class07

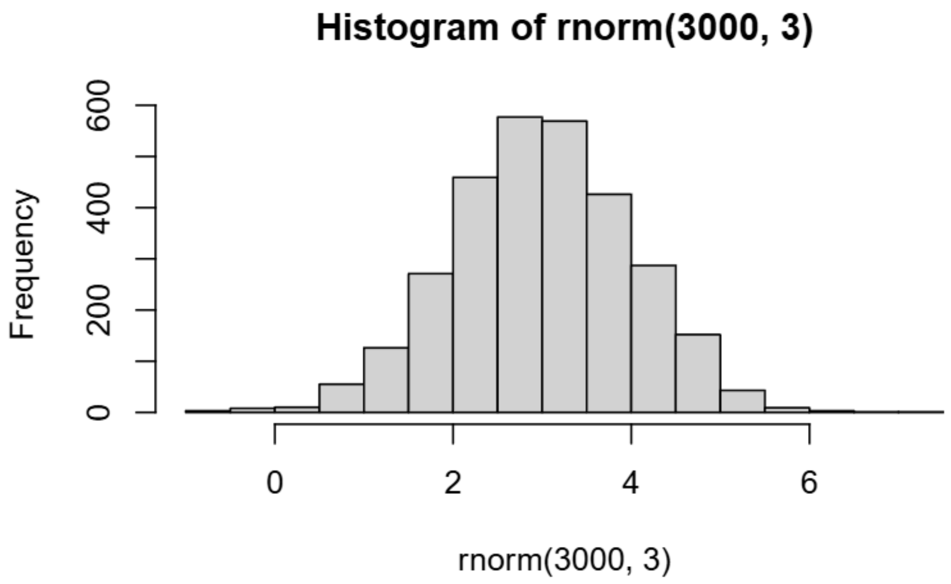
Mason Lew (PID: A17533139)

Today we will explore unsupervised machine learning methods including clustering and dimensional reduction methods.

Let's start by making up some data (where we know there are clear groups/clusters) that we can use to test out different clustering methods

we can use the `rnorm()` function to help us here:

```r
hist(rnorm(3000, 3))
```

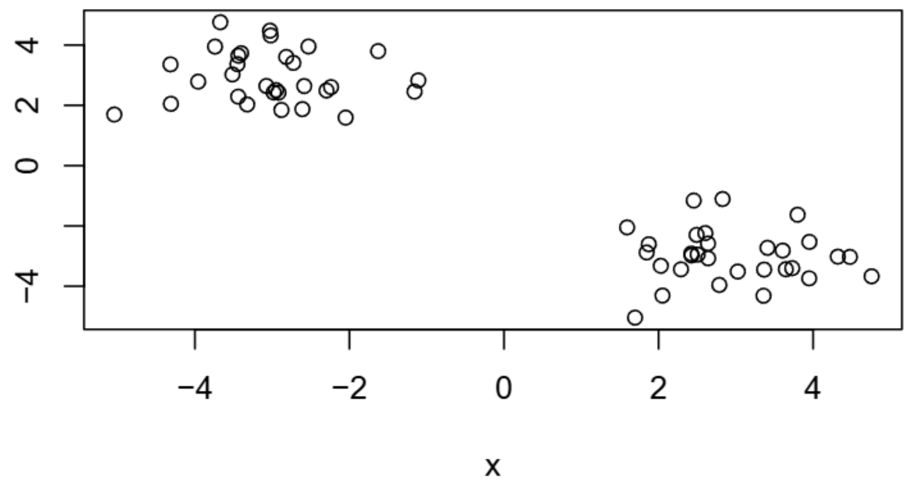


Make data with two "clusters"

```
x <- c(rnorm(30, -3),
       rnorm(30, 3))

z <- cbind(x, rev(x))
head(z)
```

```
             x
[1,] -2.608804 1.873155
[2,] -4.316237 3.358419
[3,] -3.075171 2.642164
[4,] -1.628504 3.798793
[5,] -2.297184 2.492298
[6,] -3.019553 4.319745
```

```
plot(z)
```



How big is z?

```
nrow(z)
```

```
[1] 60
```

```r
ncol(z)
```

```
[1] 2
```

K-means clustering

The main function in “base” R for K-means clustering is called `kmeans()`

```r
k <- kmeans(z, 2)
k
```

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

Cluster means:
          x
1 -3.007059  2.952554
2  2.952554 -3.007059

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] 43.88827 43.88827
 (between_SS / total_SS =  92.4 %)

Available components:

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

```r
attributes(k)
```

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

$class
[1] "kmeans"
```

> Q. How many points lie in each cluster?

```r
k$size
```

```
[1] 30 30
```

> Q. What component of our results tells us about the cluster membership (i.e. which point lie 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. Center of each cluster?

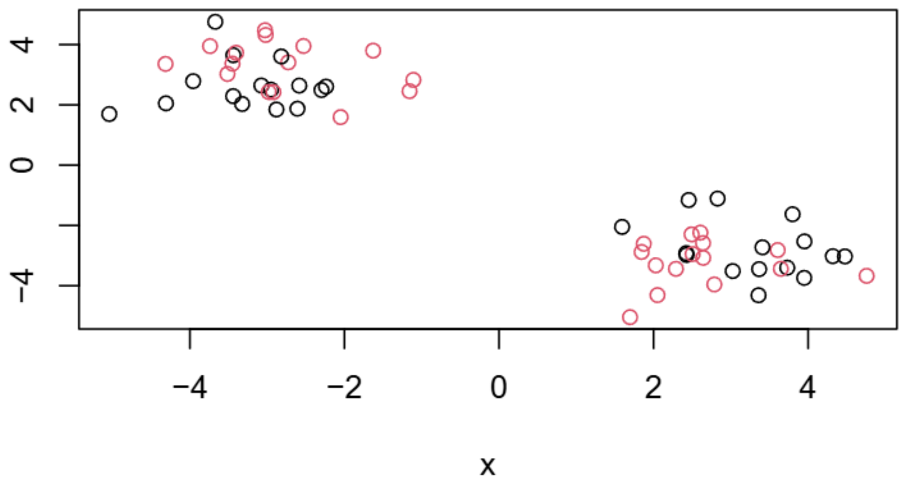
```r
k$centers
```

```
          x
1 -3.007059  2.952554
2  2.952554 -3.007059
```

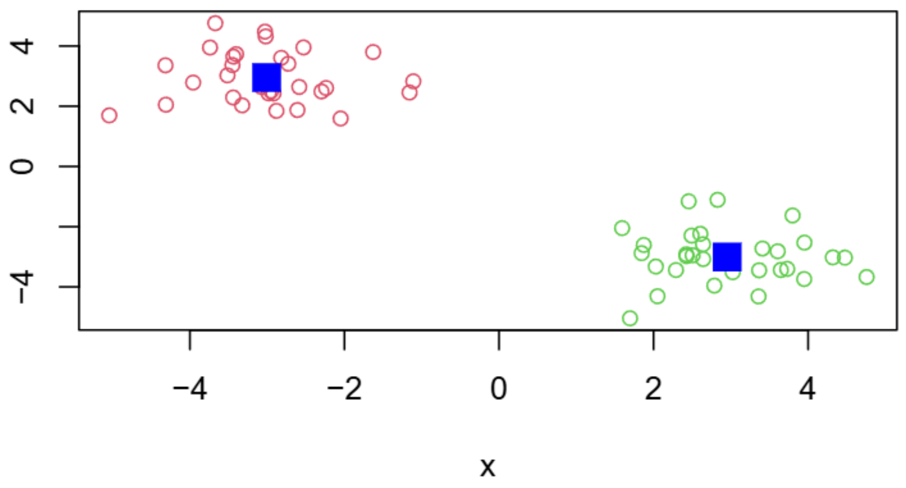
> Q. Put this reult info together and make a little "base R" plot of our clustering reult. Also add the cluster center points to this plot.

You can color by number.

```r
plot(z, col=c(1,2))
```

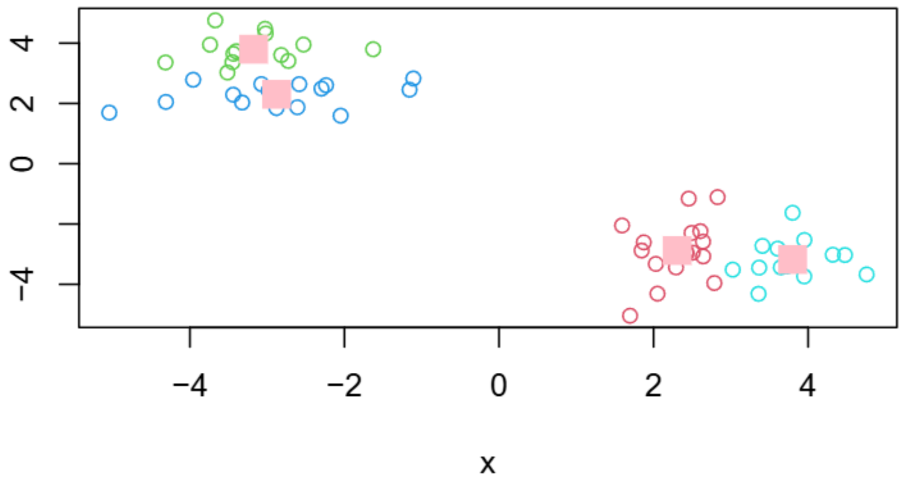


```
plot(z, col = k$cluster + 1)
points(k$centers, col = "blue", pch = 15, cex = 2)
```



Q. Run Kmeans on our input **z** and define 4 clusters making the same result visualization as above (plot of z collored by cluster membership)

```r
p <- kmeans(z, 4)

plot(z, col = p$cluster + 1)
points(p$centers, col = "pink", pch = 15, cex = 2)
```



How to tell if the k is good:

```r
p$tot.withinss
```

```
[1] 53.55179
```

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

```
[1] 87.77654
```

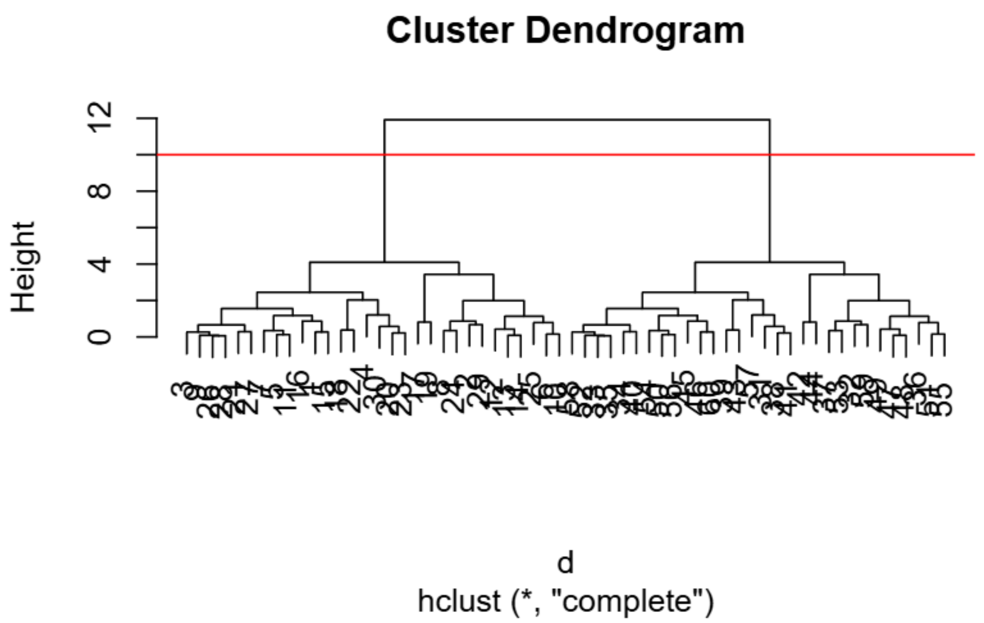
Hierarchical Clustering

The main function in base R for this called `hclust()` it will take as input a distance matrix (key point is that you can't just give your "raw" data as input - you have to first calculate a distance matrix from your data).

```r
d <- dist(z)
hc <- hclust(d)
hc
```

```

Call:
hclust(d = d)

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

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

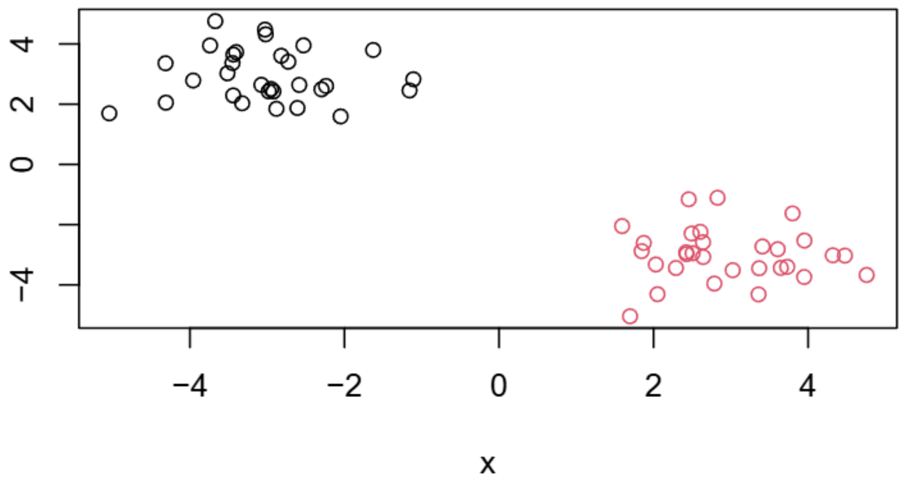


Once I inspect the "tree" I can "cut" the tree to yield my groupings or clusters. The function to do this is called `cutree()`

```r
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
```

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



Hands on with Principal Component Analysis (PCA)

Lets do a 17 dimensional data analysis of EU eating habits

Data import

```r
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
head(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
```

> 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
nrow(x)
```

```
[1] 17
```

```r
ncol(x)
```

```
[1] 4
```

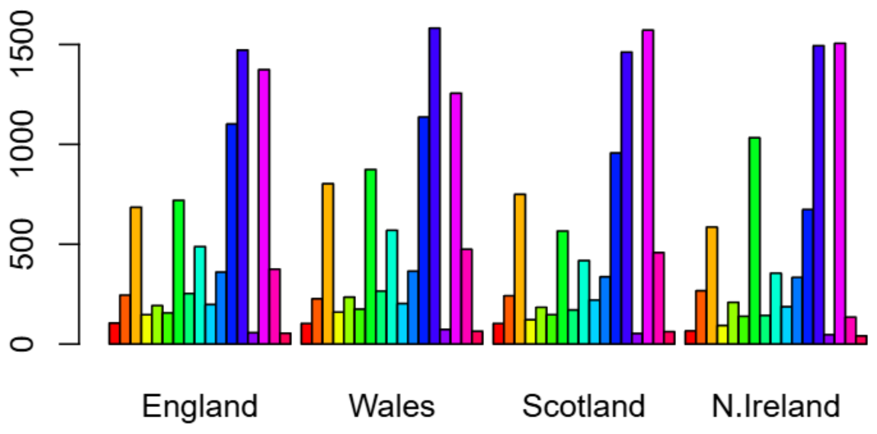
```r
dim(x)
```

```
[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?

The `row.names=1` argument setting is my preferred method of solving this issue. I would say this method is much more robust that using `x[-1]` every time I need to skip the first row.

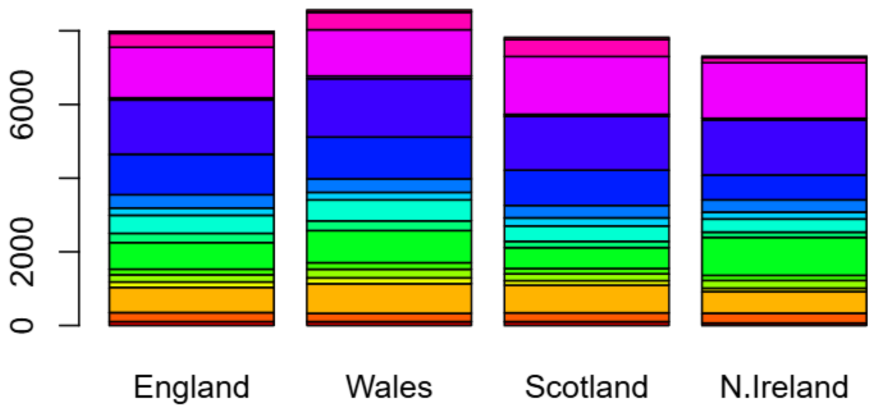
```r
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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

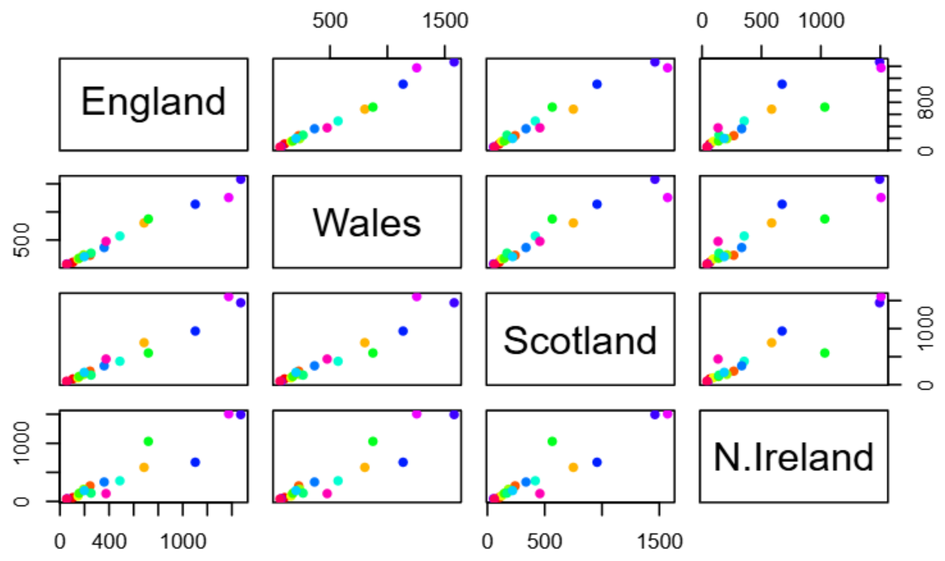
The `beside = F` argument stacks the bars within each country ontop of each other.

```r
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?

```
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?

North Ireland seems to consume less fish and more

Looking at these types of "pairwise plots" can be helpful but does not scale well and sucks!There must be a better way...

PCA to the Rescue!

The main function for PCA in base R is called `prcomp()`. This function wants the transpose of our input data - i.e. the important food categories in columns and the countries as rows.

```r
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
```

Lets see what is in our PCA result object `pca`

```r
attributes(pca)
```

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

$class
[1] "prcomp"
```

The `pca$x` result object is where we will focus first as this details how the countries are related to each other in terms of our new "axis" (a.k.a. "PCs", "eigenvectors", etc.)

```r
head(pca$x)
```

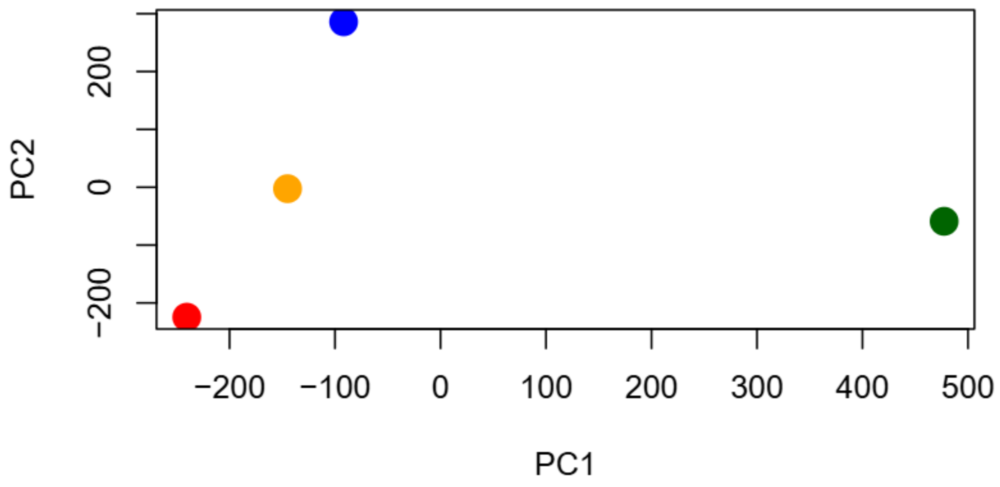
```
                 PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -4.894696e-14
Wales     -240.52915 -224.646925 -56.475555  5.700024e-13
Scotland   -91.86934  286.081786 -44.415495 -7.460785e-13
N.Ireland  477.39164  -58.901862  -4.877895  2.321303e-13
```

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(pca$x[,1], pca$x[,2], pch = 1, cex = 2,
     xlab = "PC1", ylab = "PC2", text(pca$x[,1], pca$x[,2], rownames(pca$x), col = "green"),
     dev.new(height = 500, units = 'cm'))
```

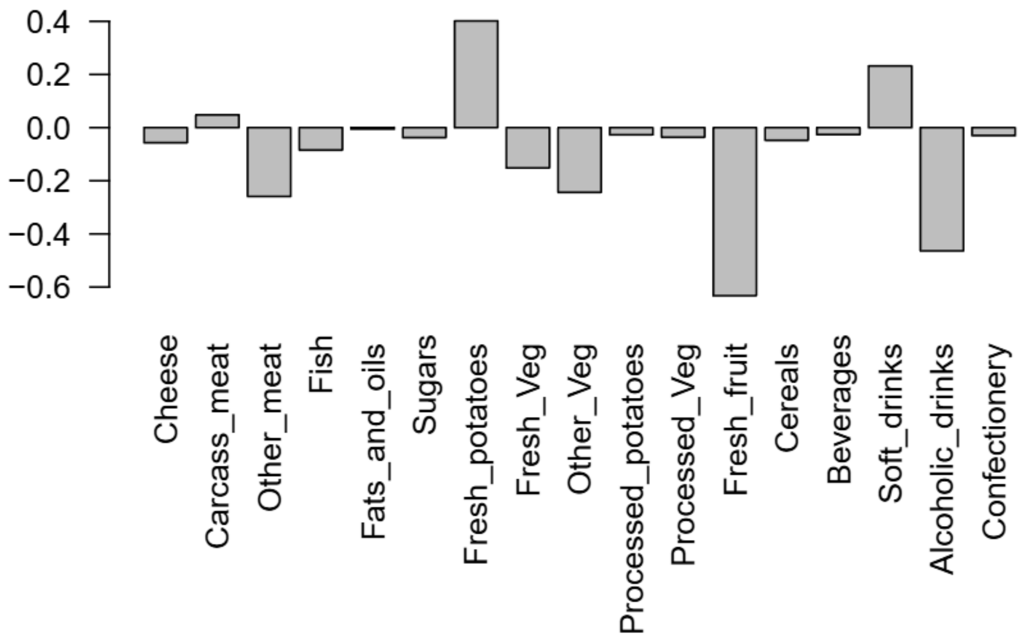
Q8. Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

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



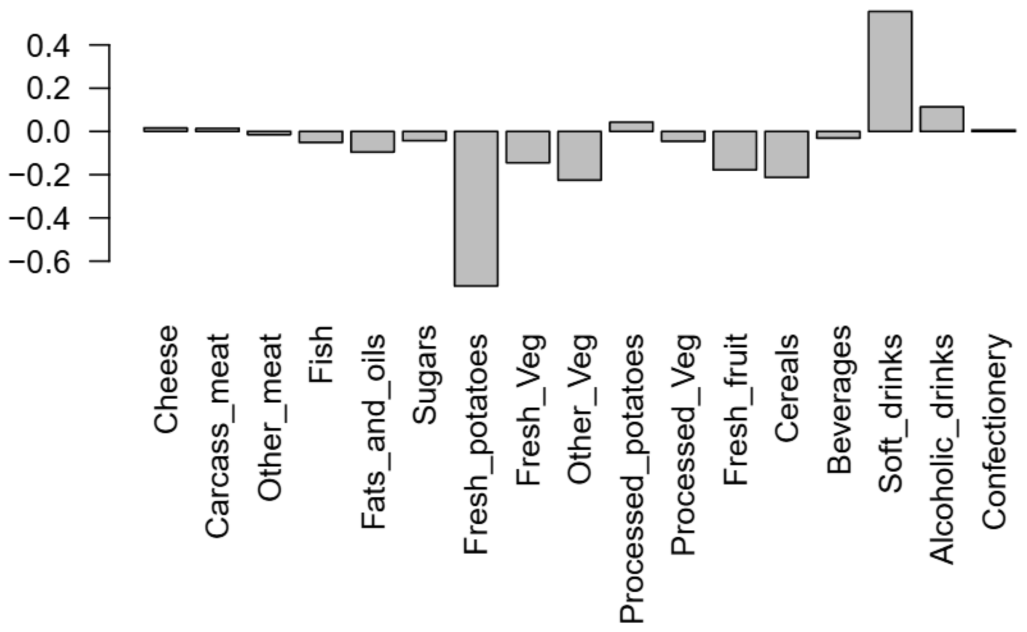
We can look at the so-called PC "loadings" result object to see how the original foods contribute to our new PCs (i.e. how the original variables contribute to our new better variables).

```
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 prominantely and what does PC2 maninly tell us about?

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



The two food groups that are the most prominently featured are, Fresh_potatoes, and Alcoholic drinks. PC2 is the second principal component which is a measure of directional variance in a perpendicular direction to PC1.

PCA of RNA-seq Data

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

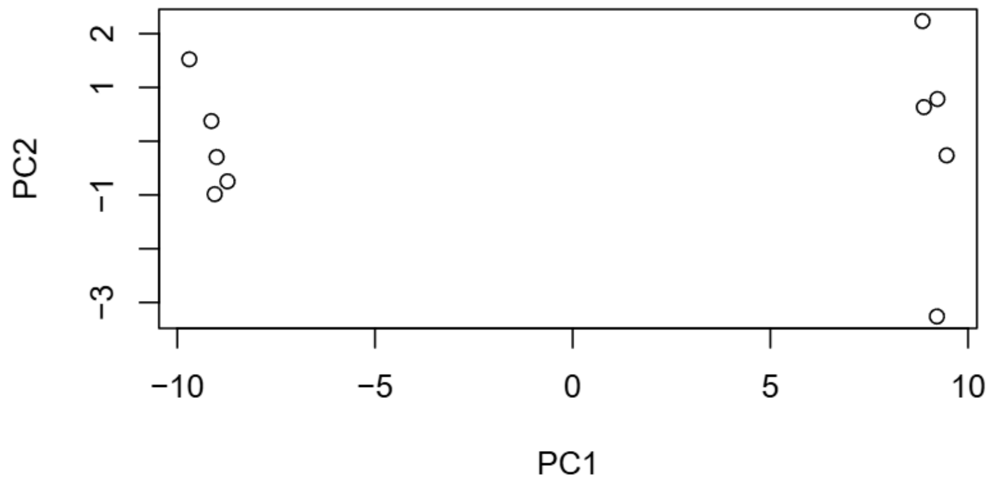
```
       wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
gene1  439 458  408  429 420  90  88  86  90  93
gene2  219 200  204  210 187 427 423 434 433 426
gene3 1006 989 1030 1017 973 252 237 238 226 210
gene4  783 792  829  856 760 849 856 835 885 894
gene5  181 249  204  244 225 277 305 272 270 279
gene6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

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

```
nrow(rna.data)
```

```
[1] 100
```

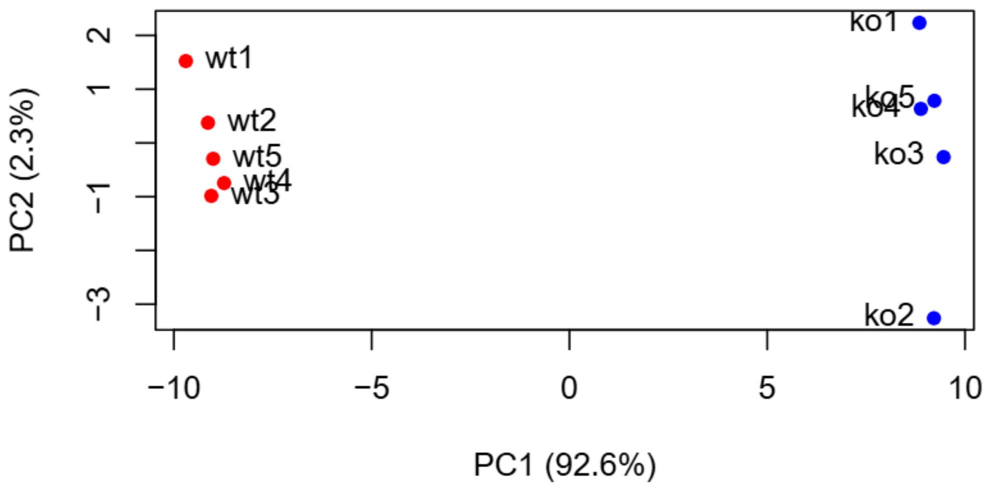
```
## Again we have to take the transpose of our data
pca <- prcomp(t(rna.data), scale=TRUE)

## Simple un polished plot of pc1 and pc2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
```



```
## Variance captured per PC
pca.var <- pca$sdev^2

## Percent variance is often more informative to look at
pca.var.per <- round(pca.var/sum(pca.var)*100, 1)
pca.var.per
```

```
 [1] 92.6  2.3  1.1  1.1  0.8  0.7  0.6  0.4  0.4  0.0
```

```r
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
colvec[grep("ko", colvec)] <- "blue"

plot(pca$x[,1], pca$x[,2], col=colvec, pch=16,
     xlab=paste0("PC1 (", pca.var.per[1], "%)"),
     ylab=paste0("PC2 (", pca.var.per[2], "%)"))

text(pca$x[,1], pca$x[,2], labels = colnames(rna.data), pos=c(rep(4,5), rep(2,5)))
```


wt1
wt2
wt5
wt4
wt3
ko1
ko5
ko4
ko3
ko2
PC2 (2.3%)
PC1 (92.6%)