Class 7: Machine Learning 1

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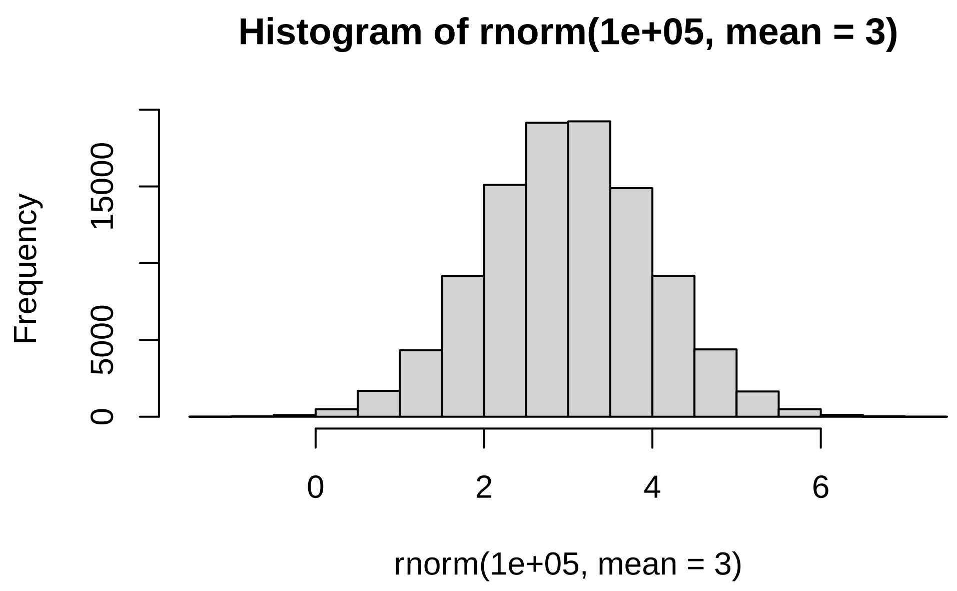
Today we will start our multi-part exploration of some key machine learning methods. We will begin with clusetering - finding groupings in data, and then dimensionallity reduction.

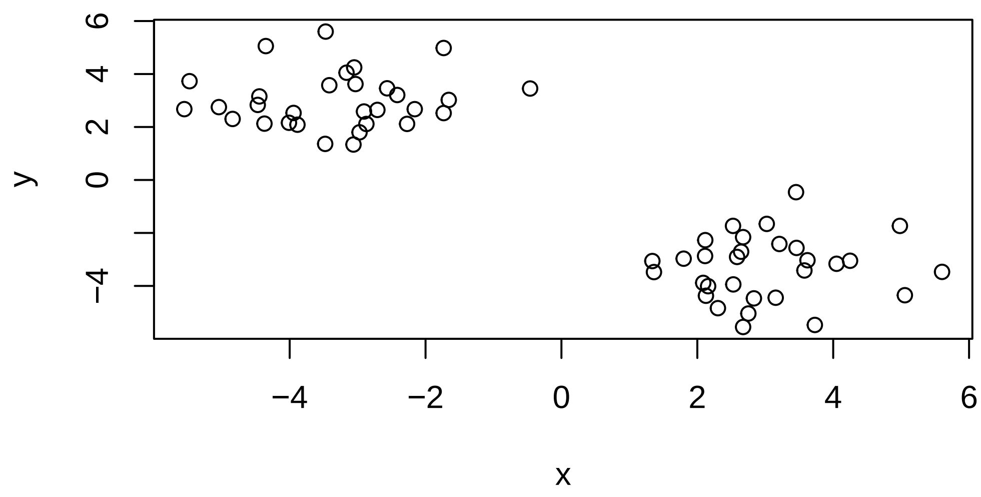
Clustering

Let's start with "k-means" cluster The main function in base R for this `kmeans()`.

```r
# Make up some data
hist(rnorm(100000, mean = 3))
```



```r
tmp <- c(rnorm(30, -3), rnorm(30, +3))
x <- cbind(x=tmp, y=rev(tmp))
plot(x)
```



Now let's try out `kmeans()`

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

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

Cluster means:
          x         y
1  2.992899 -3.317036
2 -3.317036  2.992899

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 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] 73.41066 73.41066
 (between_SS / total_SS =  89.1 %)

Available components:

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

```
attributes(km)
```

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

$class
[1] "kmeans"
```

Q. How many points in each cluster?

```
km$size
```

```
[1] 30 30
```

Q. What component of your result object details cluster assignment/membership?

```
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
```

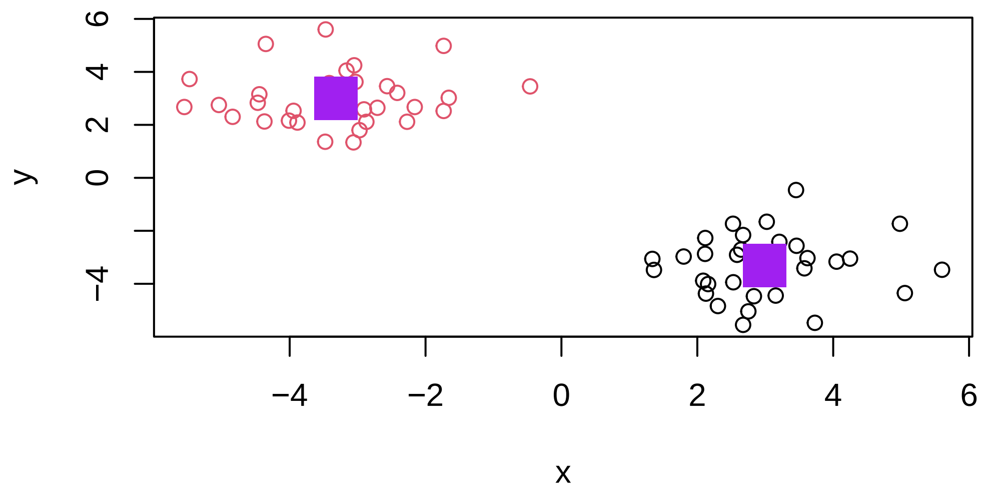
Q. What are centers/mean values of each cluster?

```
km$centers
```

```
          x         y
1  2.992899 -3.317036
2 -3.317036  2.992899
```

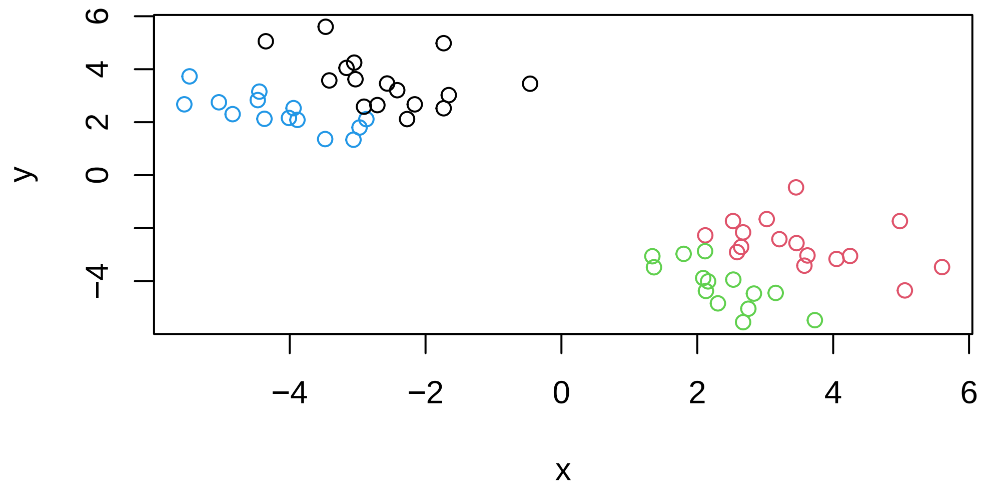
Q. Make a plot of your data showing your clustering results.

```r
plot(x, col=km$cluster)
points(km$centers, col="purple", pch=15, cex=3)
```



Q. Run `kmeans()` again and cluster in 4 groups and plot the results.

```r
km4 <- kmeans(x, centers=4)
plot(x, col=km4$cluster)
```



Hierarchical Clustering

This form of clustering aims to reveal the structure in your data by progressively grouping points into a ever smaller number of clusters.

The main function in base R for this is called `hclust()`. This function does not take our input data directly but wants a "distance matrix" that details how (dis)similar all our input points are to each other.

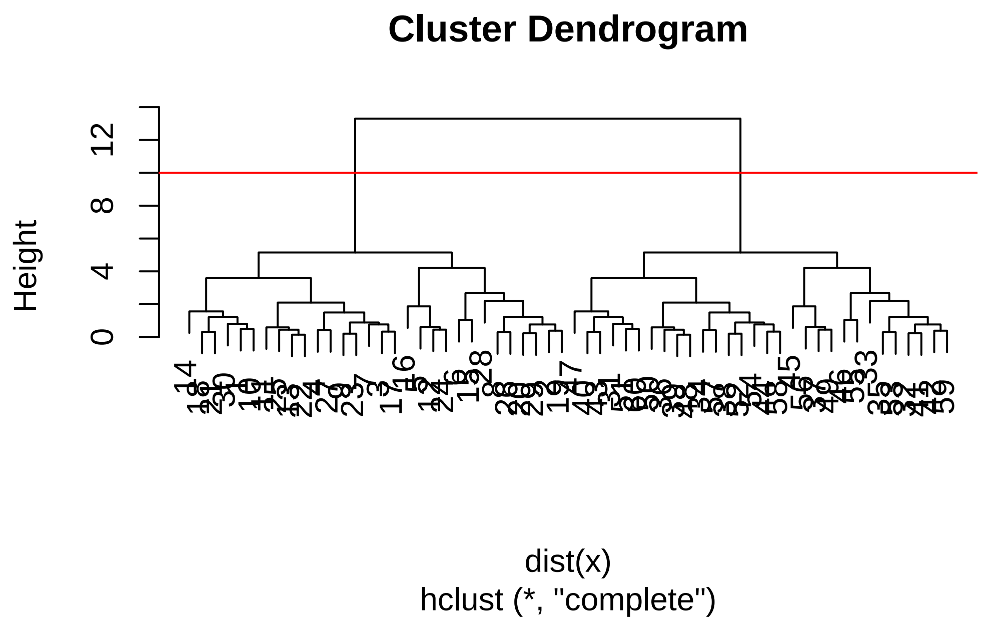
```
hc <- hclust( dist(x) )
hc
```

```
Call:
hclust(d = dist(x))

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

The print out above is not very useful (unlike that from kmeans) but there is a useful `plot()` method.

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

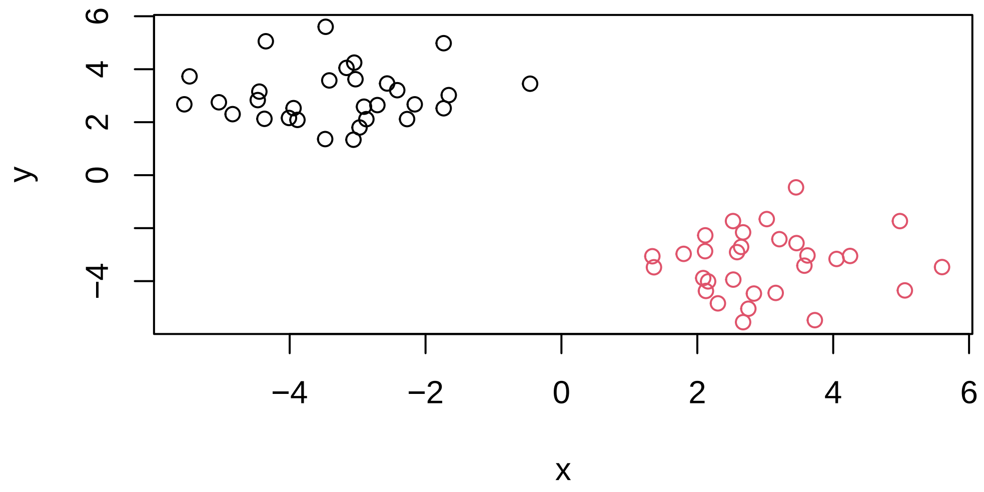


To get my main result (my cluster membership vector) I need to "cut" my tree using the function `cutree()`

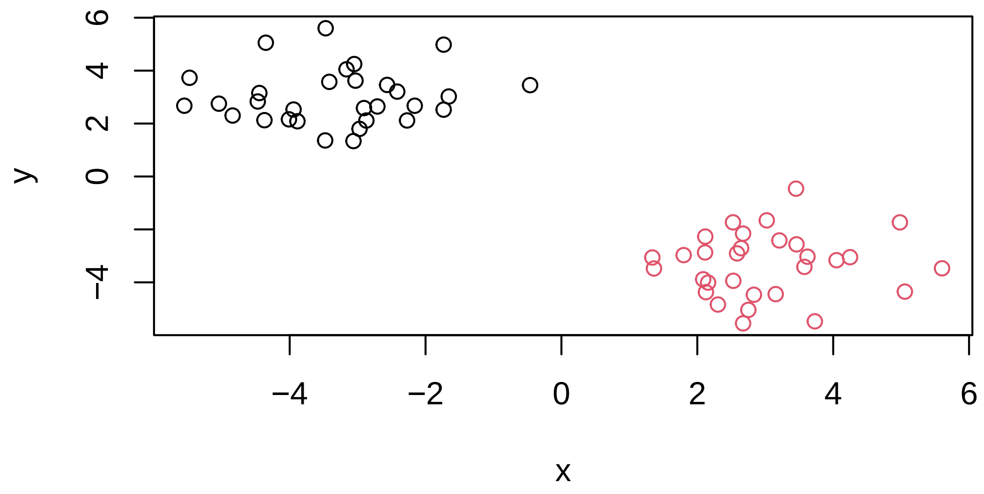
```r
grps <- cutree(hc, h=10)
grps
```

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



```
plot(x, col=cutree(hc, h=6))
```



Principal Component Analysis (PCA)

The goal of PCA is to reduce the dimensionality of a dataset down to some smaller subset of new variables (called PCs) that are useful bases for further analysis, like visualization, clustering, etc.

```r
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
```

> 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  4
```

Preview the first 6 rows

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

```
head(x)
```

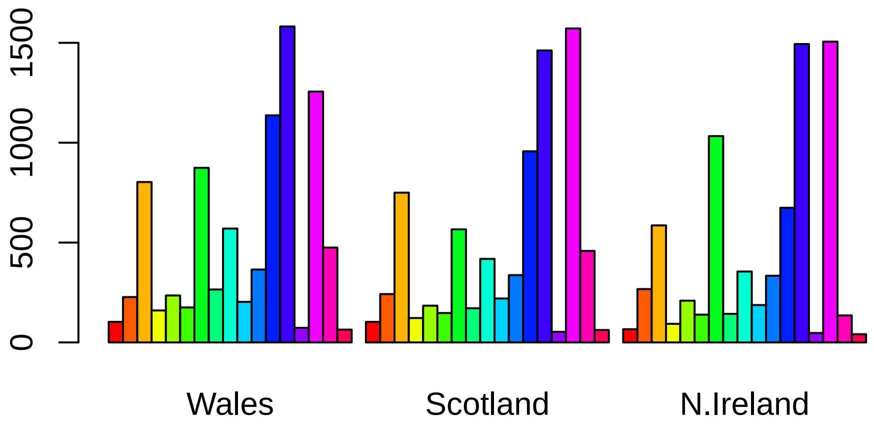
```
    Wales Scotland N.Ireland
105   103      103        66
245   227      242       267
685   803      750       586
147   160      122        93
193   235      184       209
156   175      147       139
```

> 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?

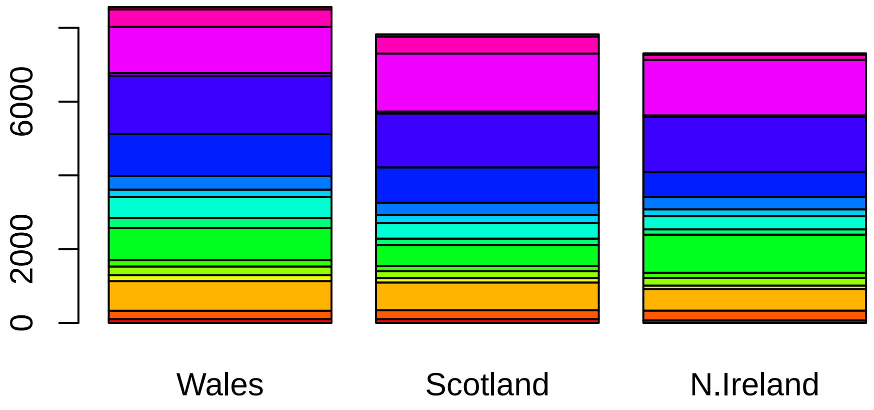
I prefer using x <- read.csv(url, row.names=1) because it looks cleaner to have the column removed while it's being read. Using the "rownames()" approach will remove the first unamed column each time, so it could lead to issues when analyzing data.

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

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

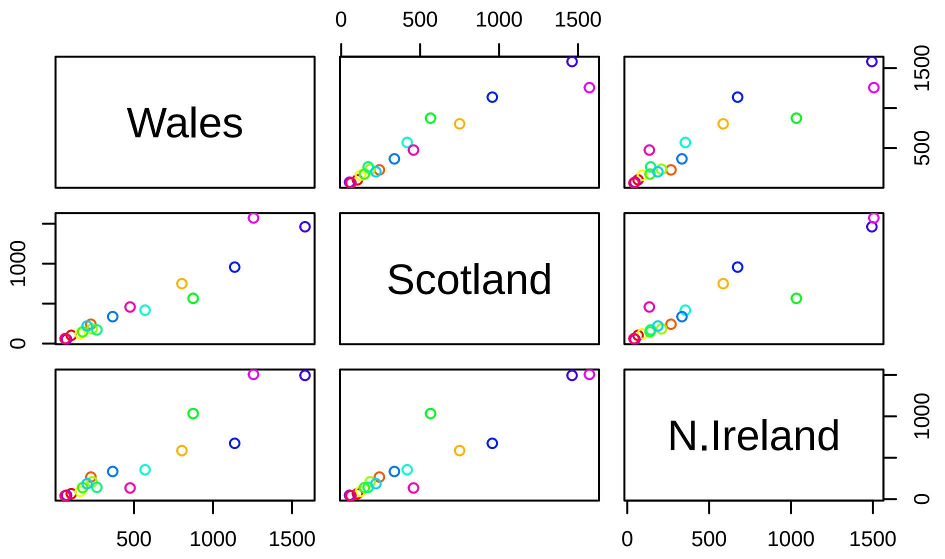


```r
barplot(as.matrix(x), col=rainbow(nrow(x)))
```



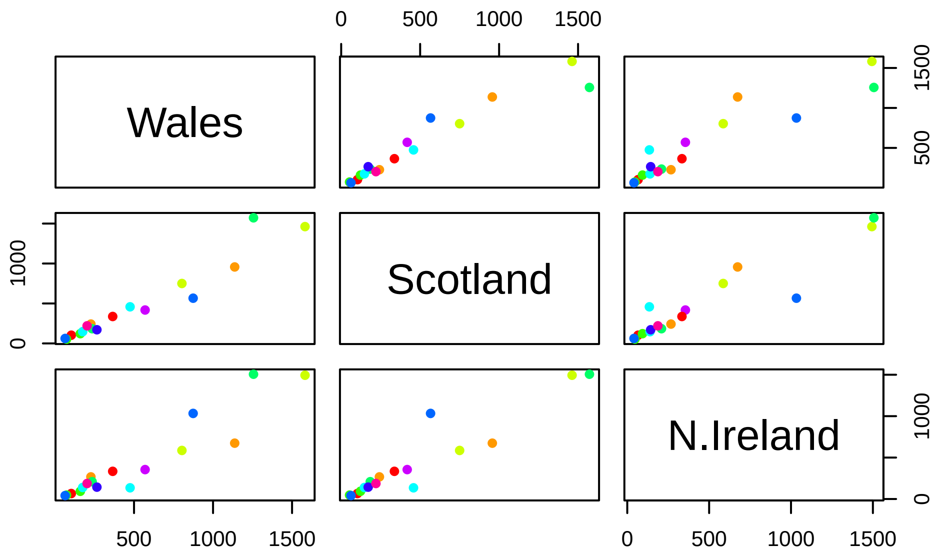
The so-called “pairs” plot can be useful for small datasets:

```
pairs(x, 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)
```



If a point lies on the diagonal line for a given plot, then the points have identical values.

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

They do not follow the diaganol line as much as the other countries of the UK.

So the pairs plot is useful for small datasets but it can be lots of work to intercept and gets untraceable for larger datasets.

So PCA to the rescue…

The main function to do PCA in base R is called `prcomp()`. This function wants the transpose of our data in this case.

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

```
Importance of components:
                            PC1      PC2       PC3
Standard deviation     379.8991 260.5533 1.459e-13
Proportion of Variance   0.6801   0.3199 0.000e+00
Cumulative Proportion    0.6801   1.0000 1.000e+00
```

```r
attributes(pca)
```

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

$class
[1] "prcomp"
```

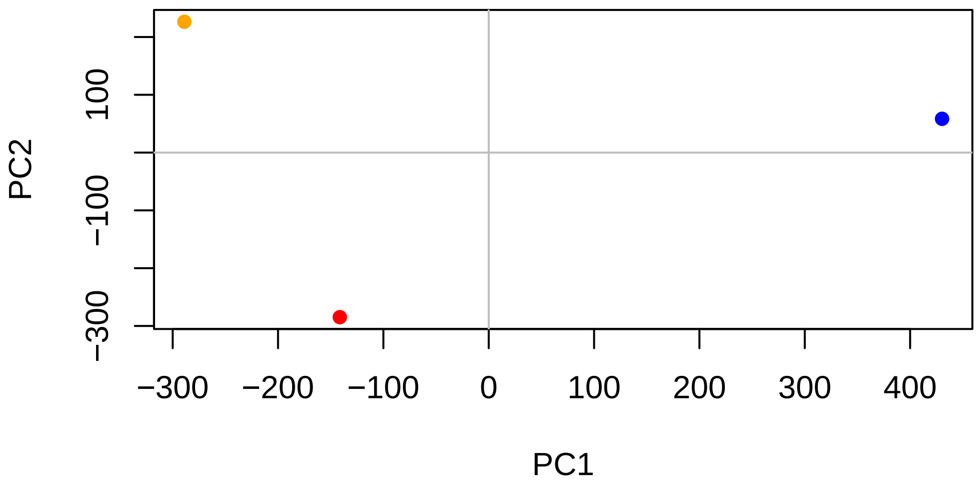
```r
pca$x
```

```
                PC1        PC2           PC3
Wales     -288.9534  226.36855  1.348366e-14
Scotland  -141.3603 -284.81172  4.627961e-13
N.Ireland  430.3137   58.44317 -1.280793e-13
```

A major PCA result viz is called a "PCA plot" (aka a score plot, biplot, PC1 vs PC2 plot, ordination plot)

> Q7. Complete the code to generate a plot of PC1 vs PC2.
>
> Q8. Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

```r
# Plot PC1 vs PC2
mycols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=mycols, pch=16,
     xlab="PC1", ylab="PC2")
abline(h=0, col="gray")
abline(v=0, col="gray")
```



Another important output from PCA is called "loadings" vector or the "rotation" componenet - this tells us how much the original variables (the foods in this case) contribute to the new PCs.

```
pca$rotation
```

```
             PC1          PC2          PC3
105  -0.05515951 -0.015926208 -0.114785683
245   0.05228588 -0.014247351  0.090388866
685  -0.29754711  0.017770827 -0.140679146
147  -0.08127351  0.050871661 -0.032506892
193  -0.01378426  0.095789177 -0.088241699
156  -0.03995614  0.043238659  0.060855246
720   0.38787509  0.714518360 -0.199098947
253  -0.13584223  0.144666425 -0.055102719
488  -0.24608178  0.226299860 -0.251953979
198  -0.03217825 -0.042547197 -0.091526858
360  -0.03250215  0.045390849  0.138275463
1102 -0.60208698  0.178285653  0.105684388
1472 -0.07242201  0.213840430 -0.673357649
57   -0.02896604  0.030761774  0.005505441
1374  0.21794320 -0.555250465 -0.560188267
```

```
375  -0.49854565 -0.110688746 -0.184979763
54   -0.03330887 -0.005704759  0.004859328
```

PCA looks to be a souper useful method for gaining some insight into high dimensional data that is difficult to examine in other ways.