Class 7: Machine Learning 1

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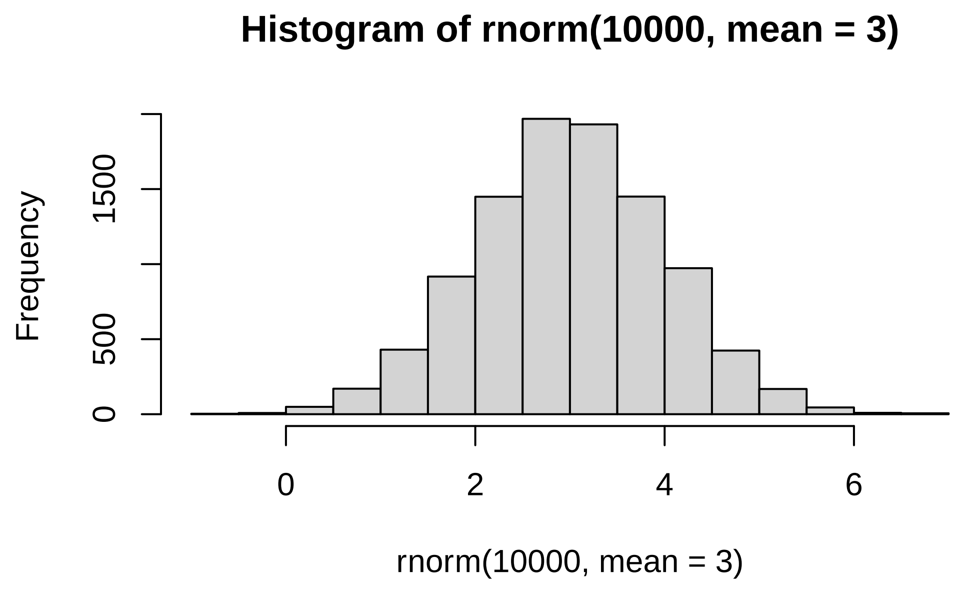
Today we will explore unsupervised machine learning methods, beginning with clustering and dimensionality reduction.

Clustering

Let's make up some data to cluster so that we know what the answer should be. The `rnorm()` function will help here.

```r
hist(rnorm(10000, mean = 3))
```



Return 30 numbers centered on -3.

```
rnorm(30, mean = -3)
```

```
 [1] -3.1334729 -3.2540254 -2.2029798 -0.4556317 -1.8410348 -3.3900962
 [7] -3.7773526 -3.5013933 -2.8390137 -2.0760867 -4.7931490 -2.8556319
[13] -1.6098052 -3.6848046 -1.4995771 -2.9471420 -2.6221567 -2.2866287
[19] -0.1237786 -4.4097363 -4.1454898 -2.4952787 -2.6383429 -3.0258054
[25] -3.1326430 -3.5473095 -2.8748996 -3.3316792 -4.2395189 -1.9419915
```

```
rnorm(30, mean = 3)
```

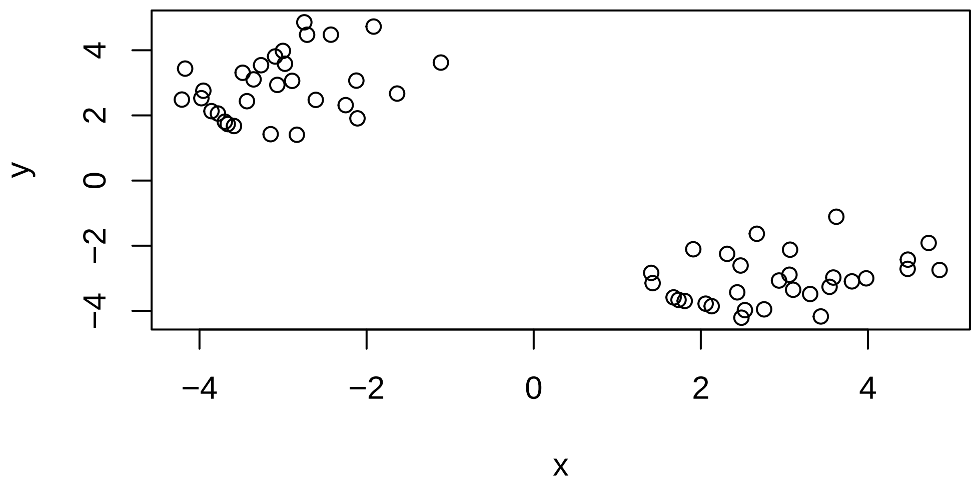
```
 [1] 2.580990 2.892710 3.407048 2.768087 3.026499 3.886969 3.049518 3.210014
 [9] 2.720161 2.564673 3.412345 3.047199 2.540965 4.129591 4.066433 1.961232
[17] 1.426716 2.330056 3.526165 3.603371 2.380431 3.400538 2.121846 3.171463
[25] 3.667982 2.479904 3.204630 2.729300 3.483269 3.229509
```

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

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

Make a plot of `x`.

```r
plot(x)
```



K-means

The main function in base R for K-means clustering is called `kmeans()`.

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

The `kmeans` function returns a list with 9 components. You can see the named components of any list with the `attributes()` function.

```r
attributes(km)
```

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

$class
[1] "kmeans"
```

How many points are in each cluster?

```r
km$size
```

```
[1] 30 30
```

Cluster assignment/membership vector

```r
km$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 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
```

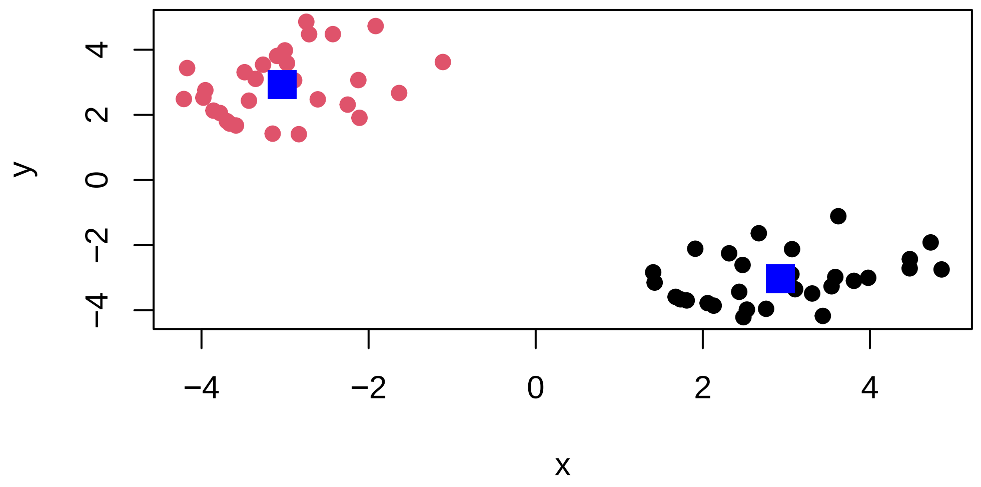
Cluster centers

```r
km$centers
```

```
          x         y
1  2.926942 -3.036133
2 -3.036133  2.926942
```

Make a plot of our `kmeans()` results showing cluster assignment using different colors for each group of points and cluster centers in blue. .

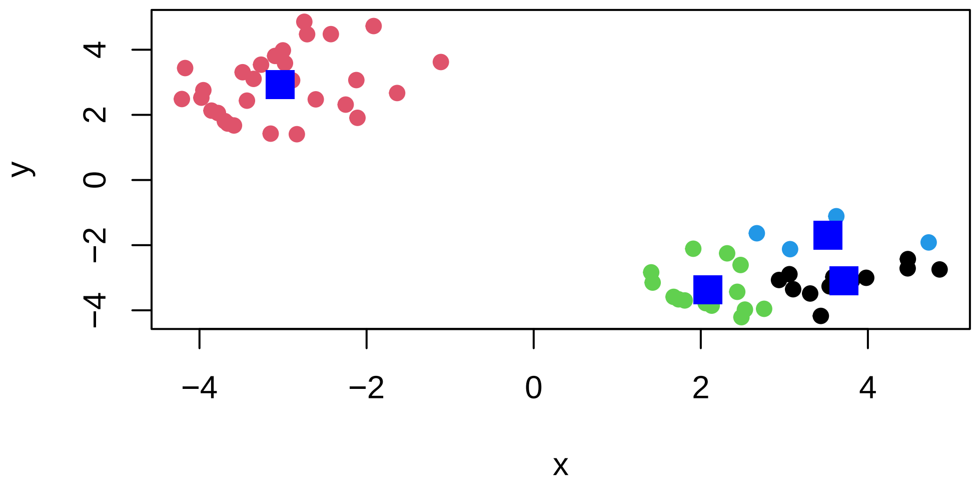
```r
plot(x, col = km$cluster, pch = 19)
points(km$centers, col = "blue", pch = 15, cex = 2)
```



Run `kmeans()` again on `x` but cluster into 4 groups and plot the same result figure.

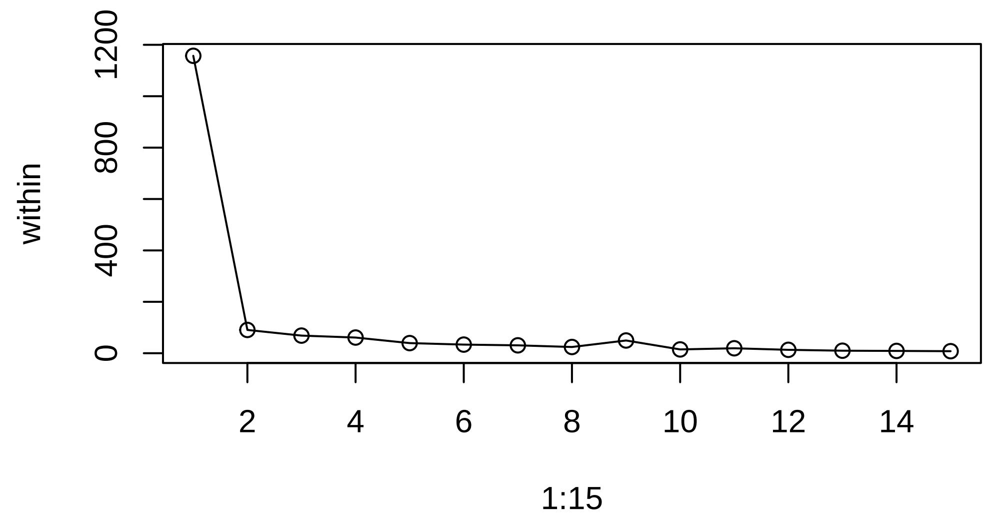
```r
km2 <- kmeans(x, centers = 4)

plot(x, col = km2$cluster, pch = 19)
points(km2$centers, col = "blue", pch = 15, cex = 2)
```



Scree plot

```
within <- numeric(15)
for (n in 1:15){
  km <- kmeans(x, centers = n)
  within[n] <- km$tot.withinss
}
plot(x = 1:15, y = within)
lines(x = 1:15, y = within)
```



> **Key point** - k-means clustering is very popular but can be misused. One big limitation is that it can impose a clustering pattern on data even if clear natural groupings don't exist - i.e., it does what you tell it to do with regard to the number of `centers`.

Hierarchical clustering

The main function in base R for hierarchical clustering is `hclust()`.

You can't just pass an input dataset as is into `hclust()`. Data must first be made into a "distance matrix", which can be done using the `dist()` function.

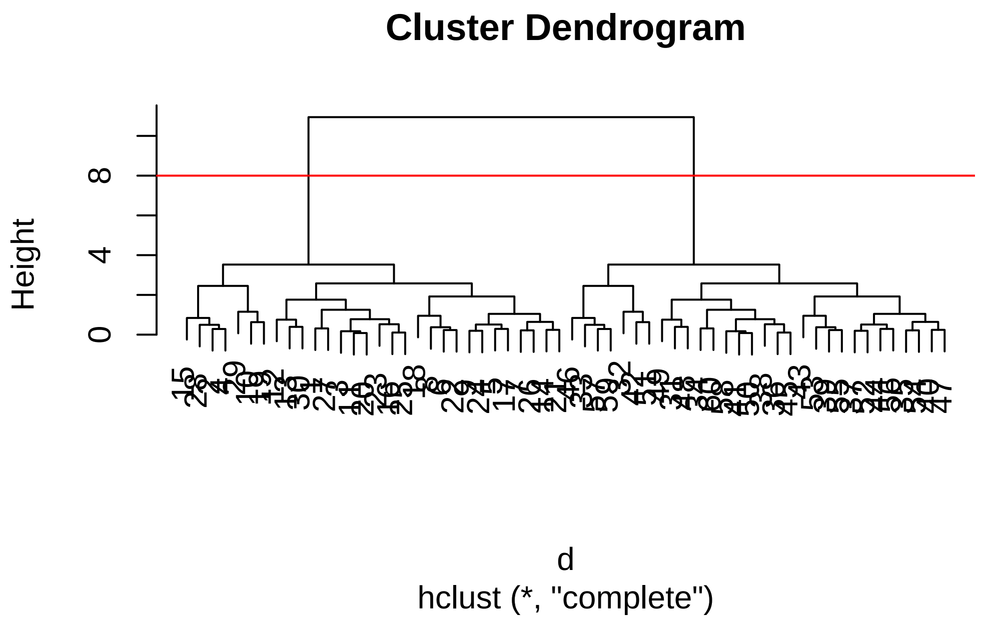
```r
d <- dist(x)
hc <- hclust(d)
hc
```

```
Call:
hclust(d = d)

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

The results of `hclust()` don't have a useful `print` method, but they do have a special `plot` method.

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

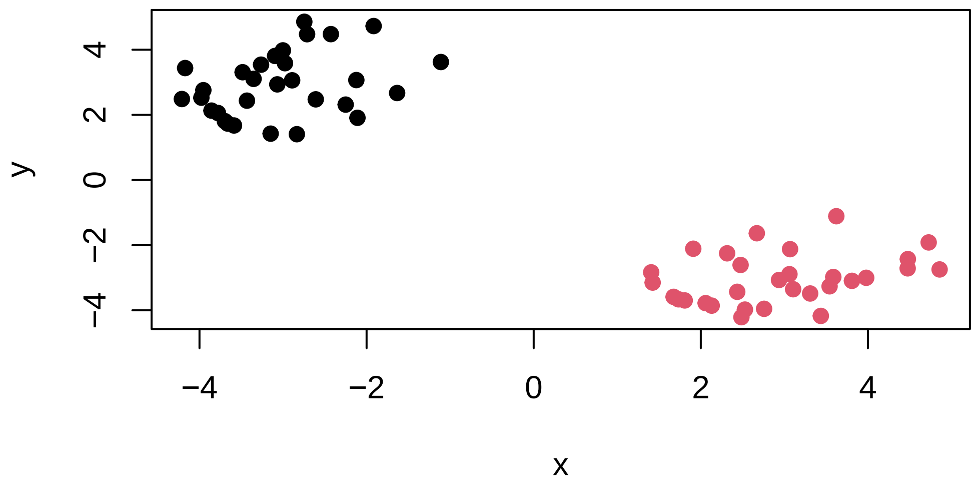


To get our main cluster assignment (membership vector), we need to "cut" the tree at the big goalposts.

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

```
grps
 1  2 
30 30 
```

```r
plot(x, col = grps, pch = 19)
```



Hierarchical clustering is distinct in that the dendrogram can reveal the potential grouping in your data (unlike k-means).

Dimensionality reduction - principal component analysis (PCA)

PCA is a common and highly useful dimensionality reduction technique used in many fields - particularly bioinformatics.

Here we will analyze some data from the UK on food consumption.

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

dim(UK_foods)
```

```
[1] 17  5
```

```
head(UK_foods)
```

```
               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
```

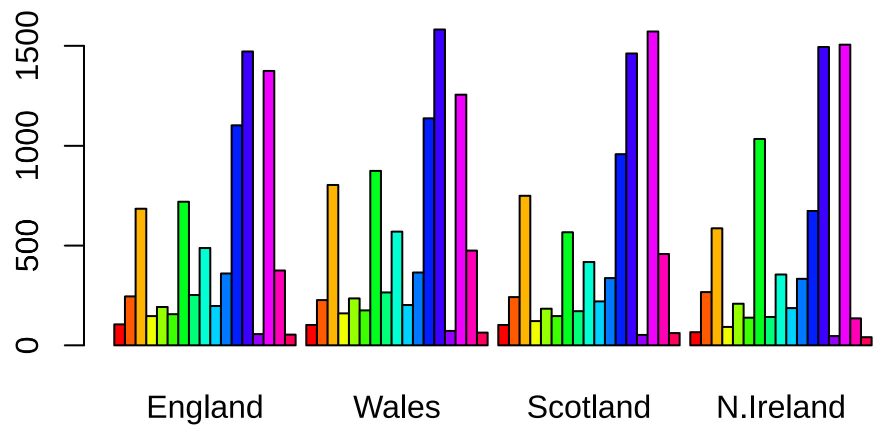
```
rownames(UK_foods) <- UK_foods[, 1]
UK_foods <- UK_foods[, -1]
head(UK_foods)
```

```
               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
```

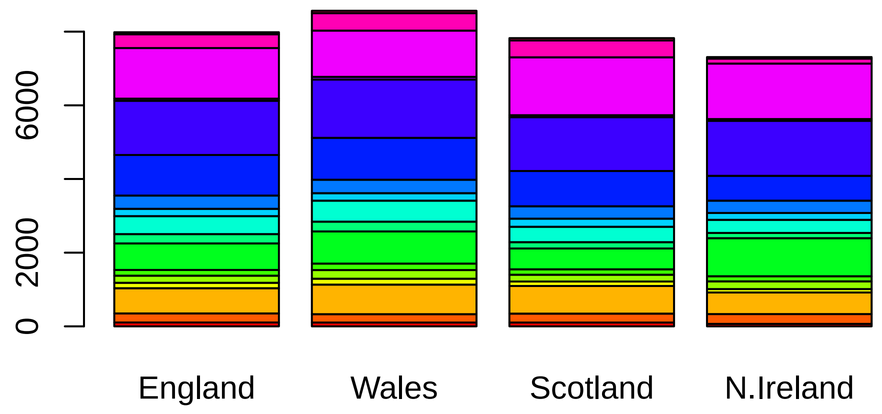
```
UK_foods <- read.csv(url("https://tinyurl.com/UK-foods"), row.names = 1)
head(UK_foods)
```

```
               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
```

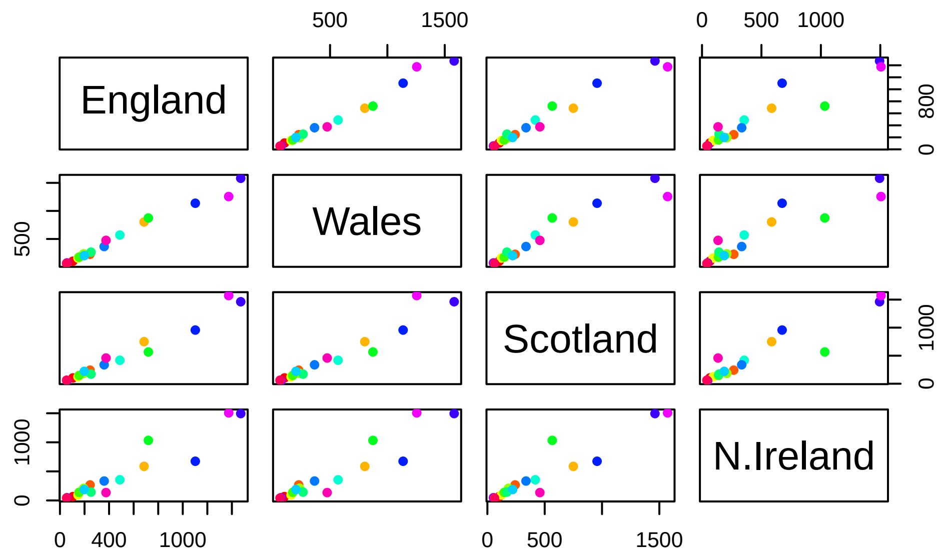
```
barplot(as.matrix(UK_foods), beside=T, col=rainbow(nrow(UK_foods)))
```



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



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



Using PCA

The main function in base R for PCA is `prcomp()`.

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

The `prcomp()` function returns a list object of our results with 5 attributes.

```r
attributes(pca)
```

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

$class
[1] "prcomp"
```

Interpreting PCA results

The two main "results" are `pca$x` and `pca$rotation`. The first of these contains the scores of the data on the new PC axis - we use these to make our PCA plot.

```r
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
```

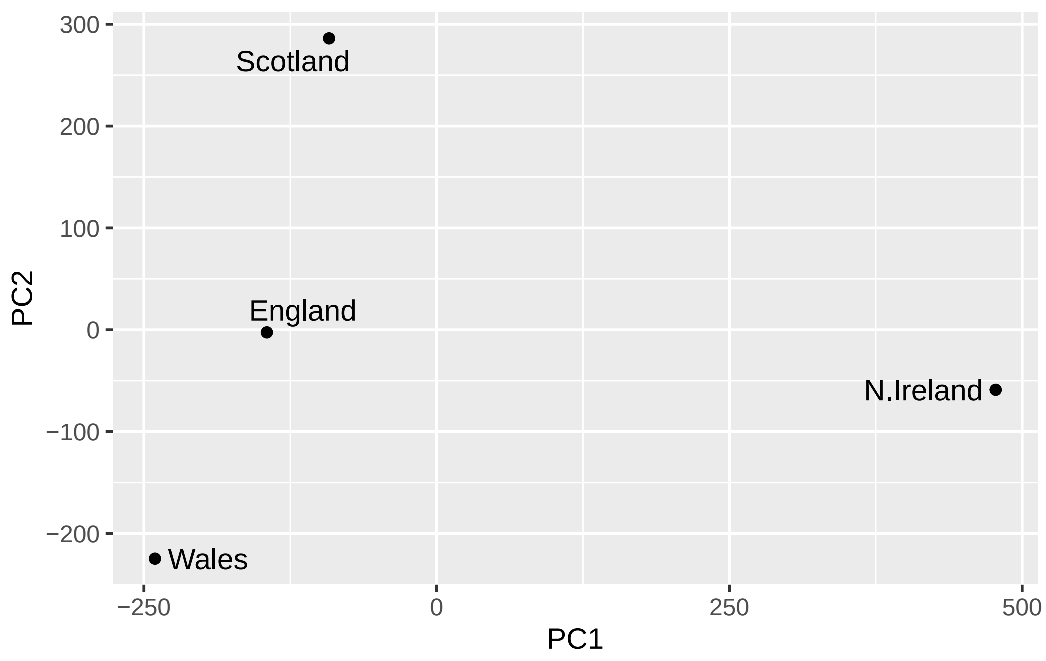
```r
library(ggplot2)
```

```
Warning: package 'ggplot2' was built under R version 4.4.3
```

```r
library(ggrepel)
```

```
Warning: package 'ggrepel' was built under R version 4.4.3
```

```r
# Make a plot of pca$x with PC1 vs PC2
ggplot(pca$x) +
  aes(x = PC1, y = PC2, label = rownames(pca$x)) +
  geom_point() +
  geom_text_repel()
```



The plot shows that England, Scotland, and Wales cluster together along the PC1 axis while Northern Ireland is on its own. England, Scotland and Wales are further apart along the PC2 axis, but the PC1 axis captures the largest proportion of the variance, so there is a larger difference between Northern Ireland and the rest of the countries.

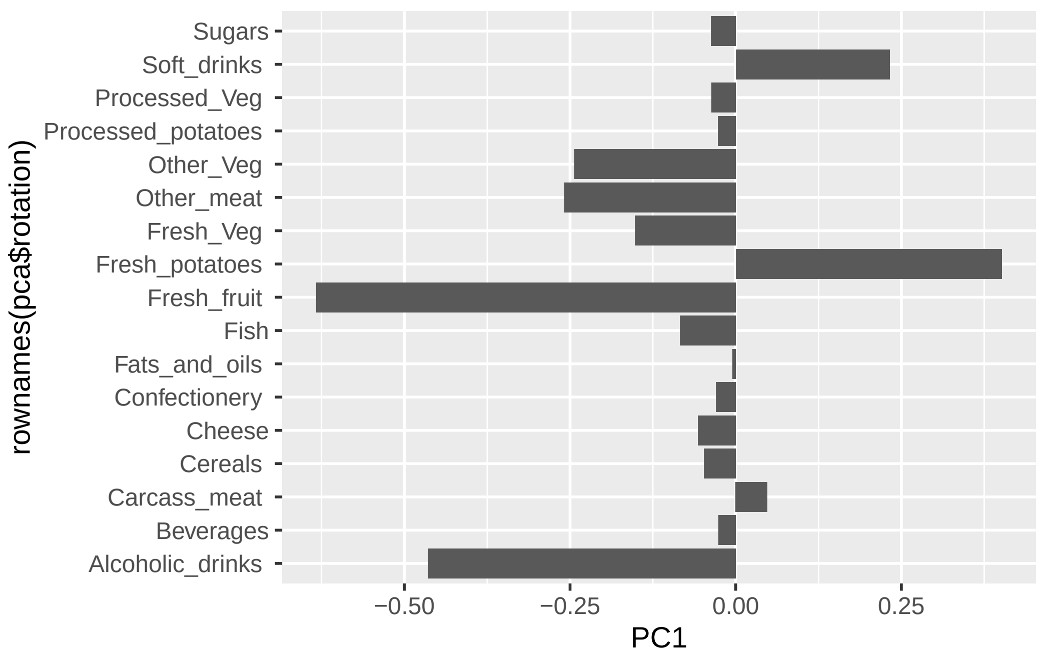
The second major result is contained in the `pca$rotation` object or component. Let's plot this to see what PCA is picking up.

```r
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
```

```
ggplot(pca$rotation) +
  aes(x = PC1, rownames(pca$rotation)) +
  geom_col()
```



The figure shows how each variable contributes to PC1. We can see that positive values for PC1 are associated with mroe soft drink and fresh potato consumption and less fresh fruit and alcohol consumption.