Class 7: Machine learning 2

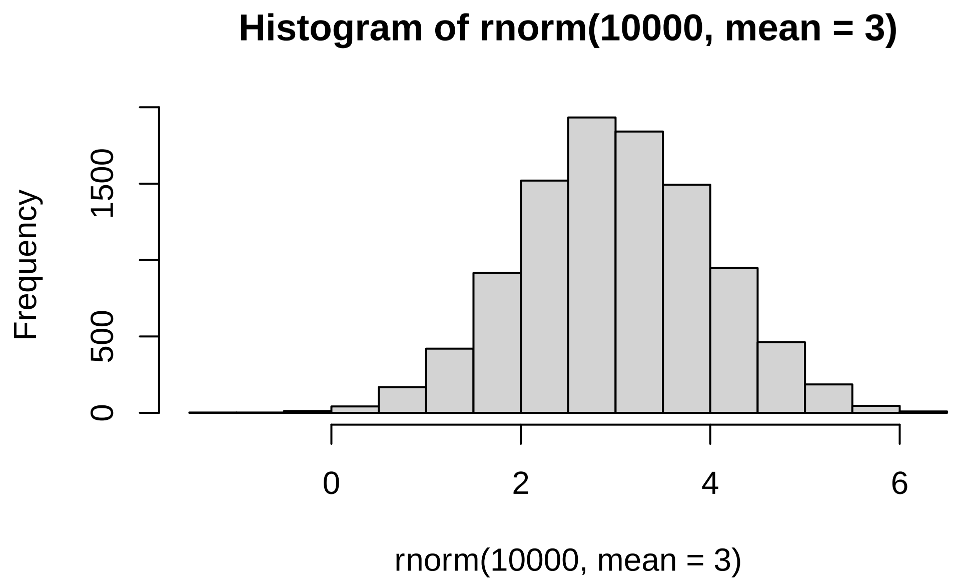
Assael Madrigal (PID: A10179083)

#Clustering k-means clusterine is very prevalent. k means that we need to tell a k - how many groups I want, later we can tell it what it should be after analysing the output but we have to start with something.

To get started let's make some data, lets see how rnorm works by plotting a histogram

```
#rnorm generates as many random numbers as I ask drawn from a normal distribution

hist(rnorm(10000, mean=3))
```



```
#so the mean is where the middle of the histogram is going to be
```

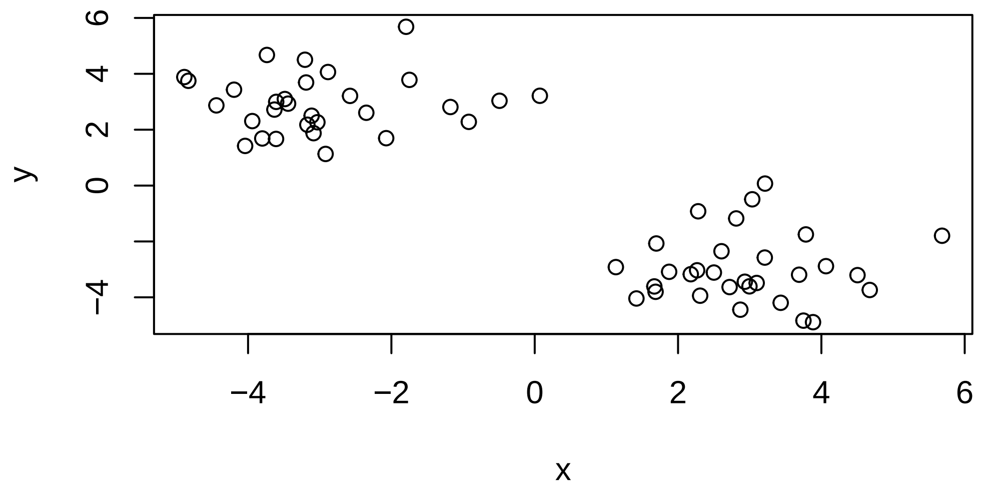
here we are going to make 2 groupings one centered around 3 and the other at -30

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

```
                x           y
 [1,]  3.88368344 -4.88962659
 [2,]  4.50401670 -3.20608635
 [3,]  2.17771563 -3.17241391
 [4,]  2.30845033 -3.94125846
 [5,]  1.87568713 -3.08629966
 [6,]  3.09716803 -3.48682628
 [7,]  1.66885452 -3.60948746
 [8,]  3.74973276 -4.83342587
 [9,]  1.13218560 -2.91836322
[10,]  2.26618438 -3.03263986
[11,]  2.71943019 -3.63285281
[12,]  1.41917840 -4.04094533
[13,]  2.99648374 -3.60736534
[14,]  2.60611441 -2.35027179
[15,]  4.06415916 -2.88471970
[16,]  2.81152556 -1.17655573
[17,]  5.68402468 -1.79511979
[18,]  1.69687925 -2.07273771
[19,]  1.68647329 -3.80172581
[20,]  4.67522726 -3.73724432
[21,]  2.28062900 -0.91999295
[22,]  2.93179458 -3.44172582
[23,]  3.78364966 -1.74836331
[24,]  3.43217575 -4.19606067
[25,]  3.21032670 -2.57716698
[26,]  3.21343697  0.07147265
[27,]  2.50009830 -3.11323793
[28,]  3.68938747 -3.19025763
[29,]  3.03551624 -0.49142900
[30,]  2.86943934 -4.44232525
[31,] -4.44232525  2.86943934
[32,] -0.49142900  3.03551624
[33,] -3.19025763  3.68938747
[34,] -3.11323793  2.50009830
[35,]  0.07147265  3.21343697
```

```
[36,] -2.57716698  3.21032670
[37,] -4.19606067  3.43217575
[38,] -1.74836331  3.78364966
[39,] -3.44172582  2.93179458
[40,] -0.91999295  2.28062900
[41,] -3.73724432  4.67522726
[42,] -3.80172581  1.68647329
[43,] -2.07273771  1.69687925
[44,] -1.79511979  5.68402468
[45,] -1.17655573  2.81152556
[46,] -2.88471970  4.06415916
[47,] -2.35027179  2.60611441
[48,] -3.60736534  2.99648374
[49,] -4.04094533  1.41917840
[50,] -3.63285281  2.71943019
[51,] -3.03263986  2.26618438
[52,] -2.91836322  1.13218560
[53,] -4.83342587  3.74973276
[54,] -3.60948746  1.66885452
[55,] -3.48682628  3.09716803
[56,] -3.08629966  1.87568713
[57,] -3.94125846  2.30845033
[58,] -3.17241391  2.17771563
[59,] -3.20608635  4.50401670
[60,] -4.88962659  3.88368344
```

```
plot(x)
```



The main function in R for K-means clustering is called `kmeans()`, kmeans(x, centers,…). The center is the number of clusters. nstart is the number of iterations kmeans will go, so one way is to keep increasing it until the answer does not change or! even better you can plot the "scree plot" and look at the elbow.

But it is still a limitation, but the advantage is that kmeans is very fast.

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

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

Cluster means:
          x         y
1 -2.977502  2.932321
2  2.932321 -2.977502

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 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] 74.34935 74.34935
 (between_SS / total_SS =  87.6 %)

Available components:

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

Q1. How many points do I need to cluster? (from k)

```
k$size
```

```
[1] 30 30
```

```
#a vector with the sizes of each cluster
```

Q2. The clustering result ie membership vector?

```
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 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
```

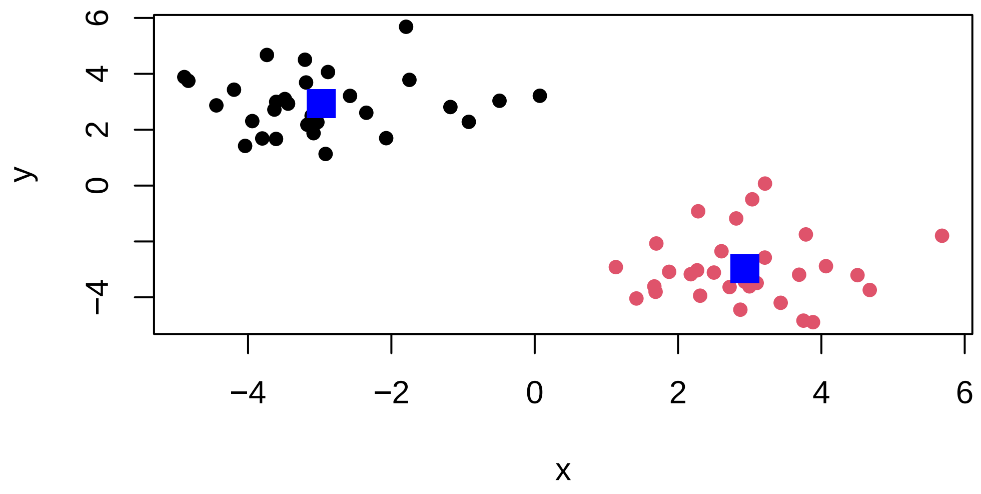
Q3. Cluster centers?

```
k$centers
```

```
          x         y
1 -2.977502  2.932321
2  2.932321 -2.977502
```

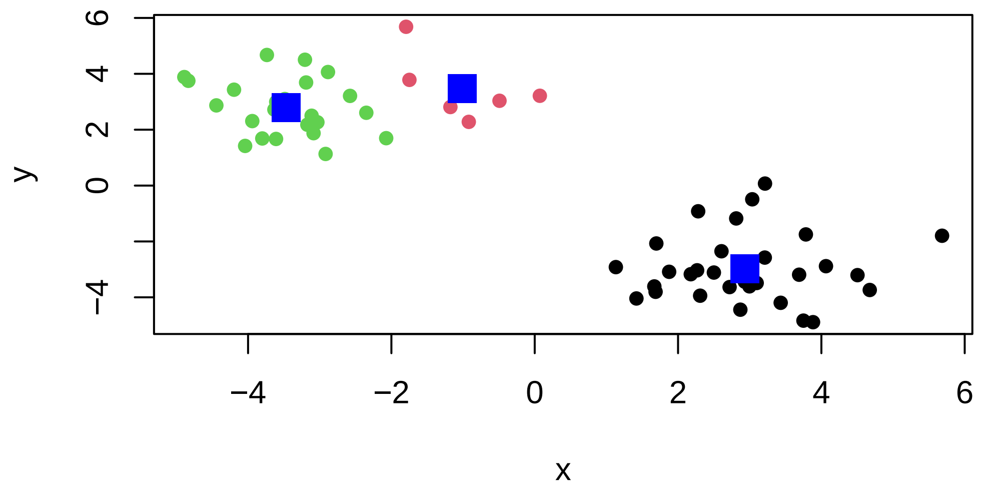
Q4. Make a plot of our data colored by clustering results with optionally the clusters centers shown

```
#col is color but if we give it an number it has a color assigned to it, so for this case
plot(x, col=k$cluster, pch=16)
points(k$centers, col="blue", pch=15, cex=2)
```



Q.5 Run kmeans again but cluster into 3 groups and plot the results

```
k3 <- kmeans(x,centers=3, nstart = 20)
plot(x, col=k3$cluster, pch=16)
points(k3$centers, col="blue", pch=15, cex=2)
```



The main problem with kmeans is that it will fit the data into the structure, so if we give it 3 clusters it will split it into 3 clusters. So on, so we have to be careful.

kmeans: - breaks observations into k-predefined number of clusters - you define the number of clusters! - help by plotting with scree plots

Heirarchical clustering

Heirarchical clustering has the advantage that it can potentially reveal structure in the data rather than imposing one as k-means will.

The main function in "base R" is `hclust()`, is follows `hclust(d, method = "complete", members = NULL)` where 'd' was produced by `dist()` or any measure of dissimilarity.

It requires a distance matrix as input, not the raw data itself

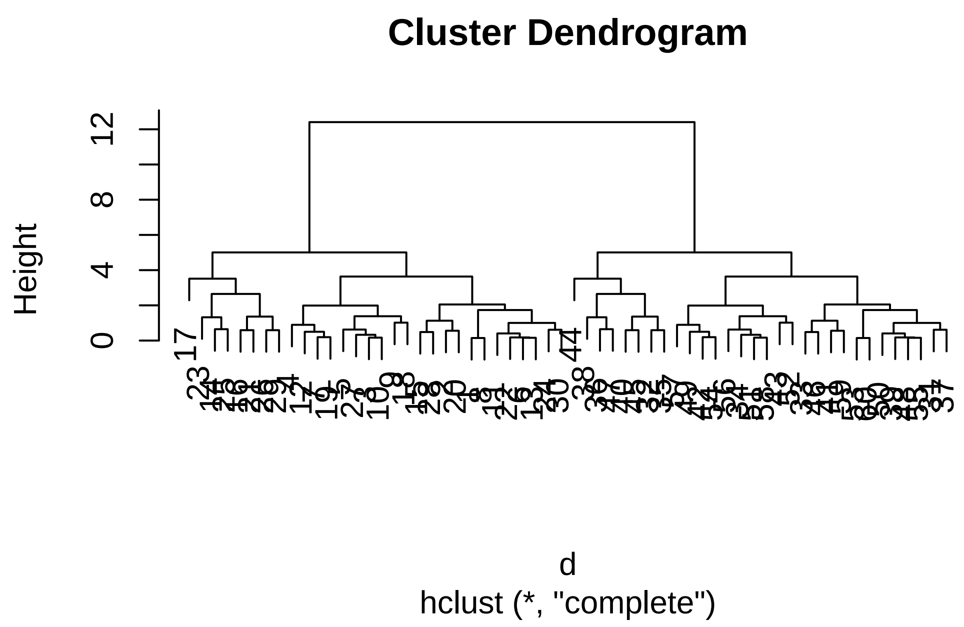
```
d<-dist(x)
hc <- hclust(d)
hc
```

```
Call:
```

```
hclust(d = d)

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

```r
plot(hc)
```



The crossbar height is how far apart the datapoints are. So in this case the largest difference is in the first 2 clusters and then the smaller clusters are very little apart from there. Y axis, height, is the distance of the two branches below it.

There are two forms of hclust: bottom up vs top down

The function to get our clusters/groups from a hclust object is called `cutree()`

```r
cutree(hc, k=2)
```

```
 [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
```

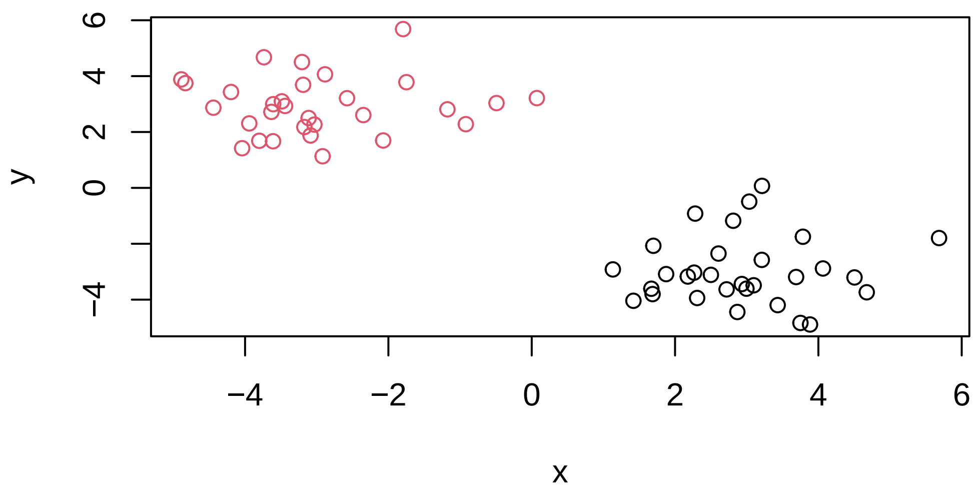
```r
#or
cutree(hc, h=8)
```

```
 [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 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
```

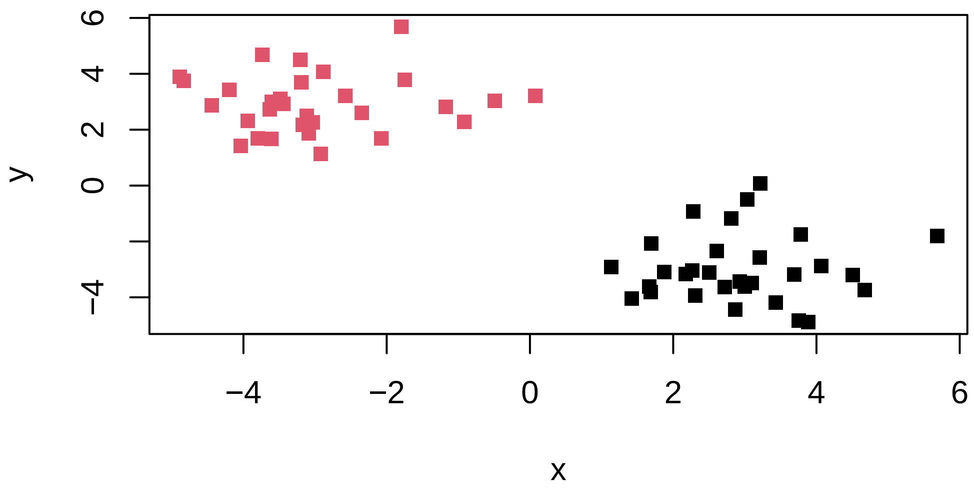
```r
grps <- cutree(hc, k=2)
```

Q. plot our hclust results in terms of our data colored by cluster membership

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



```r
plot(x, col=grps, pch=15) #pch is just the shape of the points
```



Principal Component Analysis (PCA)

UK food class lab

first import the data

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

Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?

```
## Complete the following code to find out how many rows and columns are in x?
str(x)
```

```
'data.frame':	17 obs. of  5 variables:
 $ X        : chr  "Cheese" "Carcass_meat " "Other_meat " "Fish" ...
 $ England  : int  105 245 685 147 193 156 720 253 488 198 ...
 $ Wales    : int  103 227 803 160 235 175 874 265 570 203 ...
 $ Scotland : int  103 242 750 122 184 147 566 171 418 220 ...
 $ N.Ireland: int  66 267 586 93 209 139 1033 143 355 187 ...
```

```r
dim(x)
```

```
[1] 17  5
```

```r
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
```

17 rows (observations) and 5 columns (variables) it is using the names of the food as a column so we are going to make it a name instead

```r
rownames(x)
```

```
 [1] "1"  "2"  "3"  "4"  "5"  "6"  "7"  "8"  "9"  "10" "11" "12" "13" "14" "15"
[16] "16" "17"
```

I can change them like this: but this is overwriting x every time, because it is removing a column every time.

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

a better way to do this is: when we read the data we can tell it that the row names is in column 1 `row.names=1`

```r
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
```

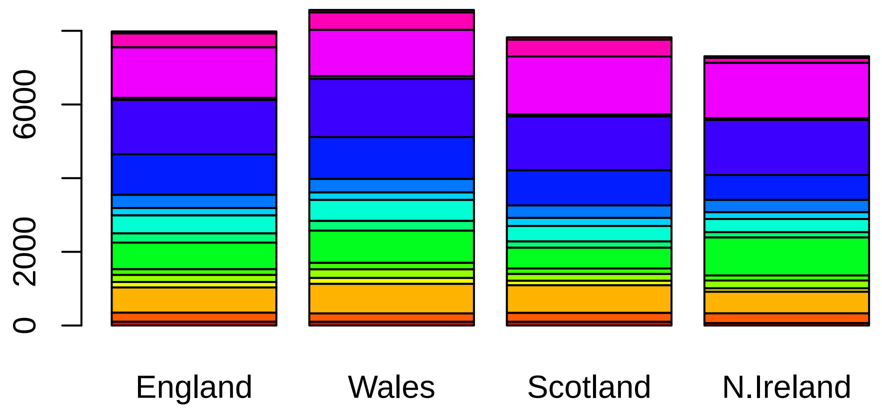
Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

I prefer assigning the row names at the same time as reading the data in. The problem may be if there are no rownames, but I would get the data first then visualize with with `head()` and then decide which column to pick for rownames

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

I just set beside to False

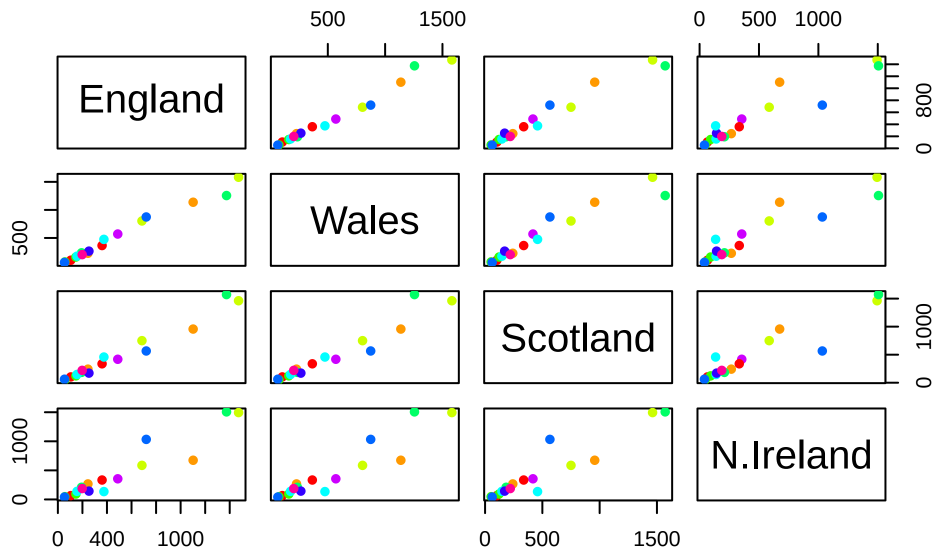
```r
barplot(as.matrix(x), beside=F,col=rainbow(nrow(x)))
```



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?

So the diagonal means they consume the same amount for that particular food. Deviation from the diagonal is what is different between them. Each graph is comparing two countries to each other, but it is mirrored. The main thing is that the difference is what we are looking for.

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



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

Based on the graphs alone it is the food represented by the blue dot, the orange dot. but it is really hard to tell.

To help me makes sense of this data… The main function for PCA in base R is called `prcomp()`

It wants the transpose (with the `t()`) of our food data for analysis

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

summary(pca)
```

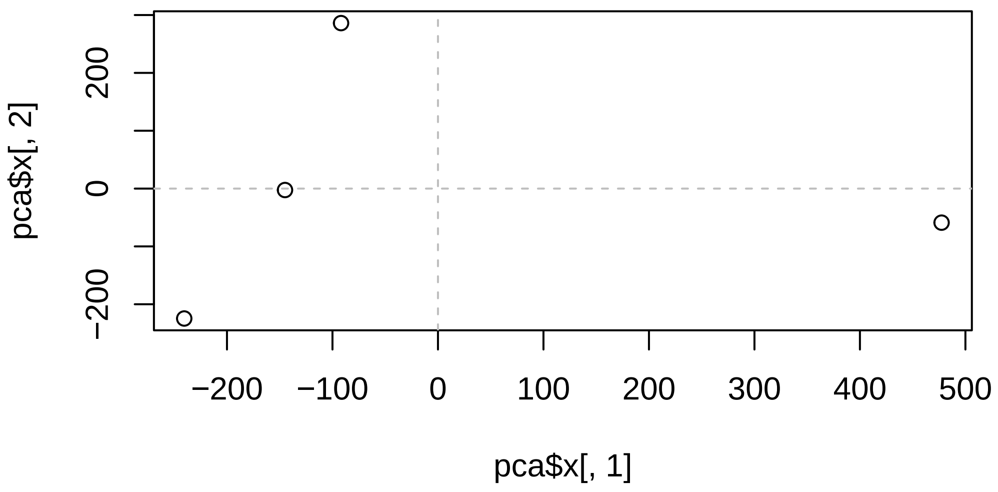
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 3.176e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

The proportion of variance is what i am looking at: 0.67 for PC1 it means that PC1 is responsible for 67% of the variance. The cumulative variance is the sum of them so for PC1 and PC2 it is 96.5%

One of the main results that folks look for is called the "score plot" a.k.a. PC plot, PC1 vs PC2 plot...

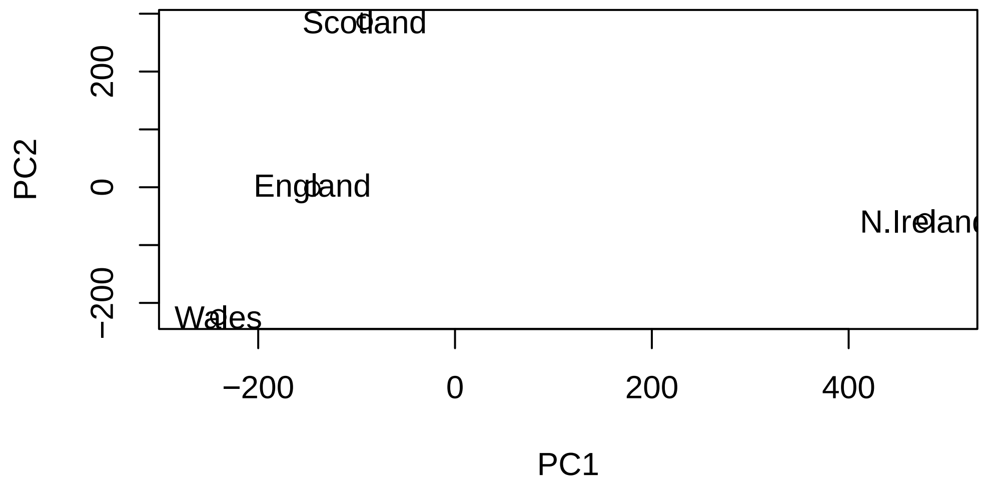
We are loooking at the distance from the point to the 0,0

```
plot(pca$x[,1], pca$x[,2])
abline(h=0, v=0, col="gray", lty=2) #adding a line just to see where0,0 is
```



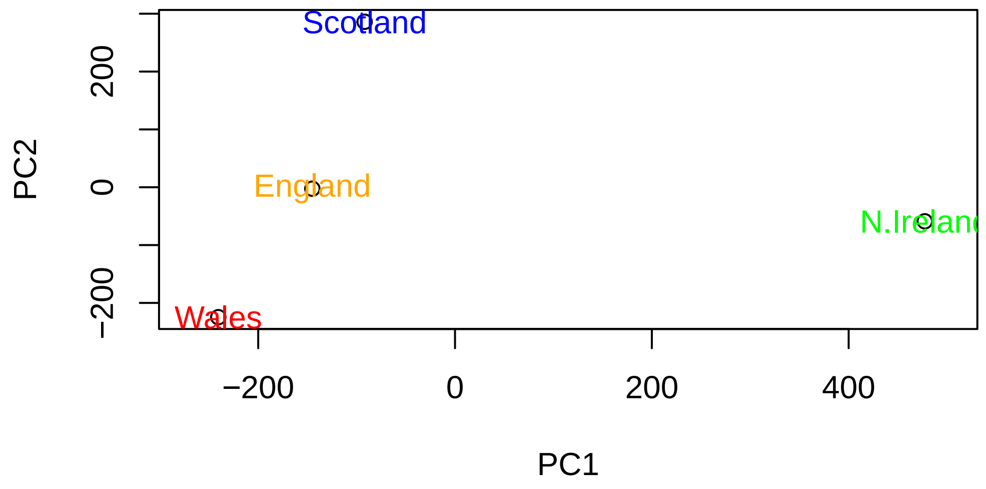
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$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.

```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x), col=c("orange","red","blue","green"))
```



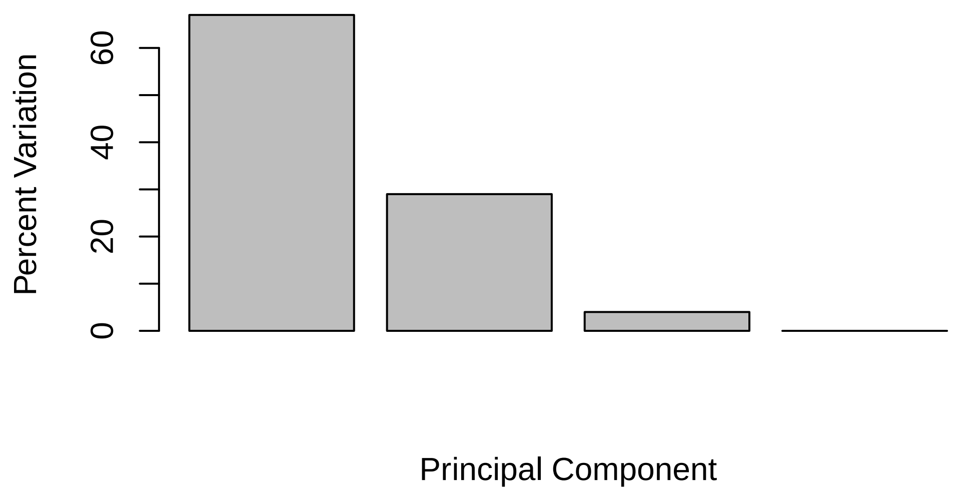
```r
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

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

```r
## or the second row here...
z <- summary(pca)
z$importance
```

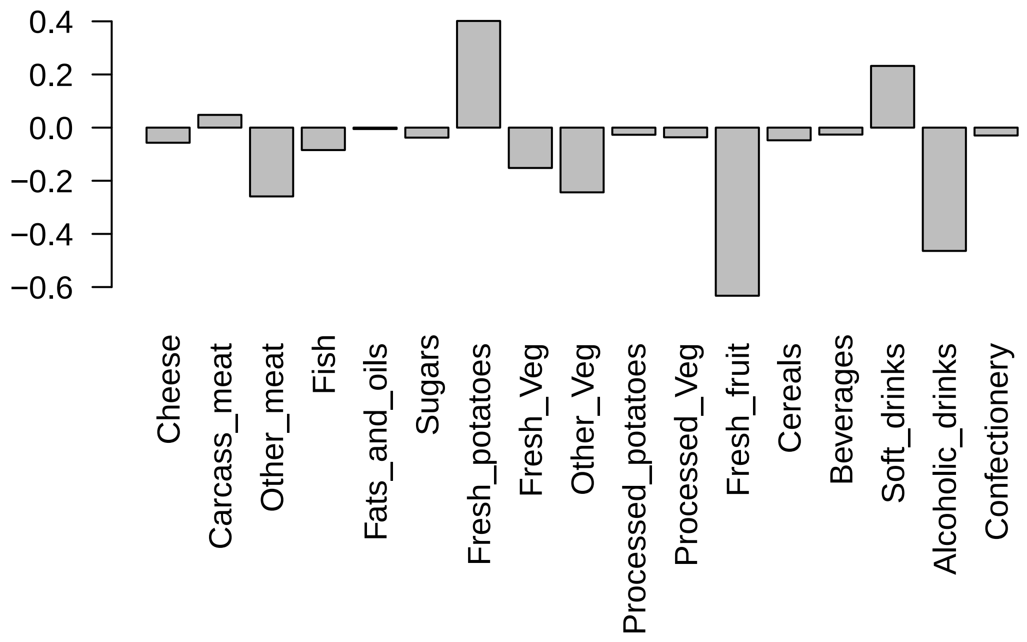
```
                             PC1       PC2      PC3          PC4
Standard deviation     324.15019 212.74780 73.87622 3.175833e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

```r
#This information can be summarized in a plot of the variances (eigenvalues) with respect
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```



To dig deeper we can see how much each variable affects the original PCA1 from the `$rotation` from `prcomp()` and summarized in `biplot()`

```r
## 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 )
```

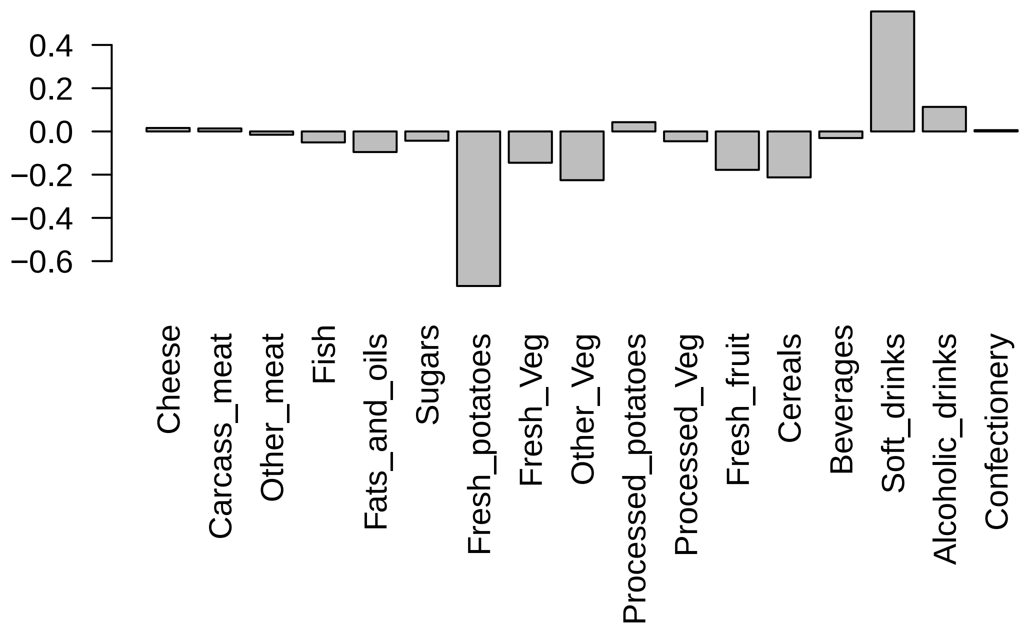


The two biggest contributors are fresh fruit and soft drinks because they are the biggest bars.

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

Fresh potatoes makes the countries go left and soft drinks right so fresh potatoes differ the most between N. Ireland and Soft drinkg makes it the most different.

```
#PC2
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```

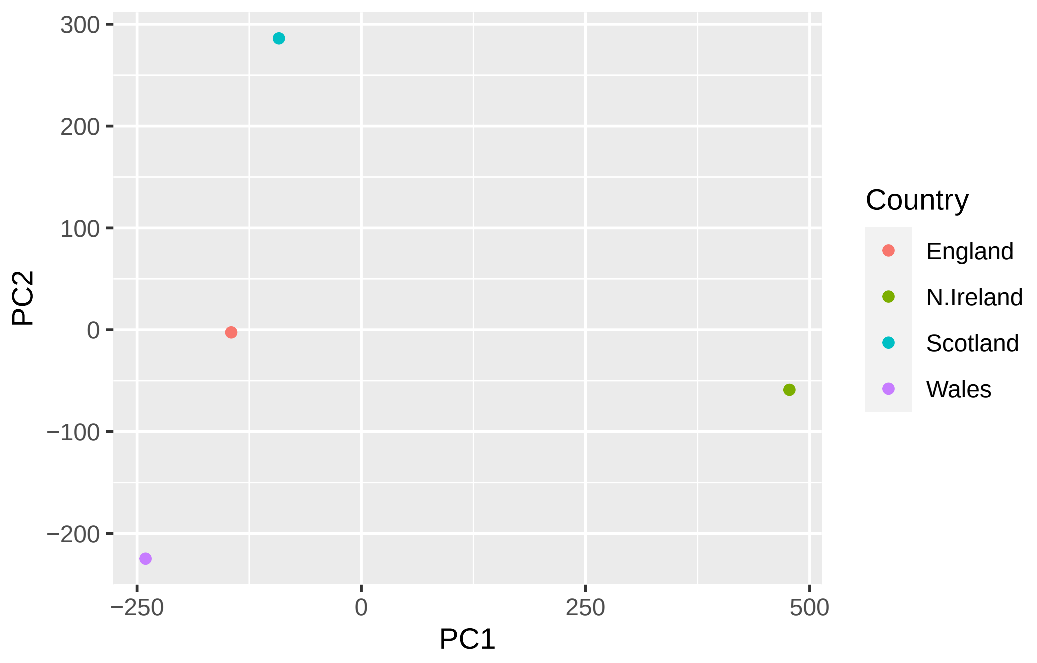


PC2 is predominantly still soft drinks but also alcoholic drinks.

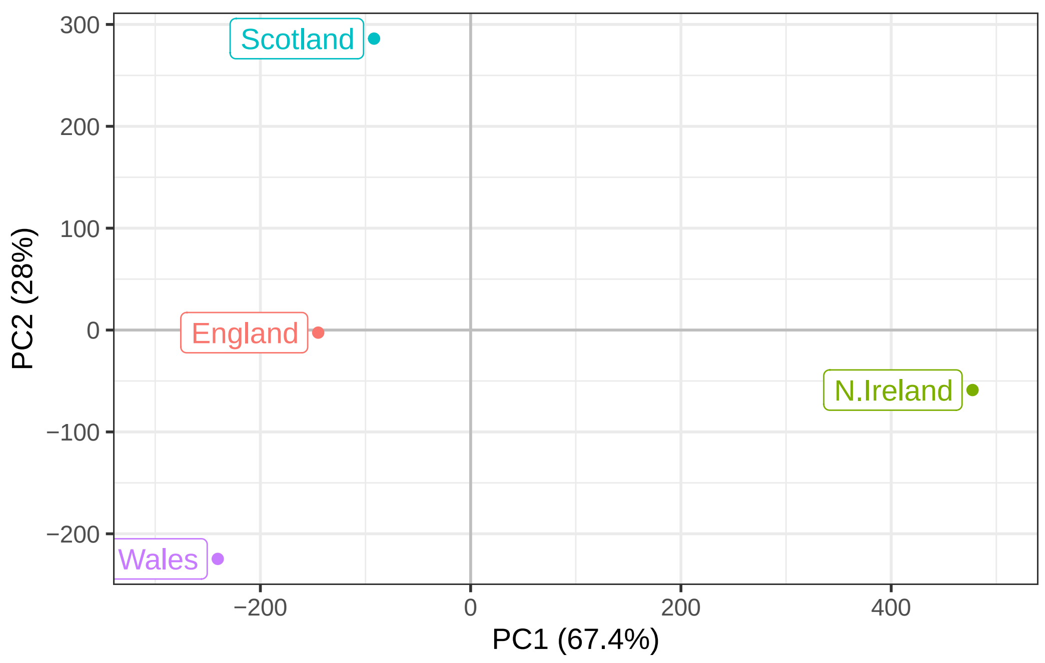
```r
library(ggplot2)

df <- as.data.frame(pca$x)
df_lab <- tibble::rownames_to_column(df, "Country")

# Our first basic plot
ggplot(df_lab) +
  aes(PC1, PC2, col=Country) +
  geom_point()
```



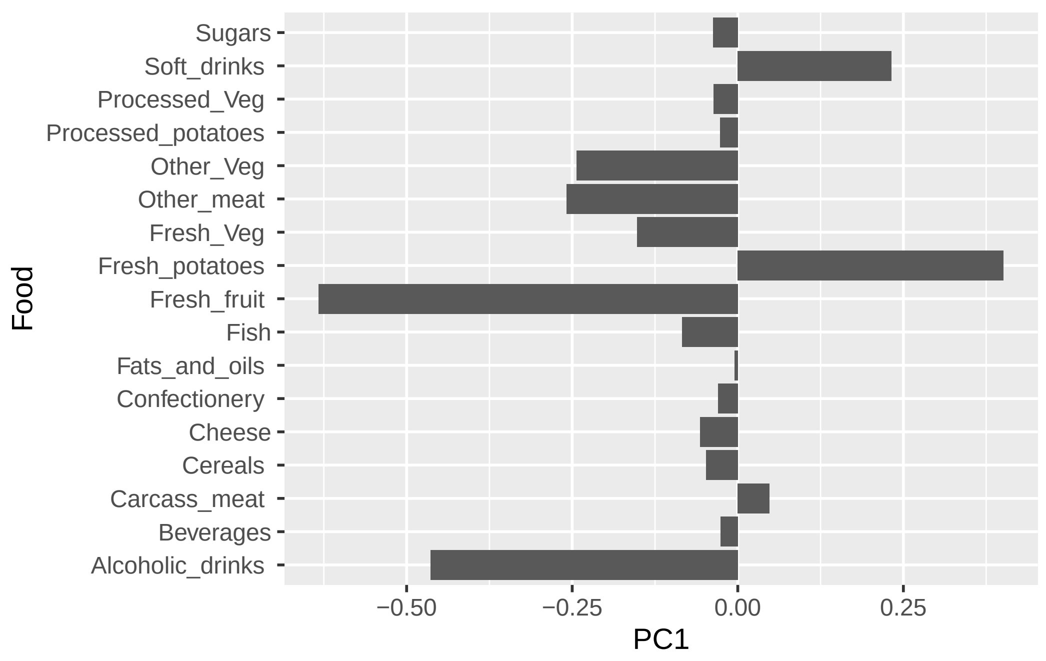
```
ggplot(df_lab) +
  aes(PC1, PC2, col=Country, label=Country) +
  geom_hline(yintercept = 0, col="gray") +
  geom_vline(xintercept = 0, col="gray") +
  geom_point(show.legend = FALSE) +
  geom_label(hjust=1, nudge_x = -10, show.legend = FALSE) +
  expand_limits(x = c(-300,500)) +
  xlab("PC1 (67.4%)") +
  ylab("PC2 (28%)") +
  theme_bw()
```



we can also make a nice ggplot for our pca

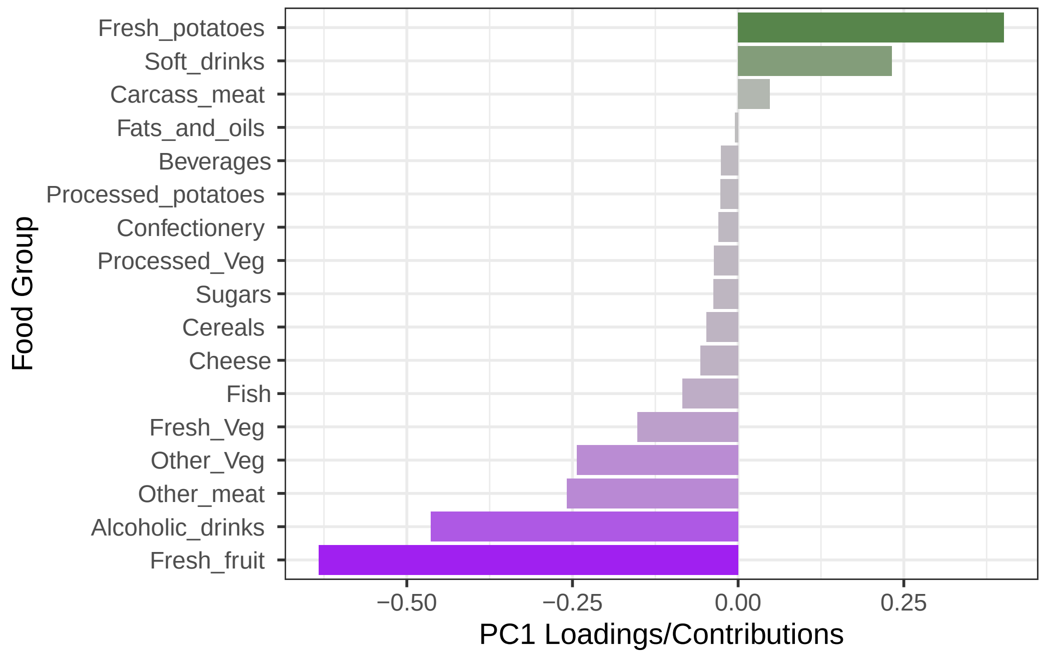
```
ld <- as.data.frame(pca$rotation)
ld_lab <- tibble::rownames_to_column(ld, "Food")

ggplot(ld_lab) +
  aes(PC1, Food) +
  geom_col()
```



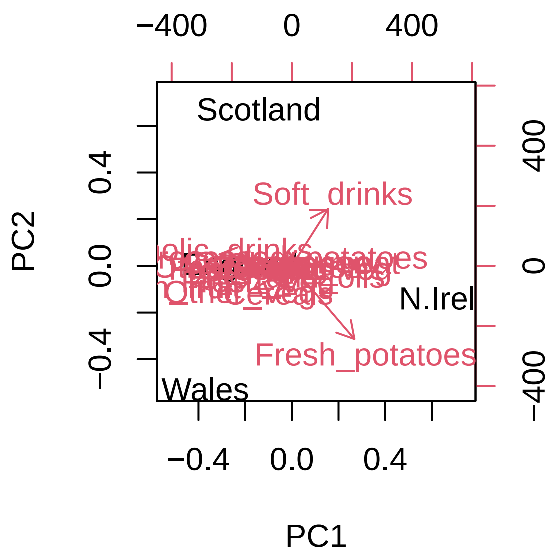
and we can also make it nicer to see by color scaling and ordering them by highest to smallest

```
ggplot(ld_lab) +
  aes(PC1, reorder(Food, PC1), bg=PC1) +
  geom_col() +
  xlab("PC1 Loadings/Contributions") +
  ylab("Food Group") +
  scale_fill_gradient2(low="purple", mid="gray", high="darkgreen", guide=NULL) +
  theme_bw()
```



another way to visualize this is by using a biplot

```
## The inbuilt biplot() can be useful for small datasets
biplot(pca)
```



PCA for RNA-seq

loading the data

```r
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?

```r
class(rna.data)
```

```
[1] "data.frame"
```

```
str(rna.data)
```

```
'data.frame':	100 obs. of  10 variables:
 $ wt1: int  439 219 1006 783 181 460 27 175 658 121 ...
 $ wt2: int  458 200 989 792 249 502 30 182 669 116 ...
 $ wt3: int  408 204 1030 829 204 491 37 184 653 134 ...
 $ wt4: int  429 210 1017 856 244 491 29 166 633 117 ...
 $ wt5: int  420 187 973 760 225 493 34 180 657 133 ...
 $ ko1: int  90 427 252 849 277 612 304 255 628 931 ...
 $ ko2: int  88 423 237 856 305 594 304 291 627 941 ...
 $ ko3: int  86 434 238 835 272 577 285 305 603 990 ...
 $ ko4: int  90 433 226 885 270 618 311 271 635 982 ...
 $ ko5: int  93 426 210 894 279 638 285 269 620 934 ...
```

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

```
[1] 100  10
```

There are 100 genes and 10 samples (columns)