# Class 7: Machine Learning 1

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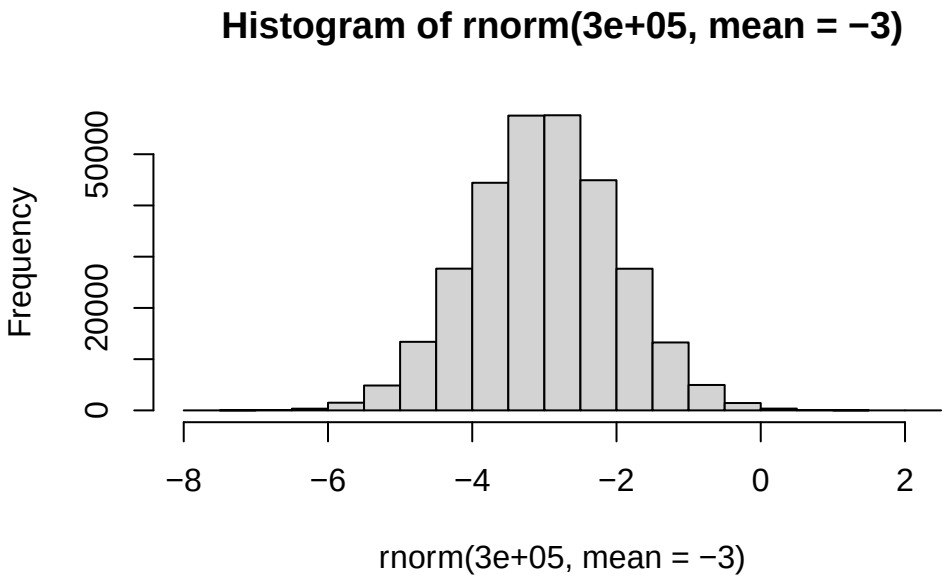
In this class, we will explore and get practice with clustering and Principal Component Analysis (PCA) #Clustering with K-means

First we will make up some data to cluster where we know what the result should be.

```
hist(rnorm(300000, mean = -3))
```

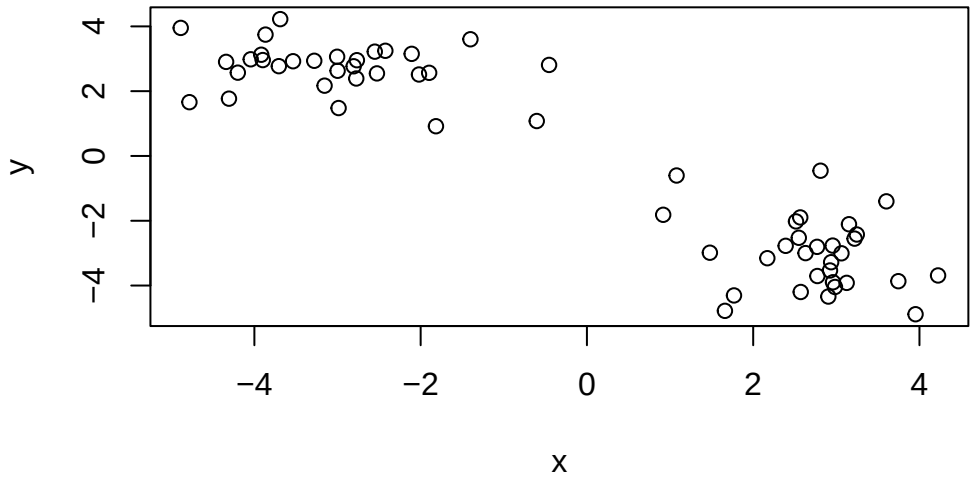



I want a little vector with two groupings in it:

```
tmp <-c(rnorm(30, -3), rnorm(30, +3))
x <- data.frame(x = tmp, y = rev(tmp))
head(x)
```

```
          x        y
1 -1.897586 2.566234
2 -2.766896 2.956173
3 -3.534633 2.923936
4 -2.525725 2.548474
5 -4.305450 1.769013
6 -2.774181 2.390898
```

```r
plot(x)
```




```r
km <- kmeans(x, centers = 2)
km
```

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

Cluster means:
          x         y
1  2.721404 -3.024728
2 -3.024728  2.721404

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] 53.52294 53.52294
 (between_SS / total_SS =  90.2 %)

Available components:

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

It's important to not just run the analysis but to be able to get your important results back in a way that we can do things with them.

Q. How do I find the cluster size?

```
km$size
```

```
[1] 30 30
```

Q. How about the cluster centers?

```
km$centers
```

```
          x         y
1  2.721404 -3.024728
2 -3.024728  2.721404
```

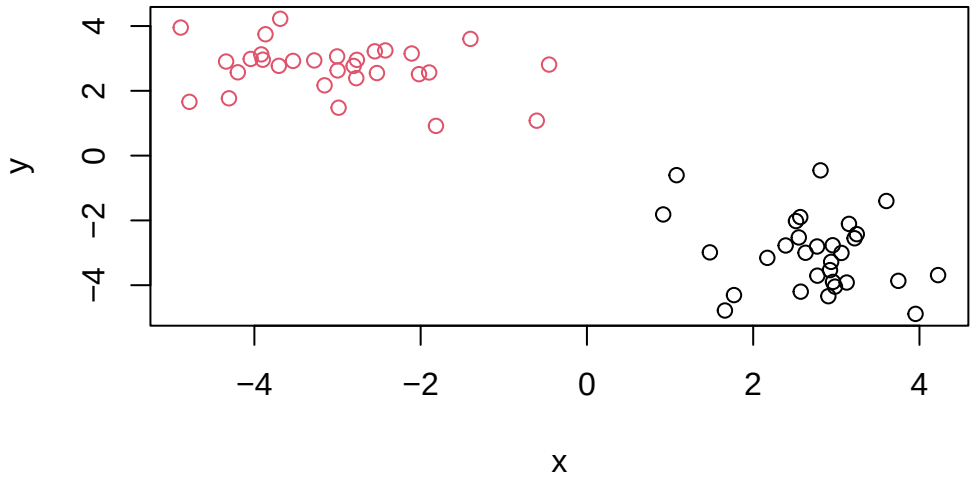
Q. How about the main result - the cluster assignment vector?

```
km$cluster
```

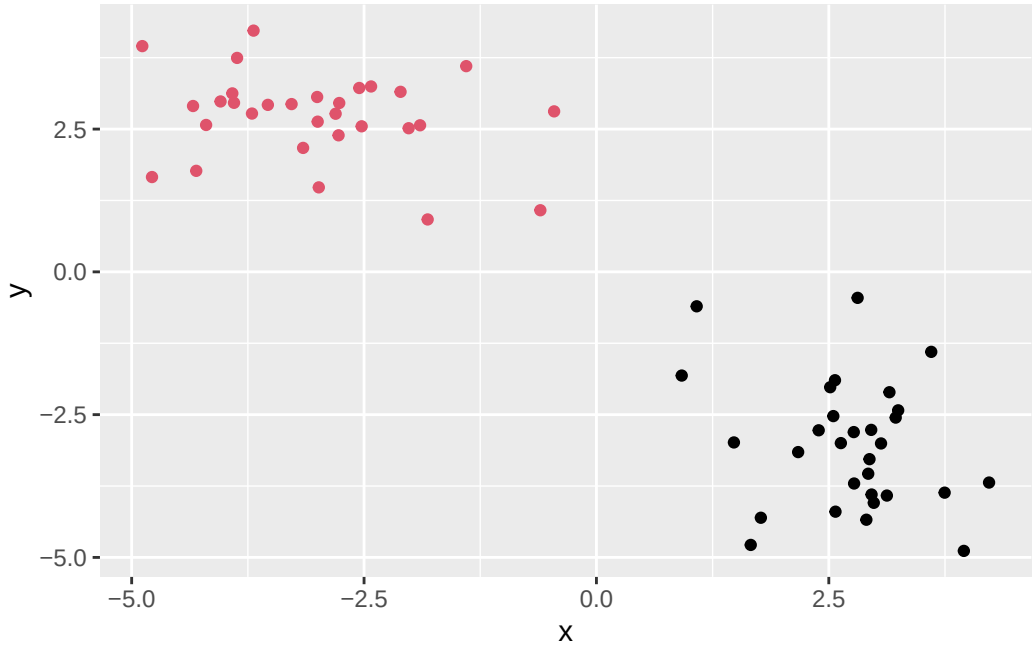
```
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

Q. Can we make a summary figure showing our clustering result? - The points colored by cluster assignament and maybe add the cluster centers as a different color?

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



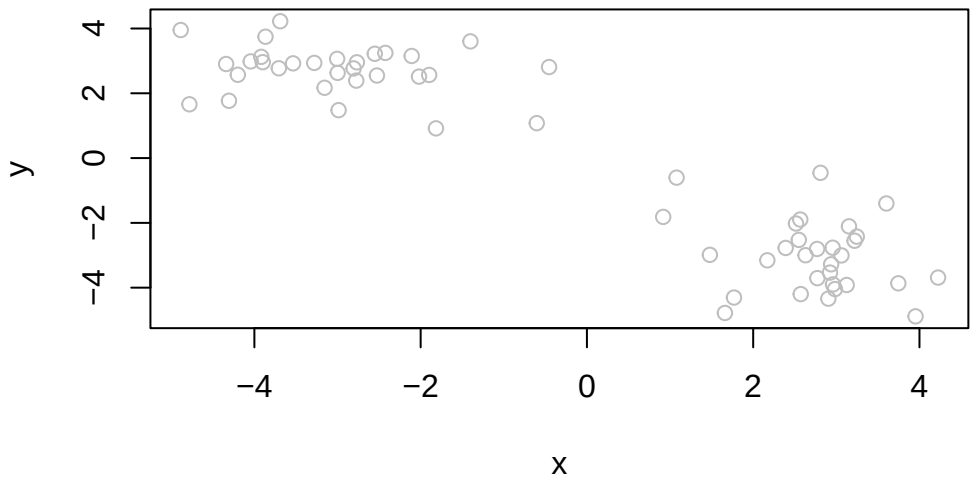

```r
library(ggplot2)
ggplot(x) +
  aes(x, y) +
  geom_point(col = km$cluster)
```




```
# Make up a color vector
mycols <- rep( "gray", 60)
mycols
```

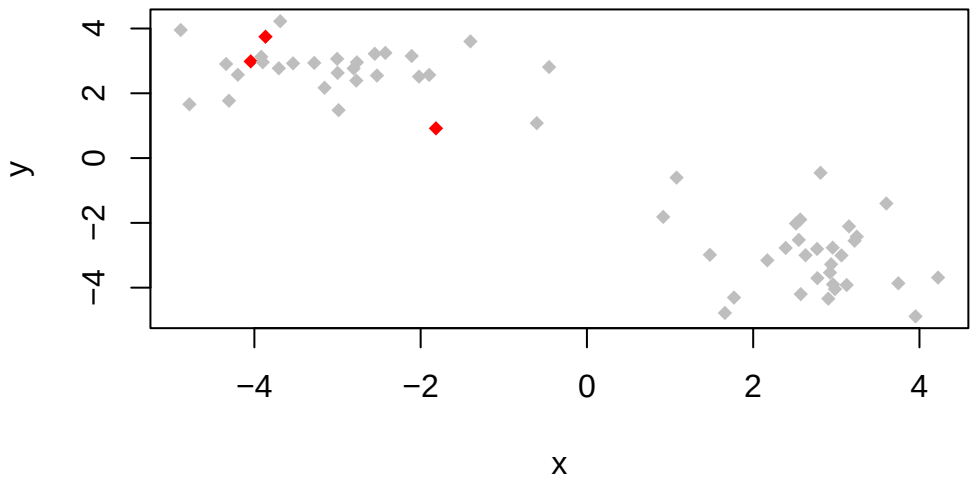
```
 [1] "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray"
[11] "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray"
[21] "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray"
[31] "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray"
[41] "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray"
[51] "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray" "gray"
```

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



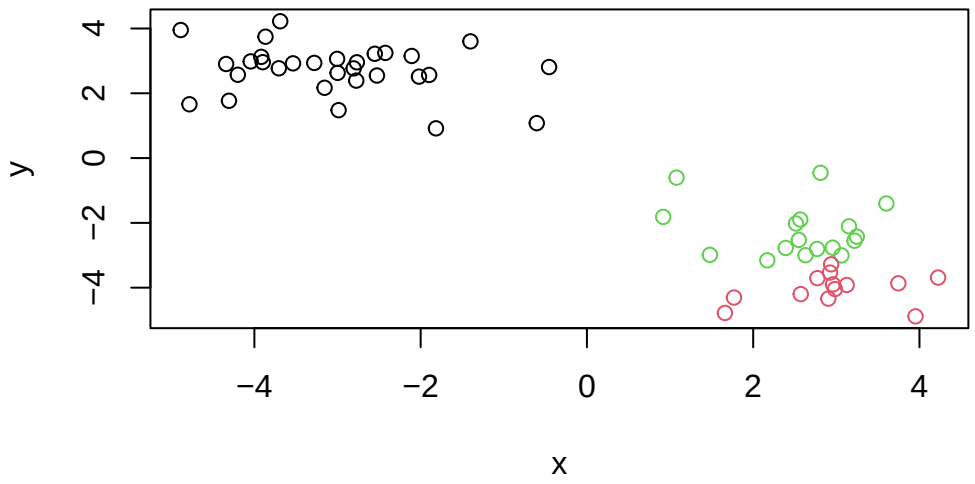

Let's highligh points 10, 12, and 20

```
mycols[c(10, 12, 20)] <- "red"
plot(x, col = mycols, pch = 18)
```




Play with different number of centers

```
km <- kmeans(x, centers = 3)
plot(x, col = km$cluster)
```



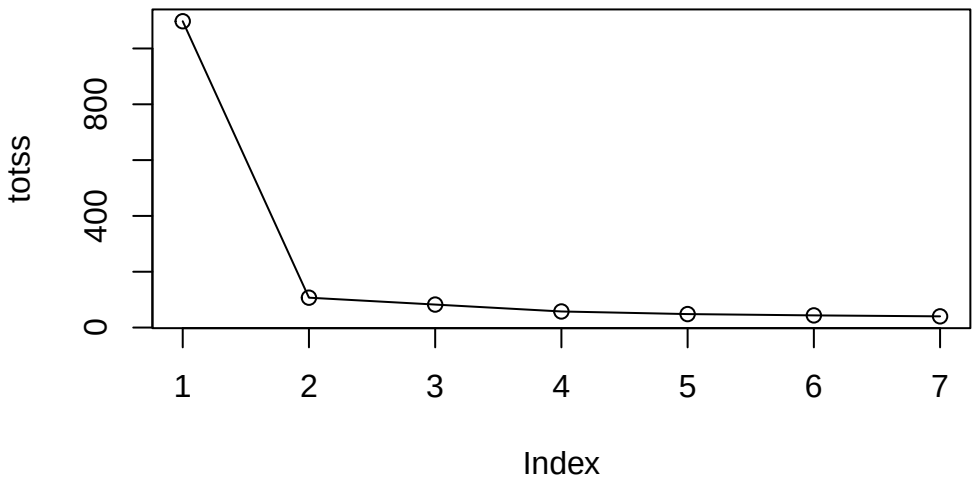

```
km$tot.withinss
```

```
[1] 82.31164
```

What we want to do is try out different number of K from 1 to 7. We cna write a `for` loop to do this for us and sotr the `$tot.withinss` each time.

```
totss <- NULL
k <- 1:7

for(i in k) {
  totss <- c(totss, kmeans(x, centers = i)$tot.withinss)
}
```

```
plot(totss, typ = "o")
```




Inflection point at 2 totss. 2 clusters is best.

#Hierarchical Clustering

We cannot just give the `hclust()` function of input data `x` like we did for `kmeans()`.

We need to first calculate a "distance matrix". the `dist()` function by default will calculate euclidean distance.

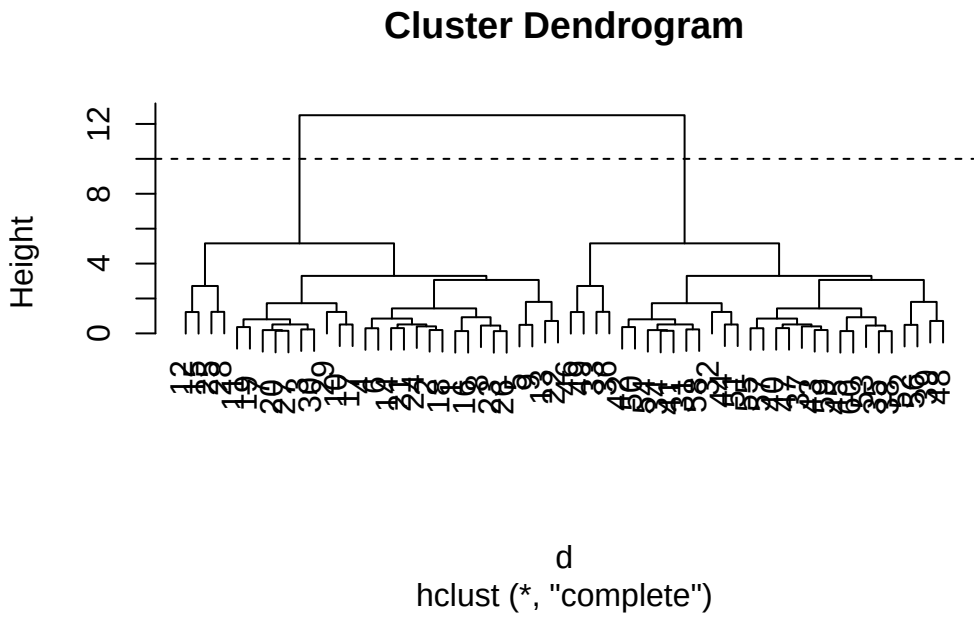
```
d <- dist(x)
hc <- hclust(d)
hc
```

```
Call:
hclust(d = d)

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

The print out is not very helpful, but the plot method is useful.

```
plot(hc)
abline(h = 10, cor = "red", lty = 2)
```

```
Warning in int_abline(a = a, b = b, h = h, v = v, untf = untf, ...): "cor" is
not a graphical parameter
```




To get my all important cluster membership vector out of a hclust object I can use the `cutree()`

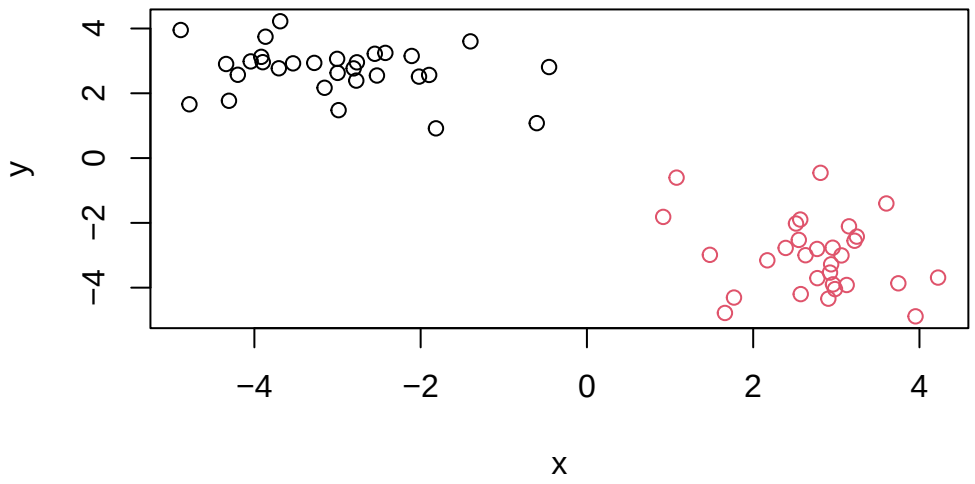
```
cutree(hc, h=10)
```

```
 [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
```

You can also set a `k=` argument to `cutree()`.

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

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




#Principal Component Analysis (PCA) PCA projects the features onto the principal components. The motivation is to reduce the feature's dimensionality.

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

## PCA of UK food

First, need ot import the data.

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

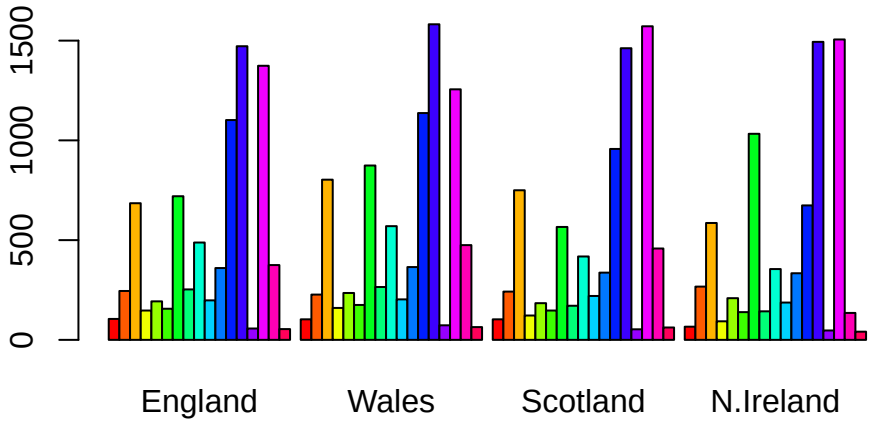
```
              England Wales Scotland N.Ireland
Cheese            105   103      103        66
Carcass_meat      245   227      242       267
Other_meat        685   803      750       586
Fish              147   160      122        93
Fats_and_oils     193   235      184       209
Sugars        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

```
dim(x)
```

```
[1] 17  4
```

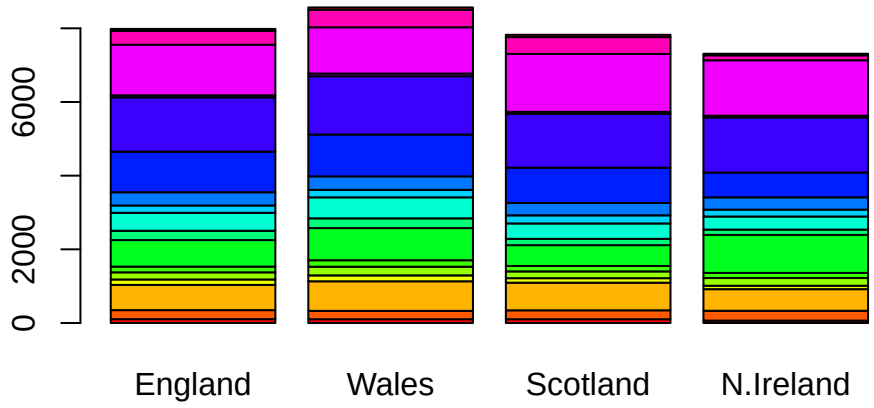
Q2. Prefer `row.names = 1` argument to `read.csv` because the other way, `x <- x[,-1]`, if you run it multiple times it will remove data.

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

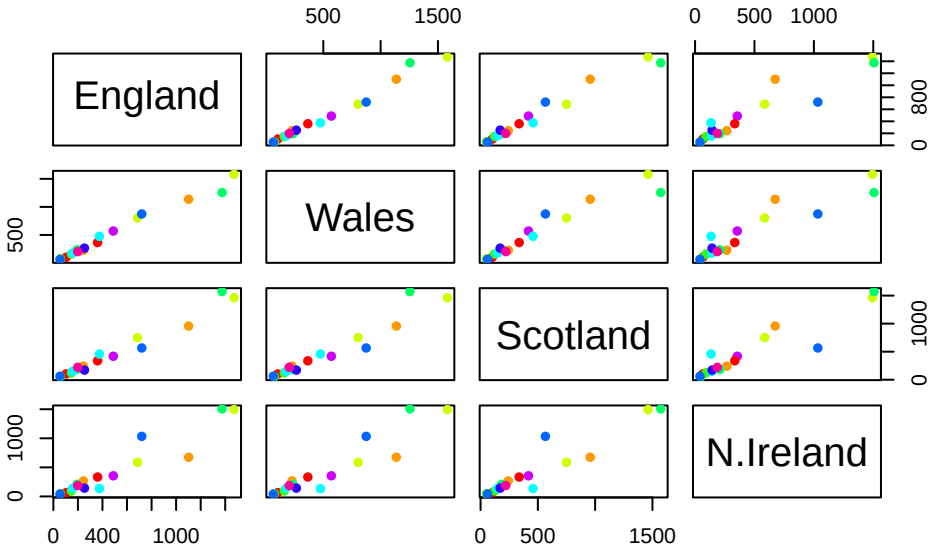



Q3. Changing the `beside =` argument from T to F gives this plot

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




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



Q5. The plots are comparing each of the countries' data with that of one other country, in a pair. A point of the diagonal means it is very similar for the two countries (the x and y coordinates are approximately the same).

Q6. The orange and blue points look most different for N. Ireland from the other countries in the UK.

For PCA, we need the transpose of our food data.

```
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
```

```
attributes(pca)
```

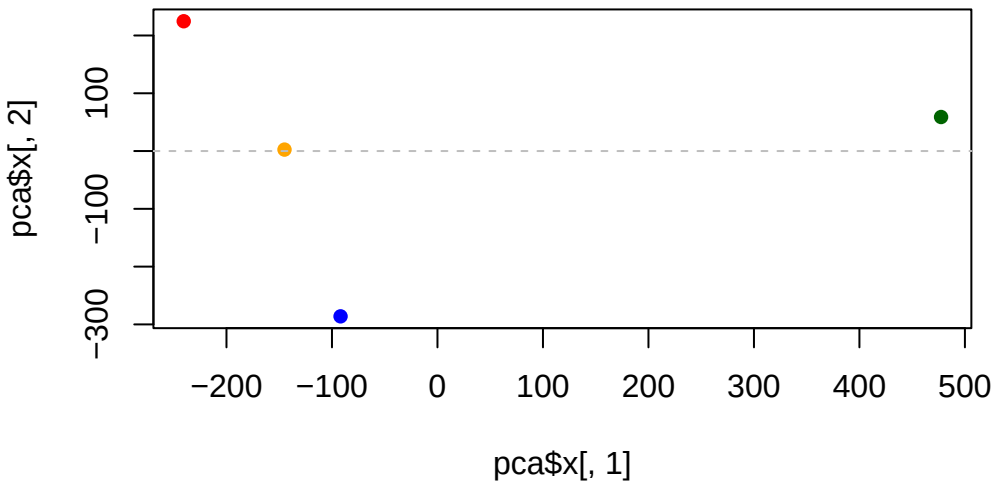
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

```
pca$x
```

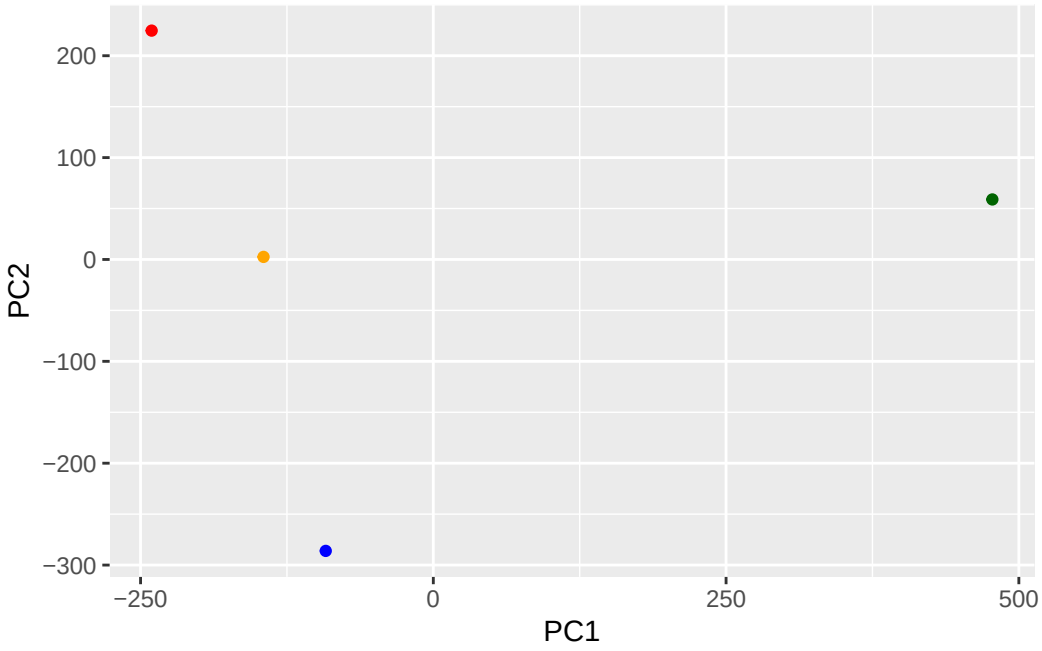
```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  2.842865e-14
Wales     -240.52915  224.646925   56.475555  7.804382e-13
Scotland   -91.86934 -286.081786   44.415495 -9.614462e-13
N.Ireland  477.39164   58.901862    4.877895  1.448078e-13
```

Make my PC1 vs PC2 plot, "score plot", "pca plot"

```
mycols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col= mycols, pch=16)
abline(h=0, col="gray", lty=2)
```

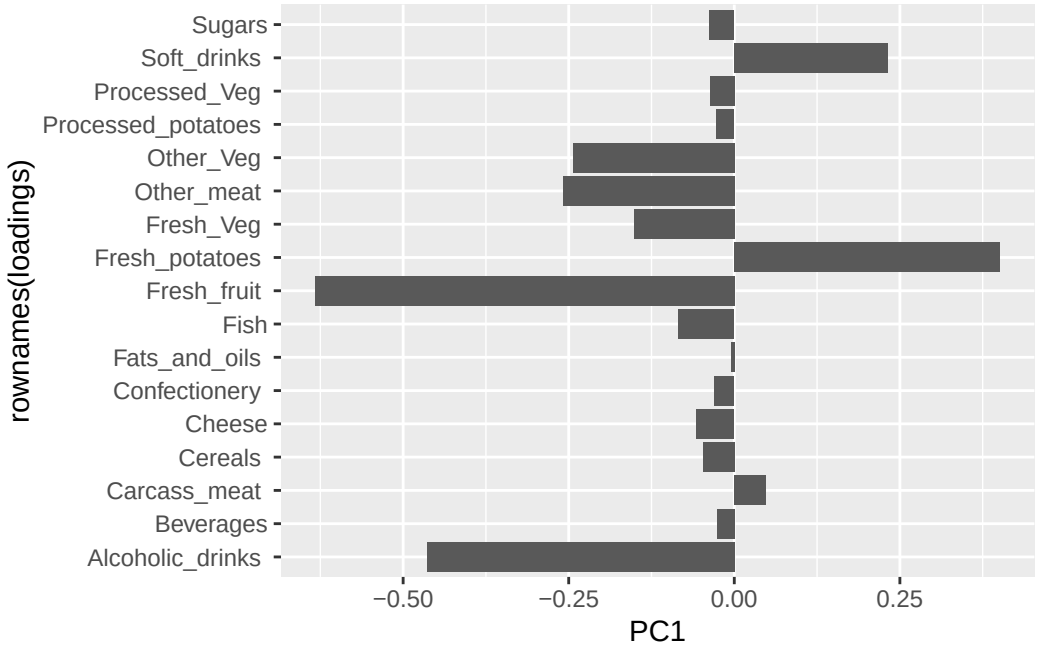



```
pc <- as.data.frame(pca$x)

ggplot(pc) +
  aes(PC1, PC2) +
  geom_point(col=mycols)
```




Let's look at how the original variables contribute to our new axis fo max variance, aka PCs

```
loadings <- as.data.frame(pca$rotation)

ggplot(loadings) +
  aes(PC1, rownames(loadings)) +
  geom_col()
```


rownames(loadings)
Sugars
Soft_drinks
Processed_Veg
Processed_potatoes
Other_Veg
Other_meat
Fresh_Veg
Fresh_potatoes
Fresh_fruit
Fish
Fats_and_oils
Confectionery
Cheese
Cereals
Carcass_meat
Beverages
Alcoholic_drinks
−0.50
−0.25
0.00
0.25
PC1