Class 7: Machine Learning 1

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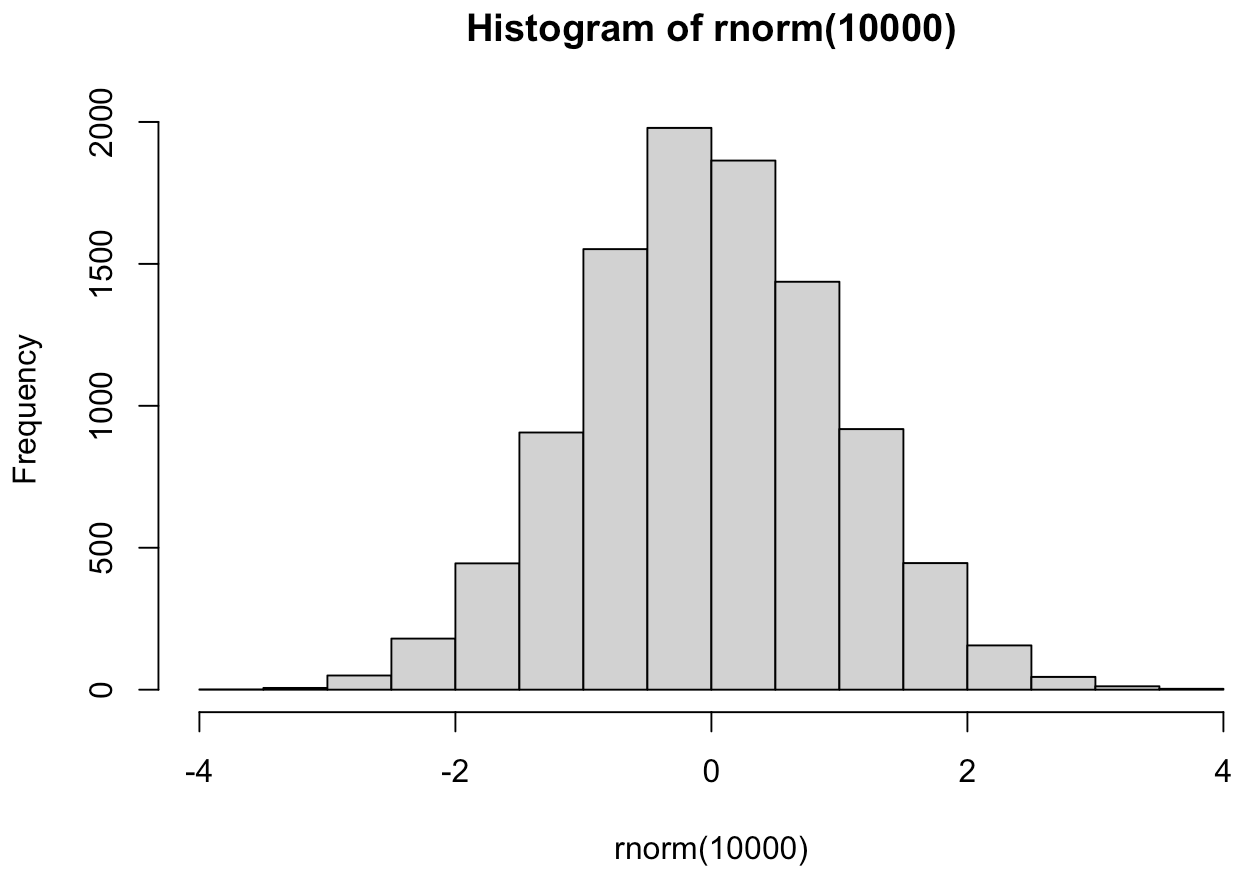
> Today we will explore unsupervised machine learning methods starting with clustering and dimensionality reduction.

Clustering

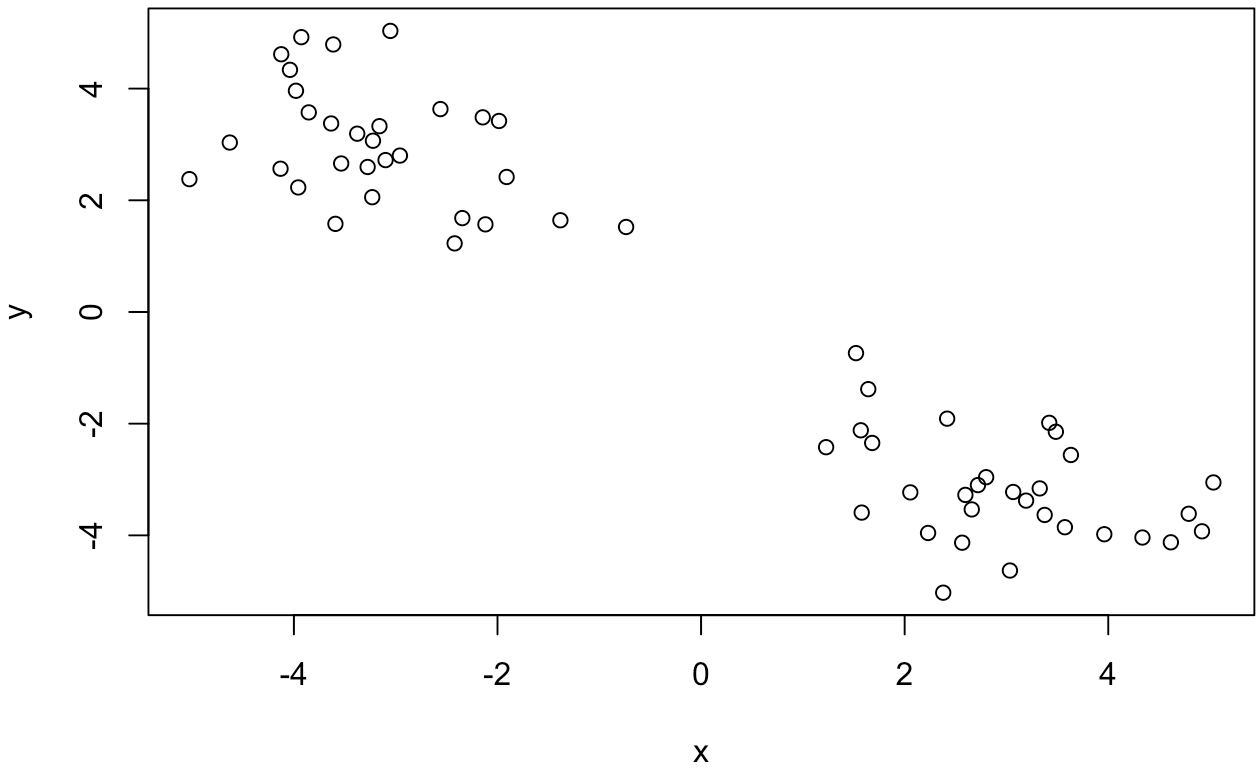
To start, let's make up some data to cluster where we know what the answer should be. The `rnorm()` function will help us here.

```
# This will create a histogram displaying 10000 randomly generated numbers.
hist(rnorm(10000))
```



And here, we create a plot with two clusters of data located at the arbitrary x values of "-3" and "3", with y values reversed.

```
# This binds the two rnorm() groups inside an object to plot
val <- c(rnorm(30, 3), rnorm(30, -3))
x <- cbind(x=val, y=rev(val))
plot(x)
```



K-means Clustering

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

```
# Only 'x' and 'centers' are required args for `kmeans()`
k <- kmeans(x, 2)
k
```

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

Cluster means:
          x         y
1  2.980318 -3.167671
2 -3.167671  2.980318

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 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] 60.75405 60.75405
 (between_SS / total_SS =  90.3 %)

Available components:

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

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

```
# This lists the 9 attributes.
attributes(k)
```

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

$class
[1] "kmeans"
```

> Q. How many points are in each cluster?

```
# Size gives the size of each cluster.
k$size
```

```
[1] 30 30
```

> Q. Cluster assignment/membership vector?

```
# This calls the vector for each cluster assignment.
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 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. Cluster centers?

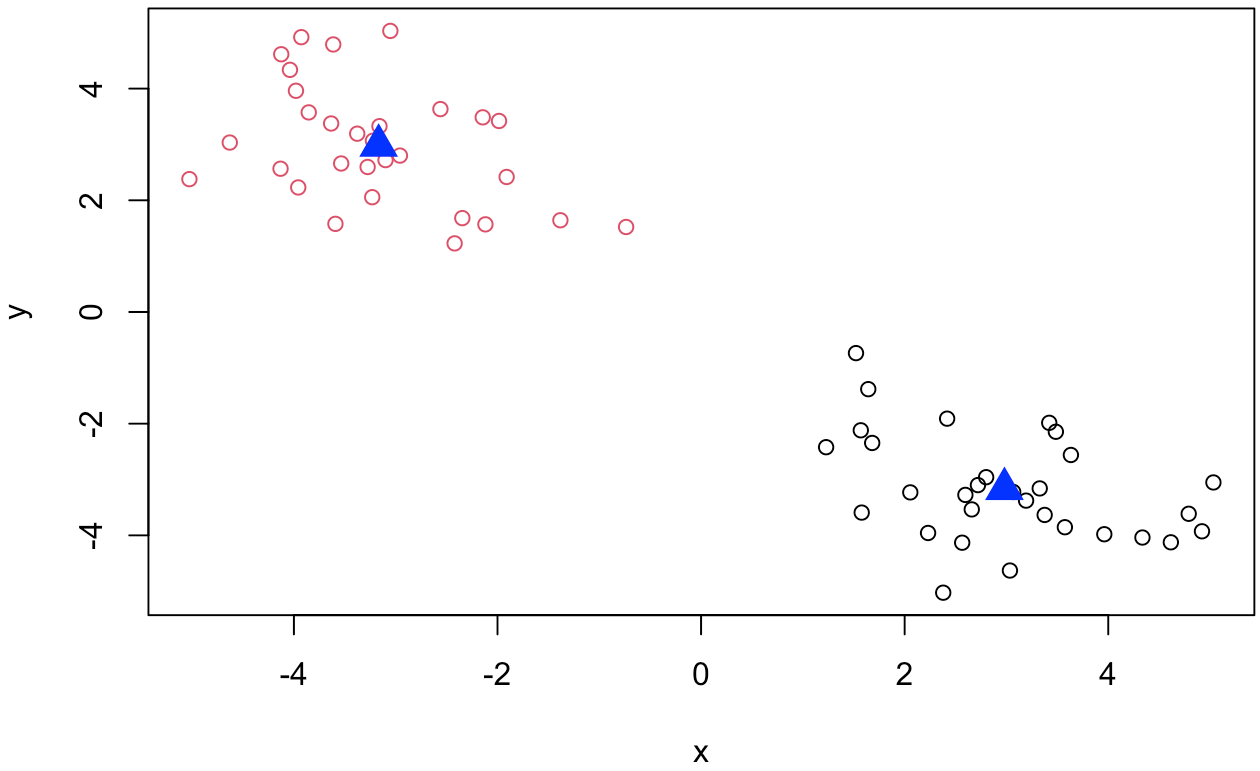
```
# This returns the coordinates of the cluster centers.
k$centers
```

```
          x         y
1  2.980318 -3.167671
```

```
2 -3.167671  2.980318
```

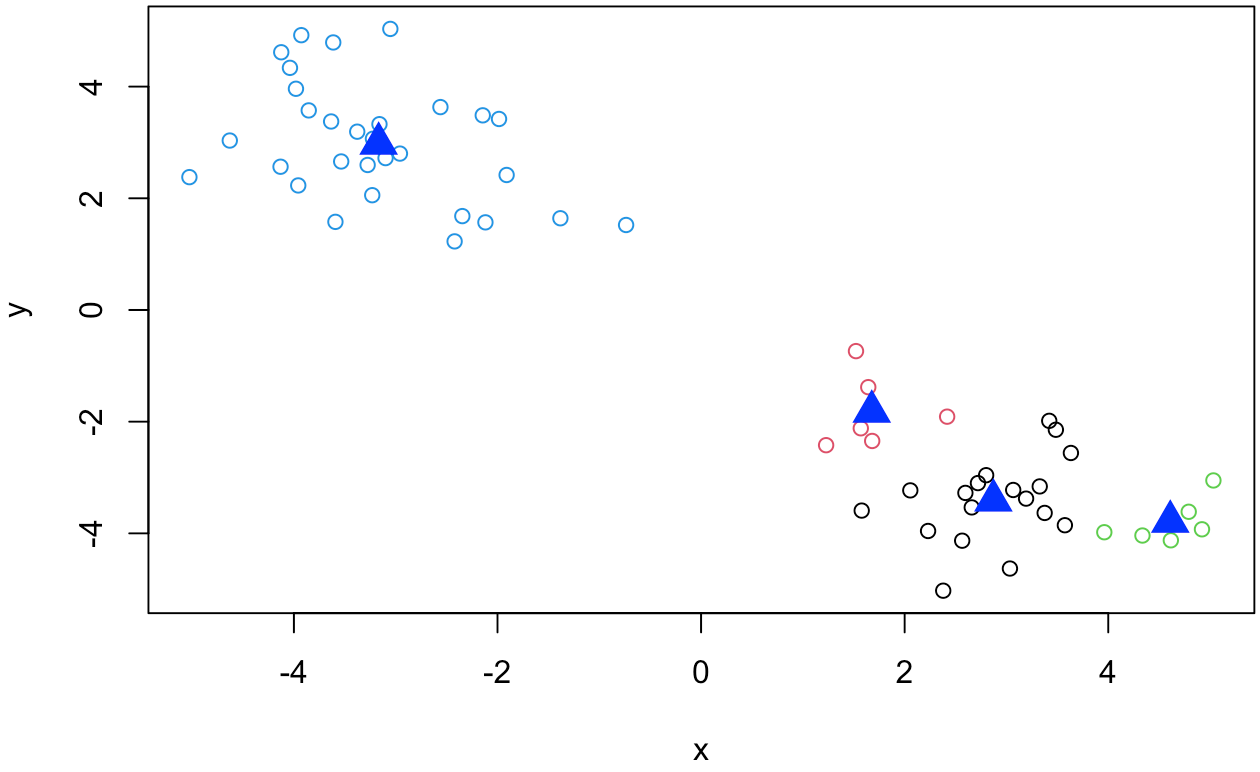
> Q. Make a plot of our `kmeans()` results showing cluster assignment with different colors for each group of points and centers in blue.

```
# Col can also be a number, so we can set it equal to k$cluster.
plot(x, col=(k$cluster))
points(k$centers, col="blue", pch=17, cex=2)
```



> Q. Run `kmeans()` again on `x` and this time cluster into four groups and plot the same result figure as above.

```
k2 <- kmeans(x,4)
plot(x, col=(k2$cluster))
points(k2$centers, col="blue", pch=17, cex=2)
```



> **Key Point**: K-means clustering is very popular but can be misused. One big limitation is that it can impose a clustering pattern on your data even if clear natural grouping doesn't exist - i.e. it does what you tell it to do in terms of `centers`.

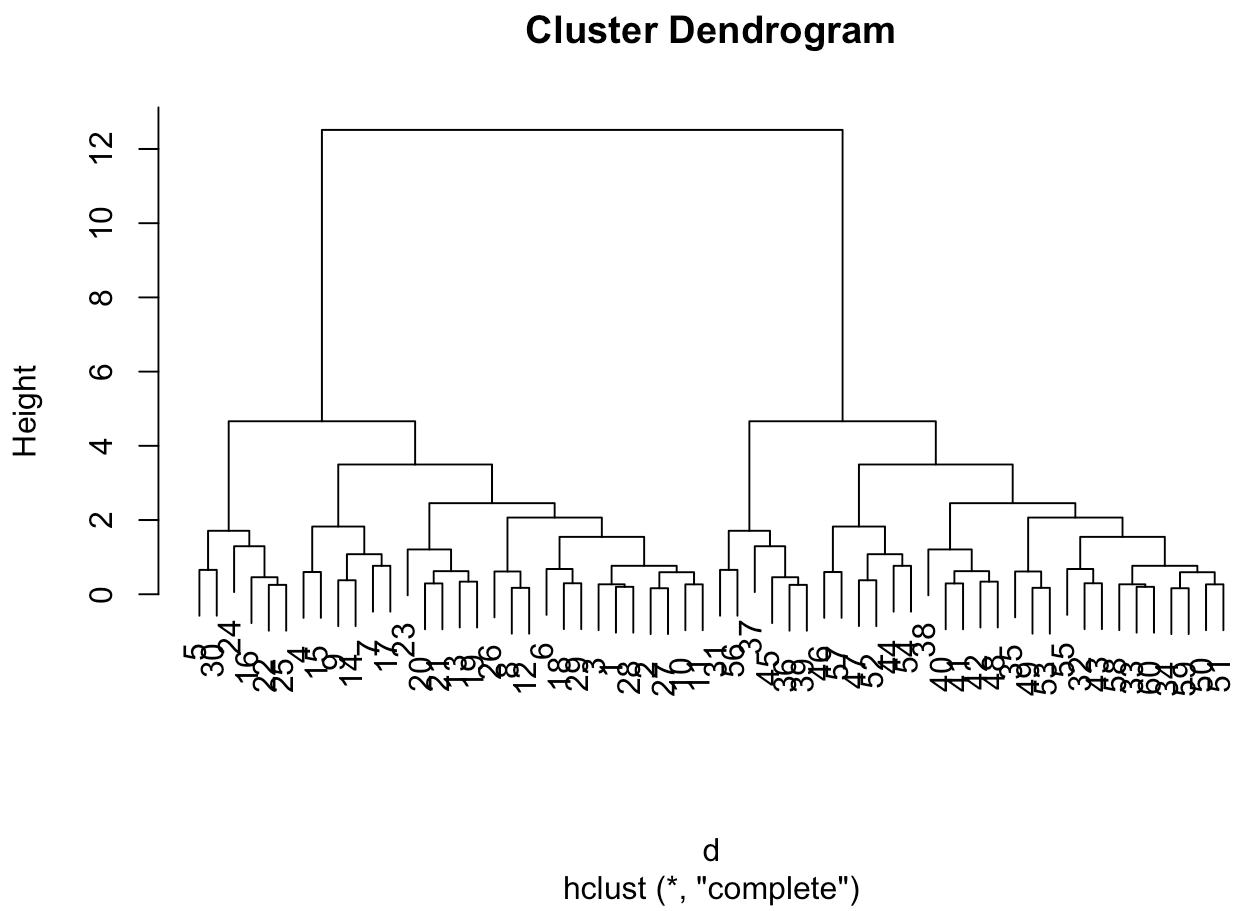
Hierarchical Clustering

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

You can't just pass our dataset into `hclust()`, more work is required, but it is more flexible than `kmeans()`.

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

```
# hclust() only has one required input, "d".
d <- dist(x)
h <- hclust(d)
plot(h)
```



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

> Q. How many large clusters are there?

```
# This will return our two original clusters!
grps <- cutree(h, h=8)
table(grps)
```

```
grps
 1  2
30 30
```

Hierarchical clustering is distinct in that the dendrogram can reveal the potential grouping in your data, unlike `kmeans()`.

Dimensionality | Principal Component Analysis

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

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

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

> (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  5
```

But what if we don't want X to be counted as a column of data?

> (Q2) Here is the preferred solution, because it is does not continually delete column names each time the code is ran:

```
# This is a non-destructive method
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
```

...and the new dimensions:

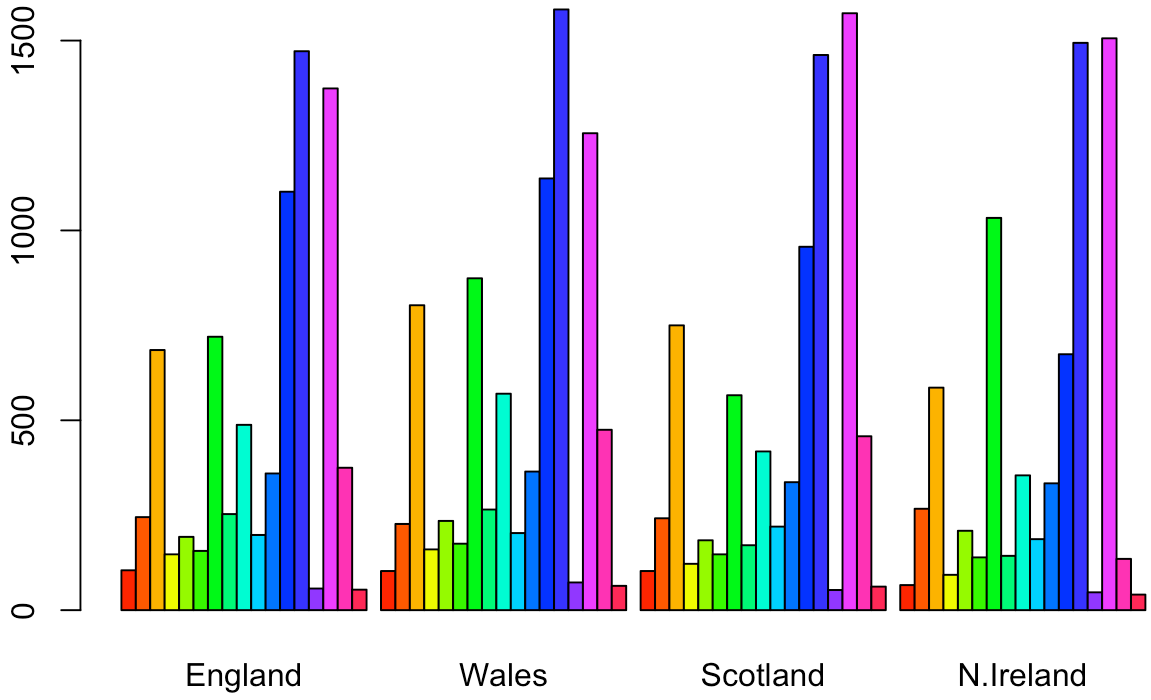
```
dim(x)
```

```
[1] 17  4
```

Spotting Major Differences

First, let's paste the original plot:

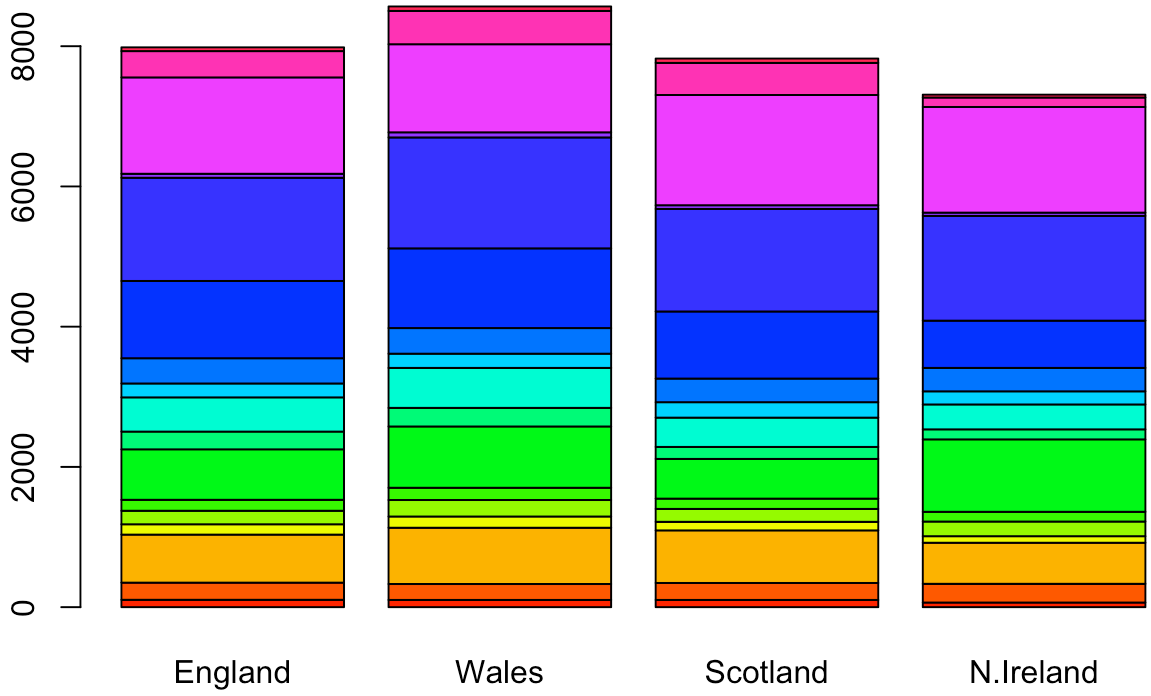
```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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

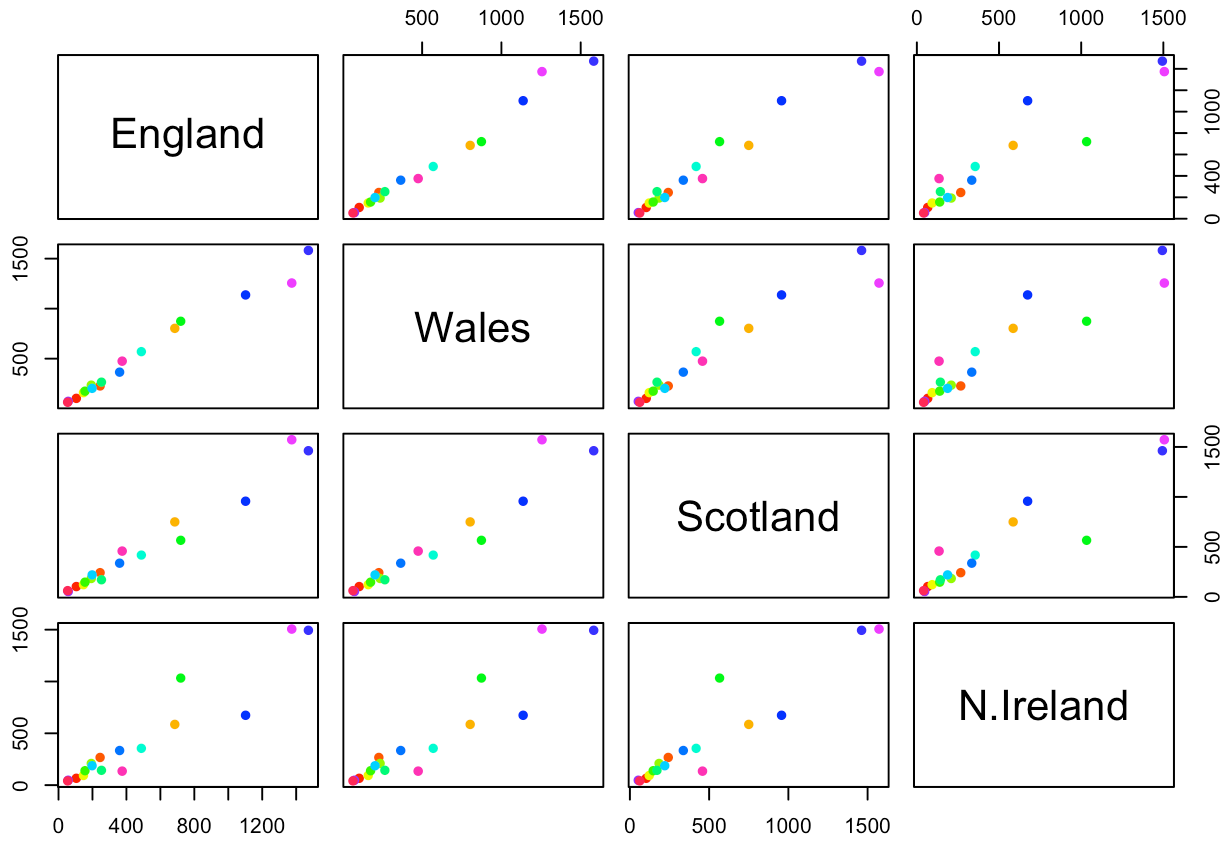
Let's make this plot different by changing one parameter:

```
# "beside" makes a side-by-side barplot, we change it to "F".
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



This plot is still not very helpful, so lets try a different conventional method — a “pairs” plot.

```
# But, this is still quite complicated...
pairs(x, col=rainbow(nrow(x)), pch=16)
```



PCA to the Rescue!

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

```
# But, this function wants this data in a specific way.
# So, lets transpose our matrix:
pca <- prcomp(t(x))
summary(pca)
```

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 2.921e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

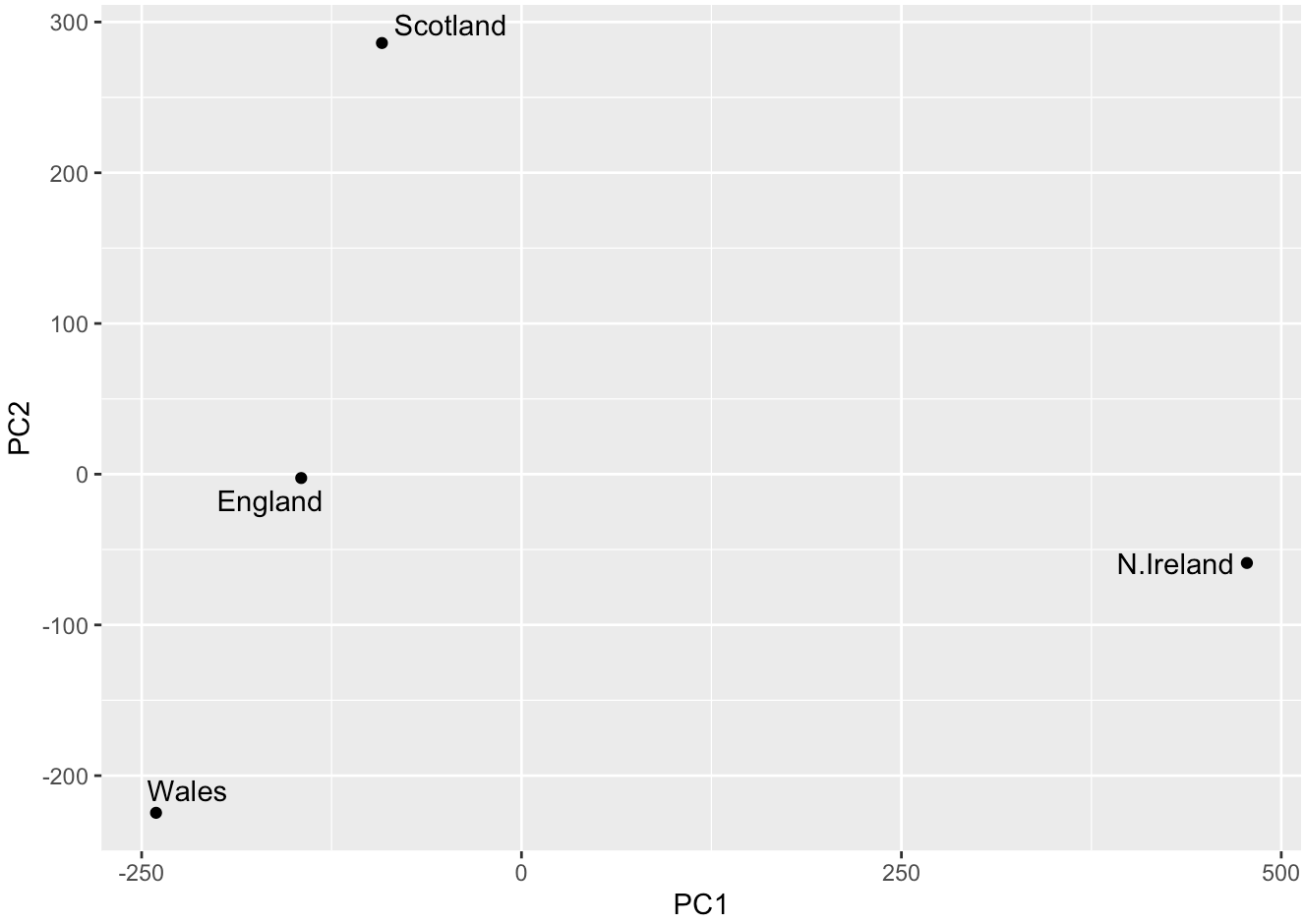
The `prcomp()` function returns a list object of our results with 5 components, according to `attributes()`.

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

> (Q7) Complete the code below to generate a plot of PC1 vs PC2.

```
# Calling the gg libraries...
library(ggplot2)
library(ggrepel)

#...then making a ggplot of PC1 vs PC2.
ggplot(pca$x) +
  aes(PC1, PC2, label=rownames(pca$x)) +
  geom_point() +
  geom_text_repel()
```



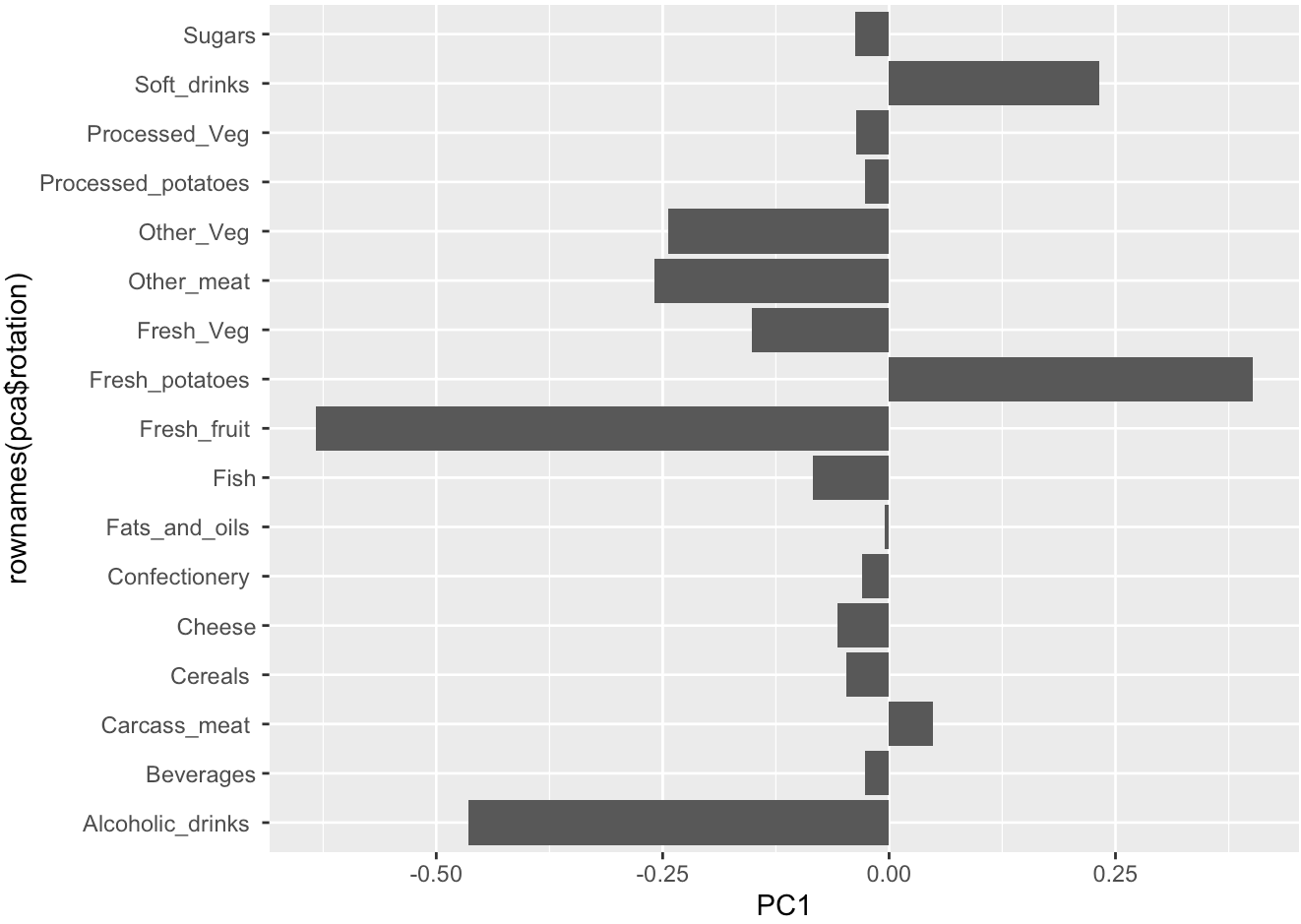
> What we can gather from this is that Wales, England, and Scotland all fall neatly along the PC1 line, but N. Ireland is significantly different. Let's see why:

We can also use `pca$rotation` to determine what in the data is leading to the variation we see in our plot.

```
# Calling the library...
library(ggplot2)

# And creating the plot.
ggplot(pca$rotation) +
```

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

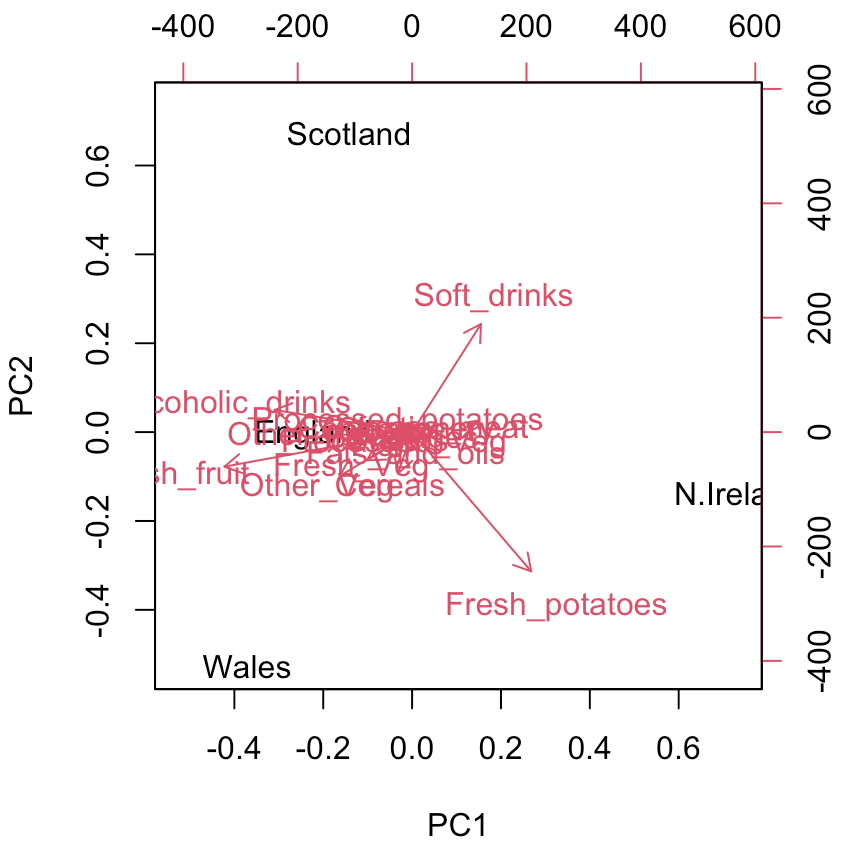


By reading both PCA plots, we can determine that:

- N. Ireland is different because they consume considerably more fresh potatoes and soft drinks.
- The rest consume considerably more alcoholic drinks and fresh fruit.

Additionally, we can see this correlation with biplots. (`biplot()` function)

```
# This is found in "base R".
biplot(pca)
```


-400
-200
0
200
400
600
Scotland
Soft_drinks
Fresh_potatoes
Wales
N.Irela
PC2
PC1
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.4
-0.2
0.0
0.2
0.4
0.6
600
400
200
0
-200
-400