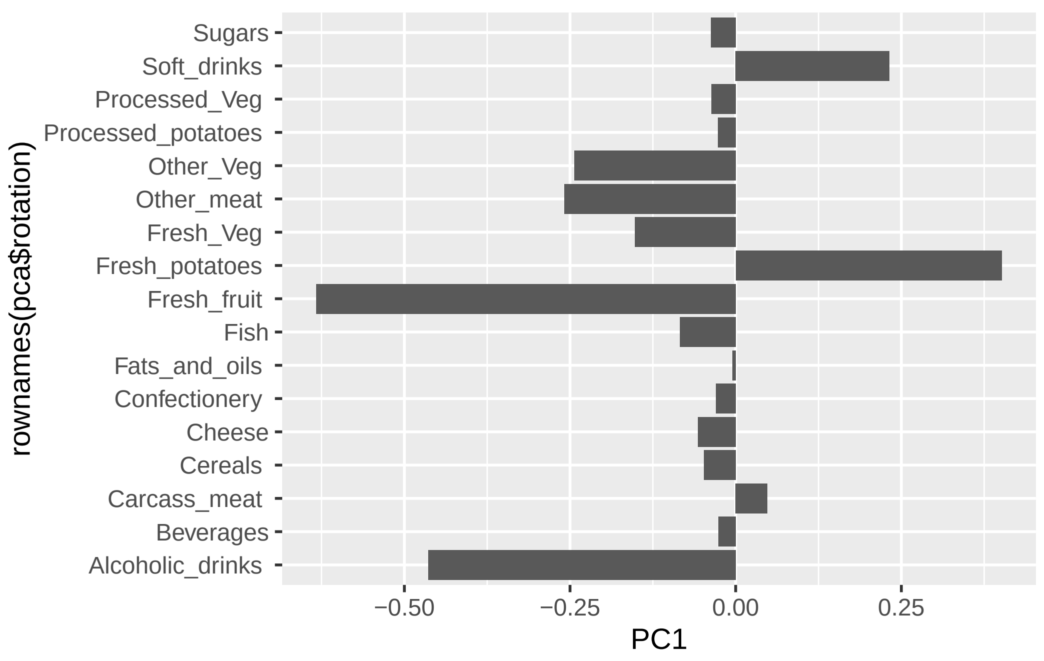
```r
my_cols <- (c("orange","red","blue","darkgreen"))
```

```r
library(ggplot2)
ggplot(pca$x) + aes(PC1,PC2)+geom_point(col=my_cols)
```



The second major result figure is called a “loadings plot” of “variable contributions plot” or “weight plot”.

```
ggplot(pca$rotation)+
  aes(PC1, rownames(pca$rotation)) + 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(pca$rotation)
−0.50
−0.25
0.00
0.25
PC1