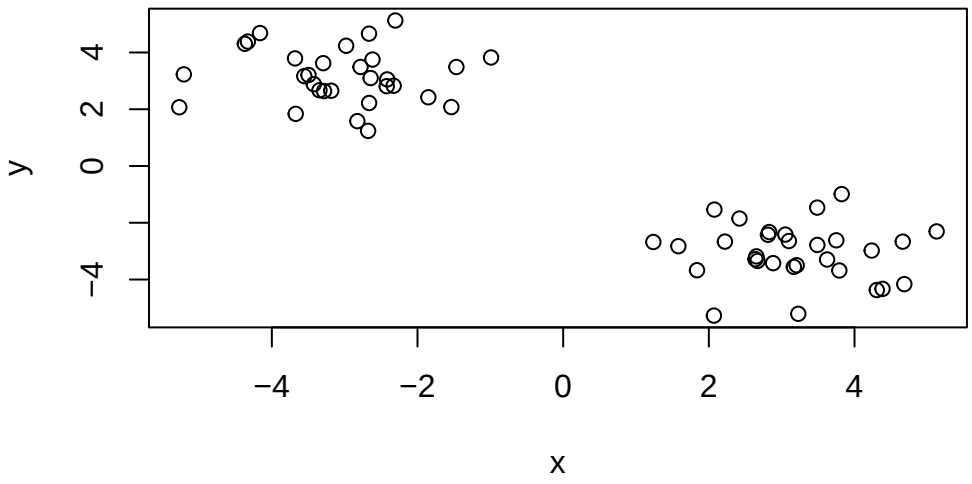
Lab Class 07 (Machine Learning 1)

Ava Limtiaco (PID: A18007672)

#First up kmeans()

Demo od using kmeans() function in base R. First make up some data with a known structure.

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



Now we have some made up data in 'x' let's see how kmeans works with this data

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

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

Cluster means:
          x         y
1  3.168062 -3.048386
2 -3.048386  3.168062

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 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] 55.94364 55.94364
 (between_SS / total_SS =  91.2 %)

Available components:

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

Q. How many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q. How we do get to the cluster membership/assignment.

```
k$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 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
```

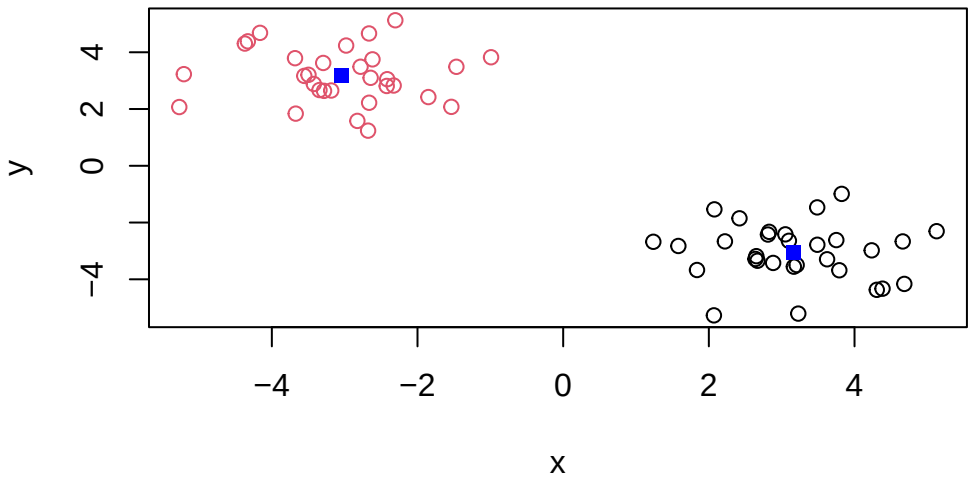
Q. What about cluster centers?

```
k$centers
```

```
          x         y
1  3.168062 -3.048386
2 -3.048386  3.168062
```

Now we got to the main results, let's use them to plot our data with the kmeans results.

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



Now for hclust()

We will cluster the same data 'x' with the 'hclust()'. In this case 'hclust()' requires a distance matrix as input.

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

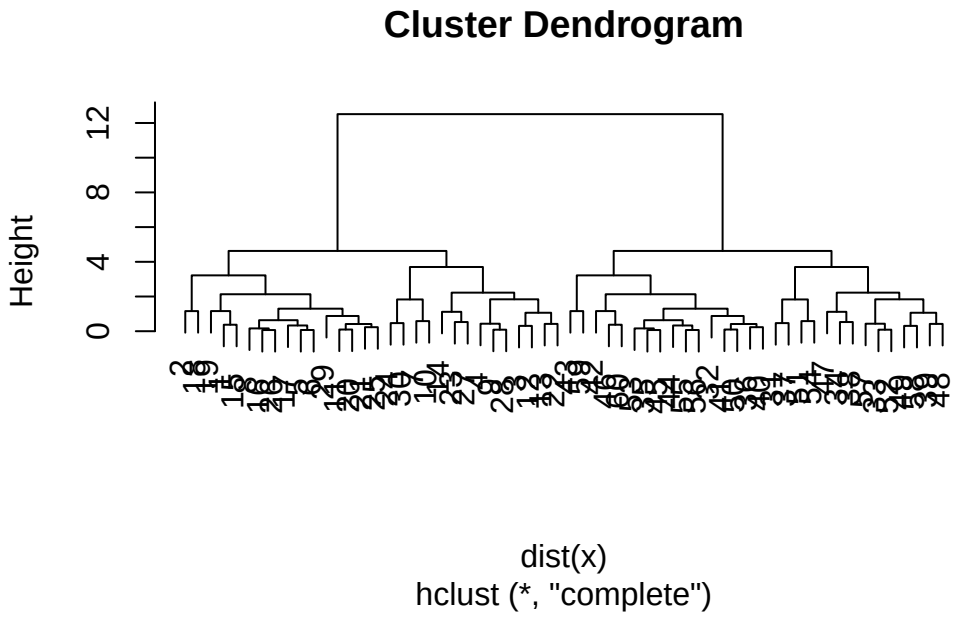
```

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

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

Let's plot our hclust result

```
plot(hc)
```



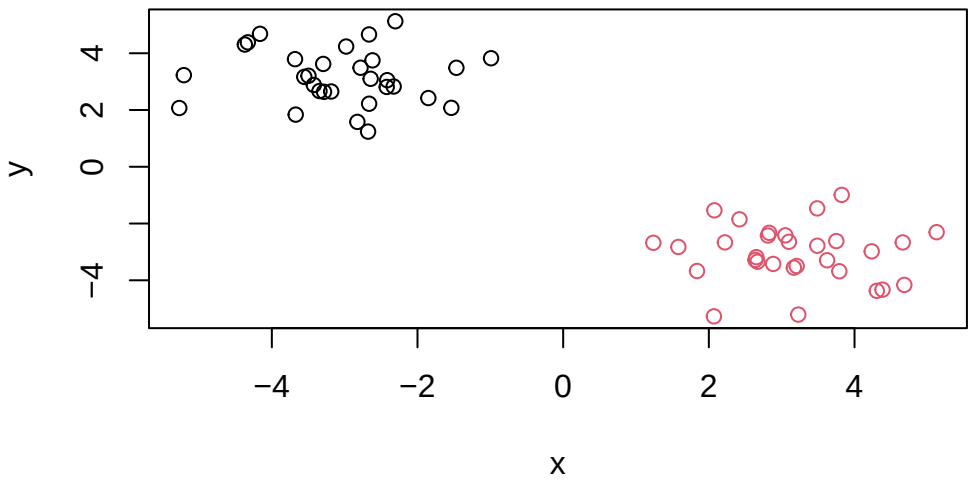
To get our cluster membership vector we need to "cut" the tree with the 'cutree()'

```
grps <- cutree(hc, h=8)
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 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
```

Now plot our data with the hclust() results

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



Principal Component Analysis (PCA)

PCA of UK food data

Read data from website and try a few visualizations.

```
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?

There are 17 rows and 4 columns. You can use 'dim(x)', 'nrow(x)', or 'ncol(x)' to find the number of rows and columns.

```
dim(x)
```

```
[1] 17  4
```

```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

```
[1] 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?

I prefer to use the 'x<-read.csv(url, row.names=1)' because it is straightforward/clear and robust compared to the other approach.

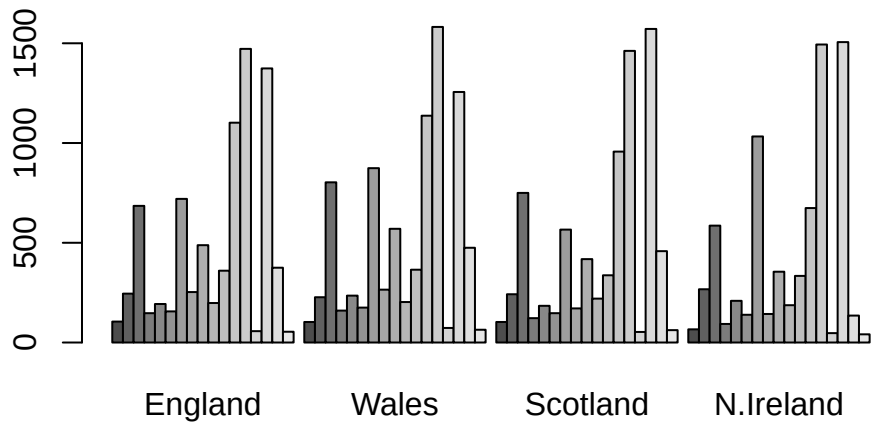
```
x <- read.csv(url)
rownames(x) <- x[,1]
x < x[,1]
```

```
                      X England Wales Scotland N.Ireland
Cheese            FALSE    TRUE  TRUE     TRUE      TRUE
Carcass_meat      FALSE    TRUE  TRUE     TRUE      TRUE
Other_meat        FALSE    TRUE  TRUE     TRUE      TRUE
```

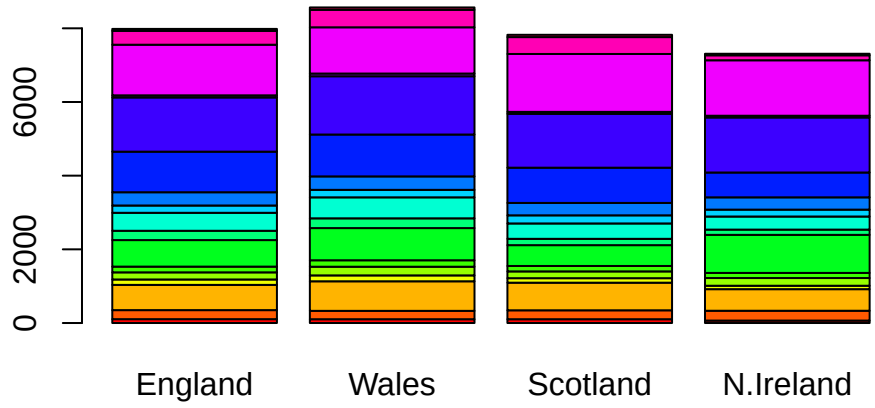
```
Fish                FALSE   TRUE  TRUE     TRUE      TRUE
Fats_and_oils       FALSE   TRUE  TRUE     TRUE      TRUE
Sugars              FALSE   TRUE  TRUE     TRUE      TRUE
Fresh_potatoes      FALSE   TRUE  TRUE     TRUE      TRUE
Fresh_Veg           FALSE   TRUE  TRUE     TRUE      TRUE
Other_Veg           FALSE   TRUE  TRUE     TRUE      TRUE
Processed_potatoes  FALSE   TRUE  TRUE     TRUE      TRUE
Processed_Veg       FALSE   TRUE  TRUE     TRUE      TRUE
Fresh_fruit         FALSE   TRUE  TRUE     TRUE      TRUE
Cereals             FALSE   TRUE  TRUE     TRUE      TRUE
Beverages           FALSE   TRUE  TRUE     TRUE      TRUE
Soft_drinks         FALSE   TRUE  TRUE     TRUE      TRUE
Alcoholic_drinks    FALSE   TRUE  TRUE     TRUE      TRUE
Confectionery       FALSE   TRUE  TRUE     TRUE      TRUE
```

```
x <- read.csv(url, row.names=1)
```

```
barplot(as.matrix(x), beside=TRUE)
```



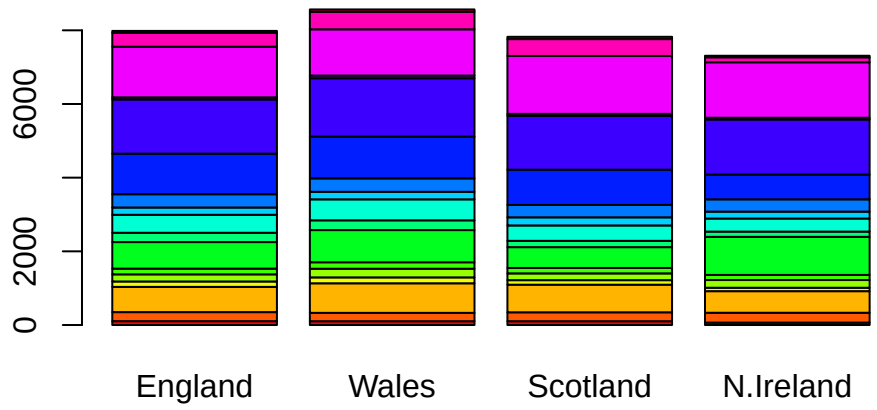

```
cols <- rainbow(nrow(x))
barplot(as.matrix(x), col=cols)
```



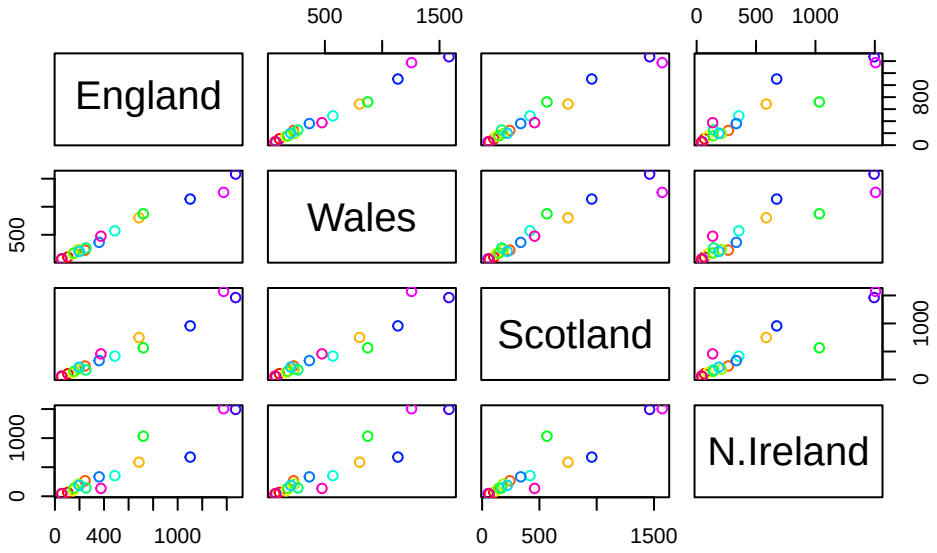
Q3.Changing what optional argument in the above barplot() function results in the following plot?

If you change the 'beside' from TRUE to FALSE.

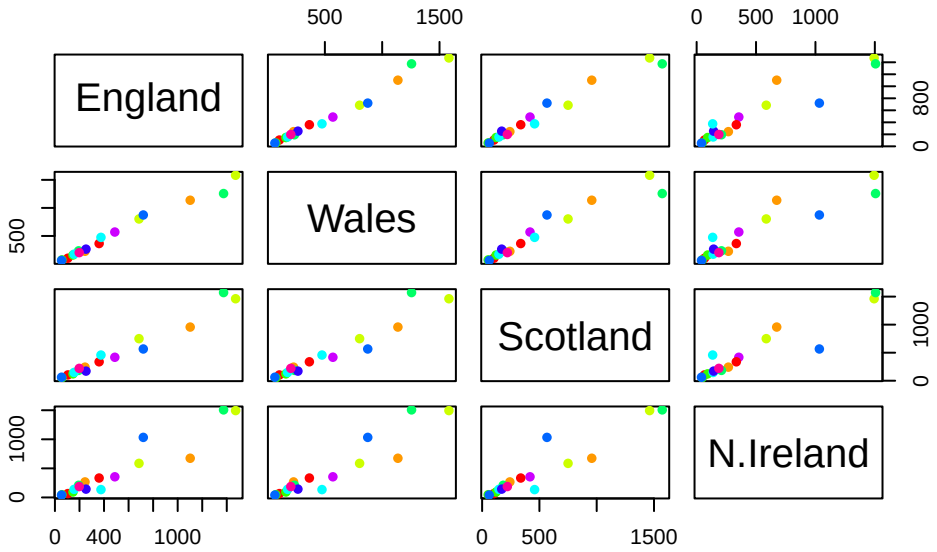
```
barplot(as.matrix(x), col=cols, beside=FALSE)
```




```
pairs(x, col=cols)
```



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



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 'col' gives the color of the plot. Each country name is lined up diagonal from each other, which just shows its being compared to itself than rather another point.

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

The main differences is that N.Ireland has higher numbers than the other countries of the UK.

PCA to the rescue!! The main base R PCA function is called 'prcomp' and we will need to give it the transpose of our input data!

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

```
Standard deviations (1, .., p=4):
[1] 3.241502e+02 2.127478e+02 7.387622e+01 2.921348e-14
```

```
Rotation (n x k) = (17 x 4):
                            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
```

This is a nice summary of how well PCA is doing

```
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
```

```
attributes(pca)
```

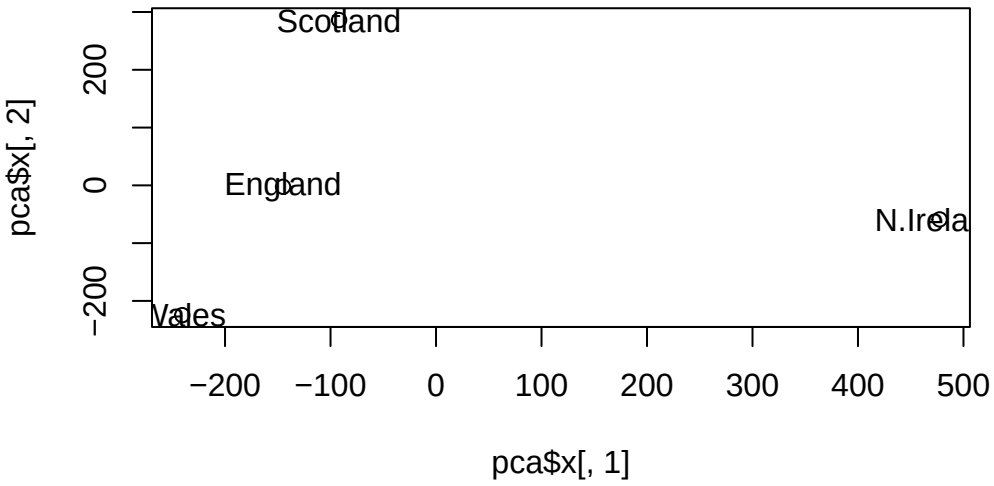
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

To make our new PCA plot (PCA score plot) we access 'pca$x'

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

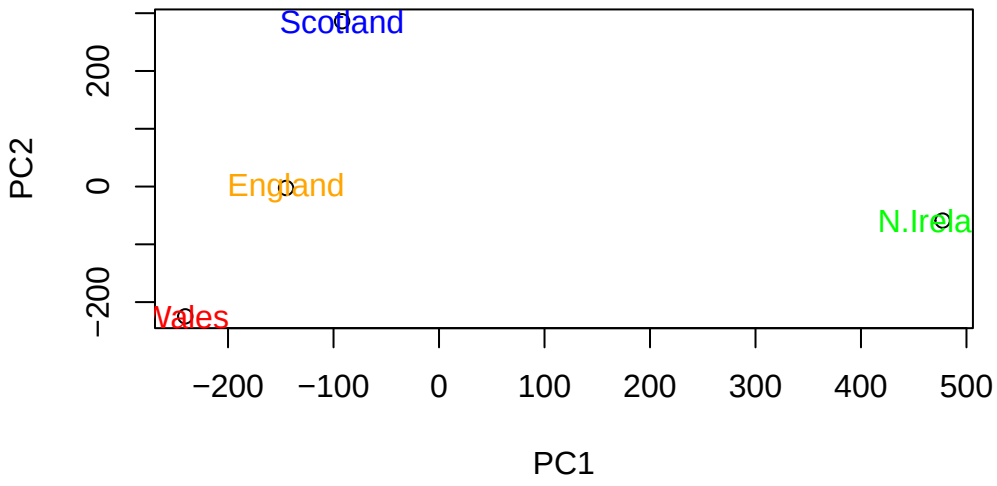
```
plot(pca$x[,1], pca$x[,2])
text(pca$x[,1], pca$x[,2], colnames(x))
```



Color up the plot

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.

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



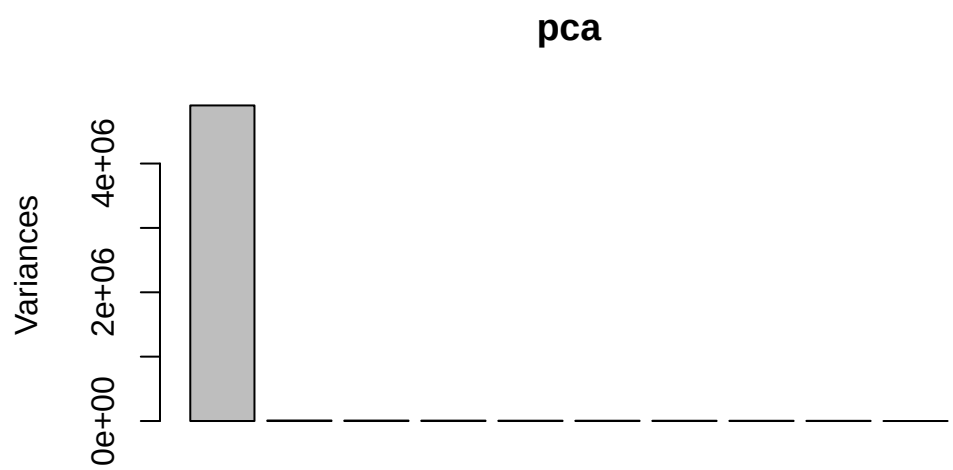
PCA of RNA-Seq data

Read input data from website

```
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
```

```
pca <- prcomp(t(rna.data))
plot(pca)
```

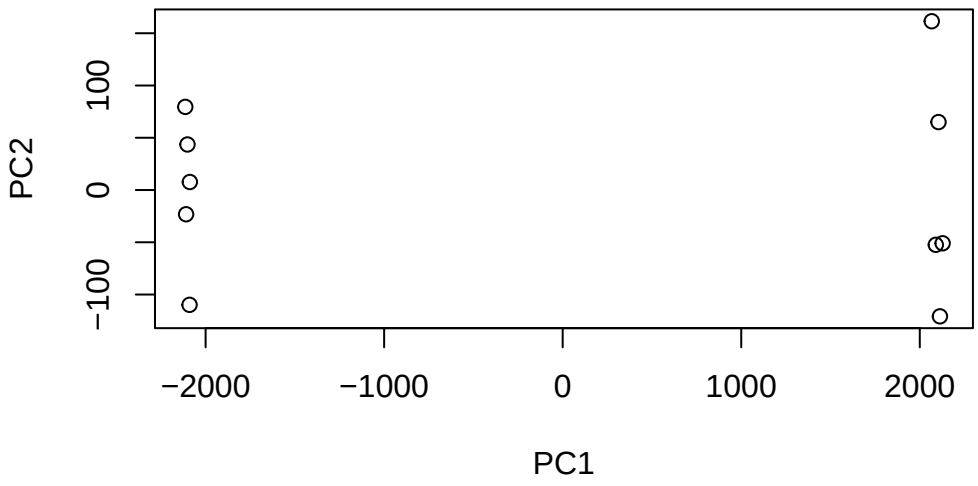



```
pca <-prcomp(t(rna.data))
summary(pca)
```

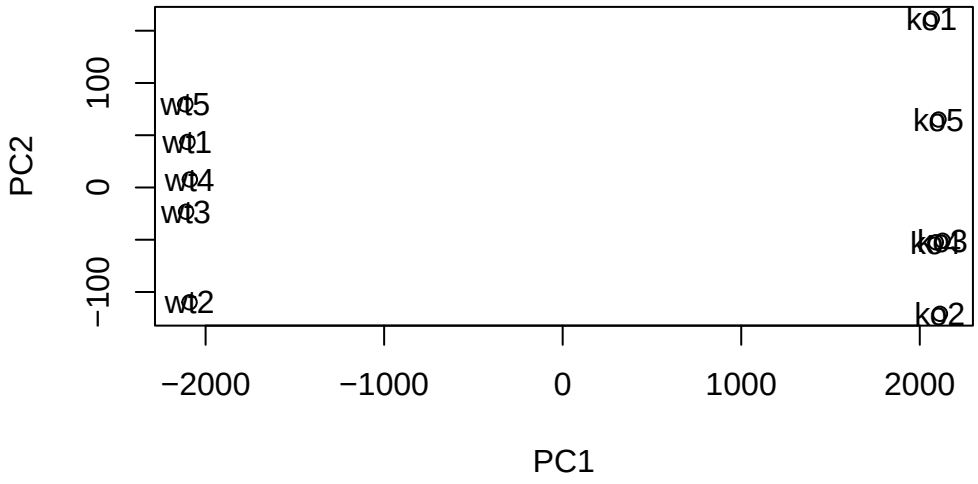
```
Importance of components:
                            PC1      PC2      PC3      PC4      PC5      PC6
Standard deviation     2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
Proportion of Variance    0.9917  0.0016  0.00144  0.00122  0.00098  0.00093
Cumulative Proportion     0.9917  0.9933  0.99471  0.99593  0.99691  0.99784
                           PC7      PC8      PC9      PC10
Standard deviation     65.29428 59.90981 53.20803 2.662e-13
Proportion of Variance  0.00086  0.00073  0.00057 0.000e+00
Cumulative Proportion   0.99870  0.99943  1.00000 1.000e+00
```

Do our PCA plot of this RNA-Seq data

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



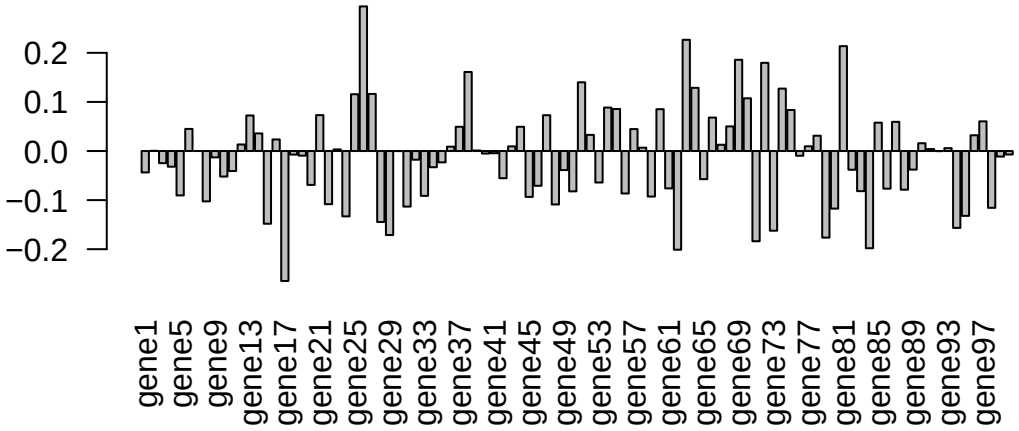

```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
text(pca$x[,1], pca$x[,2], colnames(rna.data))
```



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

It mainly tells us about the genes that are present, rather than the food group for PC2.

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



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

There are 19 genes and samples in this data set.