Class 7 Machine Learning

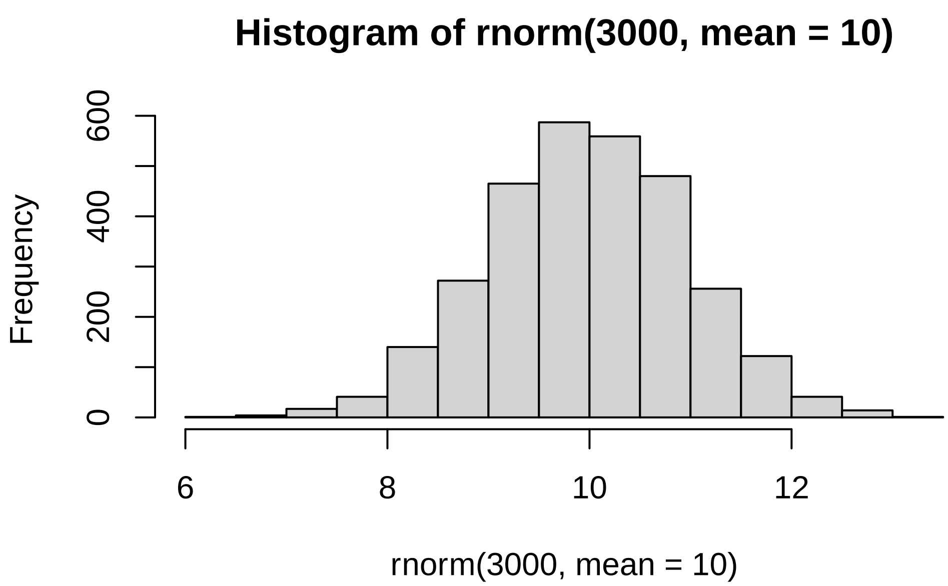
Kaliyah Adeimanu A18125684

Background

Today we will begin our exploration of important machine learning methods with a focus on **clustering** and **dimensionality reduction**

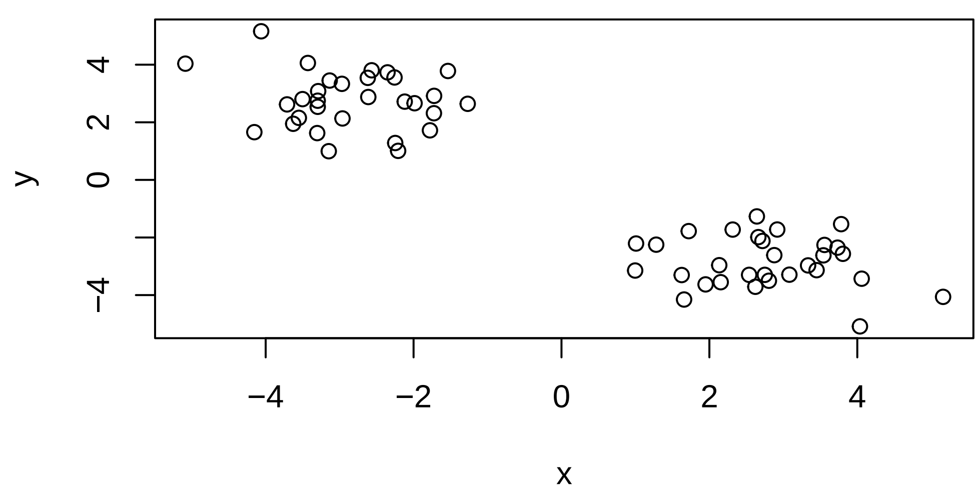
To start testing these methods let's make up some smaple data to cluster where we know what the answer should be.

```
hist(rnorm(3000, mean=10))
```



Q. Can you generate 30 numbers centered at +3 and 30 numbers at -3 taken at random from a normal distribution?

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

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



K-means clustering

The main funtion in "base R" for K-means clustering is called `kmeans()`, let's try it out:

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

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

Cluster means:
          x         y
1  2.763690 -2.850814
2 -2.850814  2.763690

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] 50.53287 50.53287
 (between_SS / total_SS =  90.3 %)

Available components:

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

> Q. What component of your kmeans result object has the cluster centers?

```r
k$centers
```

```
          x         y
1  2.763690 -2.850814
2 -2.850814  2.763690
```

> Q. What component of your kmeans result object has the cluster size (i.e.how many points are in each cluster)?

```r
k$size
```

```
[1] 30 30
```

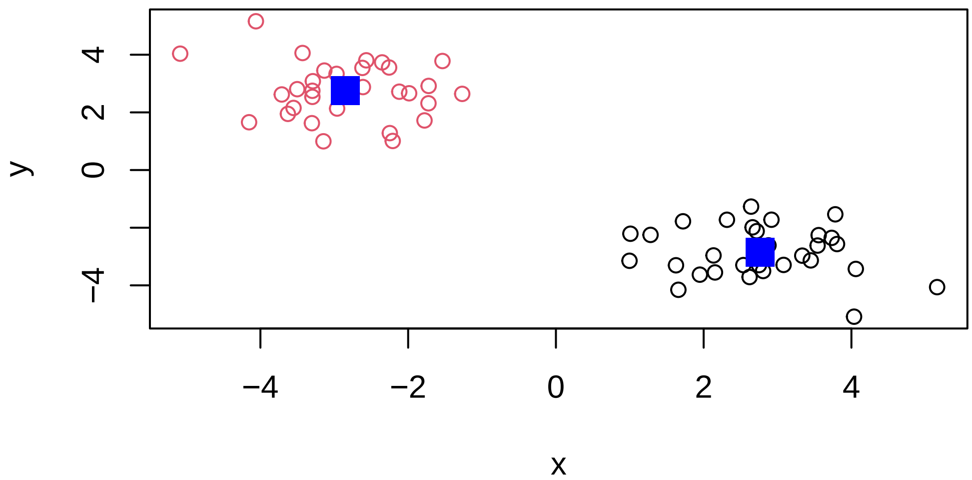
> Q. What component of your kmeans result object has the cluster membership vector (i.e. the main clustering result: which points are in which cluster)?

```r
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 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. Plot the results of clcustering (i.e. our data colored by the clustering result) along with the cluster centers.

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



Q. Can you run kmeans again and cluster into 4 clusters and plot the results just liek you did above with the coloring by cluster and the cluster cneters shown in blue

```
k2 <- kmeans(x=x, centers=4)
k2
```

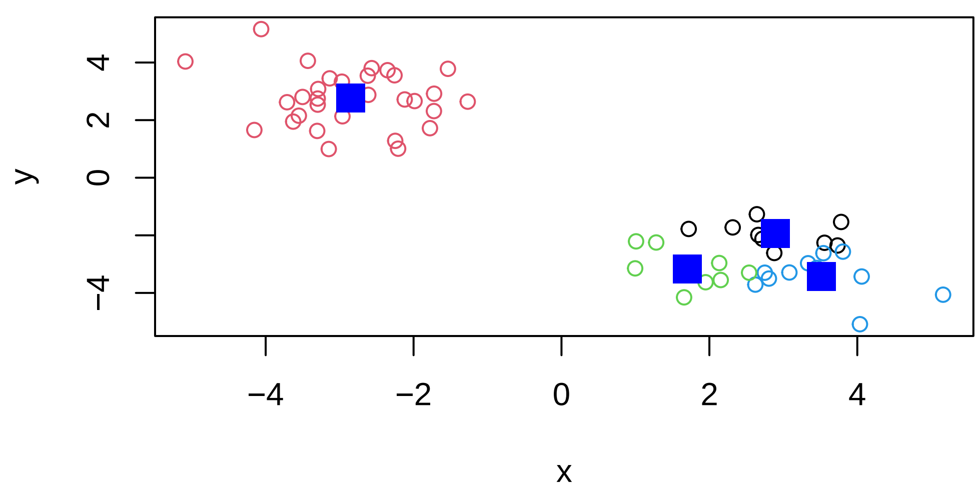
```
K-means clustering with 4 clusters of sizes 10, 30, 9, 11

Cluster means:
          x         y
1  2.892345 -1.935917
2 -2.850814  2.763690
3  1.704614 -3.166565
4  3.513249 -3.424196

Clustering vector:
 [1] 3 1 4 3 4 3 3 4 1 4 4 4 4 3 3 3 3 1 1 4 3 1 4 1 1 1 1 1 4 4 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]  5.284845 50.532875  5.486289 10.437146
 (between_SS / total_SS =  93.1 %)
```

```
Available components:

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

```r
k2$size
```

```
[1] 10 30  9 11
```

```r
plot(x,col=k2$cluster)
points(k2$centers, col="blue", pch=15, cex=2)
```



Key-point: Kmeans will always return the clustering that we ask for (this is the "K" or "centers" in K-means)

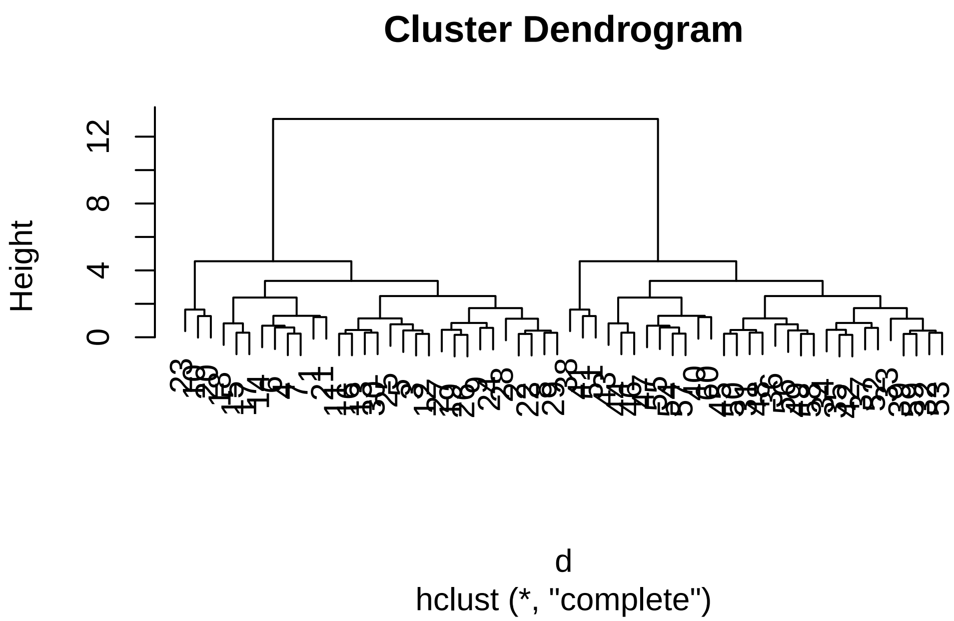
```r
k$tot.withinss
```

```
[1] 101.0657
```

Hierarchial clustering

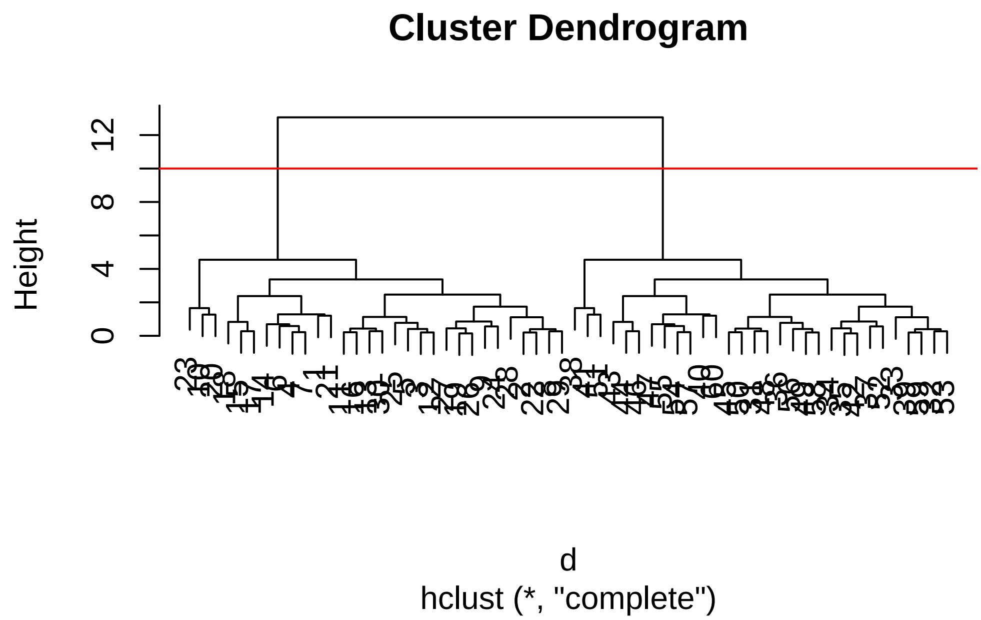
The main function for hierarchical clustering in base R is called `hclust()`. One of the main differences with respect to the `kmeans()` function is that you can not just pass your input data directly to `hclust()` - it needs a "distance matrix" as input. We can get this from lots of places including the `dist()` function.

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



We can "cut" the dendrogram or "tree" at a given height to yield our "clusters". For thsi we use the function `cutree()`

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



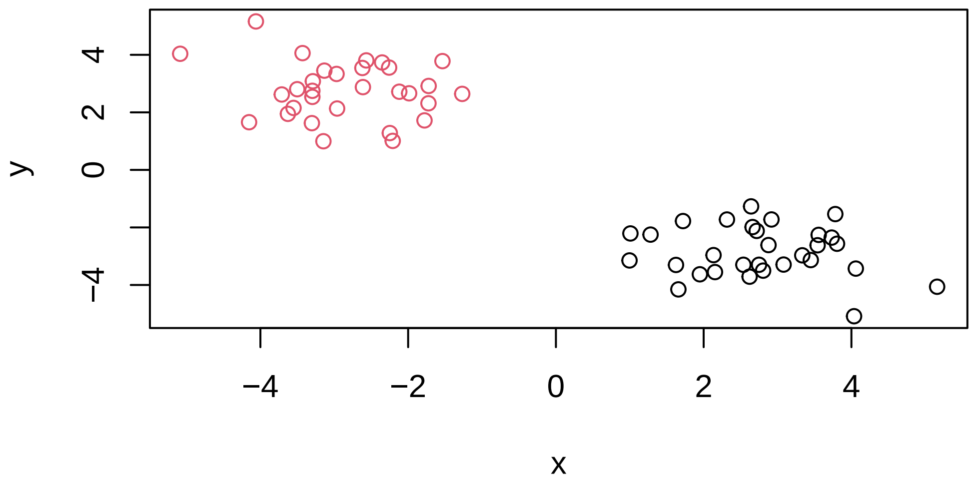

```
grps <- cutree(hc, h=10)
```

```
grps
```

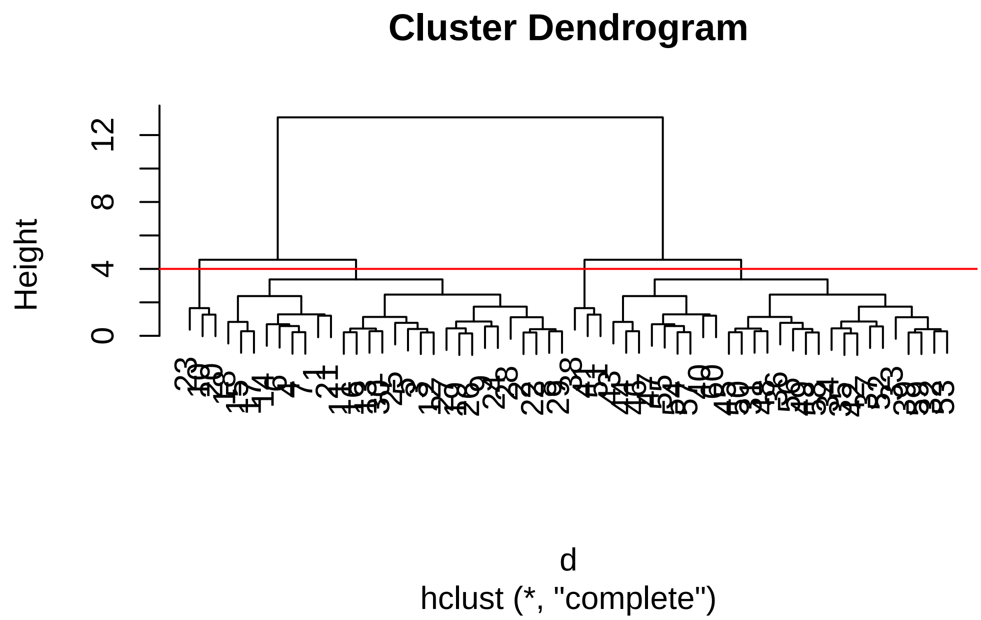
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

Q. Plot out data `x` colored by the clustering result from `hclust()` and `cutree()`

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




```r
plot(hc)
abline(h=4, col= "red")
```




```r
grps <- cutree(hc, h=4)
```

Principal Component Analysis (PCA)

PCA is a popular dimmensionality reduction technique that is widely used in bioinformatics.

PCA of UK food consumption

Read data on food consumption in UK

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

```
7       Fresh_potatoes      720   874       566       1033
8             Fresh_Veg     253   265       171        143
9             Other_Veg     488   570       418        355
10 Processed_potatoes       198   203       220        187
11        Processed_Veg     360   365       337        334
12          Fresh_fruit    1102  1137       957        674
13              Cereals    1472  1582      1462       1494
14            Beverages      57    73        53         47
15          Soft_drinks    1374  1256      1572       1506
16      Alcoholic_drinks    375   475       458        135
17        Confectionery      54    64        62         41
```

It looks like the row names are not set properly. We can fix this

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

A better way to do this is fix the row names assignment at import time:

```
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
```

17 rows and 4 columns

> 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?

```r
x <- x[,-1]
x
```

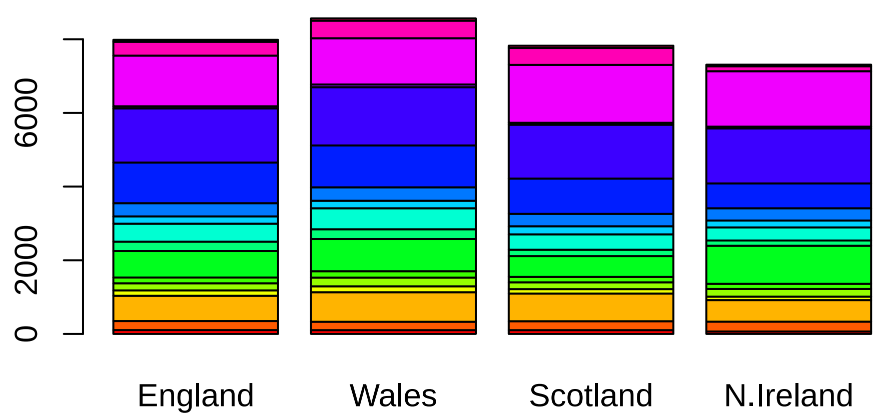
```
                    Wales Scotland N.Ireland
Cheese                103      103        66
Carcass_meat          227      242       267
Other_meat            803      750       586
Fish                  160      122        93
Fats_and_oils         235      184       209
Sugars                175 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

```
Fresh_potatoes        874     566     1033
Fresh_Veg             265     171      143
Other_Veg             570     418      355
Processed_potatoes    203     220      187
Processed_Veg         365     337      334
Fresh_fruit          1137     957      674
Cereals              1582    1462     1494
Beverages              73      53       47
Soft_drinks          1256    1572     1506
Alcoholic_drinks      475     458      135
Confectionery          64      62       41
```

There is an error is you keep running it that says there is an incorrect number of dimensions because it keeps deleting columns.

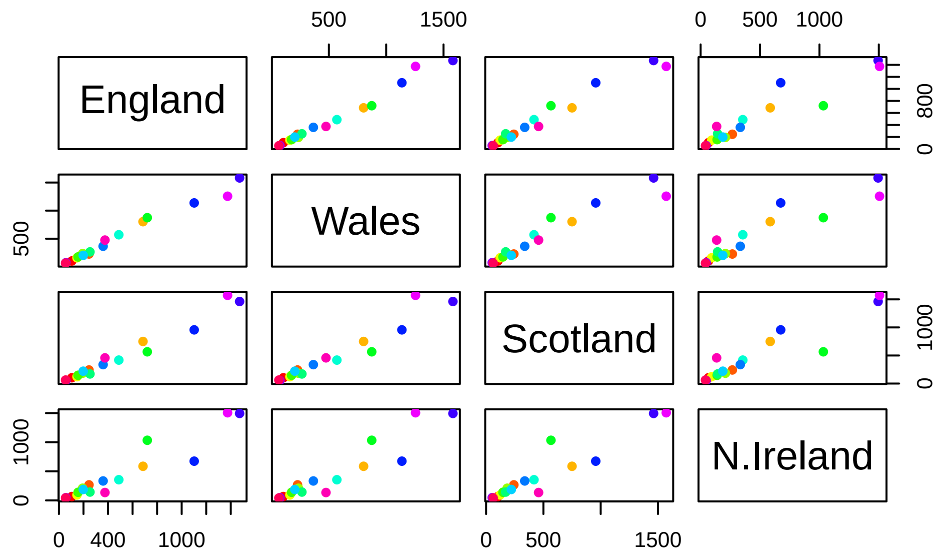
> Q3. Changing what optional argument in the above barplot() function results in the following plot?

```r
x <- read.csv(url, row.names =1)
barplot(as.matrix(x), beside=FALSE, col=rainbow(nrow(x)))
```



> Q5. We can use the pairs() function to generate all pairwise plots for our countries. 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?

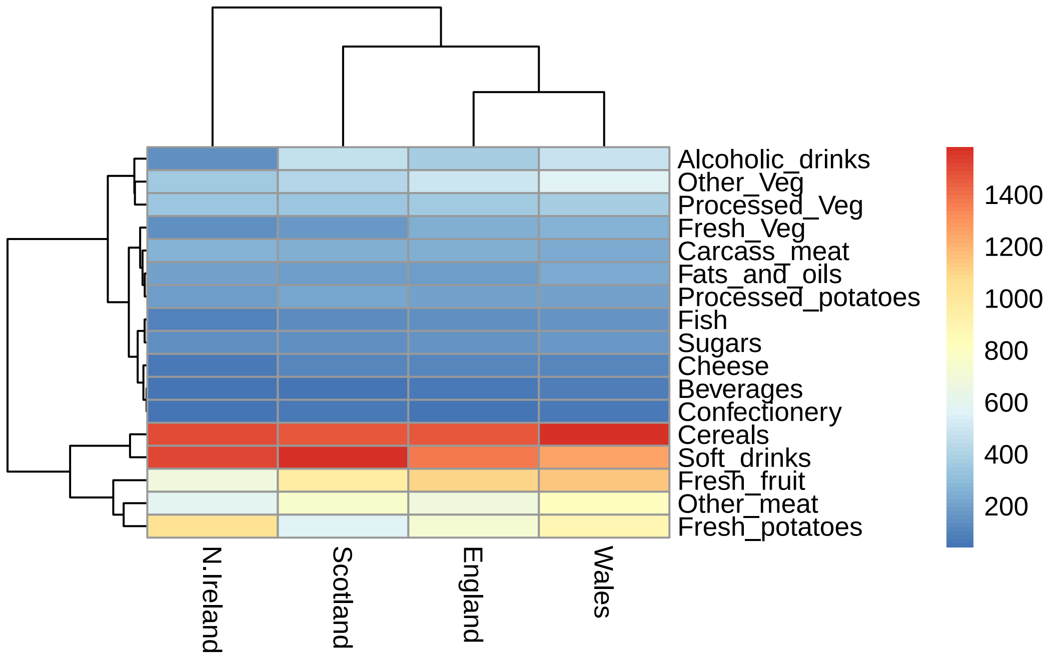
```r
pairs(x, col=rainbow(nrow(x)), pch=16)
```



The code shows each country plotted against each other. This allows us to see what countries are similar and which are not. We however do not know what food is what dot. The code makes these pair plots that compare 2 countries at a time, and have colored the foods rainbow.

> Q6. Based on the pairs and heatmap figures, which countries cluster together and what does this suggest about their food consumption patterns? Can you easily tell what the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

```r
library(pheatmap)
pheatmap( as.matrix(x))
```



The pairs figure shows that England, Wales, and Scotland all have similar food consumption, there is relatively a straight line when all of these countries are compared to each other. However that is not the cas for Northern Ireland. Northern Ireland is not as similar to the rest of the countries. The `pairs()` plot was the only plot that was useful for interpretation.

PCA to the rescue

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

```
pca <- prcomp(t(x))
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 the first PC?

67.44%

> Q. How many PCs do I need to capture at least 90% of the total variance in the dataset

2, using PC1 and PC2 together captures 96.5% of the total variance.

> Q. Plot our main PCA result. Folks can call this different things depending on their field of study e.g. "PC plot", "ordienation plot", "Score plot", "PC1 vs PC2 plot"...

```
 attributes (pca)
```

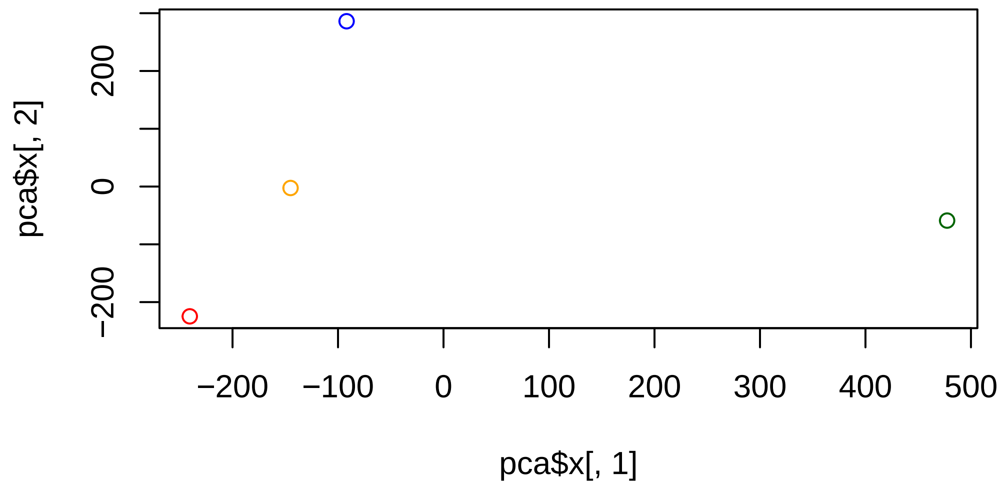
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

To generate our PCA score plot we want the **pca$x** component of the result object

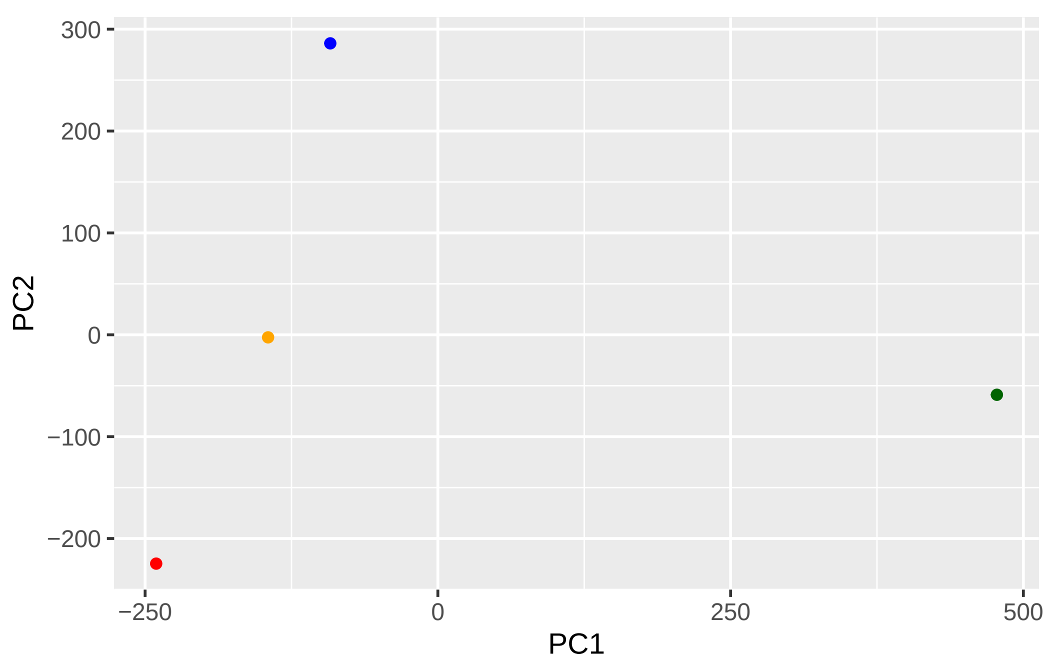
```
pca$x
```

```
                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
```

```
my_cols <- c("orange","red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=my_cols)
```



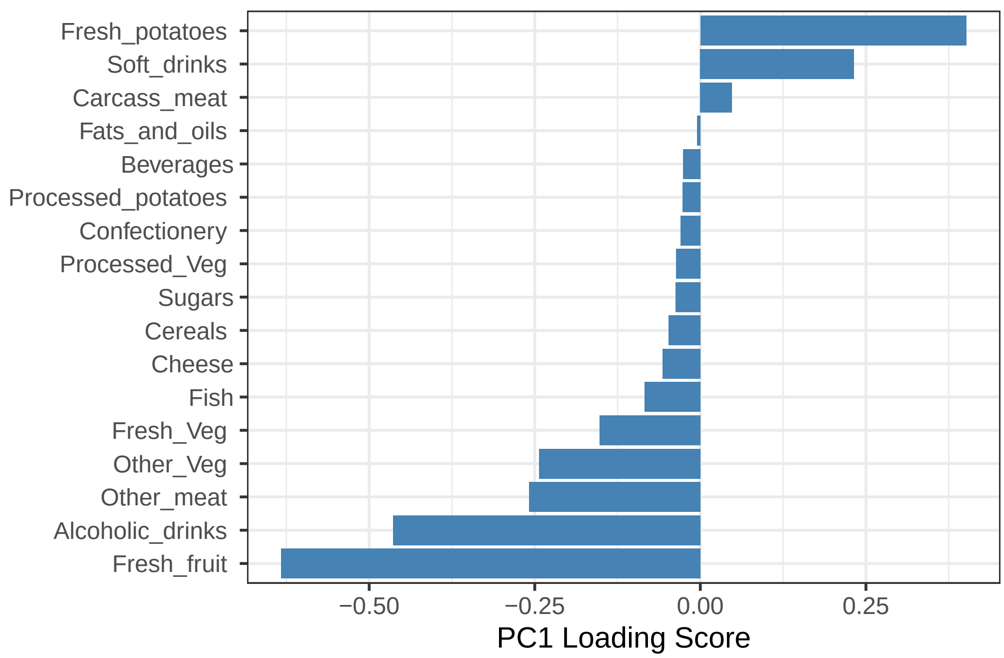

```
library(ggplot2)
ggplot(pca$x) + aes(PC1, PC2)+
  geom_point(col= my_cols)
```



Digging deeper (variable loadings)

How do the original variables (i.e. te 17 different foods) contribute to our new PCs?

```
ggplot(pca$rotation) +
  aes(x = PC1,
      y = reorder(rownames(pca$rotation), PC1)) +
  geom_col(fill = "steelblue") +
  xlab("PC1 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```



This plot shows how Ireland differs from England, Wales, and Scotland. In the above figure we can see that England, Wales and Scotland consume more of fresh fruit, alcoholic drinks etc., while Ireland consumes more potatoes and soft dirnks than the other 3 countries.