class07: Machine Learning 1

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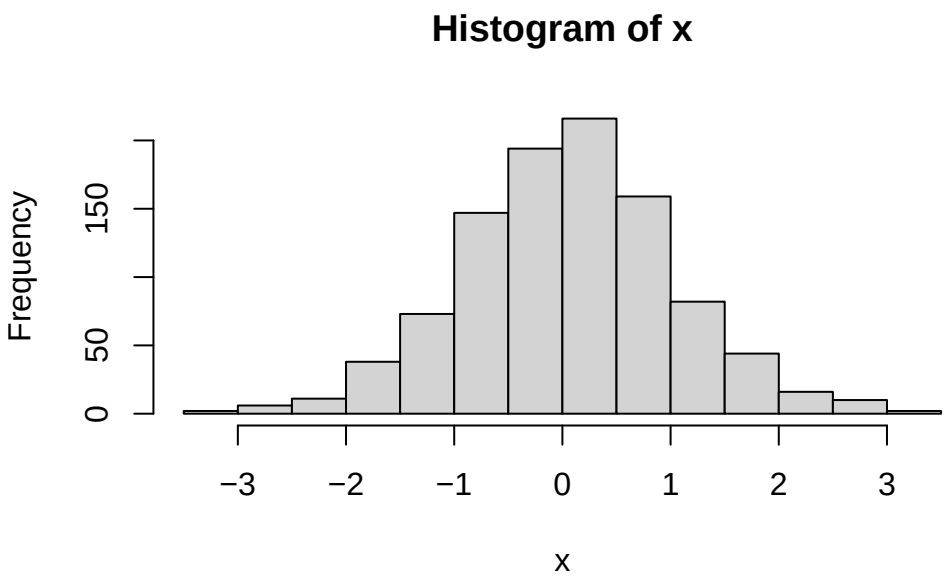
#Clustering Methods

The broad goal here is to find groups (clusters) in your input data

##Kmeans

First, let's make up some data to cluster

```
#rnorm generates a random data set that creates a normal distribution with 1000 points
x <- rnorm(1000)
hist(x)
```



Make a vector of length of 60 with 30 points cenetred on -3 and 30 points centered at +3

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

```
 [1] -2.564707 -3.178687 -3.949849 -4.285774 -2.707827 -1.661039 -2.425797
 [8] -4.239311 -2.087322 -2.567371 -2.057167 -3.101770 -3.380694 -3.593959
[15] -3.648812 -2.496706 -3.193413 -1.470624 -2.890417 -2.551546 -2.664768
[22] -3.232489 -3.256706 -2.653497 -2.955602 -3.619669 -4.676238 -3.345370
[29] -1.539865 -3.394768  4.529161  2.043800  2.203278  1.104993  3.798708
[36]  3.988852  3.017736  2.408608  3.342931  3.596817  3.119469  3.560245
[43]  3.911043  2.156519  4.025274  2.229696  3.295722  2.593097  3.843878
[50]  2.597906  3.588088  3.421639  2.732810  3.828407  3.135863  3.173958
[57]  2.548030  4.516530  2.813753  2.403883
```

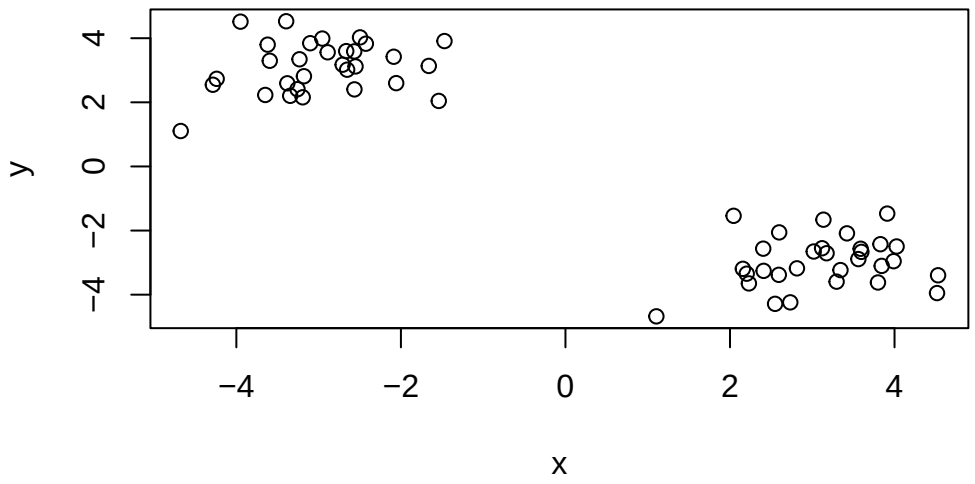
I will now make a small x and y dataset with 2 groups of points.

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

```
              x         y
 [1,] -2.564707  2.403883
 [2,] -3.178687  2.813753
 [3,] -3.949849  4.516530
 [4,] -4.285774  2.548030
 [5,] -2.707827  3.173958
 [6,] -1.661039  3.135863
 [7,] -2.425797  3.828407
 [8,] -4.239311  2.732810
 [9,] -2.087322  3.421639
[10,] -2.567371  3.588088
[11,] -2.057167  2.597906
[12,] -3.101770  3.843878
[13,] -3.380694  2.593097
[14,] -3.593959  3.295722
[15,] -3.648812  2.229696
[16,] -2.496706  4.025274
[17,] -3.193413  2.156519
[18,] -1.470624  3.911043
[19,] -2.890417  3.560245
[20,] -2.551546  3.119469
[21,] -2.664768  3.596817
[22,] -3.232489  3.342931
```

```
[23,] -3.256706  2.408608
[24,] -2.653497  3.017736
[25,] -2.955602  3.988852
[26,] -3.619669  3.798708
[27,] -4.676238  1.104993
[28,] -3.345370  2.203278
[29,] -1.539865  2.043800
[30,] -3.394768  4.529161
[31,]  4.529161 -3.394768
[32,]  2.043800 -1.539865
[33,]  2.203278 -3.345370
[34,]  1.104993 -4.676238
[35,]  3.798708 -3.619669
[36,]  3.988852 -2.955602
[37,]  3.017736 -2.653497
[38,]  2.408608 -3.256706
[39,]  3.342931 -3.232489
[40,]  3.596817 -2.664768
[41,]  3.119469 -2.551546
[42,]  3.560245 -2.890417
[43,]  3.911043 -1.470624
[44,]  2.156519 -3.193413
[45,]  4.025274 -2.496706
[46,]  2.229696 -3.648812
[47,]  3.295722 -3.593959
[48,]  2.593097 -3.380694
[49,]  3.843878 -3.101770
[50,]  2.597906 -2.057167
[51,]  3.588088 -2.567371
[52,]  3.421639 -2.087322
[53,]  2.732810 -4.239311
[54,]  3.828407 -2.425797
[55,]  3.135863 -1.661039
[56,]  3.173958 -2.707827
[57,]  2.548030 -4.285774
[58,]  4.516530 -3.949849
[59,]  2.813753 -3.178687
[60,]  2.403883 -2.564707
```

```
plot(x)
```




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

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

Cluster means:
          x         y
1  3.117690 -2.979725
2 -2.979725  3.117690

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

Within cluster sum of squares by cluster:
[1] 36.51219 36.51219
 (between_SS / total_SS =  93.9 %)

Available components:

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

Q1. From the results object, `k` how many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q2. What "component" of your resukt object details the cluster membership?

```
k$cluster
```

```
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

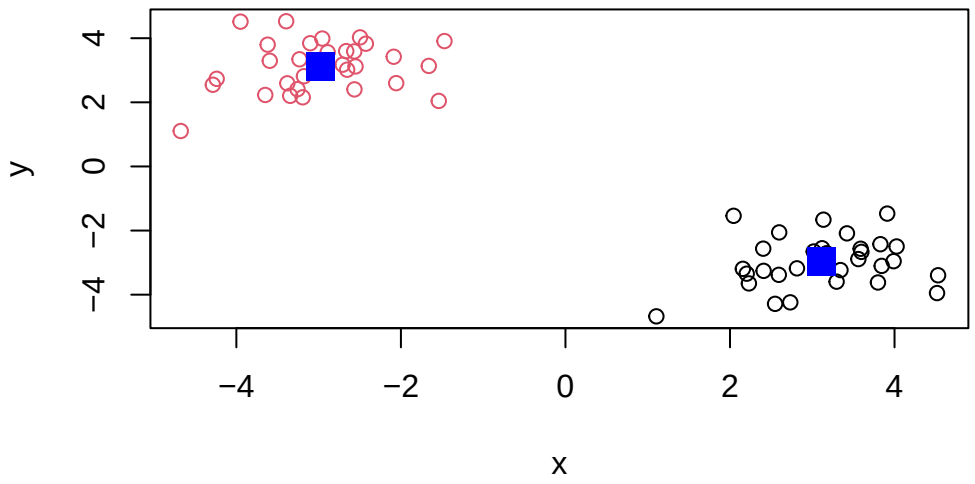
Q3. Cluster centers?

```
k$centers
```

```
          x         y
1  3.117690 -2.979725
2 -2.979725  3.117690
```

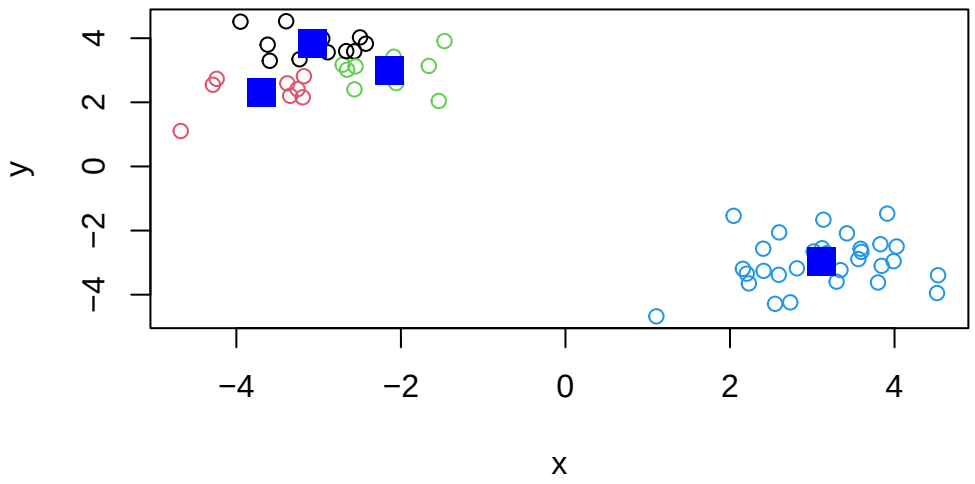
Q. Plot of our clustering results

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



We can cluster into 4 groups

```
#K means
k4 <- kmeans(x,centers = 4)

#plot results
plot(x, col = k4$cluster)
points(k4$centers, col= "blue", pch =15, cex=2)
```



A big limitation of kmeans is that it does what you ask even if you ask for silly clusters.

Hierarchical Clustering

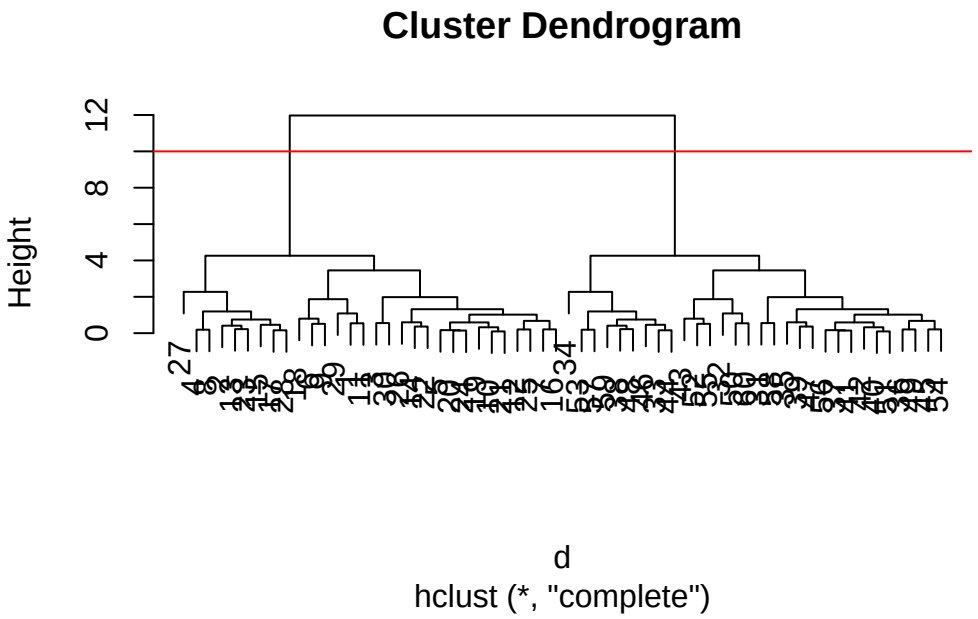
The main base R function for Hierarchical Clustering is `hclust()`. Unlike `kmeans()` you can not just pass it your data as input. You first need to calculate a distance matrix.

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

```
Call:
hclust(d = d)

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

Use `plot()` to view results

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



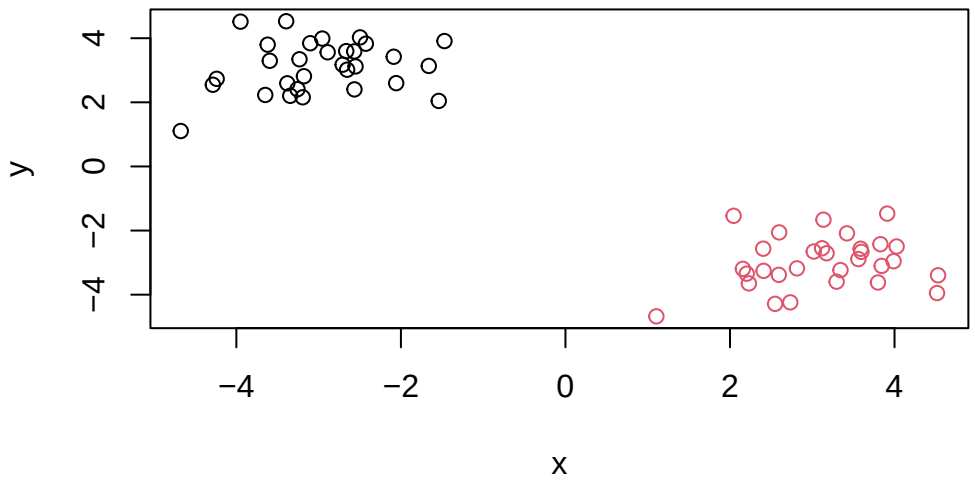
To make the "cut" and get our cluster membership ector, we can use the `cutree()` function.

```
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 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
```

Make a plot of our data colored by hclust results

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



PCA of UK Food

Here we will do Principal Component Analysis (PCA) on some food data from the UK.

```
url <- "https://tinyurl.com/UK-foods"
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
```

```
#not a good way because it can over ride itself
#rownames(x) <- x[,x]
#x <- x[,-1]
#x
```

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

```
dim(x)
```

```
[1] 17  4
```

There are 17 rows and 4 columns in the edited version because the first column was read in as the row names. I used `dim()` to see both the rows and columns with only one function.

Looking at the data

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

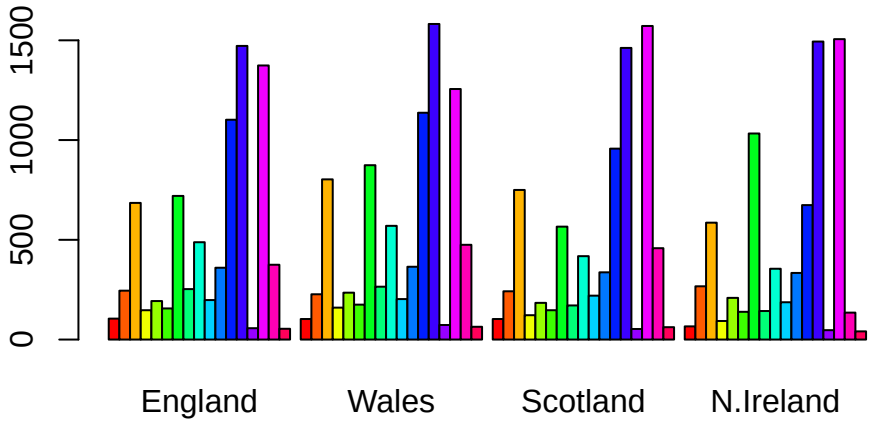
```
              England Wales Scotland N.Ireland
Cheese            105   103      103        66
Carcass_meat      245   227      242       267
Other_meat        685   803      750       586
Fish              147   160      122        93
Fats_and_oils     193   235      184       209
Sugars        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

The row.names =1 option in the `read.csv()` is a better option because it wont continue to eat at the data set if run multiple times like the other option.

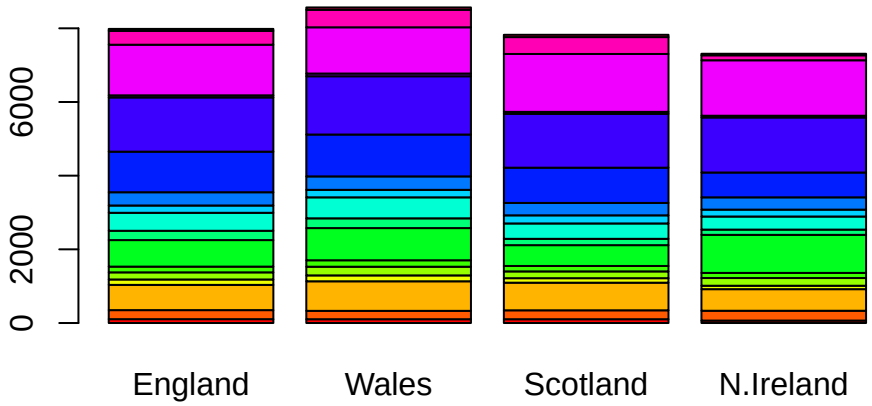
Spotting Major Differences in the data set

```
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?

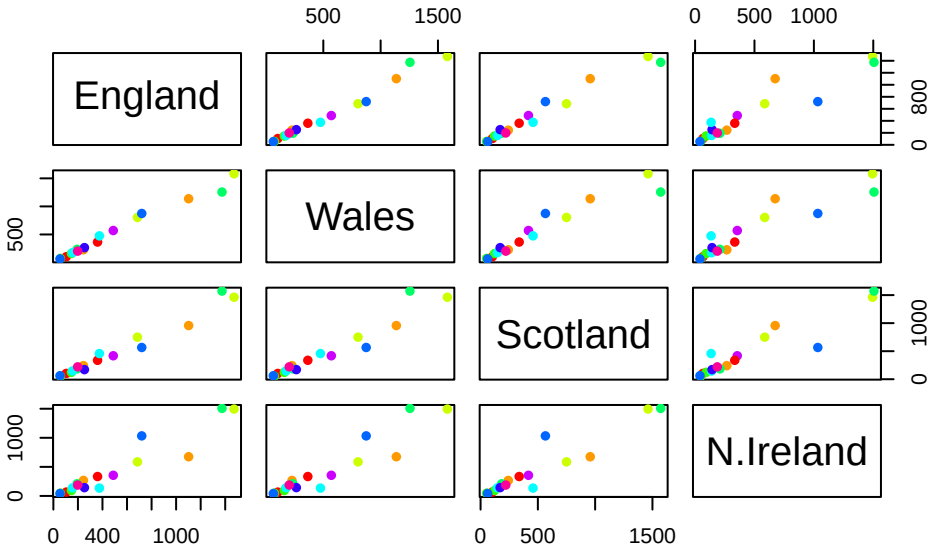
```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



Changing the `beside` argument to False results in the change of the barplot.

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)
```



These plots show the coutries plotted against each other. If the points are on a diagonal between two countries, that means the value is the same in both countries. This shows that Northern Ireland has a few points that are off the diagonal and thus it has some differences from all three.

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

It is too difficult to tell which food is the main difference but the blue and orange points tend to be off the diagonal for Northern Ireland.

##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.

```
# Use the prcomp() PCA function
#t() is used to transpose the data which makes the countries in the row names rather than
pca <- prcomp( t(x) )
#summary tables tells how well the PCA captures the variance
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%

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

To make our main "PC score plot" or "PC1 vs PC2 plot" or "PC plot" or "ordination plot".

```
attributes(pca)
```

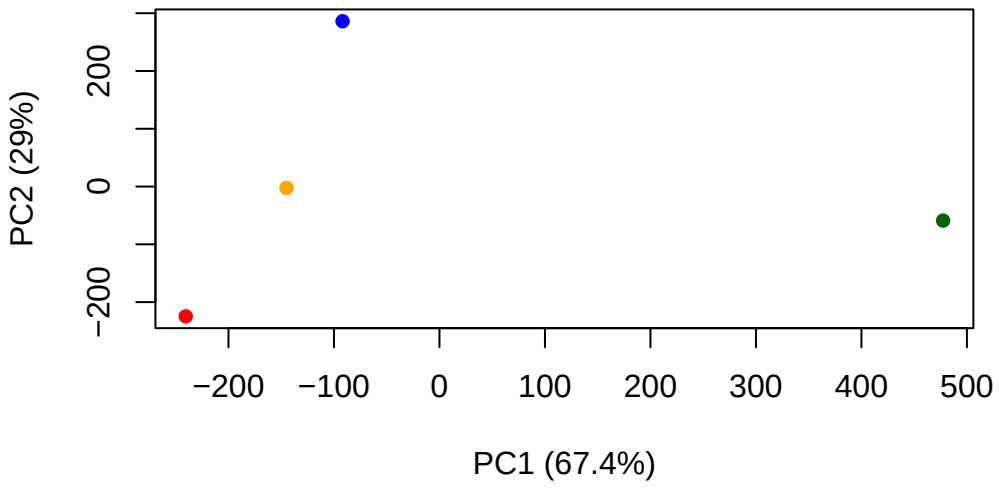
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

We are after `pca$x` result component 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
```

```
# Plot PC1 vs PC2
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 PCAs.

This is contained in the `pca$rotation` object- folks often cll 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
```

```
#greater values mean more contribution (abs value)
```

We can make a plot along PC1.

```
library(ggplot2)

contributions <- as.data.frame(pca$rotation)

ggplot(contributions) +
  aes(PC1, rownames(contributions)) +
  geom_col()
```