Class 7: Machine Learning

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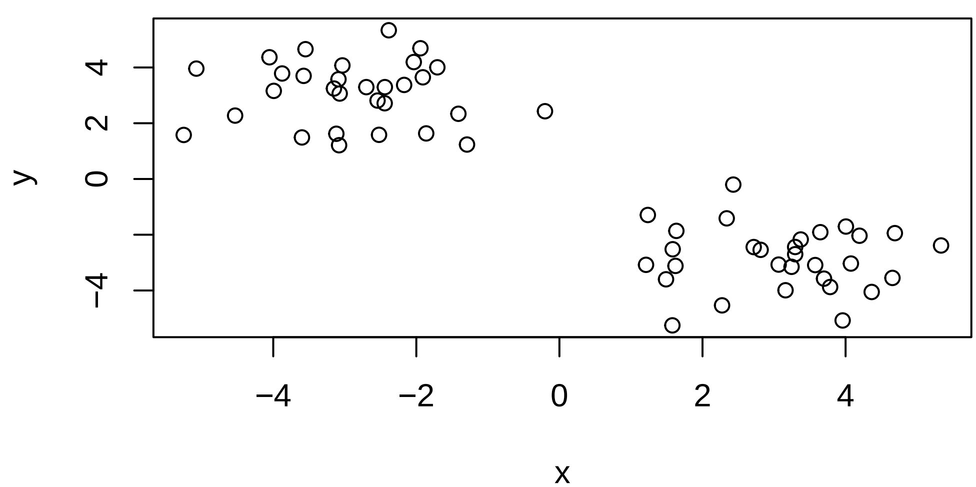
Example of K-means clustering

First step is o make up some data with a known structure, so we know what the answer should be.

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



Now we have some structured data in `x`. Let's see if k-means is able to identify the two groups.

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

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

Cluster means:
          x         y
1  3.077954 -2.853543
2 -2.853543  3.077954

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] 73.96439 73.96439
 (between_SS / total_SS =  87.7 %)

Available components:

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

Let's explore `k`:

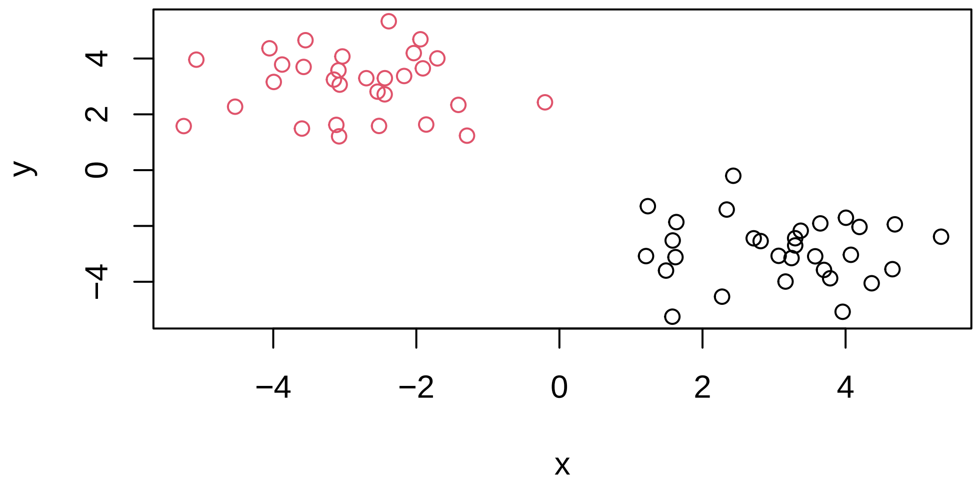
```r
k$size
```

```
[1] 30 30
```

```r
k$centers
```

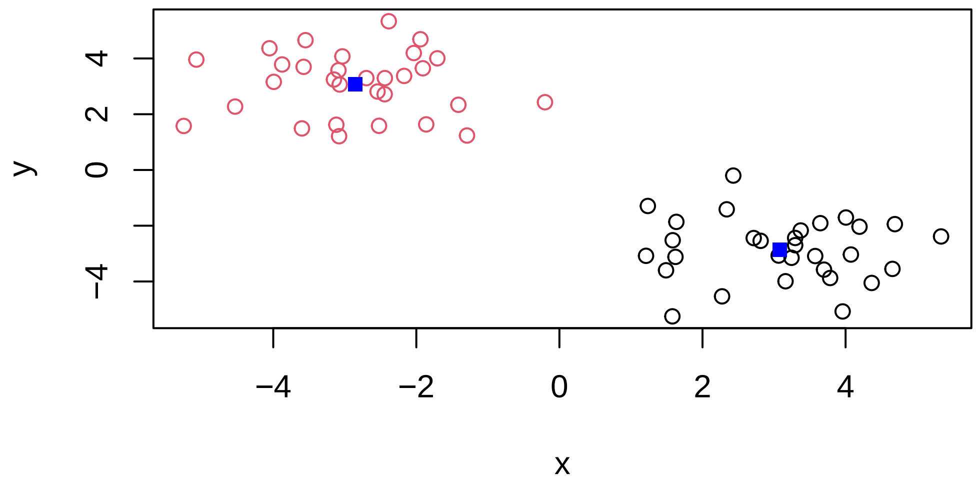
```
          x         y
1  3.077954 -2.853543
2 -2.853543  3.077954
```

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



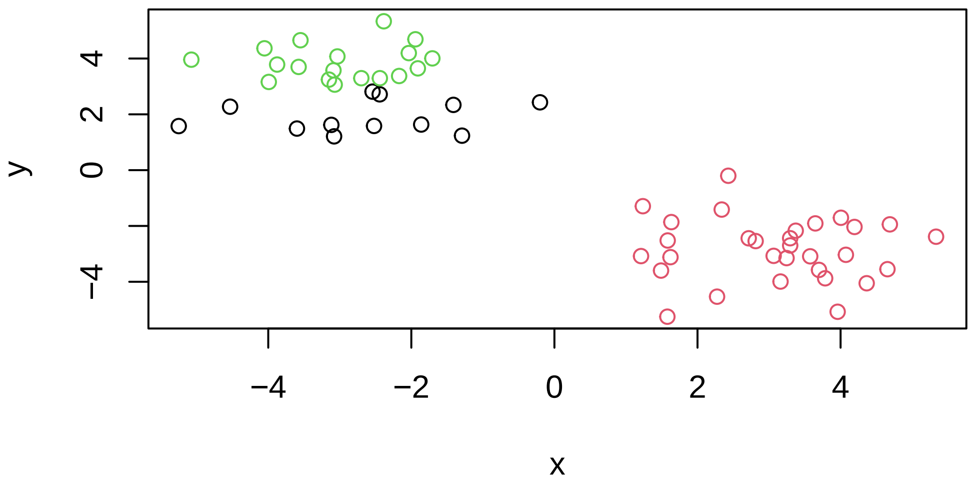
Now we can add the clusters centers:

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



An example when we select the wrong number of cluster for k-means.

```
k_3 <- kmeans(x, centers = 3, nstart = 20)
plot(x, col = k_3$cluster)
```



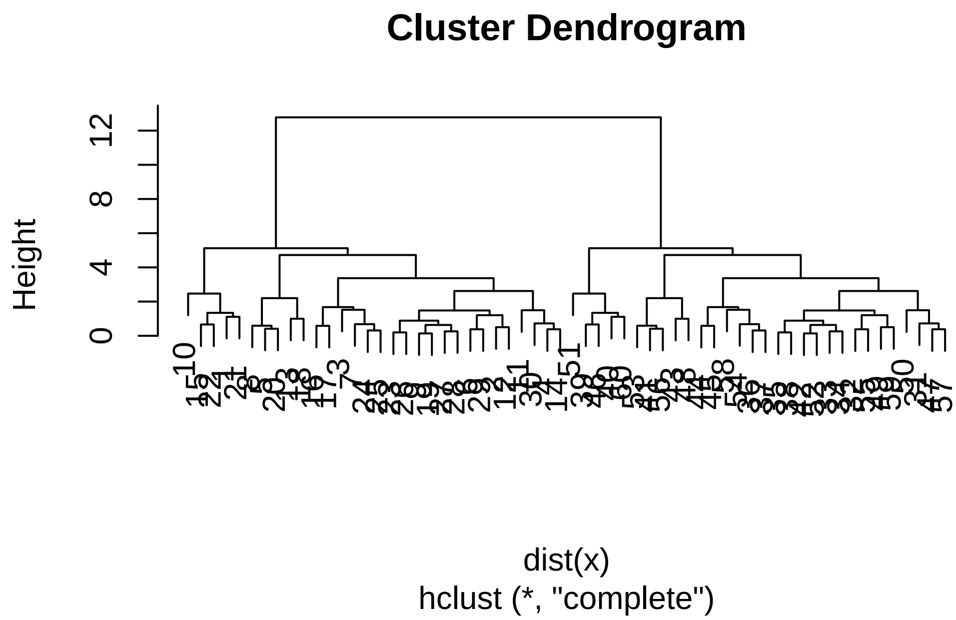
Example of Hierarchical Clustering

Let's use the same data as before, which we stored in 'x'. We will use the `'hclust()'` function.

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

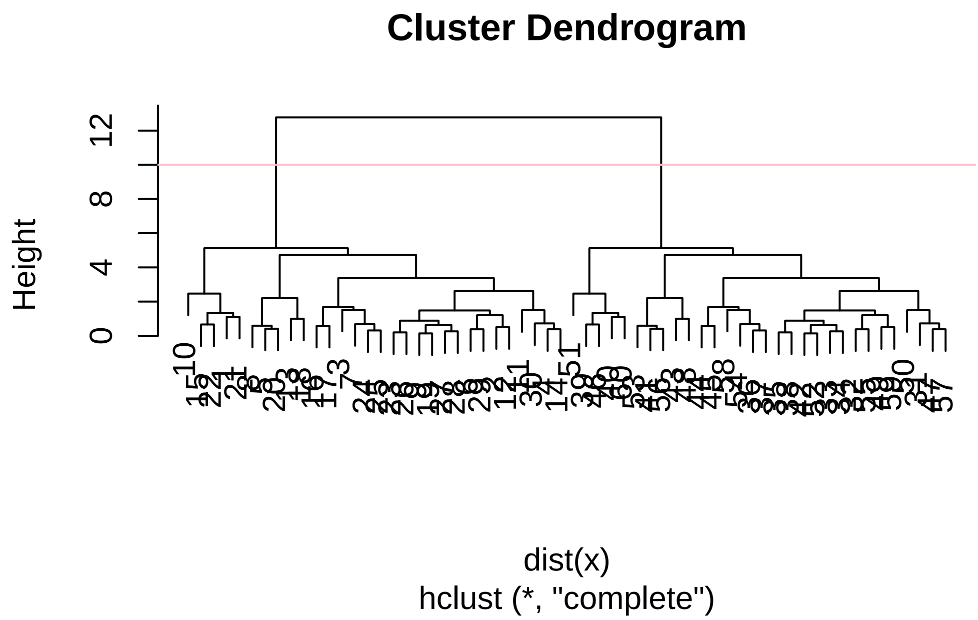
```
Call:
hclust(d = dist(x))

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

```
plot(clustering)
```



Let's add a horizontal line

```r
plot(clustering)
abline(h=10, col="pink")
```



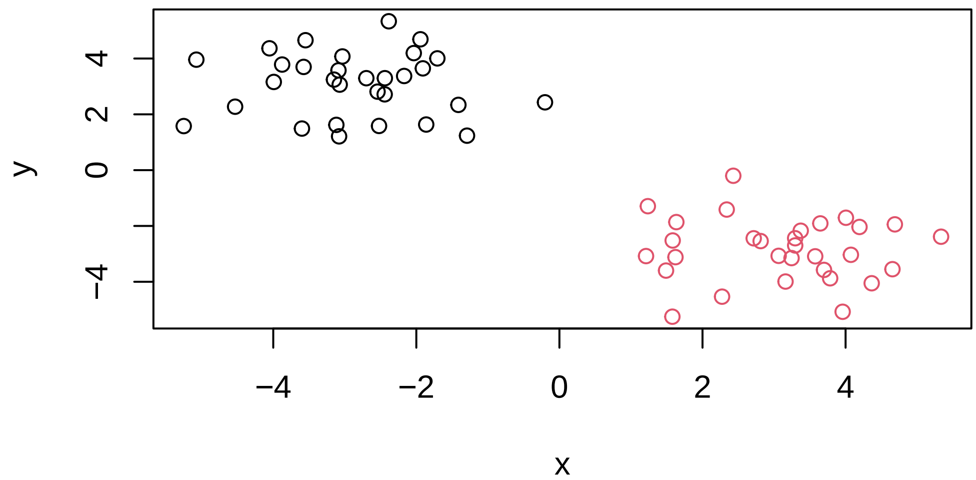
To get our results (i.e., memebership vector) we need to "cut" the tree. The function for doing that is `cutree()`.

```
subgroups <- cutree(clustering, h = 10)
subgroups
```

```
 [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
```

Plotting this…

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



You can also “cut” your tree with the number of clusters you want:

```
cutree(clustering, 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
```

Principal Component Analysis (PCA)

PCA of the UK food

First was to read the data.

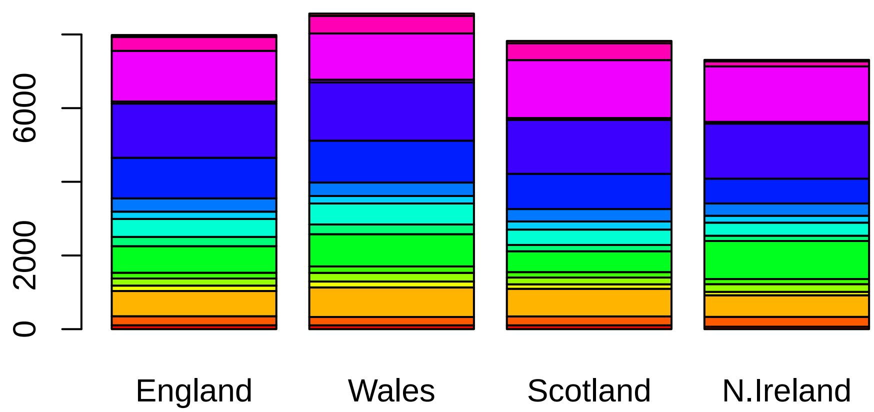
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
head(x)
```

```
               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
```

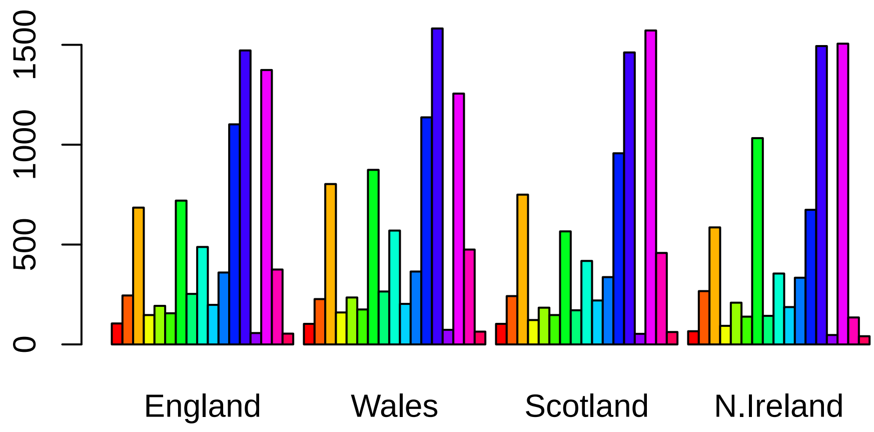
Now we can generate some basic visualizations

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



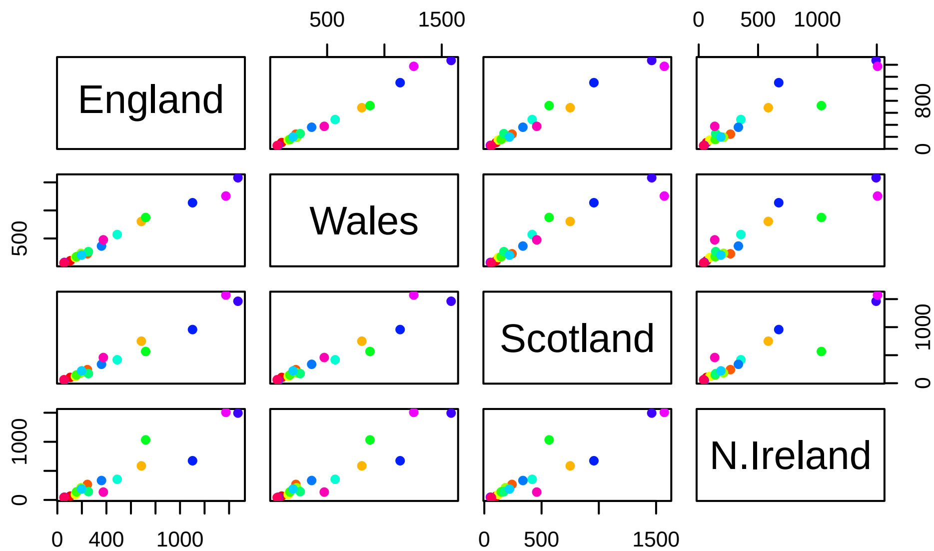
Let's refine our barplot:

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



Other visualizations that can be useful...

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



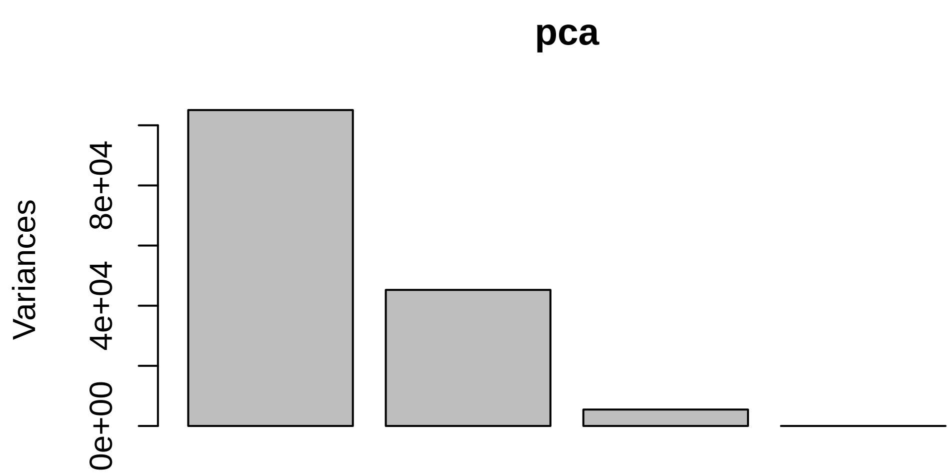
Let's apply PCA (principal components analysis). For that, we need to use the command `prcomp()`. This function expects the transpose of our data.

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

Let's plot the PCA results

```
plot(pca)
```



We need to access the results of the PCA analysis

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

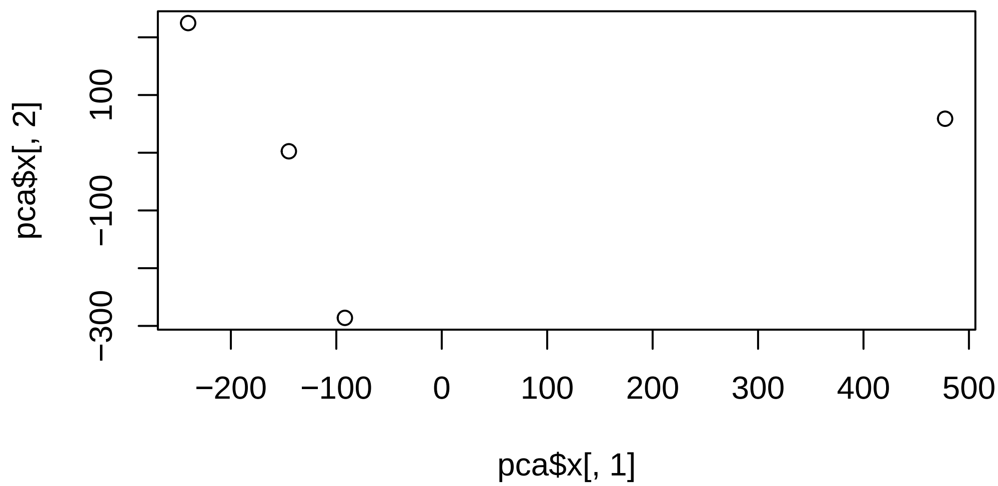
We can explore the pca$x dataframe:

```
pca$x
```

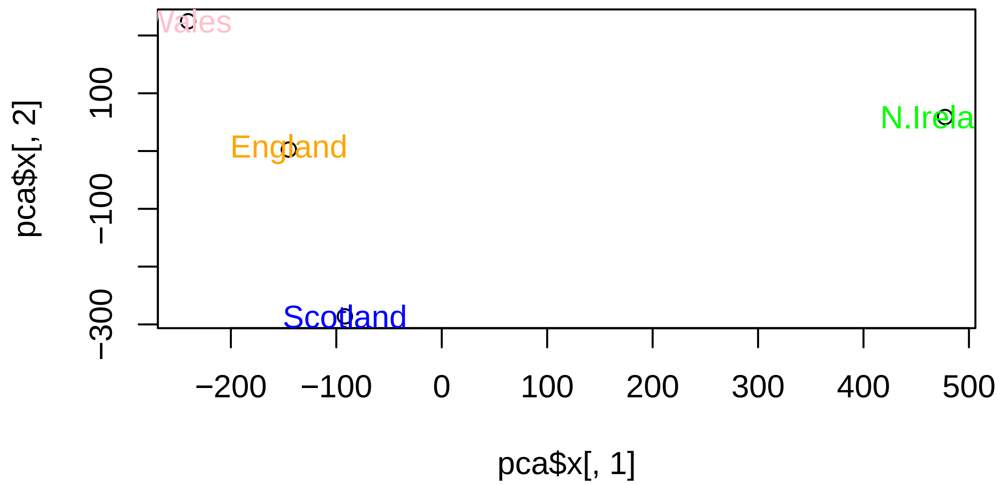
```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  2.842865e-14
Wales     -240.52915  224.646925   56.475555  7.804382e-13
Scotland   -91.86934 -286.081786   44.415495 -9.614462e-13
N.Ireland  477.39164   58.901862    4.877895  1.448078e-13
```

Plotting:

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




```
plot( x=pca$x[,1], y=pca$x[,2] )
colors_countries <- c('orange', 'pink', 'blue', 'green')
text( x=pca$x[,1], y=pca$x[,2], colnames(x), col = colors_countries)
```




```
pca$scale
```

```
[1] FALSE
```

PCA of a RNA-Seq dataset

FIrst step as always is loading the data:

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

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

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

```
[1] 100  10
```

I have 100 genes, and 10 samples.

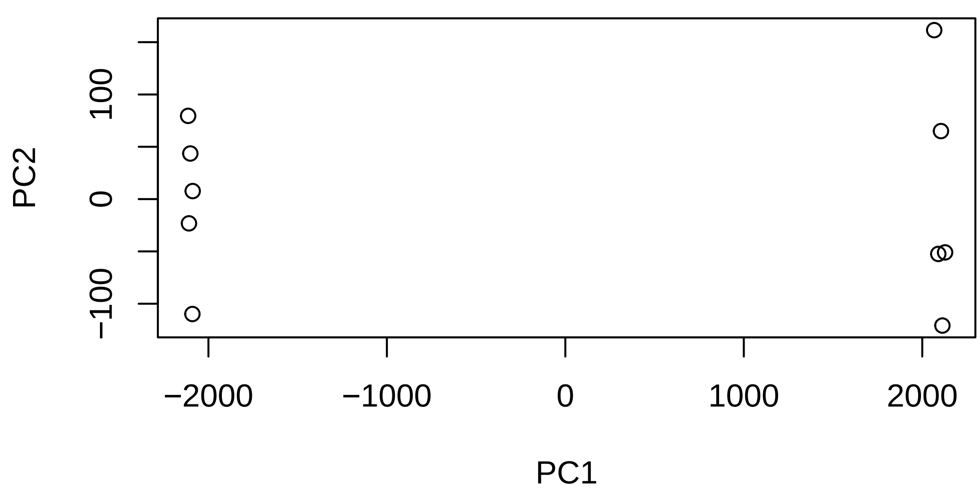
Let's apply PCA:

```r
pca_rna = prcomp( t(rna.data) )
summary(pca_rna)
```

```
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 3.142e-13
Proportion of Variance  0.00086  0.00073  0.00057 0.000e+00
Cumulative Proportion   0.99870  0.99943  1.00000 1.000e+00
```

Let's plot the principal components 1 and 2.

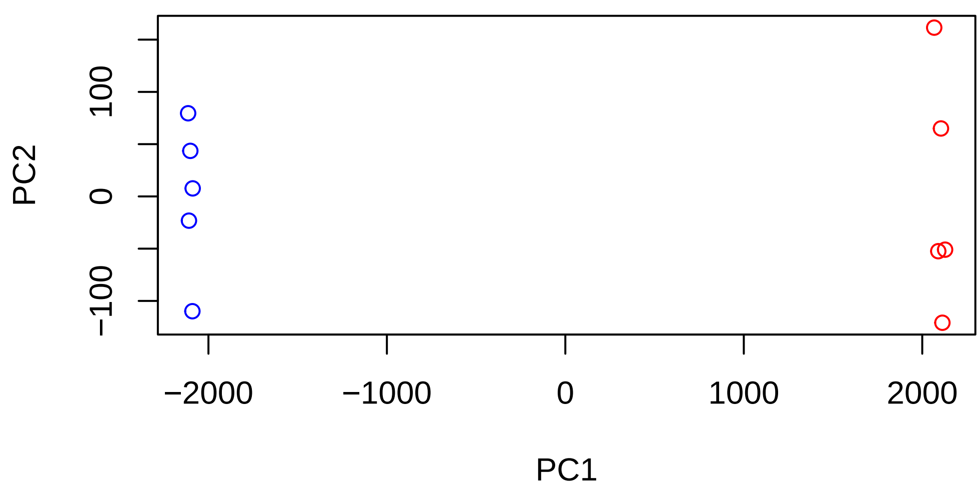
```r
plot( pca_rna$x[,1], pca_rna$x[,2],
      xlab = 'PC1', ylab = 'PC2')
```



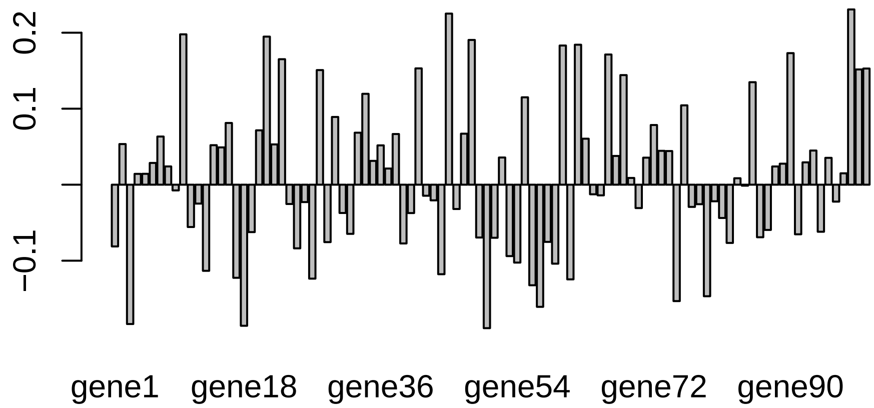

```r
cols_samples <- c( rep('blue', 5), rep('red', 5) )
cols_samples
```

```
[1] "blue" "blue" "blue" "blue" "blue" "red"  "red"  "red"  "red"  "red"
```

```r
plot( pca_rna$x[,1], pca_rna$x[,2],
      xlab = 'PC1', ylab = 'PC2',
      col = cols_samples)
```




```r
barplot(pca_rna$rotation[,1])
```




```
sort(pca_rna$rotation[,1])
```

```
     gene50      gene18       gene3      gene57      gene75      gene79
-0.188796985 -0.185668500 -0.183374164 -0.160771014 -0.153164404 -0.146803635
     gene56      gene61      gene27      gene17      gene44      gene13
-0.132330117 -0.124572881 -0.123615228 -0.122536548 -0.117808971 -0.113357525
     gene59      gene54      gene53      gene25       gene1      gene39
-0.103935563 -0.102503320 -0.093979884 -0.083761992 -0.081247810 -0.077306742
     gene82      gene29      gene58      gene51      gene49      gene86
-0.076658760 -0.075605635 -0.075274651 -0.069855142 -0.069530208 -0.069165267
     gene91      gene32      gene19      gene94      gene87      gene11
-0.065288752 -0.064721235 -0.062411218 -0.061938300 -0.059547317 -0.055698801
     gene81      gene40      gene31      gene46      gene70      gene77
-0.043780416 -0.037323670 -0.037219970 -0.031990529 -0.030784982 -0.029225446
     gene78      gene24      gene12      gene26      gene96      gene80
-0.025639741 -0.025407507 -0.024870802 -0.022868107 -0.022293151 -0.021824860
     gene43      gene42      gene65      gene64       gene9      gene84
-0.020617052 -0.014550791 -0.014052839 -0.012639567 -0.007495075 -0.001289937
     gene83      gene69       gene4       gene5      gene97      gene37
 0.008504287  0.008871890  0.014242602  0.014303808  0.014994546  0.021280555
     gene88       gene8      gene89       gene6      gene92      gene35
 0.024015925  0.024026657  0.027652967  0.028634131  0.029394259  0.031349942
```

```
     gene95      gene71      gene52      gene67      gene74      gene73
0.035342407 0.035589259 0.035802086 0.037840851 0.044286948 0.044581700
     gene93      gene15      gene36      gene14      gene22       gene2
0.044940861 0.049090676 0.051765605 0.052004194 0.053013523 0.053465569
     gene63       gene7      gene38      gene47      gene33      gene20
0.060529157 0.063389255 0.066665407 0.067141911 0.068437703 0.071571203
     gene72      gene16      gene30      gene76      gene55      gene34
0.078551648 0.081254592 0.089150461 0.104435777 0.114988217 0.119604059
     gene85      gene68      gene28      gene99     gene100      gene41
0.134907896 0.144227333 0.150812015 0.151678253 0.152877246 0.153077075
     gene23      gene66      gene90      gene60      gene62      gene48
0.165155192 0.171311307 0.173156806 0.183139926 0.184203008 0.190495289
     gene21      gene10      gene45      gene98
0.194884023 0.197905454 0.225149201 0.230633225
```