Lab 7: Unsupervised Learning

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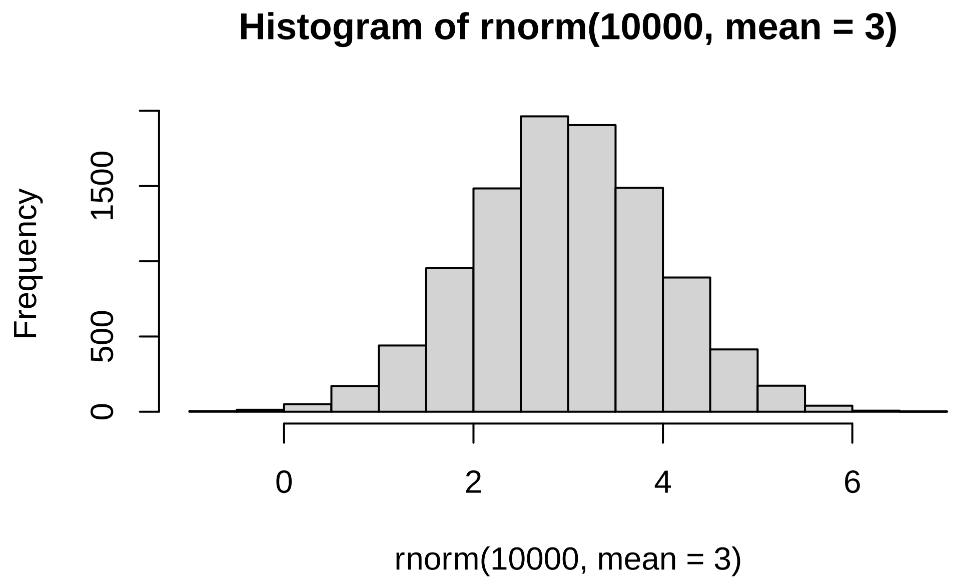
Today we will start our multi-part exploration of some key machine learning methods. We will begin with clutching - finding groupings in data, and then dimensionally reduction.

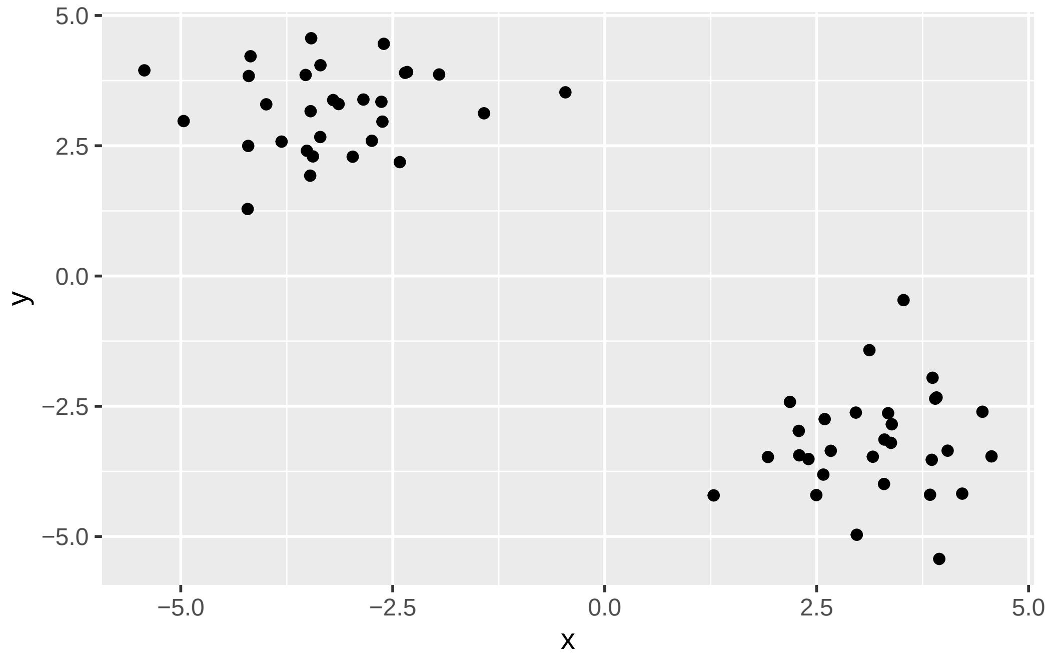
Clustering

Lets start from "k-means" cluster The main function in base R for this is `kmeans()` .

```
# Make up some data
hist(rnorm(10000, mean = 3))
```



```r
# rnorm(30, -3)
# rnorm(30, +3)

# combine two vectors
tmp <- c(rnorm(30, -3), rnorm(30, +3))

# rev means print reverse
data <- cbind(x = tmp, y = rev(tmp))
library(ggplot2)
ggplot(data, aes(x = x, y = y))+
  geom_point()
```



kmeans clustering

Now let's try `kmeans()`

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

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

```
Cluster means:
          x         y
1 -3.209497  3.192725
2  3.192725 -3.209497

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 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

Within cluster sum of squares by cluster:
[1] 47.76397 47.76397
 (between_SS / total_SS =  92.8 %)

Available components:

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

> Q. How many points in each cluster?

```r
km$size
```

```
[1] 30 30
```

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

```r
km$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 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
```

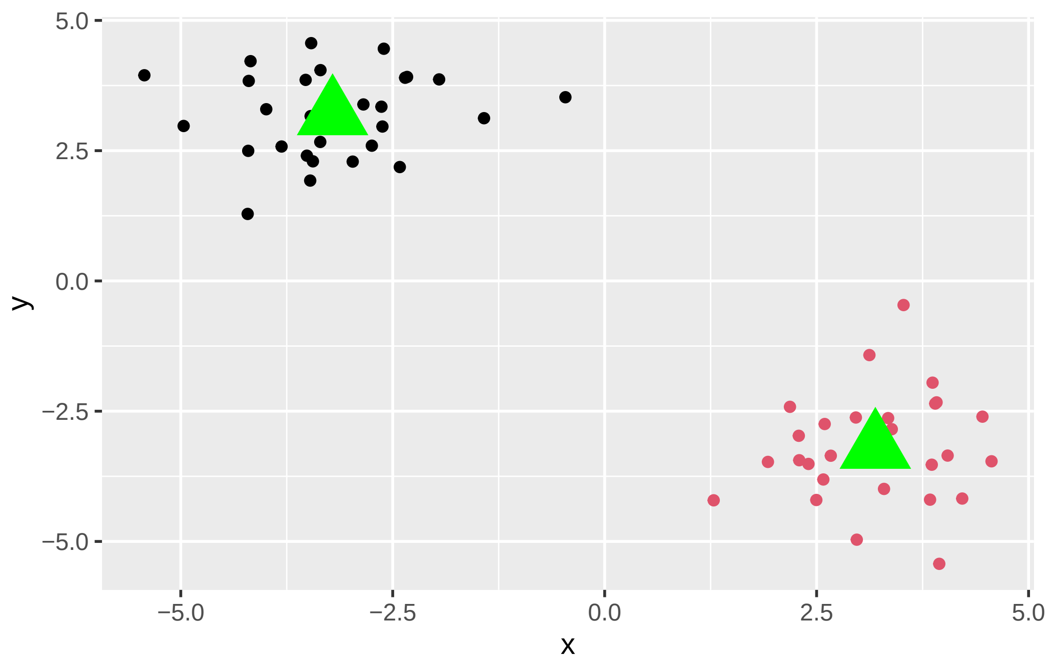
> Q. What are centers/mean value of each center?

```r
km$centers
```

```
          x         y
1 -3.209497  3.192725
2  3.192725 -3.209497
```

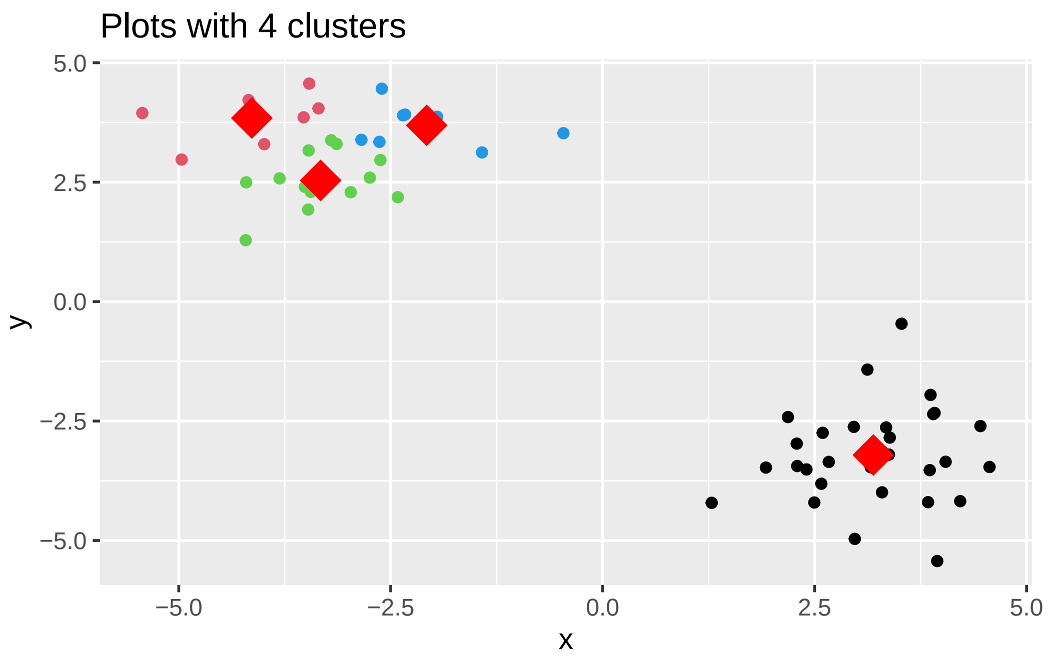
> Q. Make a plot of your data showing your cluster results (grouping/ cluster and cluster center)

```r
ggplot(data, aes(x = x, y = y))+
  geom_point(col = km$cluster) +
  geom_point(data = km$centers, color = 'green', size = 9, shape = 17)
```



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

```r
km4 <- kmeans(data, centers = 4)

ggplot(data, aes(x = x, y = y))+
  geom_point(col = km4$cluster) +
  geom_point(data = km4$centers, color = 'red', size = 7, shape = 18) +
  labs(title = 'Plots with 4 clusters')
```



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.

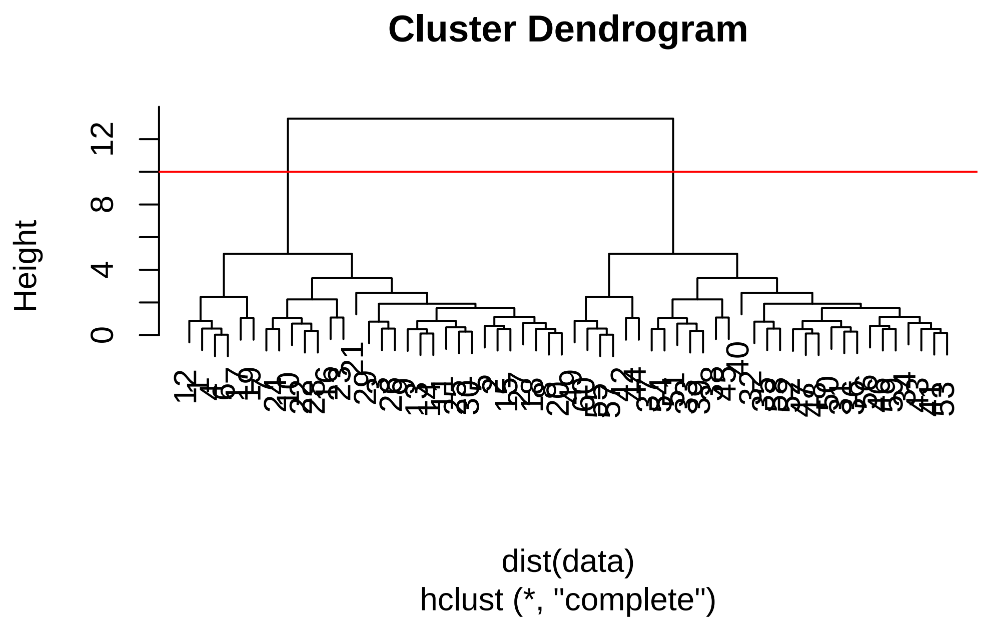
The main function in base R for this is `hclust()`. This function does not take our input data directly but wants "distance matrix" that details how (dis)similar all our input points are to each other.

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

```

Call:
hclust(d = dist(data))

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

The print out above is not very useful, but there is a useful `plot()` method.

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

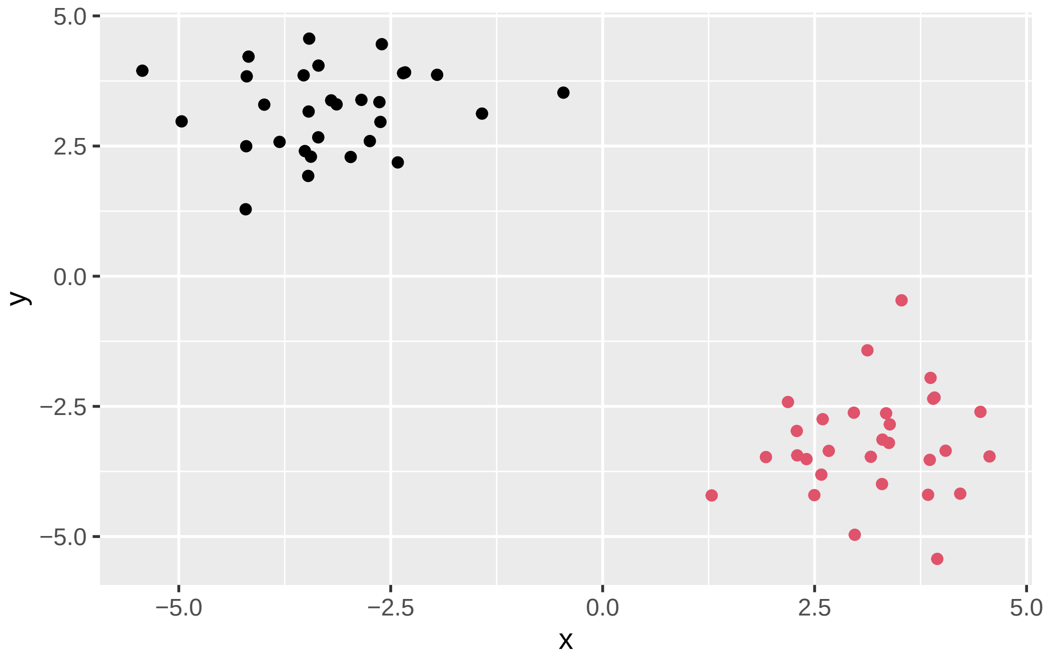


To get my main result (my cluster membership vector) I need to "cut" my tree use `cutree()`

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

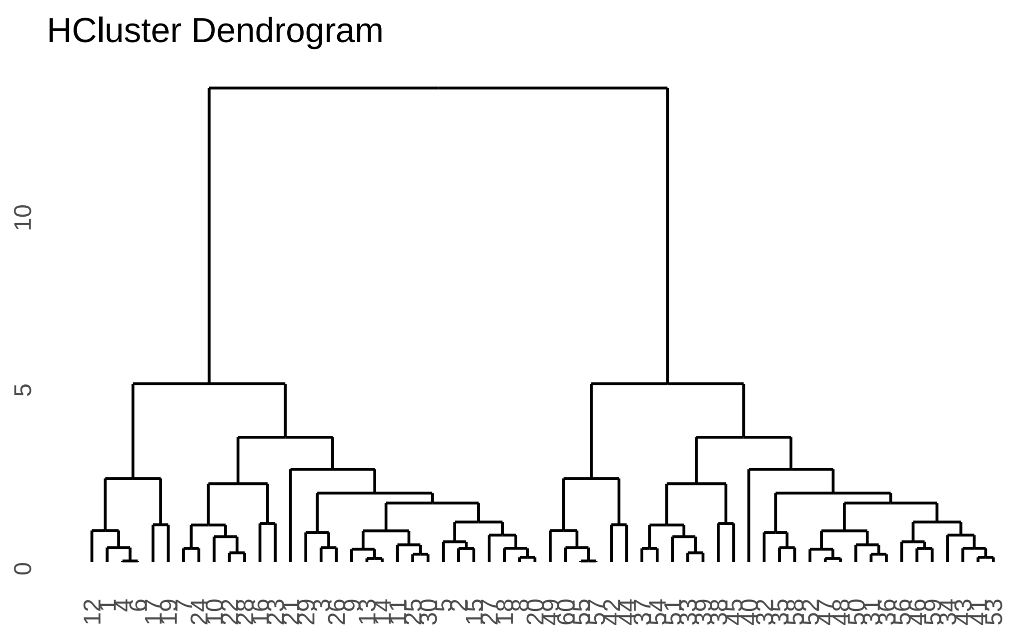
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

```r
ggplot(data, aes(x, y)) +
  geom_point(col = cut)
```



Use ggplot to plot dendrogram

```
library(ggdendro)
hhc <- dendro_data(hc, type = "rectangle")
ggdendrogram(hc, rotate = FALSE) +
  labs(title = 'HCluster Dendrogram')
```



1. PCA of UK food data

Import and Read data

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

> 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
# Complete the following code to find out how many rows and columns are in x?
dim(x)
```

```
[1] 17  5
```

Preview the first 6 rows

```r
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
```

Remove the name column

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

Or you can do

```
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
```

```
dim(x)
```

```
[1] 17  4
```

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?

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

```
               Wales Scotland N.Ireland
Cheese           103      103        66
Carcass_meat     227      242       267
Other_meat       803      750       586
Fish             160      122        93
Fats_and_oils    235      184       209
Sugars           175      147       139
```

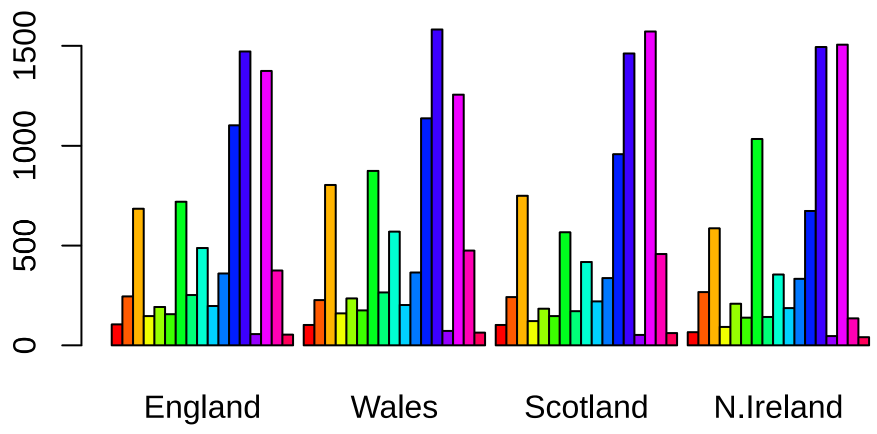
This method is less robust because it would "cut" the data if you do it several times

```
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
```

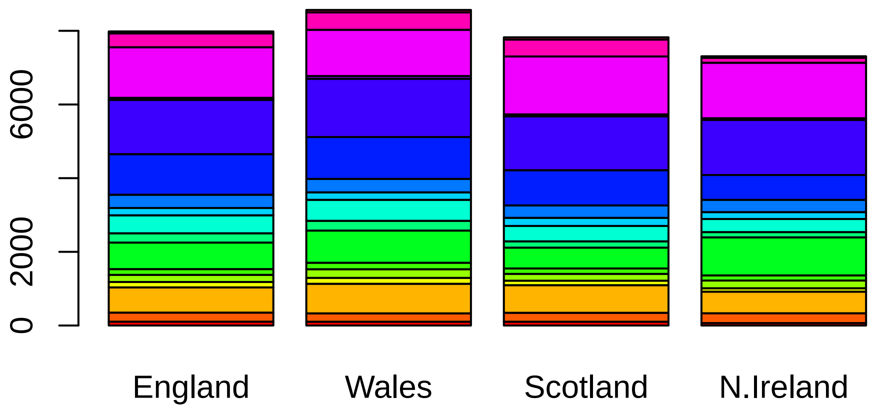
Spotting major differences and trends

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



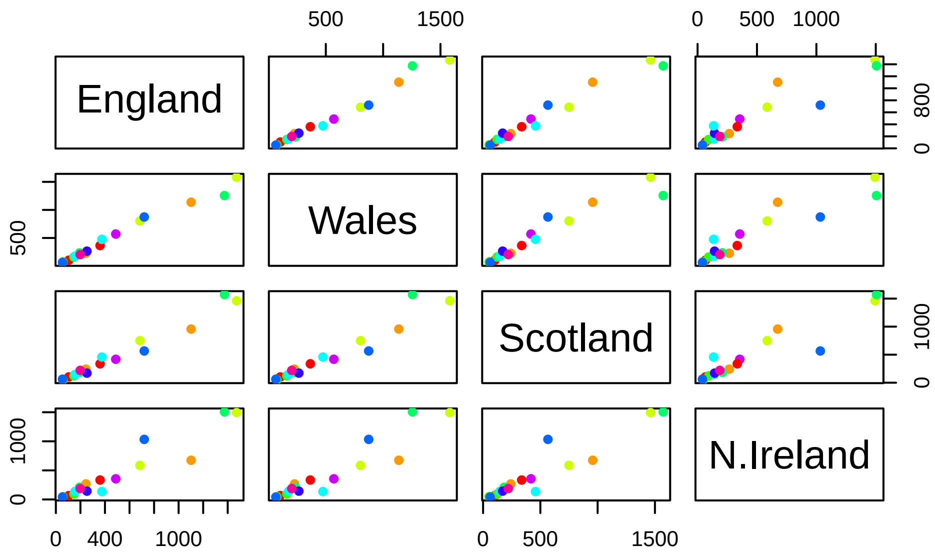
Q3: Changing what optional argument in the above barplot() function results in the following plot?

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



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?

```r
pairs(x, col=rainbow(10), pch=16)
```



So the paris plot is useful for small datasets but it can be lots of work to interpret.

Each plot is comparing two regions in terms of food raw data. Each data point is each food consumed in grams (per person, per week for the two region in x and y axis.

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

PCA to the rescue

Using `prcomp()`

```r
# Use the prcomp() PCA function
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
```

```r
attributes(pca)
```

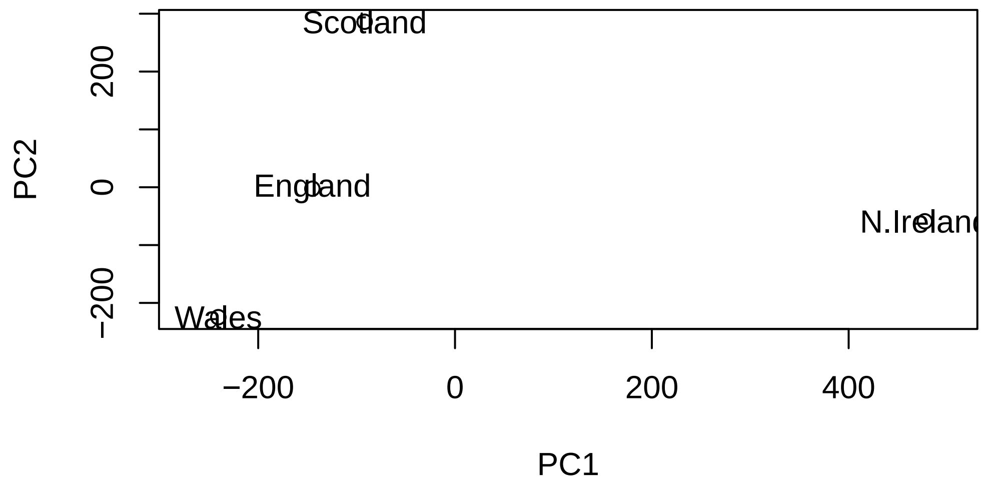
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

```r
pca$x
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -9.152022e-15
Wales     -240.52915 -224.646925 -56.475555  5.560040e-13
Scotland   -91.86934  286.081786 -44.415495 -6.638419e-13
N.Ireland  477.39164  -58.901862  -4.877895  1.329771e-13
```

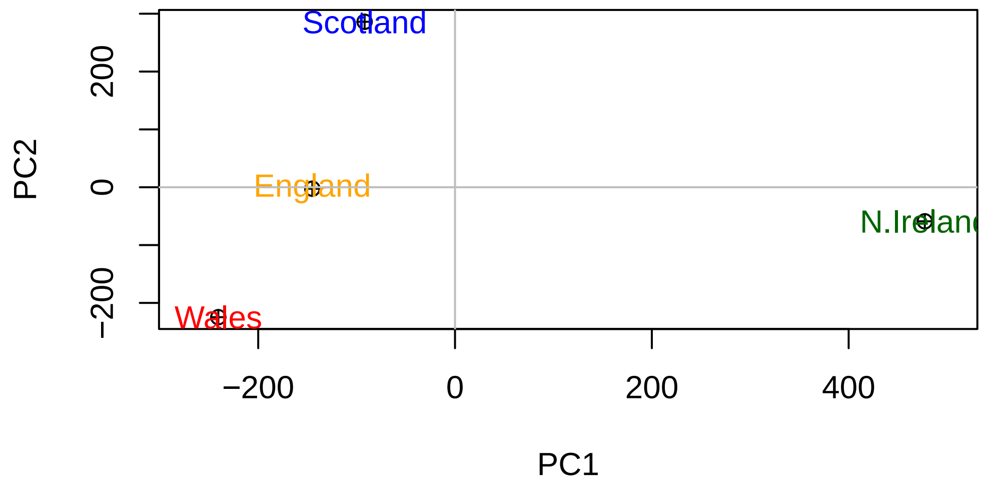
> Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```r
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x))
```



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.

```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500), pch = 10)
text(pca$x[,1], pca$x[,2], colnames(x), col = c('orange', 'red', 'blue', 'darkgreen'))
abline(h = 0, col = "grey")
abline(v = 0, col = "grey")
```



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

```
pca$rotation
```

```
                            PC1          PC2         PC3          PC4
Cheese              -0.056955380  0.016012850  0.02394295 -0.409382587
Carcass_meat         0.047927628  0.013915823  0.06367111  0.729481922
Other_meat          -0.258916658 -0.015331138 -0.55384854  0.331001134
Fish                -0.084414983 -0.050754947  0.03906481  0.022375878
Fats_and_oils       -0.005193623 -0.095388656 -0.12522257  0.034512161
Sugars              -0.037620983 -0.043021699 -0.03605745  0.024943337
Fresh_potatoes       0.401402060 -0.715017078 -0.20668248  0.021396007
Fresh_Veg           -0.151849942 -0.144900268  0.21382237  0.001606882
Other_Veg           -0.243593729 -0.225450923 -0.05332841  0.031153231
Processed_potatoes  -0.026886233  0.042850761 -0.07364902 -0.017379680
Processed_Veg       -0.036488269 -0.045451802  0.05289191  0.021250980
Fresh_fruit         -0.632640898 -0.177740743  0.40012865  0.227657348
Cereals             -0.047702858 -0.212599678 -0.35884921  0.100043319
Beverages           -0.026187756 -0.030560542 -0.04135860 -0.018382072
Soft_drinks          0.232244140  0.555124311 -0.16942648  0.222319484
```

```
Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.273126013
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001890737
```

PCA is a super useful method for gaining insight into high dimensional data

PCA of RNA-seq data

```r
url2 <- "https://tinyurl.com/expression-CSV"
rna.data <- read.csv(url2, row.names=1)
head(rna.data)
```

```
       wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
gene1  439 458  408  429 420  90  88  86  90  93
gene2  219 200  204  210 187 427 423 434 433 426
gene3 1006 989 1030 1017 973 252 237 238 226 210
gene4  783 792  829  856 760 849 856 835 885 894
gene5  181 249  204  244 225 277 305 272 270 279
gene6  460 502  491  491 493 612 594 577 618 638
```