Class 7: Machine Learning 1

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2022-10-19

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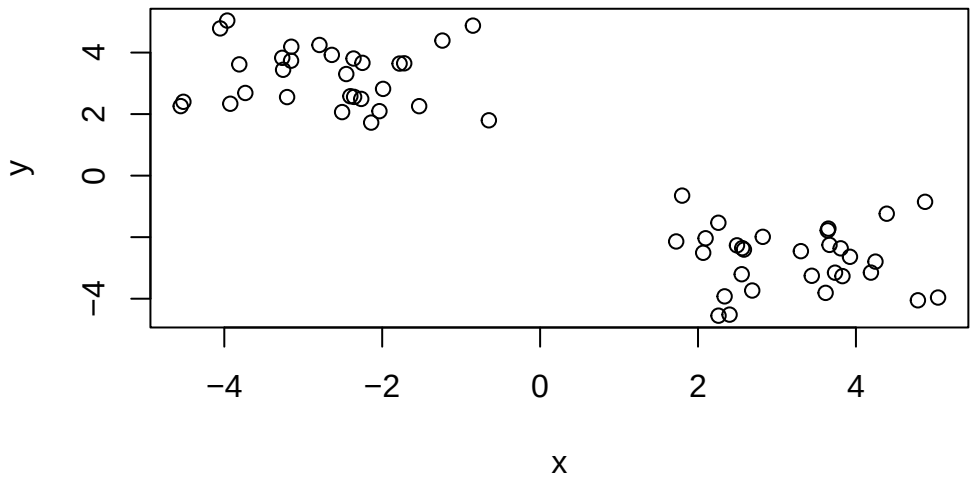
K-means clustering

K –> the number of clusters you get. You have to tell it how many clusters you want.

Let's make up some data to cluster.

```
#rnorm --> will pick numbers from a normal distribution
#you can adjust where the mean falls by adding a number in the second position
```

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




```
#rev function reverses your vector
rev(c("a", "b", "C"))
```

```
[1] "C" "b" "a"
```

The function to do k-means clustering in base R is called 'kmeans()'.

```
#for kmeans(), need to worry about x and centers (see the help page)
#x is the data you're clustering
#centers is the number of clusters you want
km <- kmeans(x, centers=4, nstart=20)
km
```

```
K-means clustering with 4 clusters of sizes 16, 16, 14, 14

Cluster means:
```

```
          x         y
1 -1.908435  2.983088
2  2.983088 -1.908435
3  3.503167 -3.572646
4 -3.572646  3.503167

Clustering vector:
 [1] 1 1 1 4 1 4 1 4 1 4 1 1 4 1 4 4 4 1 1 1 1 4 1 4 1 4 1 4 4 4 3 3 3 2 3 2 3 2
[39] 3 2 2 2 2 3 3 3 2 3 2 2 3 2 3 2 3 2 3 2 2 2

Within cluster sum of squares by cluster:
[1] 18.41869 18.41869 15.68063 15.68063
 (between_SS / total_SS =  94.1 %)

Available components:

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

What "component" of your result object details:

- cluster size? –> "size"

```
#size will tell you how many points in each cluster
km$size
```

```
[1] 16 16 14 14
```

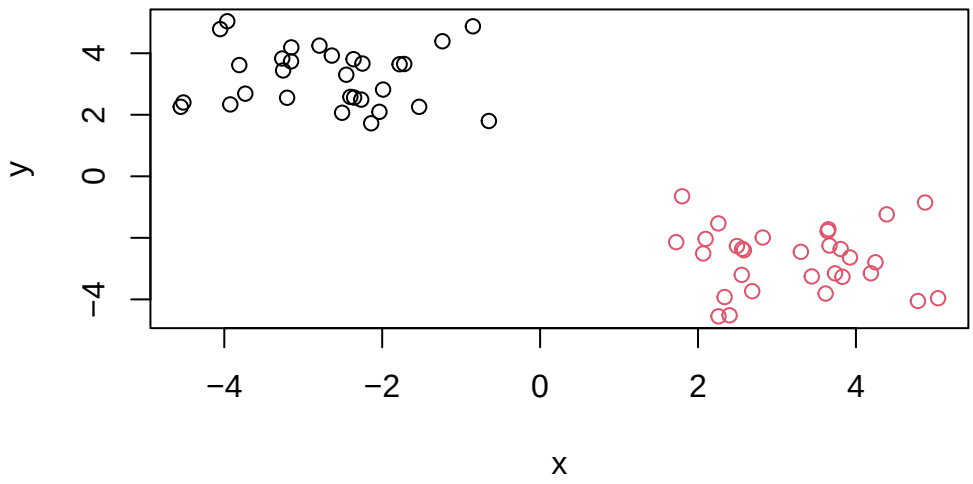
- cluster assignment/membership? –> "cluster"

```
km$cluster
```

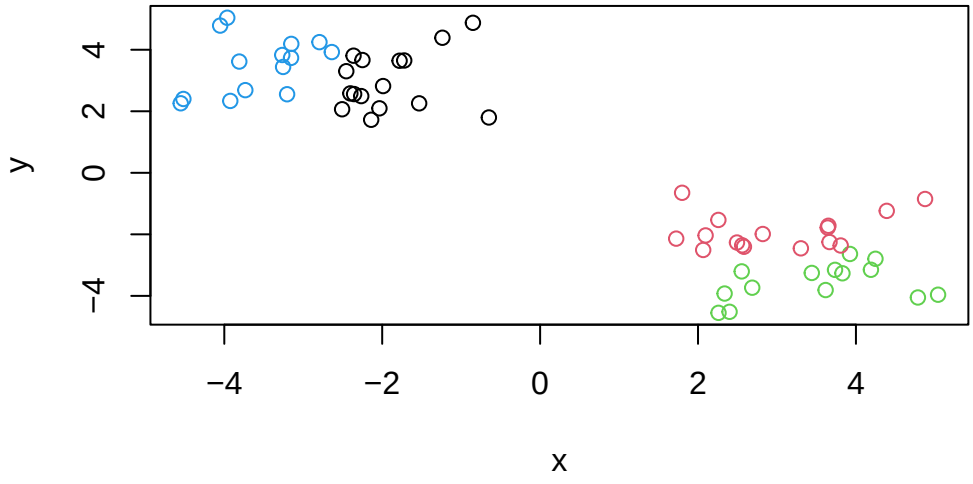
```
 [1] 1 1 1 4 1 4 1 4 1 4 1 1 4 1 4 4 4 1 1 1 1 4 1 4 1 4 1 4 4 4 3 3 3 2 3 2 3 2
[39] 3 2 2 2 2 3 3 3 2 3 2 2 3 2 3 2 3 2 3 2 2 2
```

Q. Plot x colored by the kmeans cluster assignment and add cluster centers as blue points?

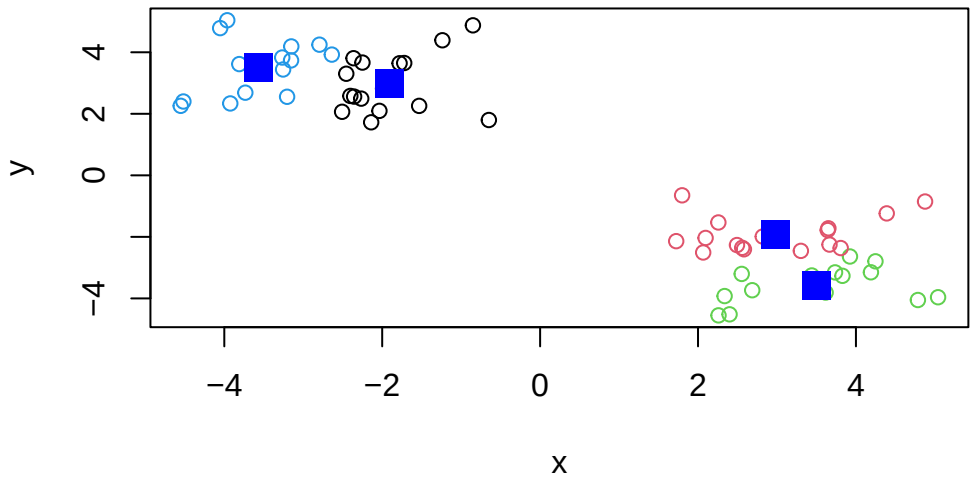
```
plot(x, col=c(rep(1,30), rep(2,30)))
```




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



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




```
km$centers
```

```
          x         y
1 -1.908435  2.983088
2  2.983088 -1.908435
3  3.503167 -3.572646
4 -3.572646  3.503167
```

#Hierarchical Clustering

The 'hclust()' function performs hierarchical clustering. The big advantage here is that I don't need to tell it "k", the number of clusters…

To run 'hclust()' I need to provide a distance matrix as input (not the original data).

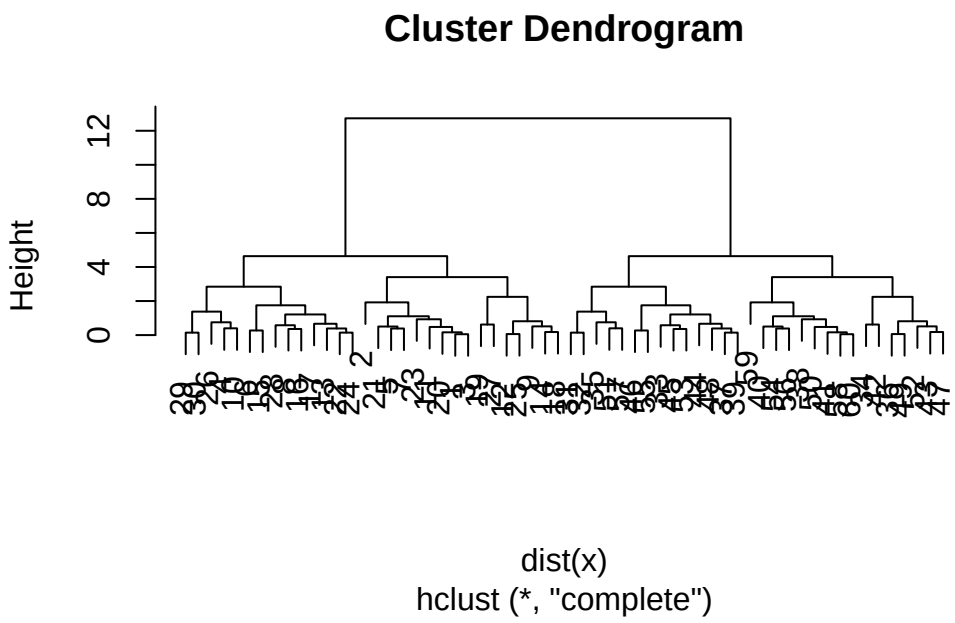
For kmean(), it assumes Euclidean distance

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

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

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

```
plot(hc)
```




```
#looking for where the biggest jump is
```

To get my 'main" result (cluster membership), I want to "cut" this tree to yield "branches" whose leaves are the members of the cluster.

```
#h= the height you want to cut the tree at
cutree(hc, h=8)
```

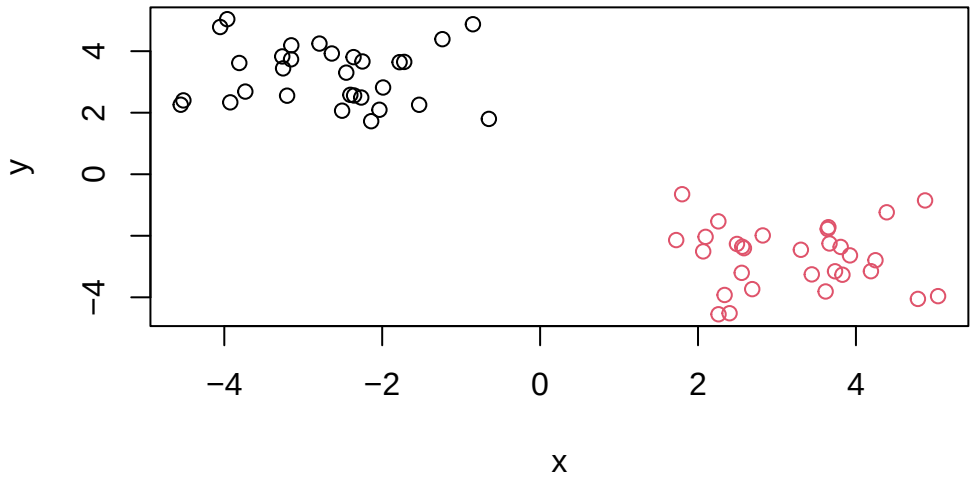
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

More often we will use 'cutree()' with k=2 for example

```
#can also do, give me cut that will give me # clusters
grps <-cutree(hc, k=2)
```

Make a plot of our 'hclust()' results i.e. our data colored by cluster assignment

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



Principal component analysis (PCA)

Read data for UK food trends from online

```
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
```

Q1. How many rows and columns?

```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

```
[1] 5
```

```
dim(x)
```

```
[1] 17  5
```

```
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
```

We are getting 5 columns–> we want the column with the foods to be our index

```
# Note how the minus indexing works
rownames(x) <- x[,1] #makes the first column the row titles
head(x)
```

```
                          X England Wales Scotland N.Ireland
Cheese                Cheese     105   103      103        66
Carcass_meat    Carcass_meat     245   227      242       267
Other_meat        Other_meat     685   803      750       586
Fish                    Fish     147   160      122        93
Fats_and_oils  Fats_and_oils     193   235      184       209
Sugars                Sugars     156   175      147       139
```

```
#need to get rid of the "X" column which is now duplicated
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
```

```
dim(x)
```

```
[1] 17  4
```

Explore the data-- basically plot, plot, and plot again

```
#another way to set the correct row names
x<- read.csv(url, row.names=1)
head(x)
```

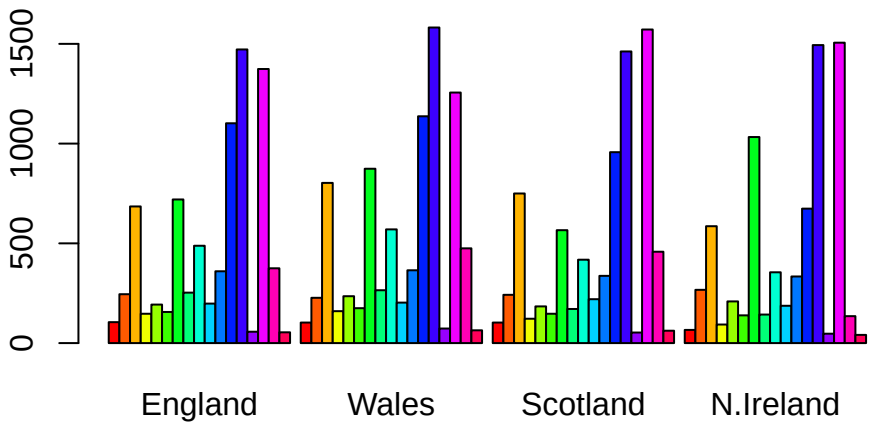
```
              England Wales Scotland N.Ireland
Cheese            105   103      103        66
Carcass_meat      245   227      242       267
Other_meat        685   803      750       586
```

```
Fish               147    160       122        93
Fats_and_oils      193    235       184       209
Sugars             156    175       147       139
```

Q2. Which approach to solving the "row-names problem" do you prefer and why?

I prefer the second approach using "row.names=1". This way you don't have to worry about your matrix changing if you accidentally run your code again.

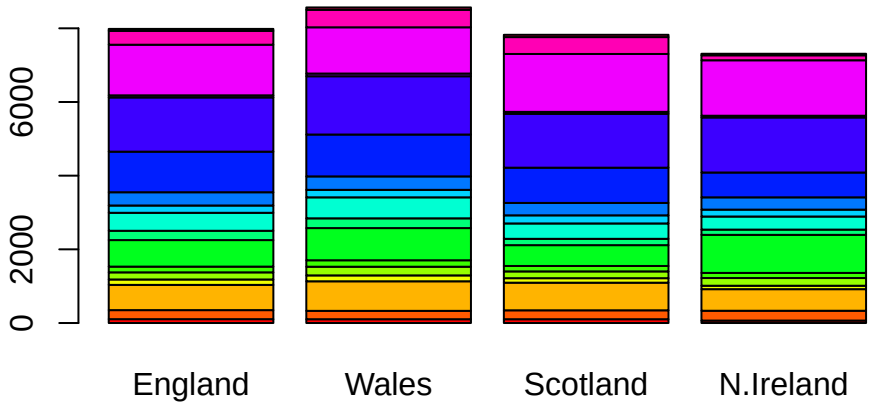
```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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

Setting beside to False

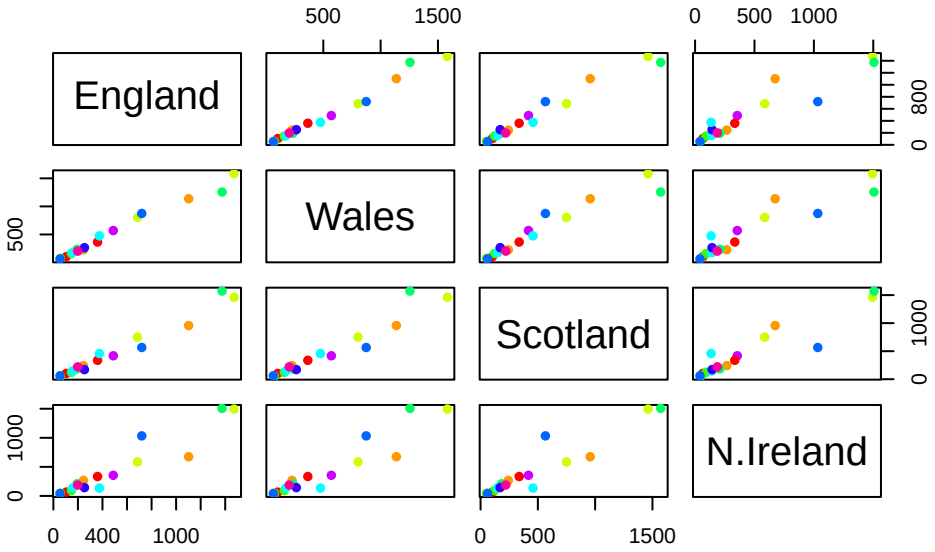
```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



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?

If a point lies on the diagonal, then that food has the same frequency in both countries displayed.

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



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

#PCA to the rescue!

The main function in base R to do PCA is called 'prcomp()'.

One annoying thing about prcomp() function is that it expects the transpose of our data as input. –> in this case, it wants the foods to be columns, and the countries to be rows

```
t(x)
```

```
           Cheese Carcass_meat  Other_meat  Fish Fats_and_oils  Sugars
England       105           245         685  147            193    156
Wales         103           227         803  160            235    175
Scotland      103           242         750  122            184    147
N.Ireland      66           267         586   93            209    139
           Fresh_potatoes  Fresh_Veg  Other_Veg  Processed_potatoes
England               720        253        488                 198
Wales                 874        265        570                 203
Scotland              566        171        418                 220
N.Ireland            1033        143        355                 187
```

```
          Processed_Veg  Fresh_fruit  Cereals  Beverages Soft_drinks
England             360         1102     1472         57         1374
Wales               365         1137     1582         73         1256
Scotland            337          957     1462         53         1572
N.Ireland           334          674     1494         47         1506
          Alcoholic_drinks  Confectionery
England                375             54
Wales                  475             64
Scotland               458             62
N.Ireland              135             41
```

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

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 4.189e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
#most important bit is the variance
```

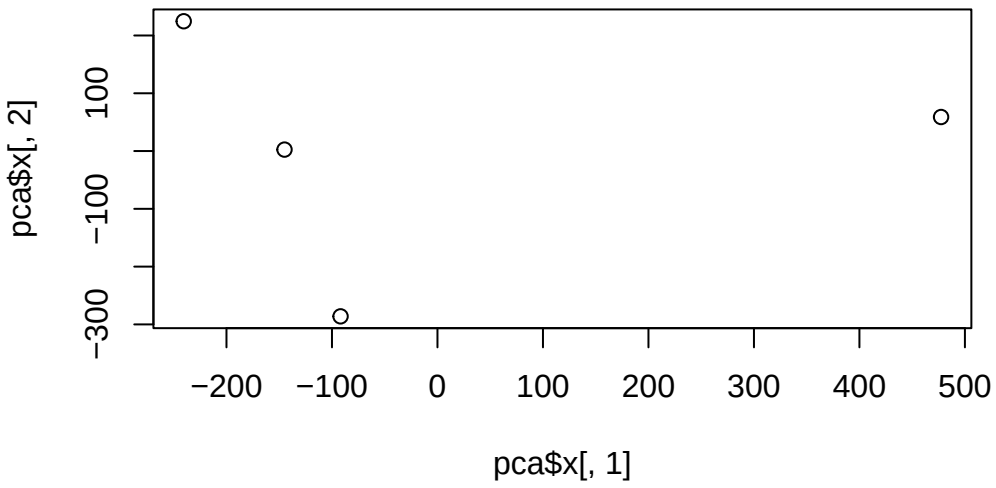
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points

The object returned by 'prcomp()' has our results that include a $x component. This is our "scores" along the PCs (i.e. the plot of our data along the new PC axis).

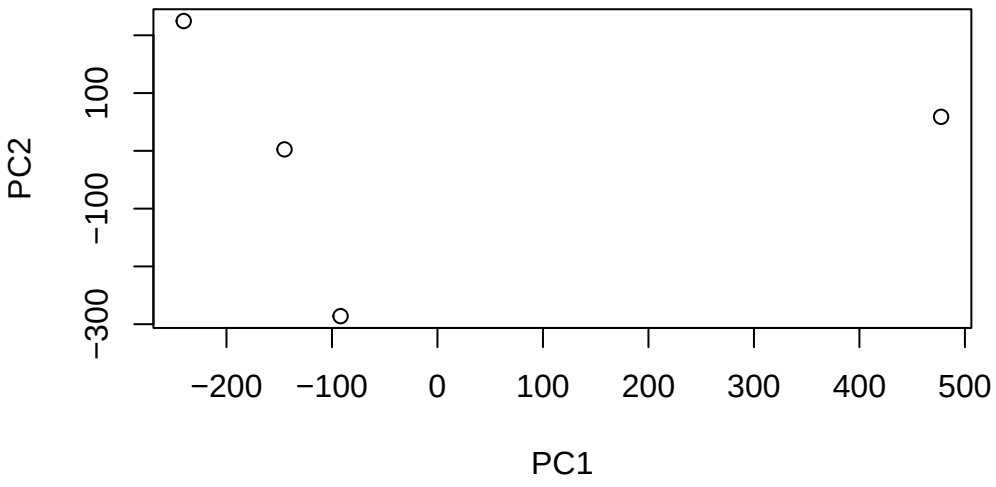
```
pca$x
```

```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  2.842865e-14
Wales     -240.52915  224.646925   56.475555  7.804382e-13
Scotland   -91.86934 -286.081786   44.415495 -9.614462e-13
N.Ireland  477.39164   58.901862    4.877895  1.448078e-13
```

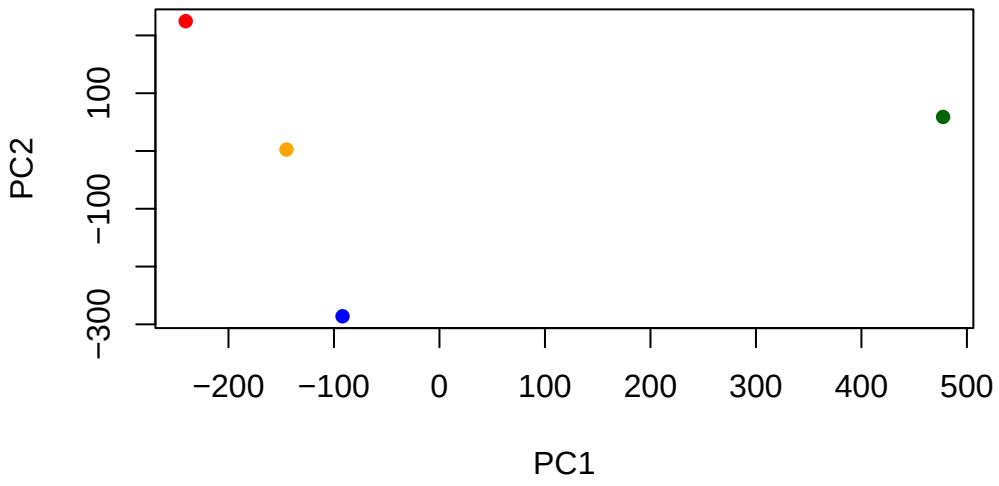
```
plot(pca$x[,1], pca$x[,2])
```



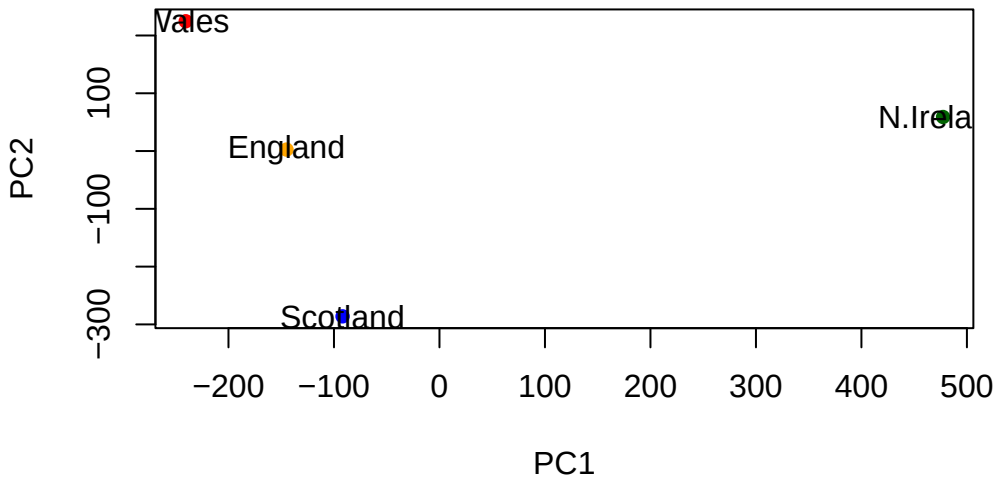

```
plot(pca$x[,1], pca$x[,2],
     xlab="PC1", ylab="PC2")
```



```
plot(pca$x[,1], pca$x[,2],
     xlab="PC1", ylab="PC2",
     col=c("orange", "red", "blue", "darkgreen"),
           pch=16)
```

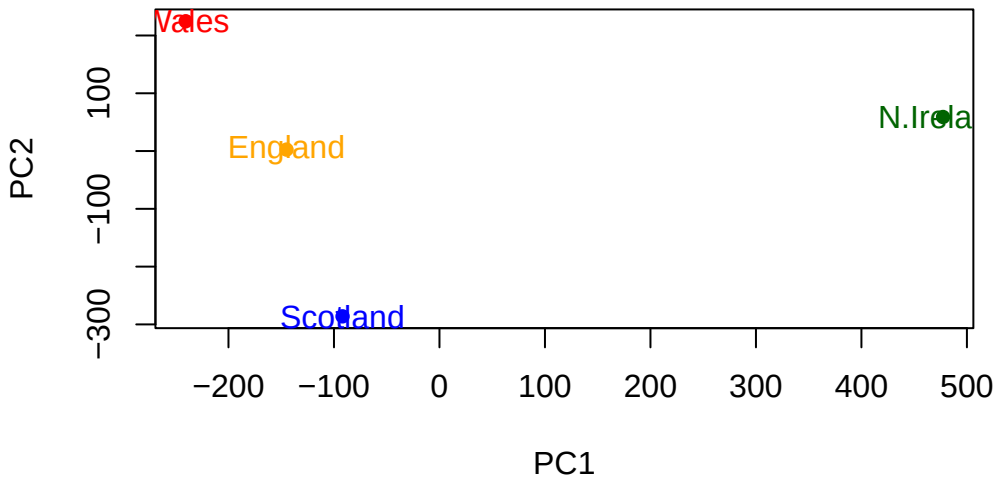



```
plot(pca$x[,1], pca$x[,2],
     xlab="PC1", ylab="PC2",
     col=c("orange", "red", "blue", "darkgreen"),
           pch=16)
text(pca$x[,1], pca$x[,2], colnames(x))
```



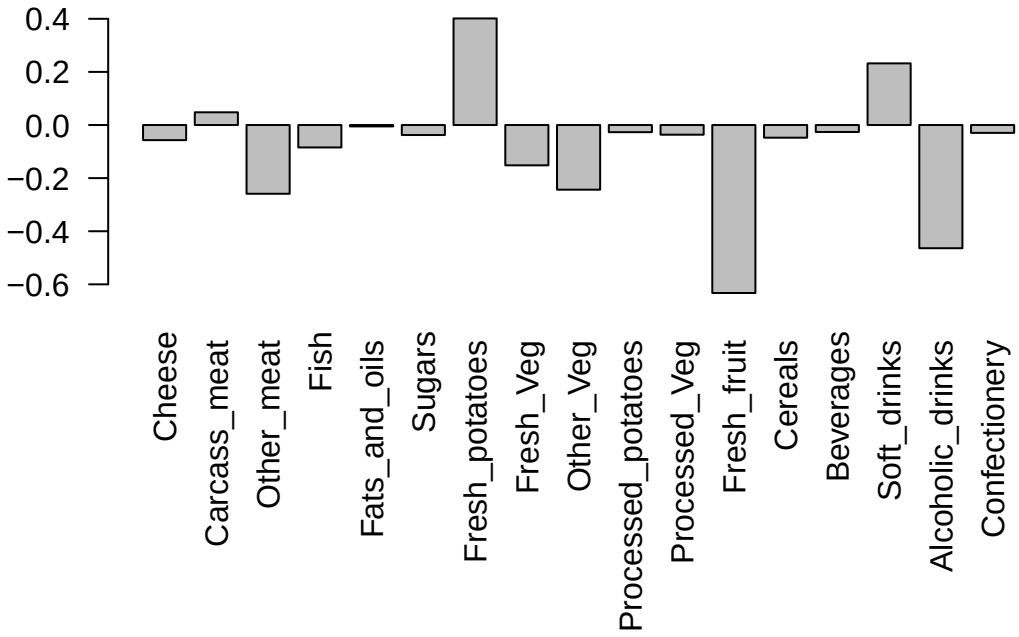
Q8. Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

```
plot(pca$x[,1], pca$x[,2],
     xlab="PC1", ylab="PC2",
     col=c("orange", "red", "blue", "darkgreen"),
           pch=16)
text(pca$x[,1], pca$x[,2], colnames(x), col=c("orange", "red", "blue", "darkgreen"))
```



Digging Deeper: Variable Loadings

```
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```


0.4
0.2
0.0
−0.2
−0.4
−0.6
Cheese
Carcass_meat
Other_meat
Fish
Fats_and_oils
Sugars
Fresh_potatoes
Fresh_Veg
Other_Veg
Processed_potatoes
Processed_Veg
Fresh_fruit
Cereals
Beverages
Soft_drinks
Alcoholic_drinks
Confectionery