Class 7: Machine Learning 1

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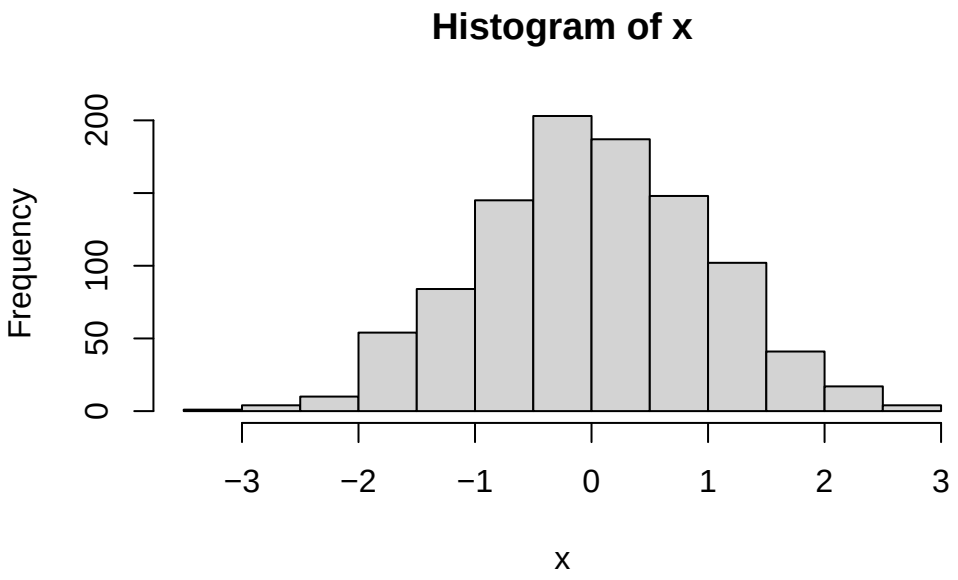
Clustering Methods

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] -3.30148314 -2.23211205 -5.22980332 -5.57722023 -2.84316094 -3.83500133
 [7] -0.90352558 -4.11334918 -4.38573154 -2.82409798 -2.49472520 -4.37371447
[13] -4.33350030 -3.28146119 -4.23594252  0.06057436 -2.79877630 -5.16504362
[19] -1.91989112 -2.00076335 -3.24352786 -3.80907680 -3.27851833 -2.87049230
[25] -2.22448866 -3.17069506 -2.47567598 -3.01417182 -2.95624190 -3.24611903
[31]  3.93837087  2.22374823  5.04319823  3.38182938  4.56424599  3.04557143
[37]  2.10468364  3.58145240  1.13732009  2.07057667  2.96269294  5.08661264
[43]  2.85829095  4.20414048  2.44672403  3.13937821  3.49636201  2.96727120
[49]  3.30482983  2.50016454  1.63992143  3.73383871  2.93879456  2.88037212
[55]  3.15305497  4.01693655  3.59277198  3.16423891  2.31631220  3.57881594
```

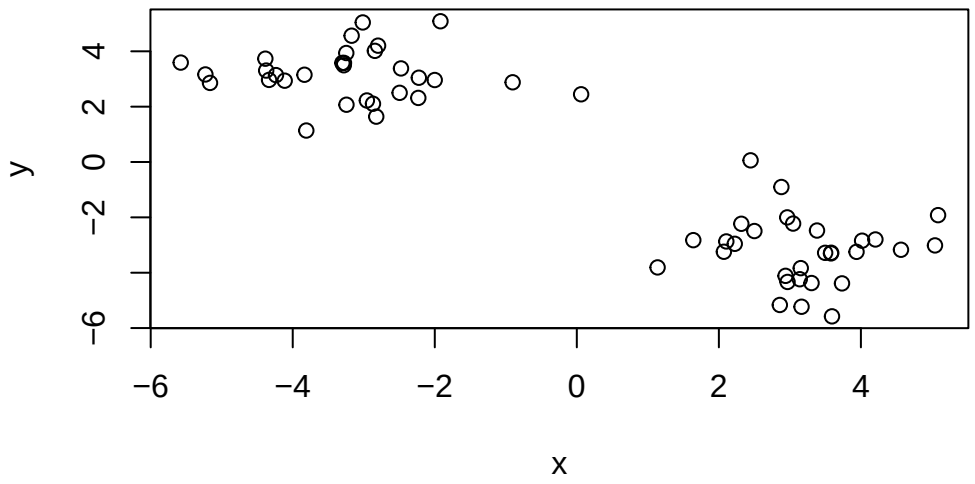
I will now make a wee x an y dataset with 2 groups of points.

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

```
                x           y
 [1,] -3.30148314  3.57881594
 [2,] -2.23211205  2.31631220
 [3,] -5.22980332  3.16423891
 [4,] -5.57722023  3.59277198
 [5,] -2.84316094  4.01693655
 [6,] -3.83500133  3.15305497
 [7,] -0.90352558  2.88037212
 [8,] -4.11334918  2.93879456
 [9,] -4.38573154  3.73383871
[10,] -2.82409798  1.63992143
[11,] -2.49472520  2.50016454
[12,] -4.37371447  3.30482983
[13,] -4.33350030  2.96727120
[14,] -3.28146119  3.49636201
[15,] -4.23594252  3.13937821
[16,]  0.06057436  2.44672403
[17,] -2.79877630  4.20414048
[18,] -5.16504362  2.85829095
[19,] -1.91989112  5.08661264
[20,] -2.00076335  2.96269294
[21,] -3.24352786  2.07057667
```

```
[22,] -3.80907680  1.13732009
[23,] -3.27851833  3.58145240
[24,] -2.87049230  2.10468364
[25,] -2.22448866  3.04557143
[26,] -3.17069506  4.56424599
[27,] -2.47567598  3.38182938
[28,] -3.01417182  5.04319823
[29,] -2.95624190  2.22374823
[30,] -3.24611903  3.93837087
[31,]  3.93837087 -3.24611903
[32,]  2.22374823 -2.95624190
[33,]  5.04319823 -3.01417182
[34,]  3.38182938 -2.47567598
[35,]  4.56424599 -3.17069506
[36,]  3.04557143 -2.22448866
[37,]  2.10468364 -2.87049230
[38,]  3.58145240 -3.27851833
[39,]  1.13732009 -3.80907680
[40,]  2.07057667 -3.24352786
[41,]  2.96269294 -2.00076335
[42,]  5.08661264 -1.91989112
[43,]  2.85829095 -5.16504362
[44,]  4.20414048 -2.79877630
[45,]  2.44672403  0.06057436
[46,]  3.13937821 -4.23594252
[47,]  3.49636201 -3.28146119
[48,]  2.96727120 -4.33350030
[49,]  3.30482983 -4.37371447
[50,]  2.50016454 -2.49472520
[51,]  1.63992143 -2.82409798
[52,]  3.73383871 -4.38573154
[53,]  2.93879456 -4.11334918
[54,]  2.88037212 -0.90352558
[55,]  3.15305497 -3.83500133
[56,]  4.01693655 -2.84316094
[57,]  3.59277198 -5.57722023
[58,]  3.16423891 -5.22980332
[59,]  2.31631220 -2.23211205
[60,]  3.57881594 -3.30148314
```

```
plot(x)
```




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

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

Cluster means:
          x         y
1 -3.202591  3.169084
2  3.169084 -3.202591

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 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

Within cluster sum of squares by cluster:
[1] 67.18885 67.18885
 (between_SS / total_SS =  90.1 %)

Available components:

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

Q. From your results object 'k' how many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q. What "component" of your result object details the 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 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
```

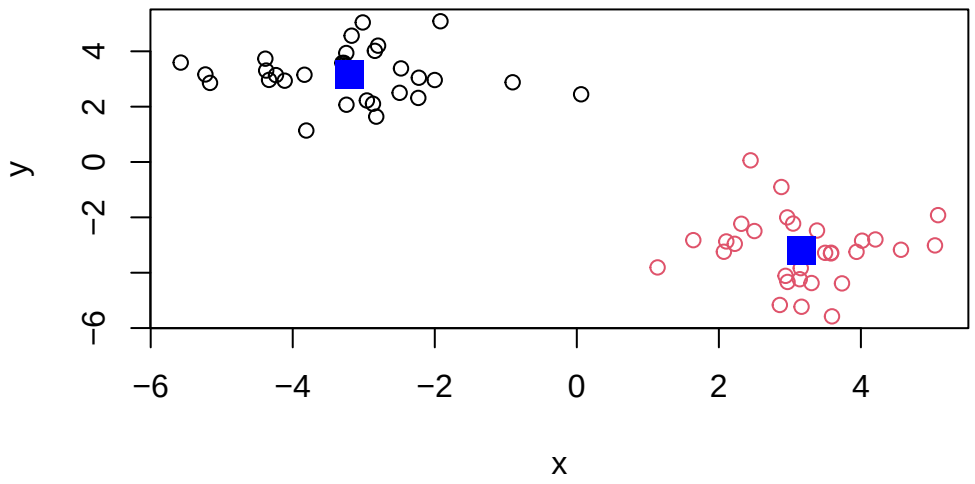
Cluster centers?

```
k$centers
```

```
          x         y
1 -3.202591  3.169084
2  3.169084 -3.202591
```

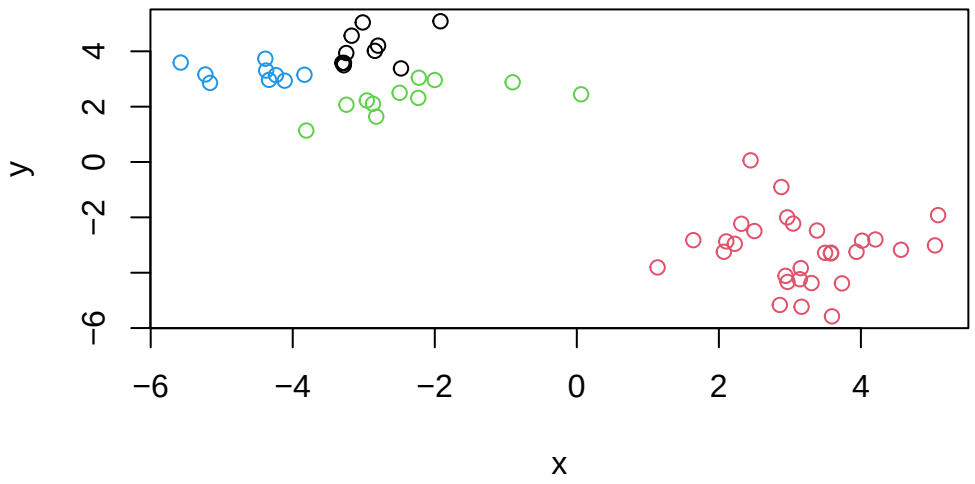
Q. Plot of our clustering results

```
plot(x, col=k$cluster)
points(k$center, 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

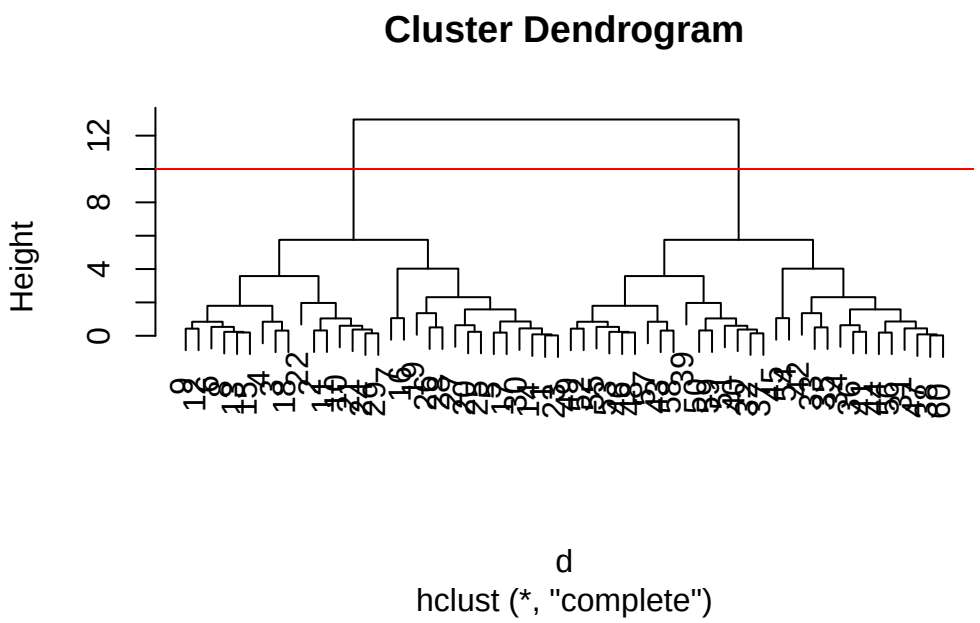
The main base R function for Hierarchial Clustering is 'hclust()'. Unlike 'kmeans()' you can not just pass it your data as input. You first need to calculate a distance matrix.

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

```
Call:
hclust(d = d)

Cluster method   : complete
Distance         : euclidean
Number of objects: 60
```

Use 'plot()' to see results.

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



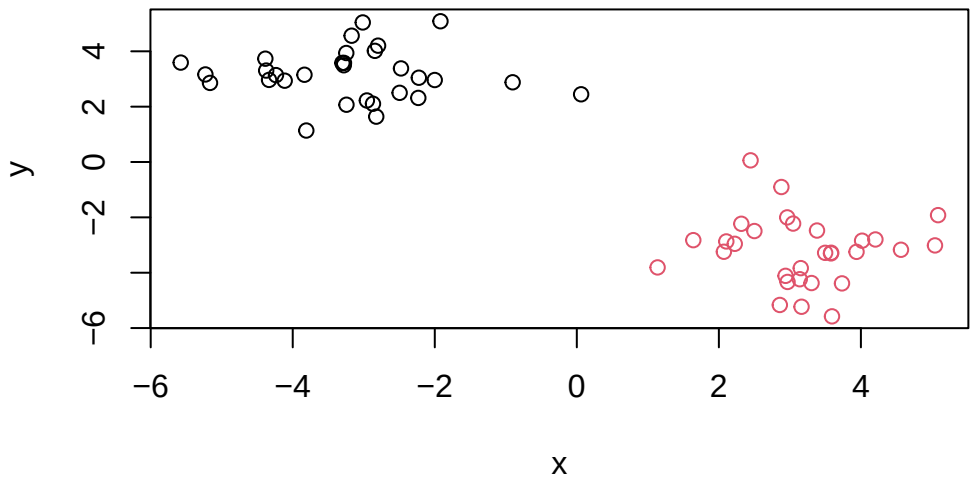
To make the "cut" and get our cluster membership vector we can use the 'cutree()' function.

```
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 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
```

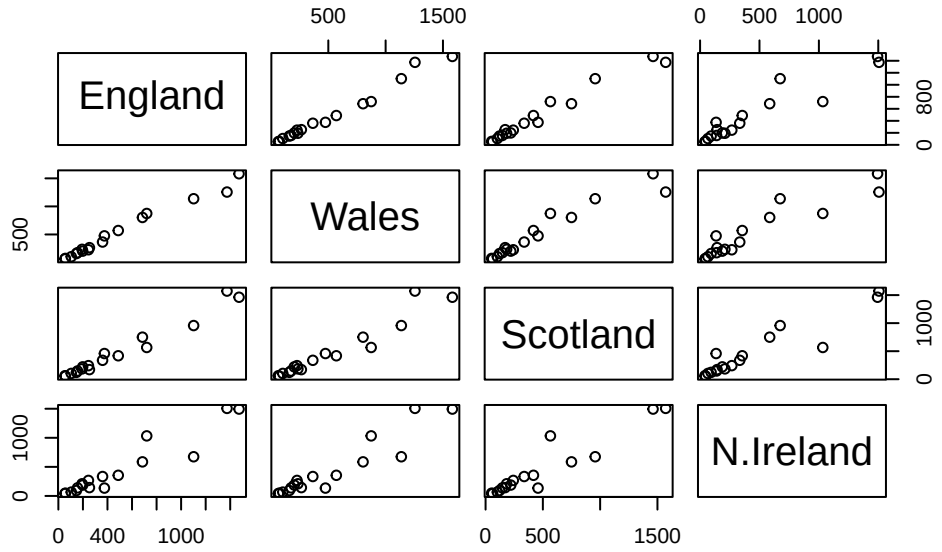
Make a plot of our data colored by hclust results

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



PCA of UK Food Data

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




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

```
     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
720    874      566      1033
253    265      171       143
488    570      418       355
198    203      220       187
360    365      337       334
1102  1137      957       674
1472  1582     1462      1494
57      73       53        47
1374  1256     1572      1506
375    475      458       135
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?

```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

```
[1] 3
```

```
dim(x)
```

```
[1] 17  3
```

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?

- I prefer the second method since the first method can give errors if we run it multiple times.

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

```
    Scotland N.Ireland
103      103        66
227      242       267
803      750       586
160      122        93
235      184       209
175      147       139
```

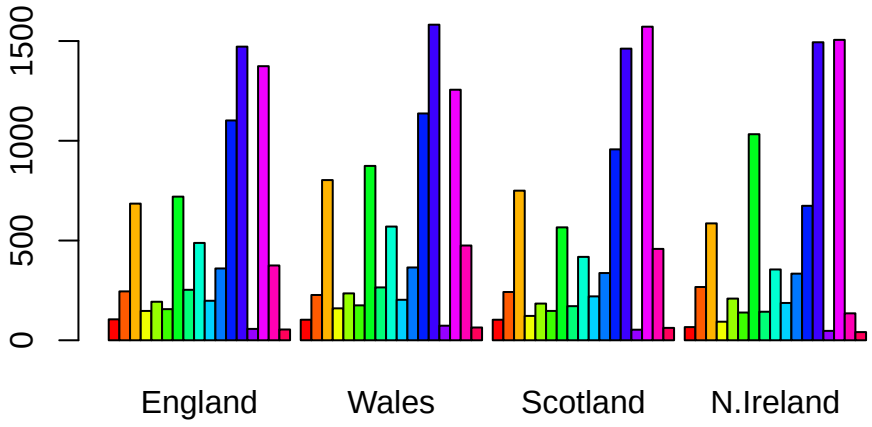
```
x <- read.csv(url, row.names=1)
head(x)
```

```
                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
```

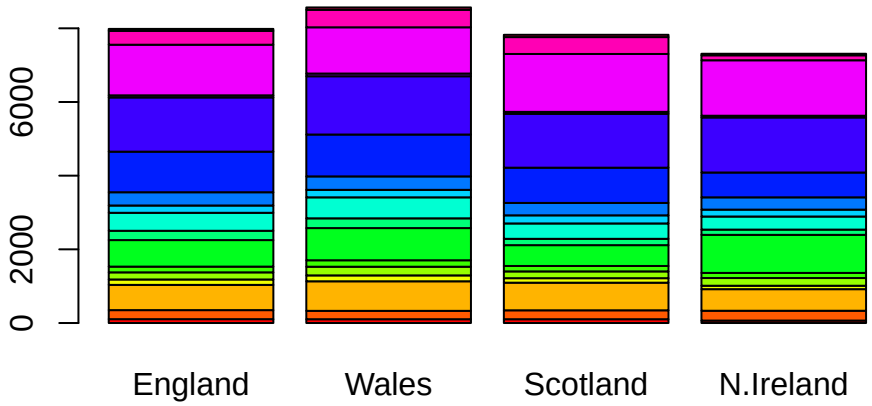
Q3: Changing what optional argument in the above barplot() function results in the following plot?

- beside=T to beside=F
- if FALSE, the columns of height are portrayed as stacked bars, and if TRUE the columns are portrayed as juxtaposed bars.

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

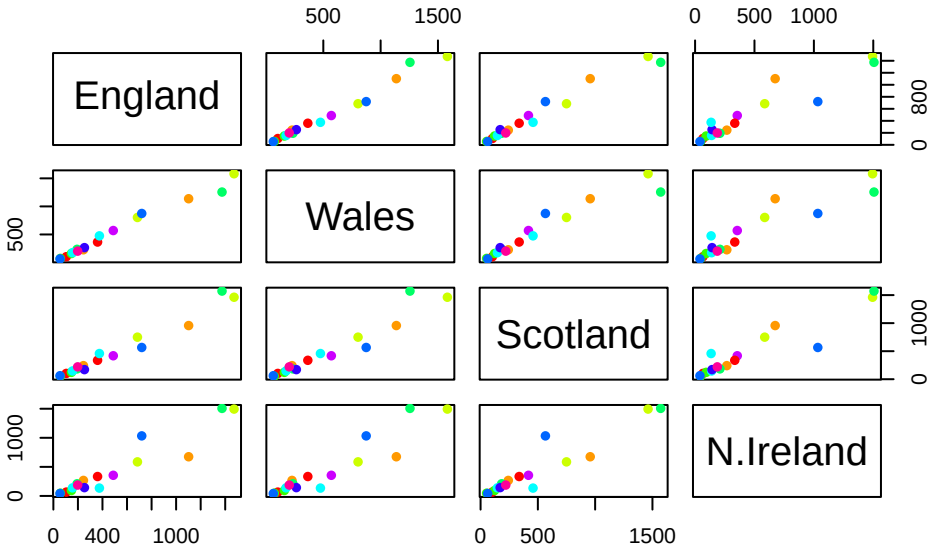



```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



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?

```
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 columns.

```
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
```

Q. How much variance is captured in 2 PCs?

- 96.5%

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

```
attributes(pca)
```

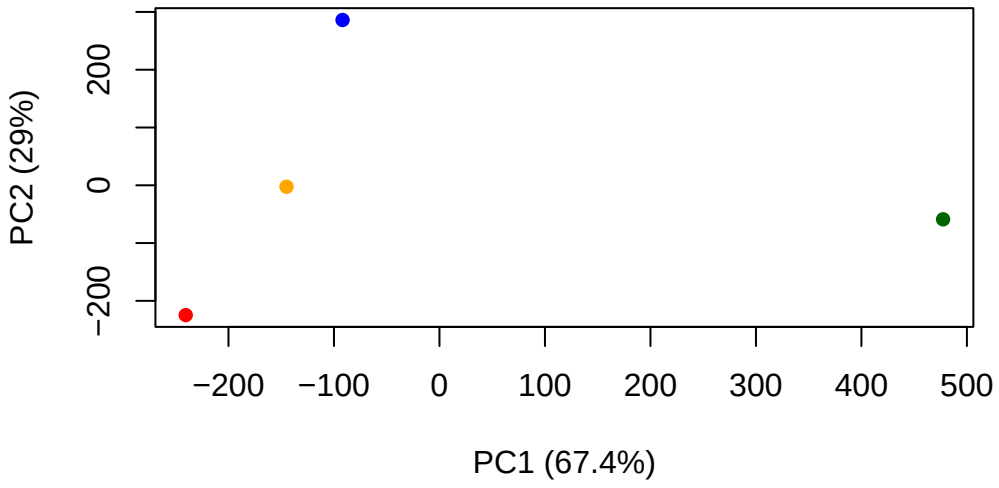
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

We are after the 'pca$x' result componenet to make our main PCA plot.

```
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
```

```
mycols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=mycols, pch=16,
     xlab="PC1 (67.4%)", ylab="PC2 (29%)")
```



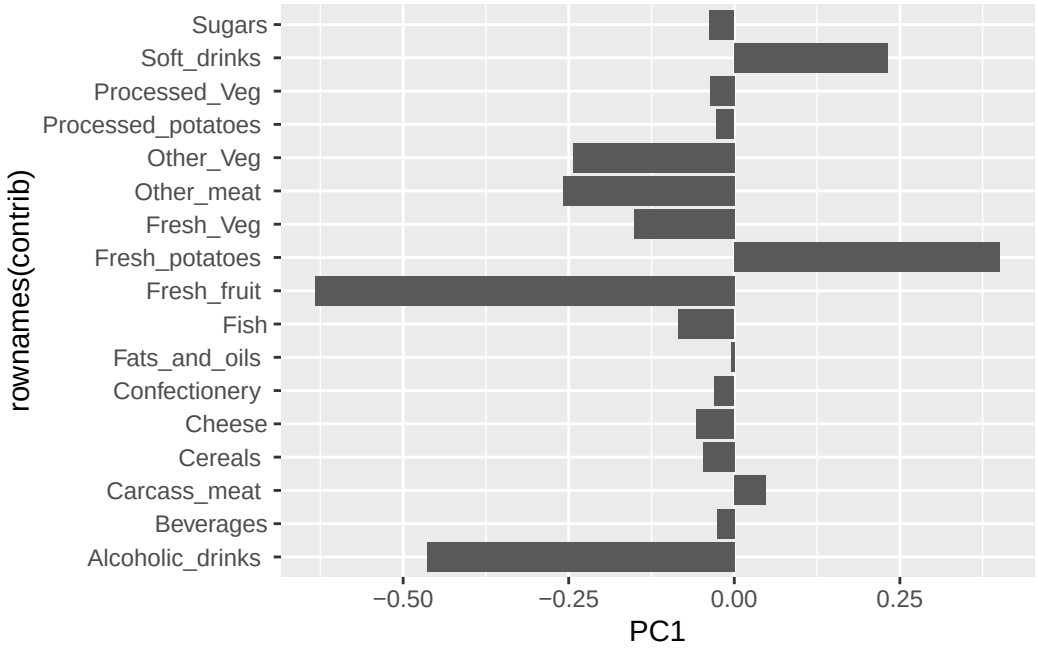
Another important result from PCA is how the original variables (in this case the foods) contribute to the PCs. This is contained in the 'pca$rotation' object - folks often call this the "loadings" or "contributions" to the PCs

```
pca$rotation
```

```
                          PC1          PC2         PC3          PC4
Cheese             -0.056955380  0.016012850  0.02394295 -0.694538519
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
```

We can make a plot along PC1.

```
library(ggplot2)
contrib <- as.data.frame(pca$rotation)
ggplot(contrib) +
  aes(PC1, rownames(contrib)) +
  geom_col()
```


rownames(contrib)
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
−0.50
−0.25
0.00
0.25
PC1