Class07

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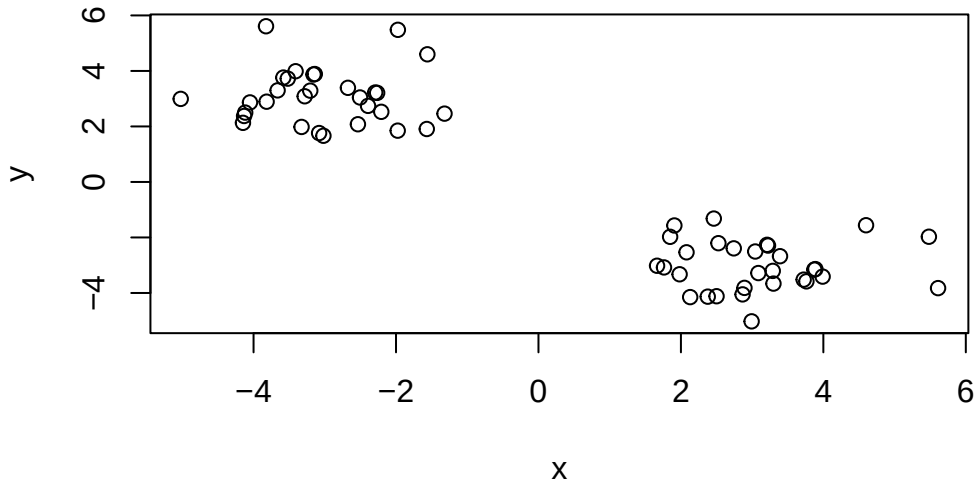
Example of K-means clustering

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

```
tmp <- c( rnorm(30, mean = -3), rnorm(30, mean = 3))

tmp
```

```
 [1] -1.318840 -3.139945 -2.292040 -5.022647 -2.206585 -3.662239 -3.519670
 [8] -4.132914 -2.392941 -2.534755 -4.148910 -3.326058 -1.559615 -3.158746
[15] -3.204317 -3.079850 -1.567982 -4.050482 -2.675170 -1.976201 -4.117288
[22] -3.409732 -1.973913 -3.019207 -2.505563 -3.825097 -3.581838 -2.264687
[29] -3.816681 -3.281927  3.087319  2.892237  3.209686  3.761985  5.610593
[36]  3.043669  1.664909  5.481754  3.989764  2.500497  1.848445  3.391406
[43]  2.865719  1.908092  1.762407  3.289631  3.872871  4.599365  1.981990
[50]  2.130156  2.078930  2.742149  2.376879  3.723546  3.299216  2.526489
[57]  2.992858  3.223002  3.888434  2.461687
```

```
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.

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

k
```

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

Cluster means:
          x         y
1 -3.025528  3.073523
2  3.073523 -3.025528

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 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] 52.68448 52.68448
 (between_SS / total_SS =  91.4 %)
```

```
Available components:

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

Let's explore K:

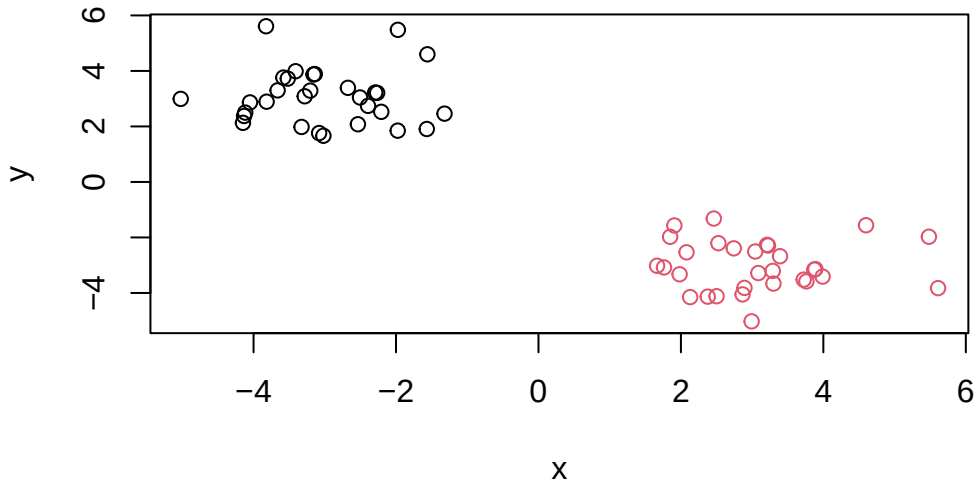
```
#We're exploring the size of k.

k$size
```

```
[1] 30 30
```

```
#We're exploring the centers of k.

k$centers
```

```
          x         y
1 -3.025528  3.073523
2  3.073523 -3.025528
```

```
#Now we plot the variable x and the clusters for k (k$clusters)

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

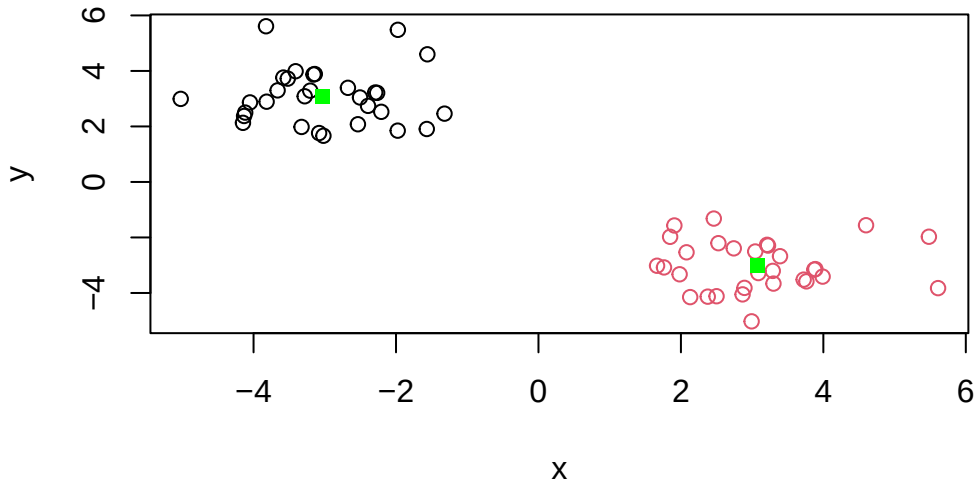



```
#We're exploring the cluster of k.

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 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
```

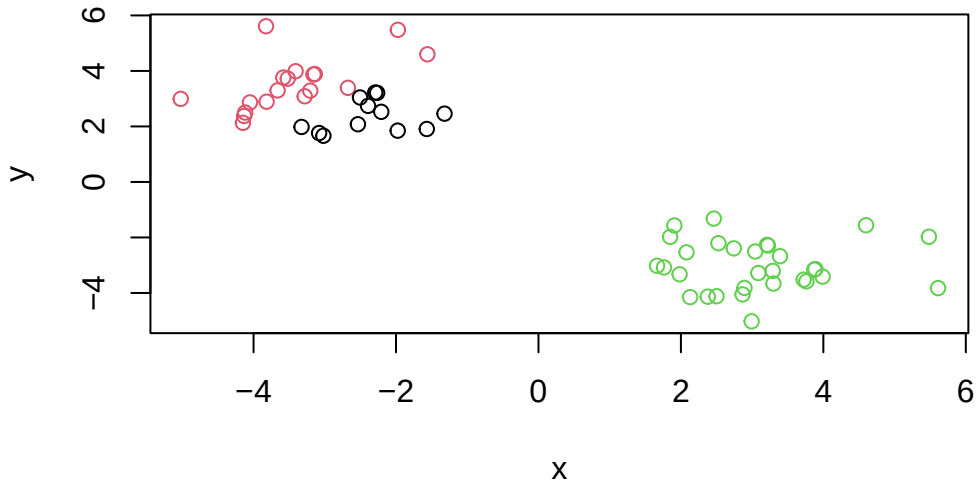
Now we can add the clusters centers:

```
#Using the plot of variable x and k$clusters

plot(x, col = k$cluster)

# We want to look at points 15 in the centers data.
# To higlight these points we use the function for color col = 'green'
points(k$centers, col = 'green', pch = 15)
```



An example,

```
k_3 <- kmeans(x, centers = 3, nstart = 20)

plot(x, col = k_3$cluster)
```



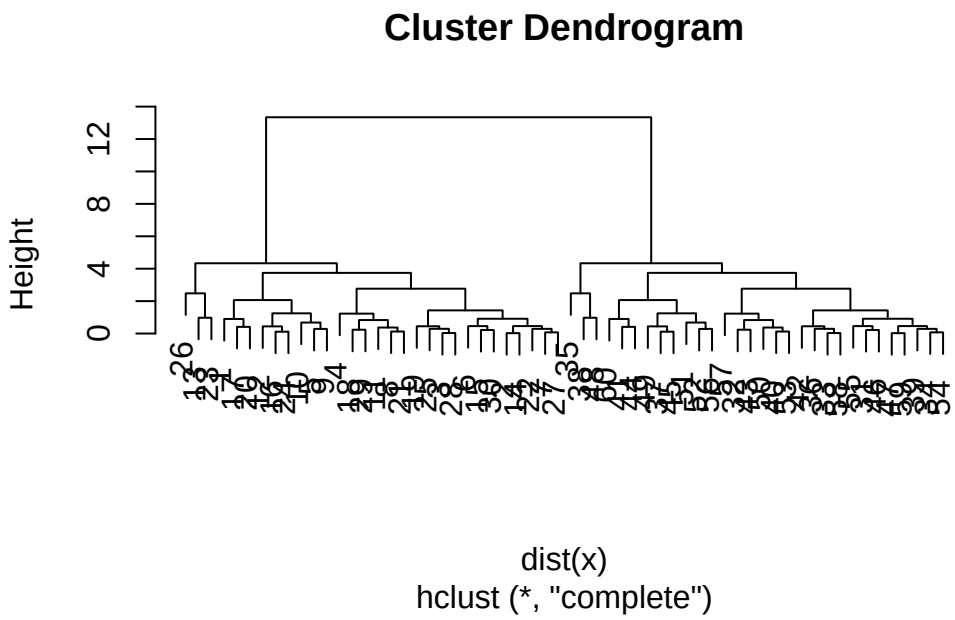
Example of Hierarchical Clustering

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

```
# By using the hclust() function we can cluster the data in dist(x).
clustering <- hclust(dist(x))

# Now we check that the new information was stored in clustering.
clustering
```

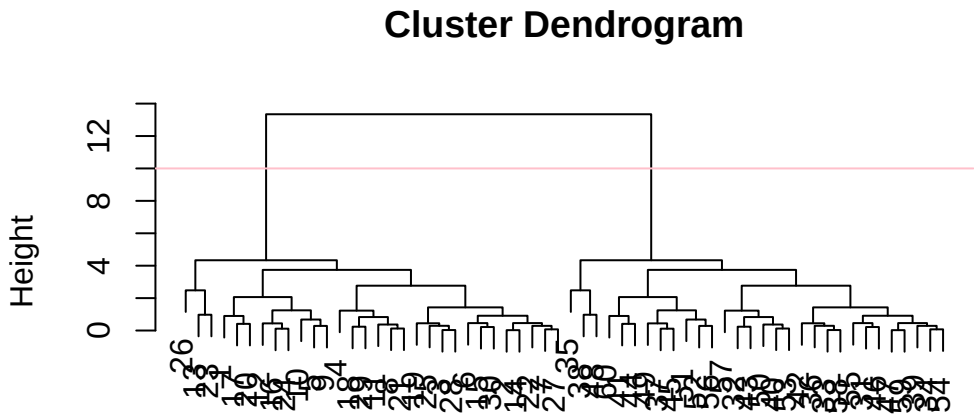
```
Call:
hclust(d = dist(x))

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

```
# We want to plot the clustering data.
plot(clustering)
```



Let's add a horizontal line

```
# Now that we have ploted the clustering data, we want to add a line
plot(clustering)

# We add a line by using the function abline(). However, we have to specify the height (10
abline(h = 10, col = 'pink')
```



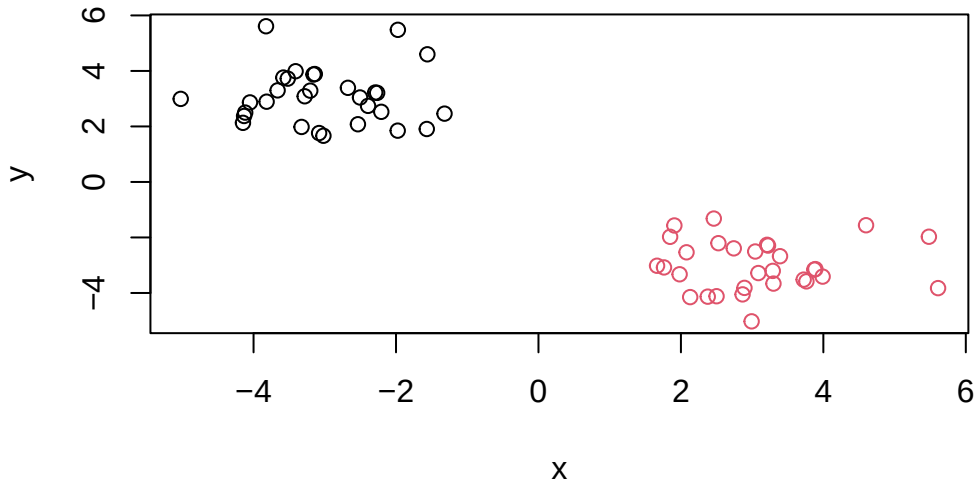
To get our results (i.e., membership vector) we need to "cut" the tree. The function for doing that is cutree().

```
# We want to store the vector under subgroup.
# We also specified that we want a height of 10.
subgroups <- cutree(clustering, h = 10)

# Check that the cutree function was stored in subgroups
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 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
```

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 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
```

Principal Compnent Analysis (PCA)

PCA of UK food data

First was to read the data

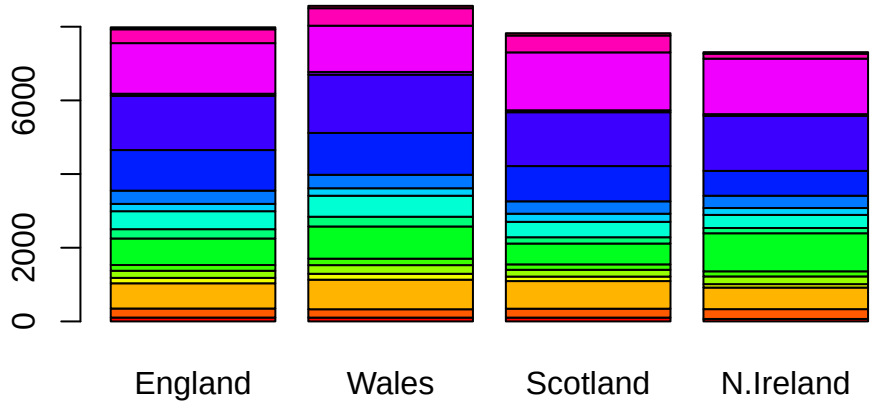
```
url <- "https://tinyurl.com/UK-foods"

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

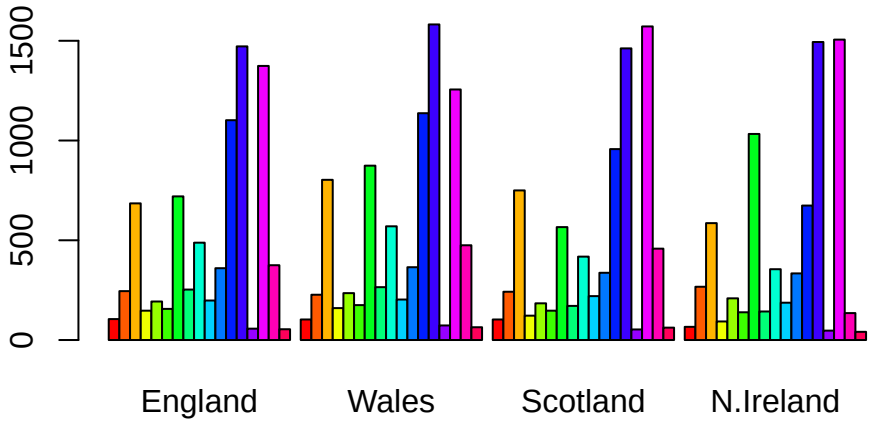
Now we can generate some basic visualizations

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



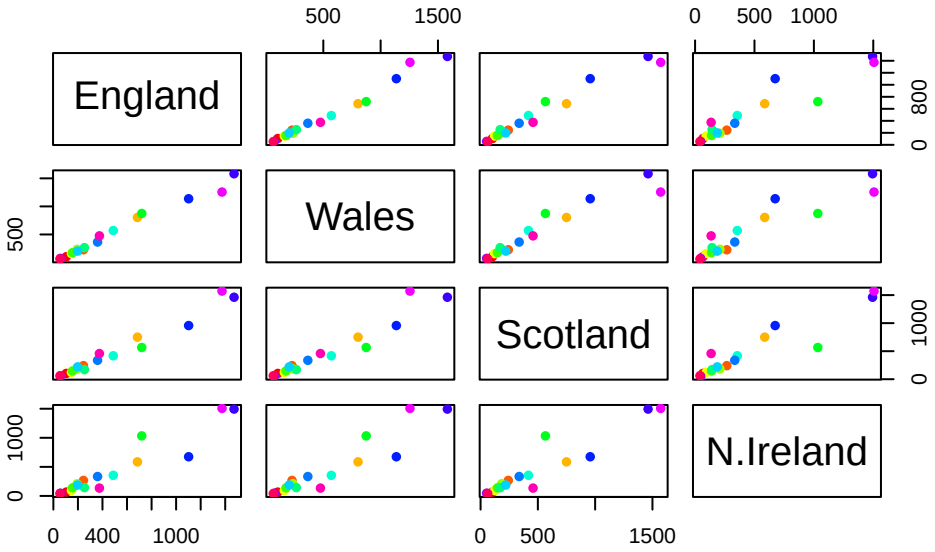
Let's refine our barplot

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



Other visualizations that can be useful…

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



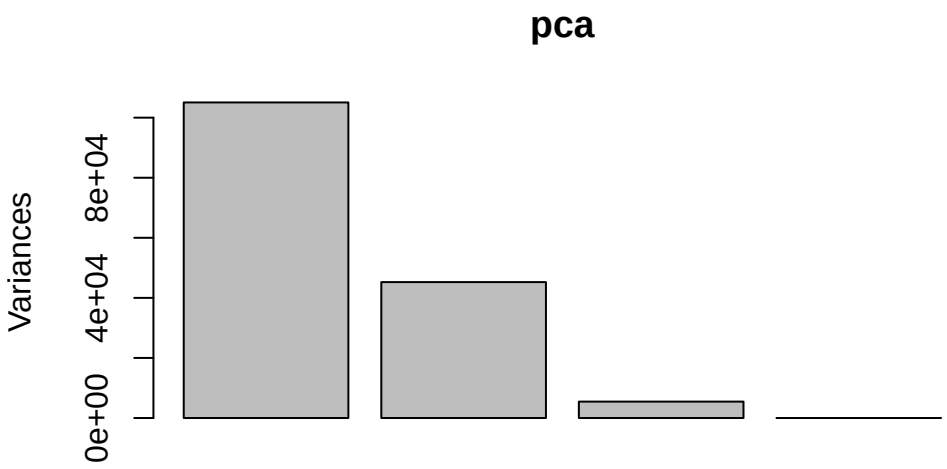
Let's apply PCA (principal components analysis). For that, we need to use the command prcomp(). This function expects the transpose of our data.

```
# 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 5.552e-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"
```

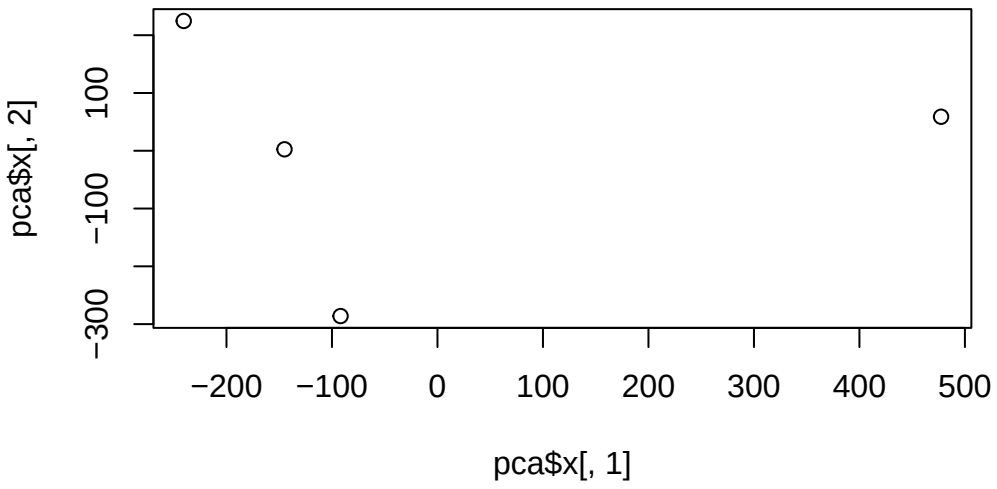
We can explore the pca$x dataframe:

```
pca$x
```

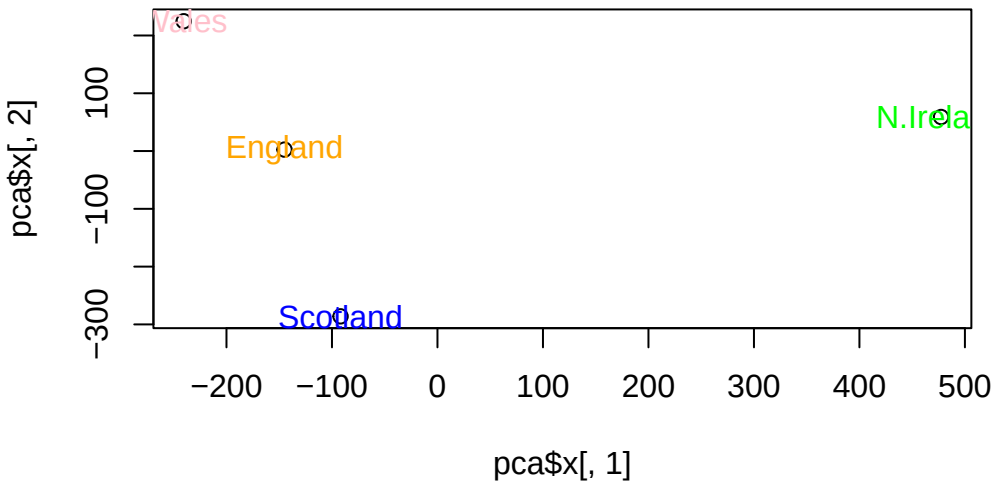
```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  1.042460e-14
Wales     -240.52915  224.646925   56.475555  9.556806e-13
Scotland   -91.86934 -286.081786   44.415495 -1.257152e-12
N.Ireland  477.39164   58.901862    4.877895  2.872787e-13
```

Plotting:

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




```r
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 RNA-seq data set

First is as always is loading the 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?

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

```
[1] 100  10
```

I have 100 genes, and 10 samples.

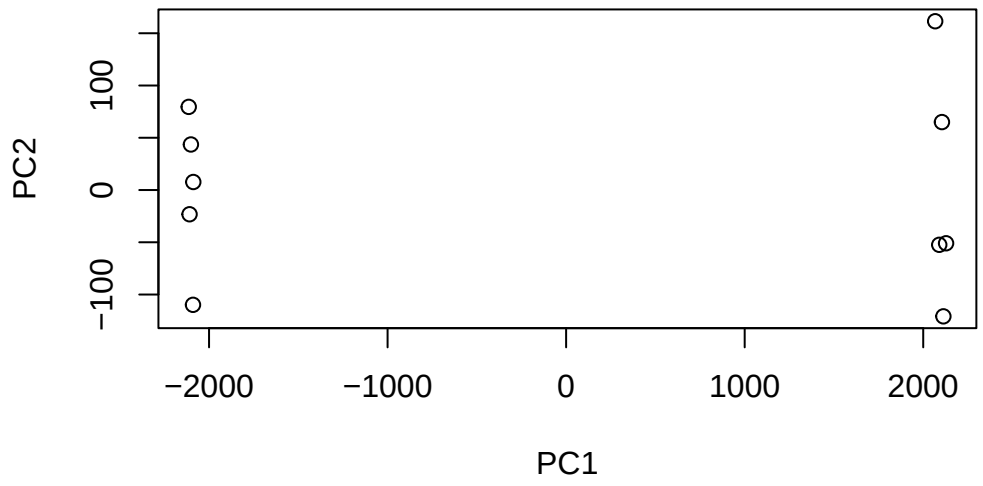
Let's apply PCA:

```
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 2.715e-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.

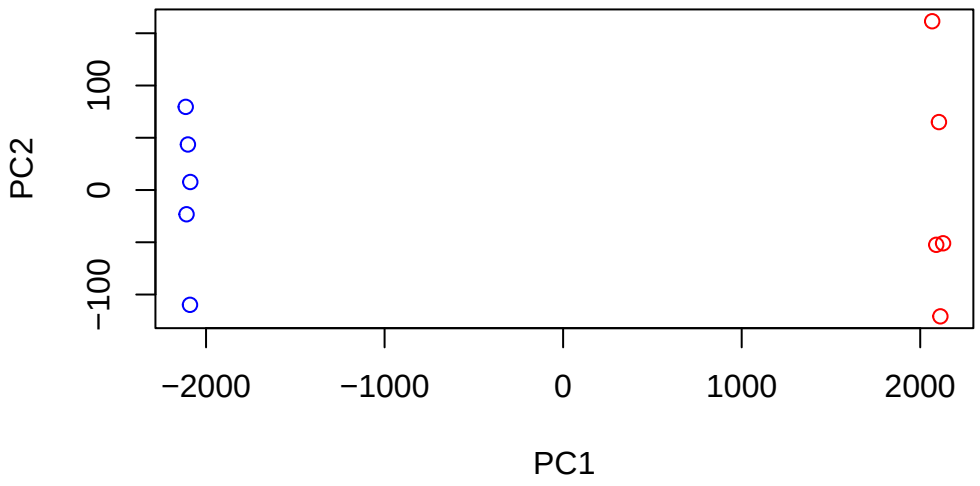
```
plot(pca_rna$x[,1], pca_rna$x[,2], xlab = 'PC1', ylab = 'PC2')
```



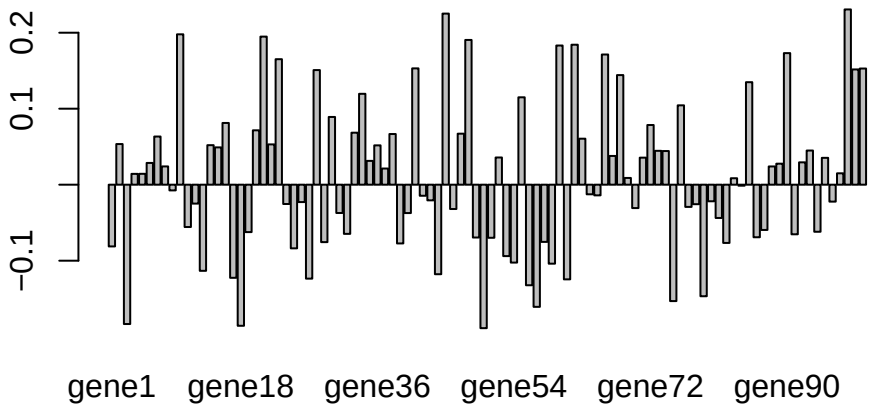

```
#We only want the information in the column of names for the rna.data
#colnames(rna.data)

#We want to change the color of the column names, where the left points will be colored bl

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

#We enter the cols_samples as a variable.

cols_samples
```

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

```
#Now we put everything together in the plot, so we have the color of the samples updated.

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




```
#We want to plot pca_rna$rotation into a barplot

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




```
# We're sorting the data for pca_rna$rotation

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		