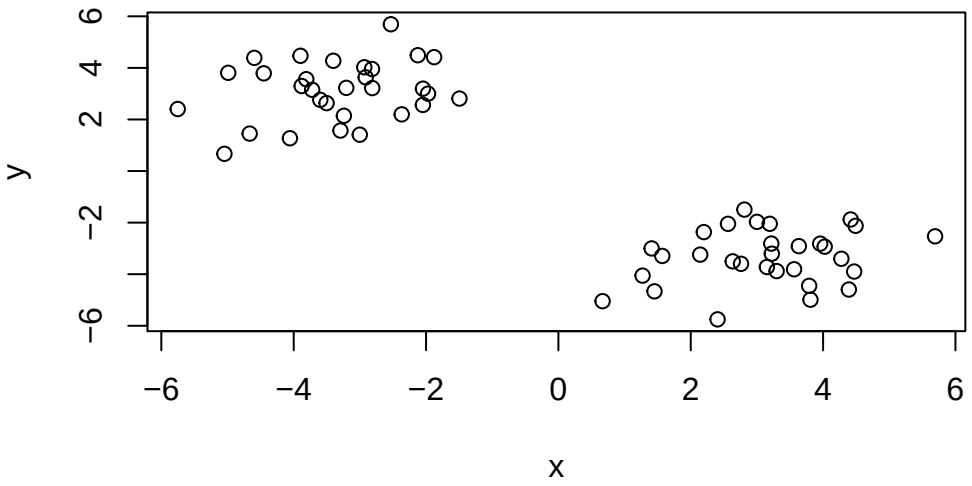
Class 7: Machine Learning

4/26/23

Example of K-means clustering

First step is to make some data with a known structure, so we know what the answer should be.

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



Now we have some structured data in the variable `x`. Let's see if k-means is able to identify the two groups.

```
k <- kmeans(x,centers=2, nstart = 20)
k
```

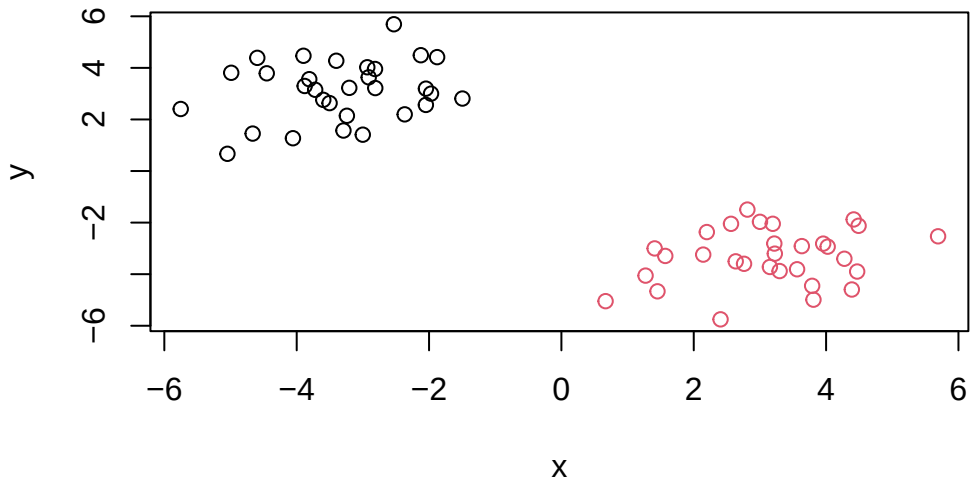
```
K-means clustering with 2 clusters of sizes 30, 30

Cluster means:
          x         y
1 -3.334816  3.115979
2  3.115979 -3.334816

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] 71.02871 71.02871
 (between_SS / total_SS =  89.8 %)

Available components:

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

Let's explore `k`:

```
k$centers
```

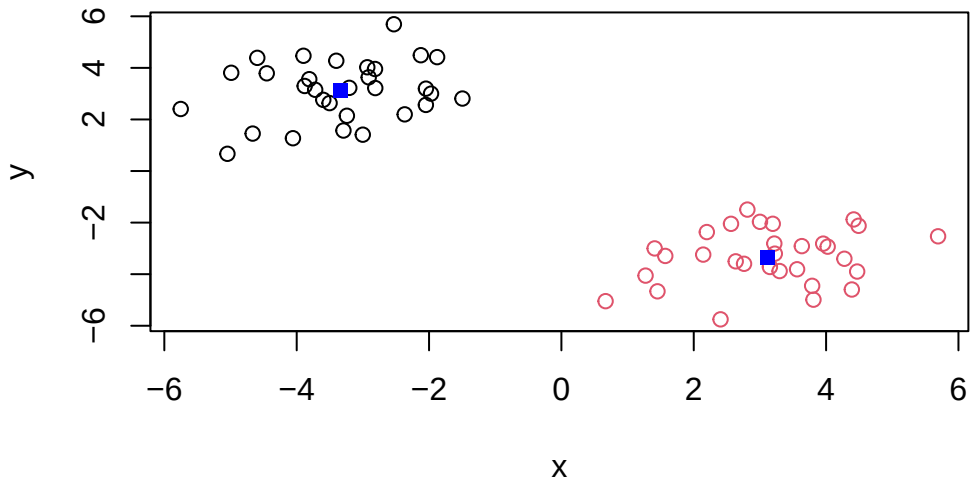
```
          x         y
1 -3.334816  3.115979
2  3.115979 -3.334816
```

```
plot(x, col = k$cluster)
```



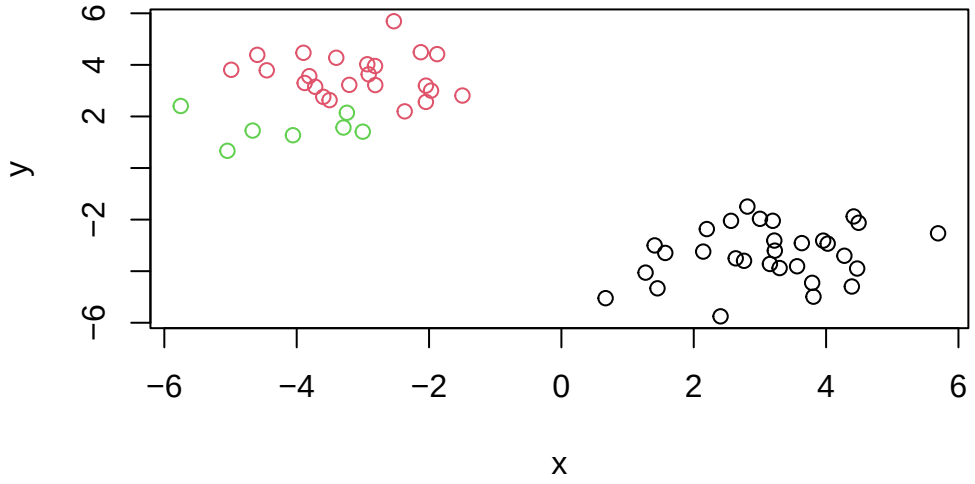
Now we can add the clusters' centers:

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



An example when we select the wrong number of cluster for k-means.

```
k_3 <- kmeans(x, centers = 3, nstart = 20)
plot(x, col = k_3$cluster)
```



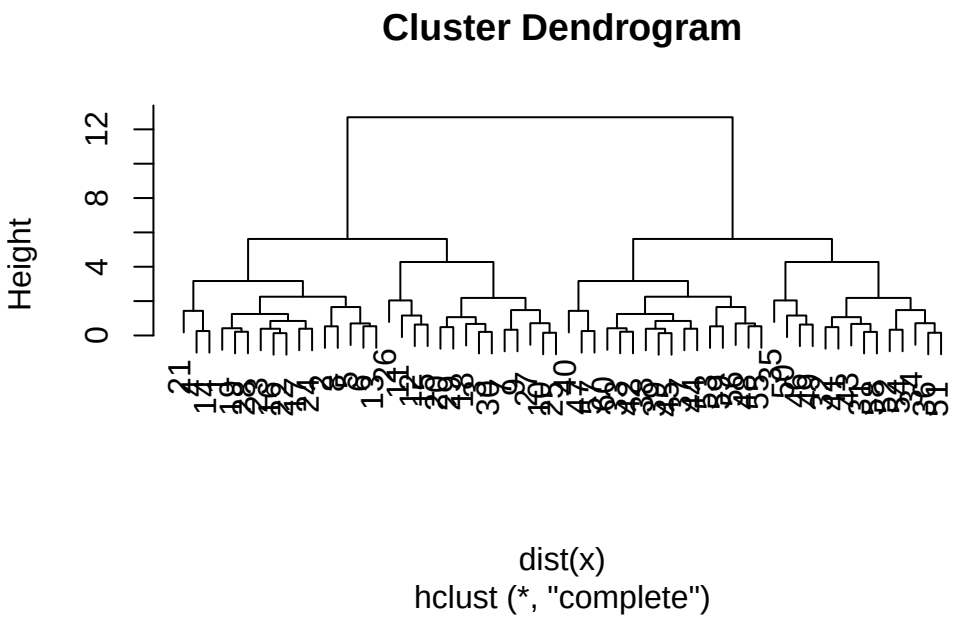
Example of Hierarchical Clustering

Let's use the same data as before, which we stored in `x`. We will use the `hclust()` function.

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

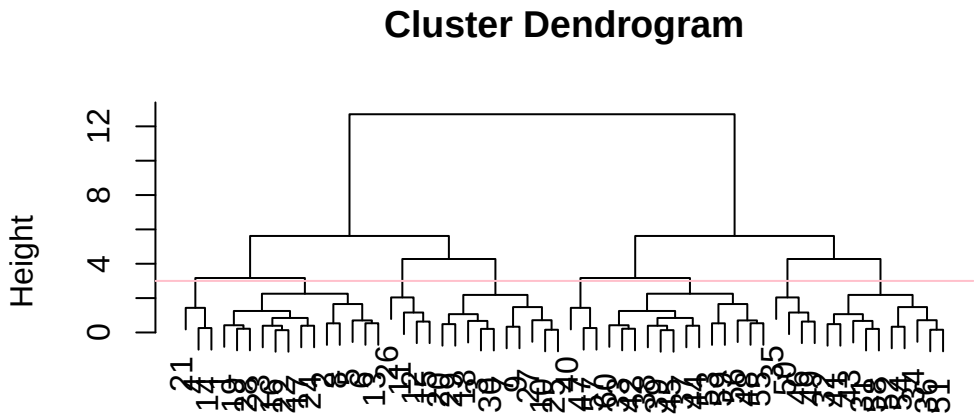
```
Call:
hclust(d = dist(x))

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

```
plot(clustering)
```



Let's add a horizontal line

```
plot(clustering)
abline(h= 3, col= 'pink')
```



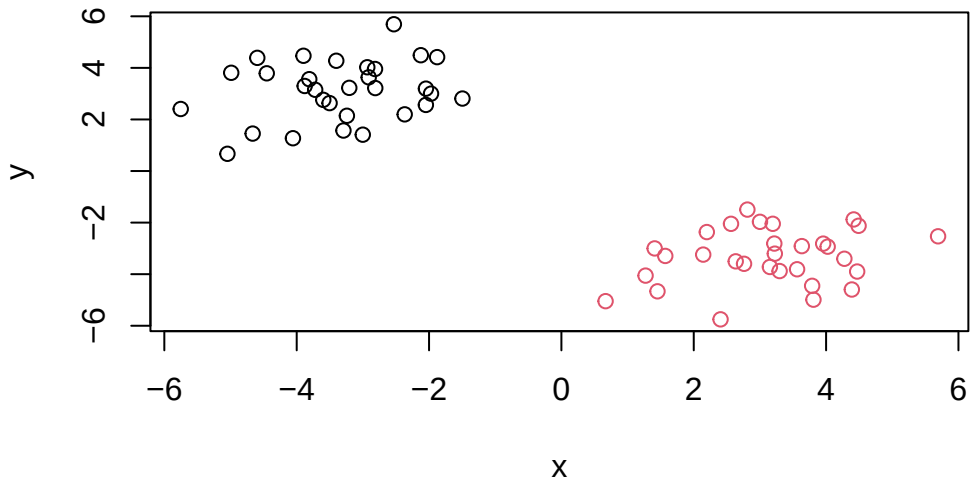
To get our results (i.e., membership vector) we need to "cut" the tree. The function for doing that is `cutree()`.

```
subgroups <- cutree(clustering, h=10)
subgroups
```

```
 [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
```

Plotting this...

```
plot(x, col = subgroups)
```



You can also "cut" your tree with the number of clusters you want:

```
subgroups <- cutree(clustering, k=2)
```

Principal Component Analysis (PCA)

PCA of UK Food Data

First, we read the data:

```
url <- "https://tinyurl.com/UK-foods"
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
```

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  4
```

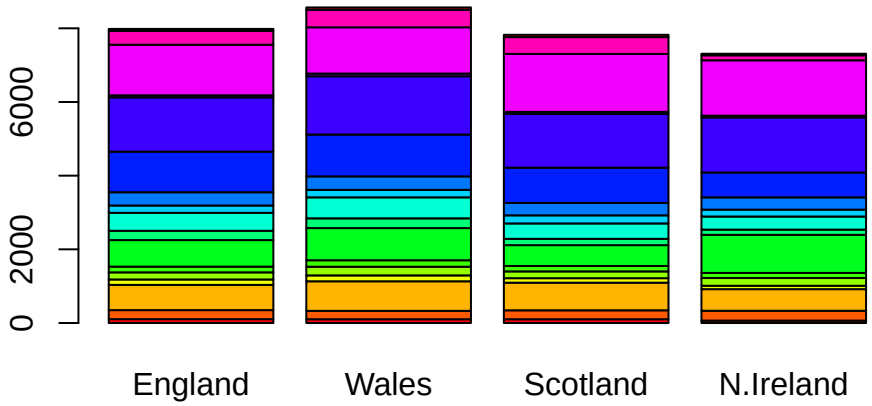
There are 17 rows and 4 columns.

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?

I prefer using the `row.names` function in the code when using `read.csv`, as it uses less steps and leaves less room for error. The first approach (x <- x[,-1] approach) requires more code and, if ran multiple times, will continue to eliminate columns.

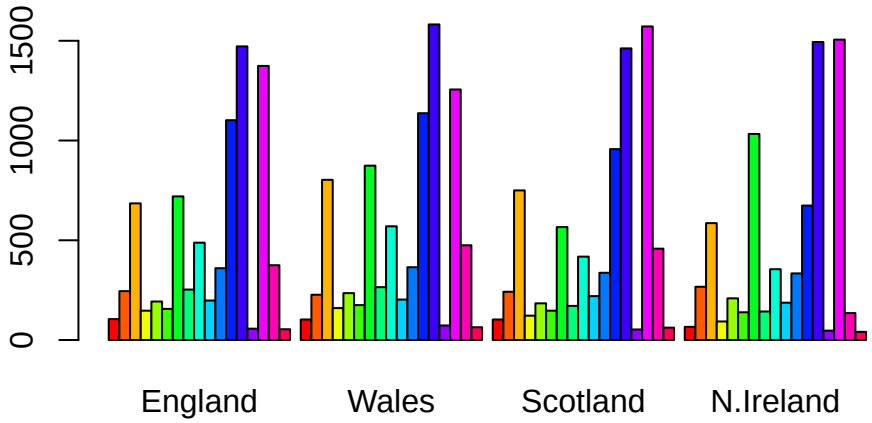
Now we can generate some basic visualizations:

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



Let's redefine our barplot:

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



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

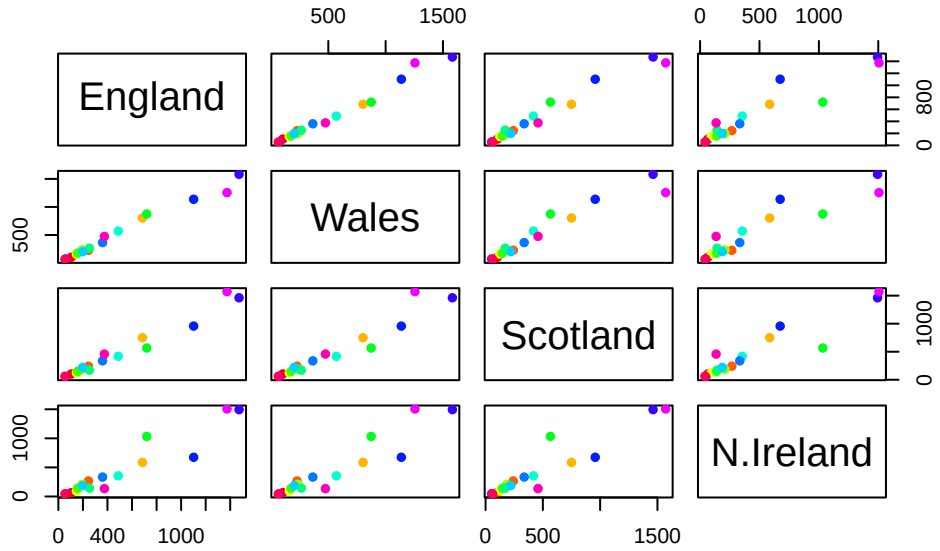
Removing the `beside = T` argument in the barplot() function generates the stacked column chart rather than the individual bar chart.

Other visualizations that can be useful…

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?

The code pairs together each of the countries individually, and plots the data from each country against the other. One country's data is represented on the y-axis, and the other on the x-axis. Each point that lies on the diagonal means there is a 1:1 ratio between that particular data point (food group) between the two countries (the amount of that particular food is consumed at equal amounts between the two countries). If a data point is higher on the y-axis, that means that food group is more represented in the country defined on the y-axis, and if a data point is further to the right on the x-axis, that means that food group is more represented in the country defined on the x-axis.

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



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

N. Ireland consistently consumes more fresh potatoes than all of the other countries of the UK in terms of this data-set.

Let's apply PCA (principal component analysis). For that, we need to use the command `prcomp()`. This function expects the transpose of our data.

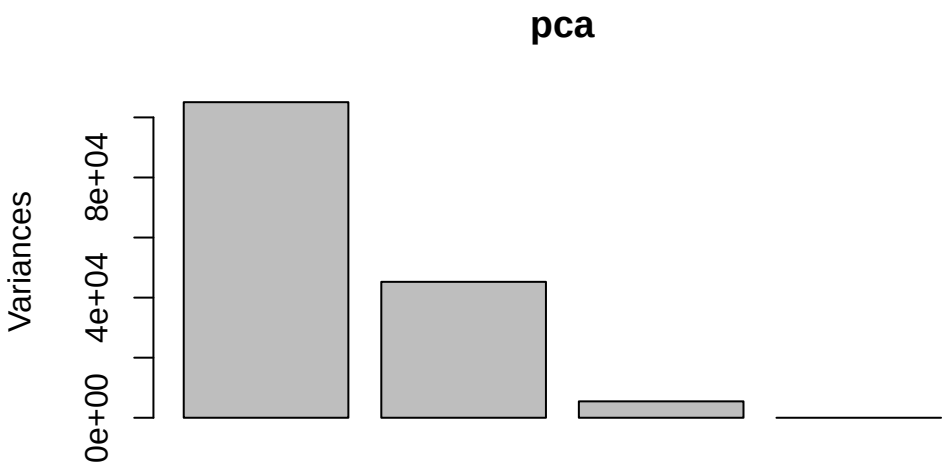
```
#transpose_matrix <- t(x)
#pca <- prcomp( transpose_matrix )

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

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 5.552e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
```

```
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

Let's plot the PCA results:

```
plot(pca)
```



We need to access the results of the PCA analysis:

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

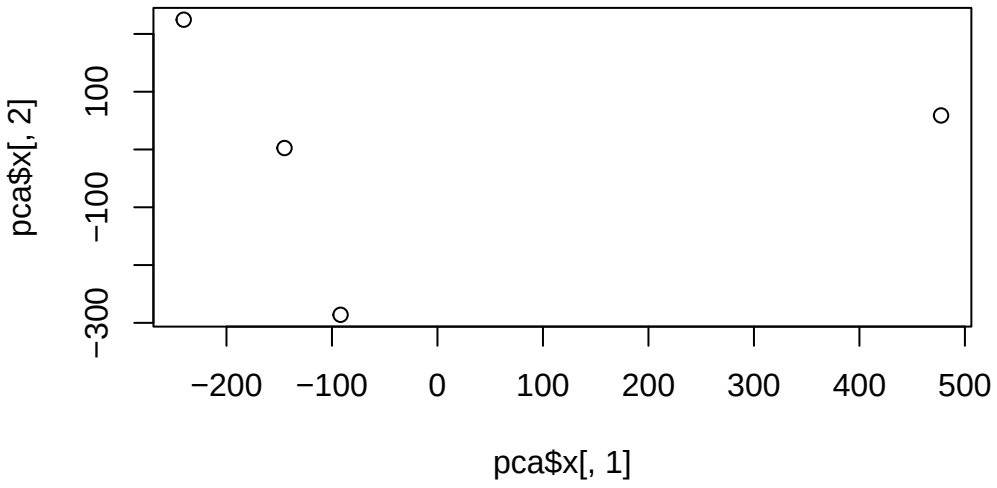
We can explore the pca$x dataframe:

```
pca$x
```

```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  1.042460e-14
Wales     -240.52915  224.646925   56.475555  9.556806e-13
Scotland   -91.86934 -286.081786   44.415495 -1.257152e-12
N.Ireland  477.39164   58.901862    4.877895  2.872787e-13
```

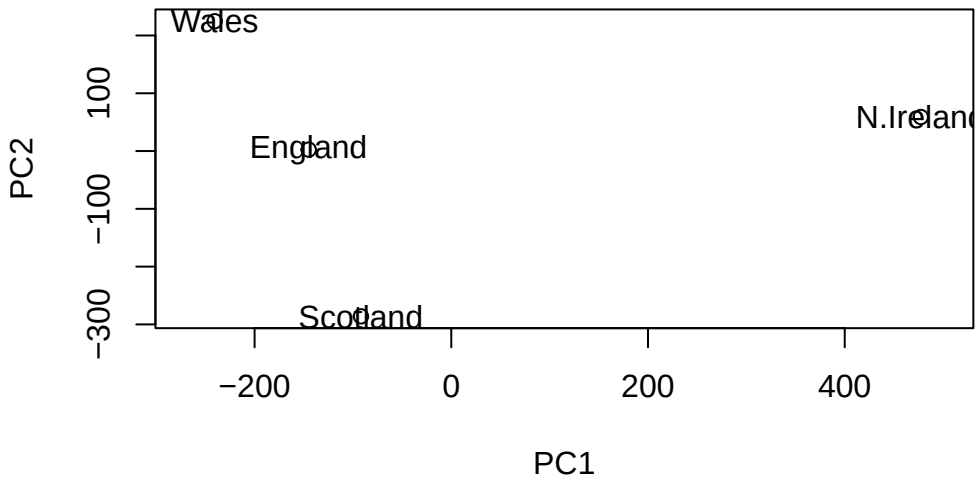
Plotting:

```
plot( x=pca$x[,1], y=pca$x[,2])
```



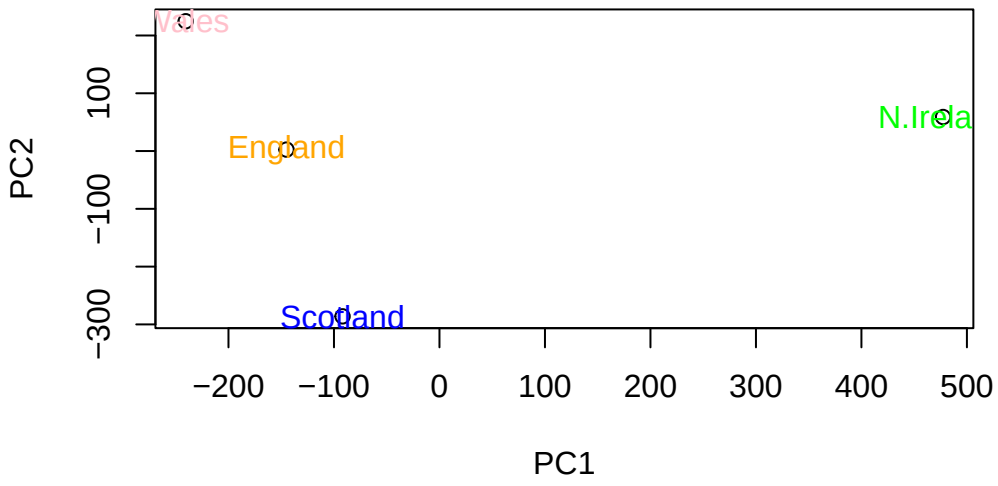
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
plot( x=pca$x[,1], y=pca$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.

```
#colnames(x)
#rownames(pca$x)

plot( x=pca$x[,1], y=pca$x[,2],xlab="PC1", ylab="PC2",)
colors_countries <- c('orange','pink','blue','green')
text( x=pca$x[,1], y=pca$x[,2],colnames(x), col= colors_countries)
```



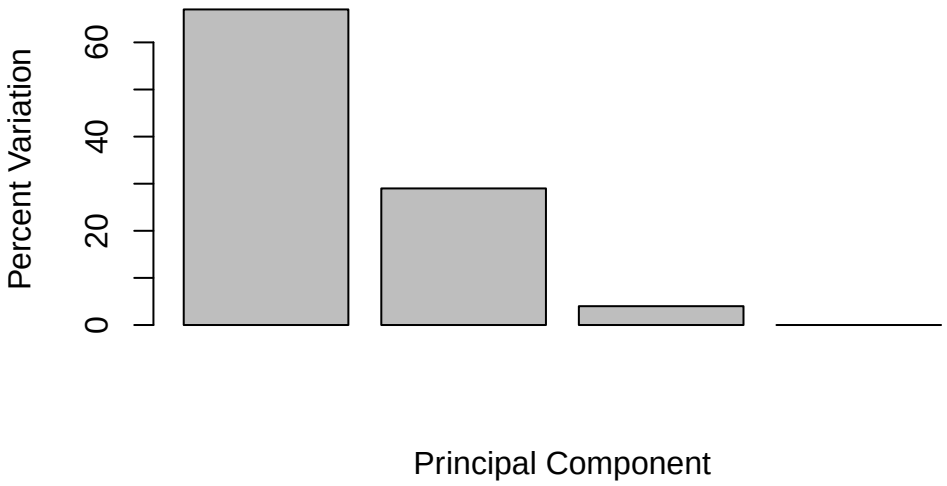

```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

```
[1] 67 29  4  0
```

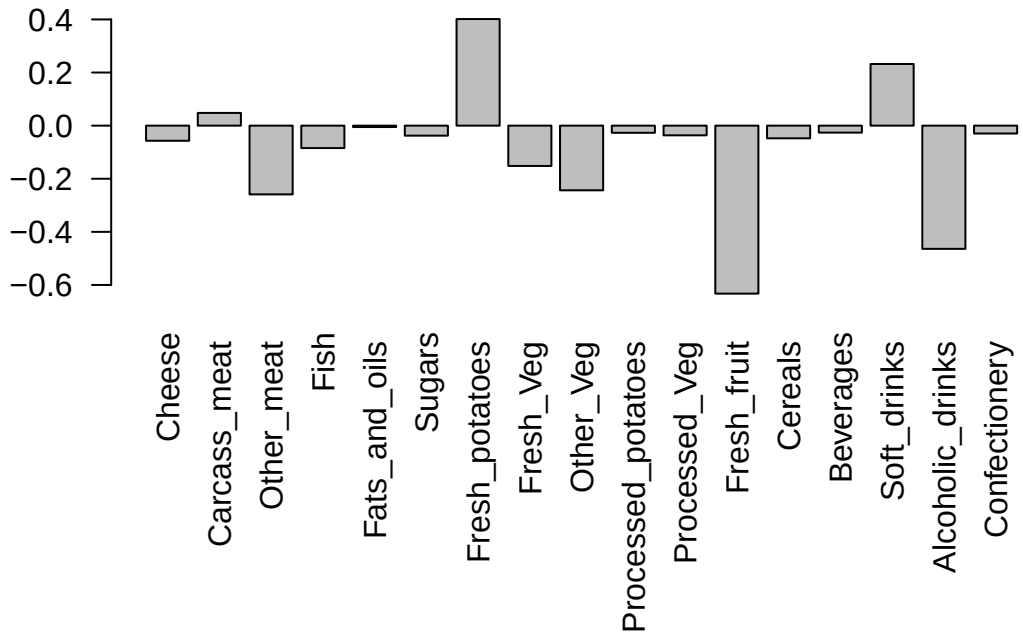
```
z <- summary(pca)
z$importance
```

```
                             PC1       PC2      PC3           PC4
Standard deviation     324.15019 212.74780 73.87622 5.551558e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

```
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```

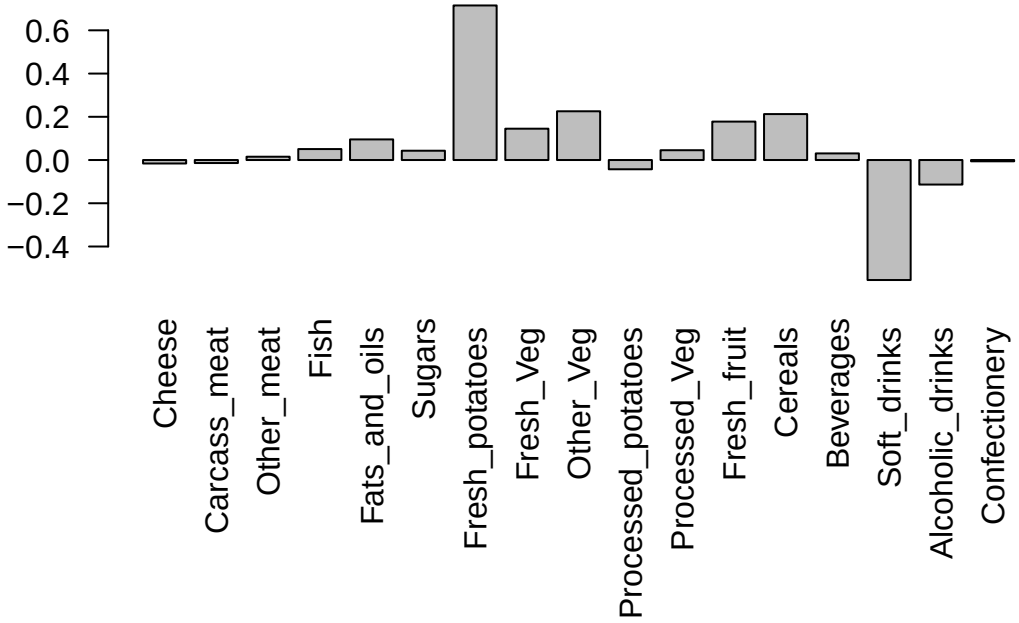



```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```



Q9: Generate a similar 'loadings plot' for PC2. What two food groups feature predominantly and what does PC2 mainly tell us about?

```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```



The two food groups that are predominantly featured are fresh potatoes (positive) and soft drinks (negative). PC2 mainly tells us about what groups are similar and what groups are still most variable within the remaining variance not accounted for by PC1. This chart shows that soft drinks are more variable whereas fresh potatoes are more similar in the context of PC2.

PCA of a RNA-Seq dataset

```
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
```

Q10: How many genes and samples are in this data set?

```
dim( rna.data )
```

```
[1] 100  10
```

I have 100 genes, and 10 samples.

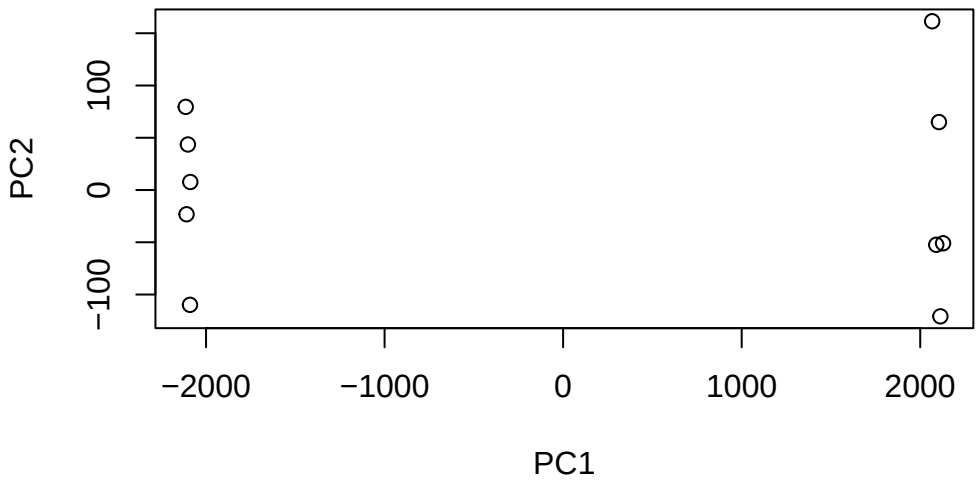
Let's apply PCA:

```
pca_rna = prcomp(t(rna.data))
summary(pca_rna)
```

```
Importance of components:
                            PC1     PC2      PC3      PC4      PC5      PC6
Standard deviation     2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
Proportion of Variance    0.9917  0.0016  0.00144  0.00122  0.00098  0.00093
Cumulative Proportion     0.9917  0.9933  0.99471  0.99593  0.99691  0.99784
                           PC7      PC8      PC9      PC10
Standard deviation     65.29428 59.90981 53.20803 2.715e-13
Proportion of Variance  0.00086  0.00073  0.00057 0.000e+00
Cumulative Proportion   0.99870  0.99943  1.00000 1.000e+00
```

Let's plot the principal components 1 and 2.

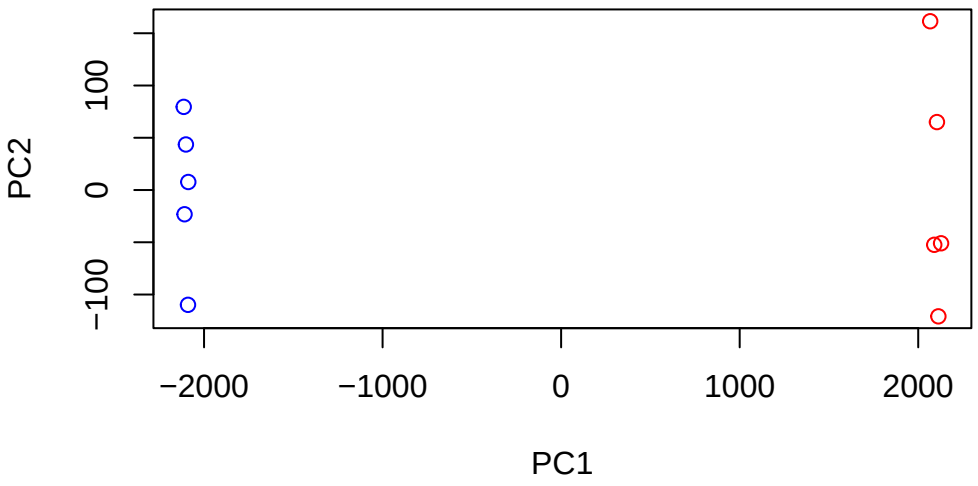
```
plot( pca_rna$x[,1], pca_rna$x[,2],
      xlab = 'PC1', ylab = 'PC2')
```



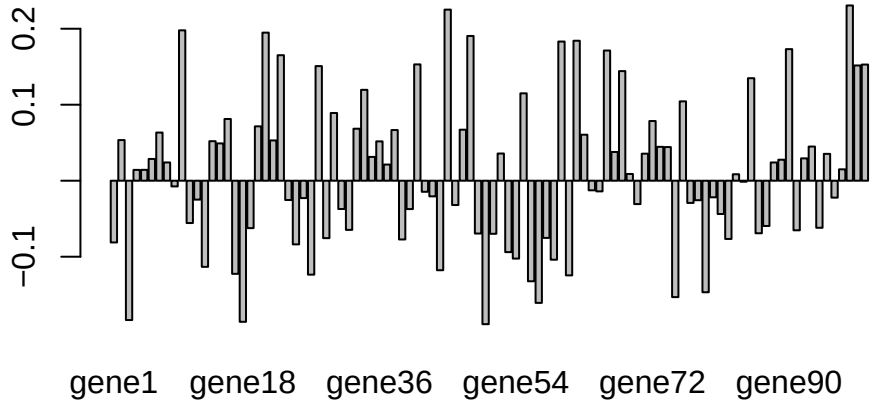

```
#colnames(rna.data)
cols_samples <- c(rep('blue',5), rep('red',5) )
cols_samples
```

```
[1] "blue" "blue" "blue" "blue" "blue" "red"  "red"  "red"  "red"  "red"
```

```
plot( pca_rna$x[,1], pca_rna$x[,2],
      xlab = 'PC1', ylab = 'PC2',
      col = cols_samples)
```




```
barplot(pca_rna$rotation[,1])
```



```
sort(pca_rna$rotation[,1])
```

```
      gene50       gene18        gene3       gene57       gene75       gene79
-0.188796985 -0.185668500 -0.183374164 -0.160771014 -0.153164404 -0.146803635
      gene56       gene61       gene27       gene17       gene44       gene13
-0.132330117 -0.124572881 -0.123615228 -0.122536548 -0.117808971 -0.113357525
      gene59       gene54       gene53       gene25        gene1       gene39
-0.103935563 -0.102503320 -0.093979884 -0.083761992 -0.081247810 -0.077306742
      gene82       gene29       gene58       gene51       gene49       gene86
-0.076658760 -0.075605635 -0.075274651 -0.069855142 -0.069530208 -0.069165267
      gene91       gene32       gene19       gene94       gene87       gene11
-0.065288752 -0.064721235 -0.062411218 -0.061938300 -0.059547317 -0.055698801
      gene81       gene40       gene31       gene46       gene70       gene77
-0.043780416 -0.037323670 -0.037219970 -0.031990529 -0.030784982 -0.029225446
      gene78       gene24       gene12       gene26       gene96       gene80
-0.025639741 -0.025407507 -0.024870802 -0.022868107 -0.022293151 -0.021824860
      gene43       gene42       gene65       gene64        gene9       gene84
-0.020617052 -0.014550791 -0.014052839 -0.012639567 -0.007495075 -0.001289937
      gene83       gene69        gene4        gene5       gene97       gene37
 0.008504287  0.008871890  0.014242602  0.014303808  0.014994546  0.021280555
      gene88        gene8       gene89        gene6       gene92       gene35
 0.024015925  0.024026657  0.027652967  0.028634131  0.029394259  0.031349942
      gene95       gene71       gene52       gene67       gene74       gene73
 0.035342407  0.035589259  0.035802086  0.037840851  0.044286948  0.044581700
      gene93       gene15       gene36       gene14       gene22        gene2
 0.044940861  0.049090676  0.051765605  0.052004194  0.053013523  0.053465569
      gene63        gene7       gene38       gene47       gene33       gene20
 0.060529157  0.063389255  0.066665407  0.067141911  0.068437703  0.071571203
      gene72       gene16       gene30       gene76       gene55       gene34
 0.078551648  0.081254592  0.089150461  0.104435777  0.114988217  0.119604059
      gene85       gene68       gene28       gene99      gene100       gene41
 0.134907896  0.144227333  0.150812015  0.151678253  0.152877246  0.153077075
      gene23       gene66       gene90       gene60       gene62       gene48
 0.165155192  0.171311307  0.173156806  0.183139926  0.184203008  0.190495289
      gene21       gene10       gene45       gene98
 0.194884023  0.197905454  0.225149201  0.230633225
```