Machine Learning 1

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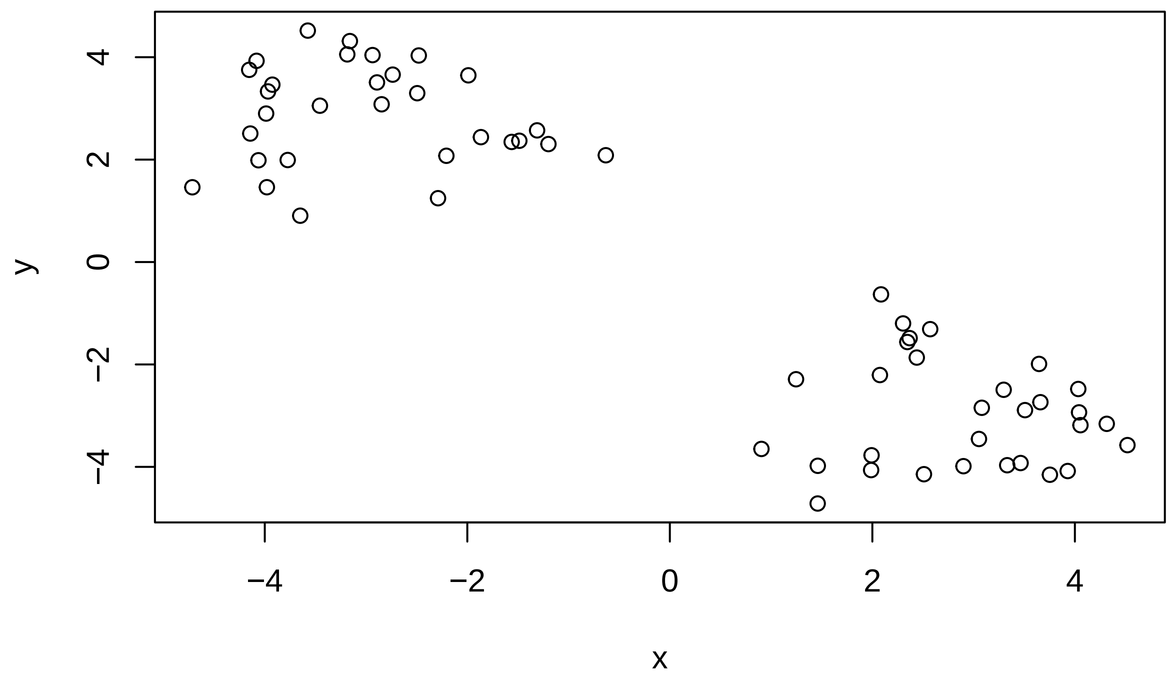
First up kmeans()

Demo of using kmeans() function in base R. First make up some data with a known structure.

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



Now we have some made up data in `x` let's see how kmeans works with this data.

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

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

```
##           x         y
## 1  2.877792 -2.958028
## 2 -2.958028  2.877792
##
## 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] 61.1301 61.1301
##  (between_SS / total_SS =  89.3 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

Q. How many points are in each cluster?

```r
k$size
```

```
## [1] 30 30
```

Q. How do we get to the cluster membership/assignment?

```r
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
```

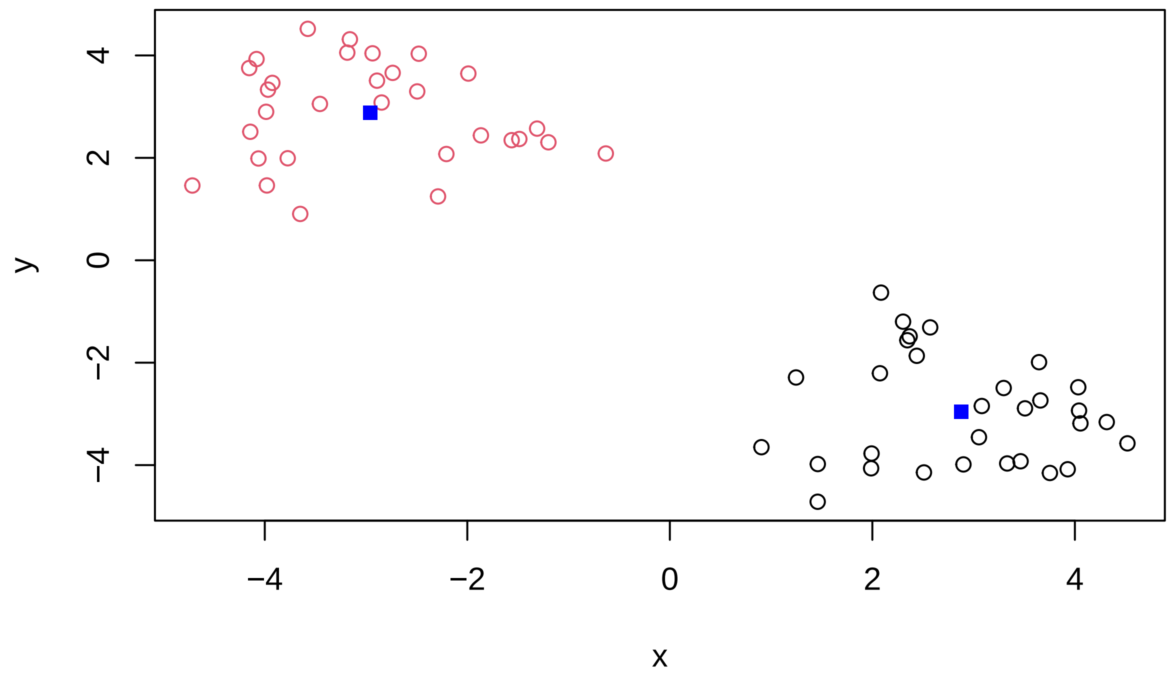
Q. What about cluster centers?

```r
k$centers
```

```
##           x         y
## 1  2.877792 -2.958028
## 2 -2.958028  2.877792
```

Now we got to the main results let's use them to plot our data with the kmeans result

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



Now for Hierarchical Clustering - hclust()

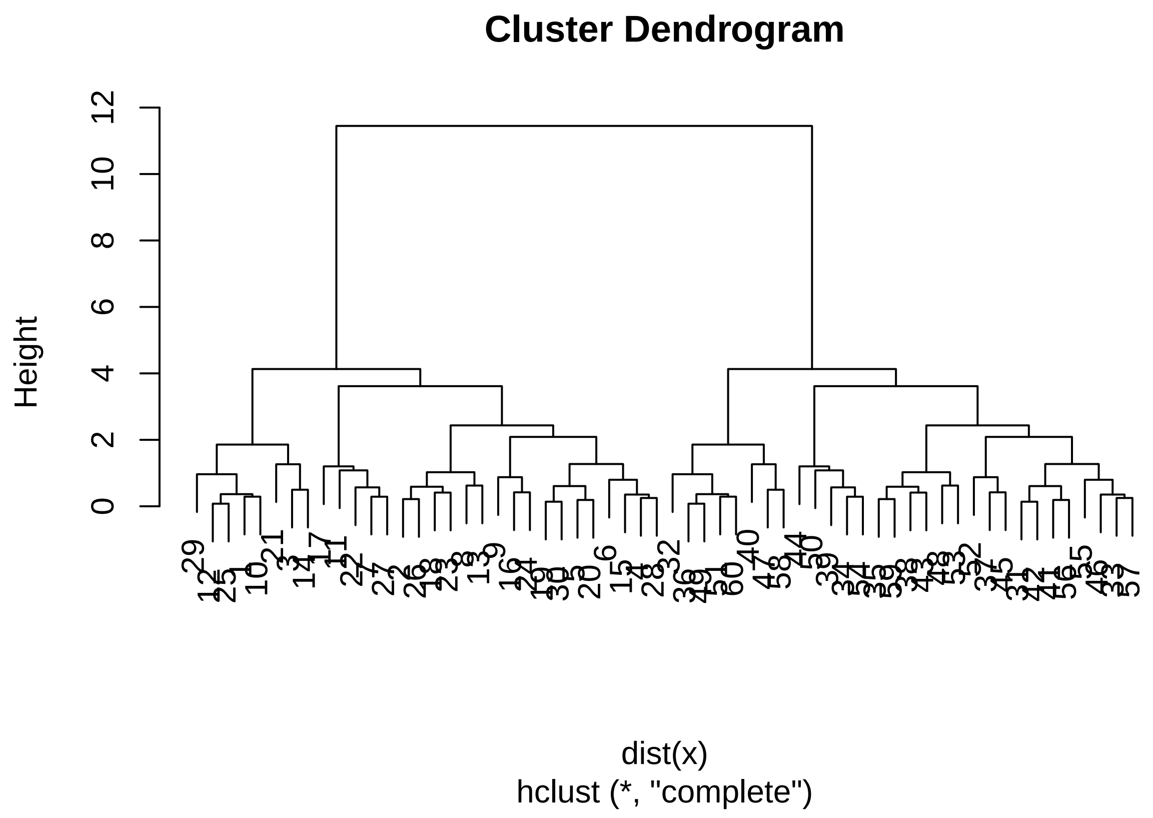
We will cluster the same data `x` with the `hclust()`. In this case `hclust()` requires a distance matrix as input.

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

```
##
## Call:
## hclust(d = dist(x))
##
## Cluster method   : complete
## Distance         : euclidean
## Number of objects: 60
```

Let's plot our hclust result

```
plot(hc)
```



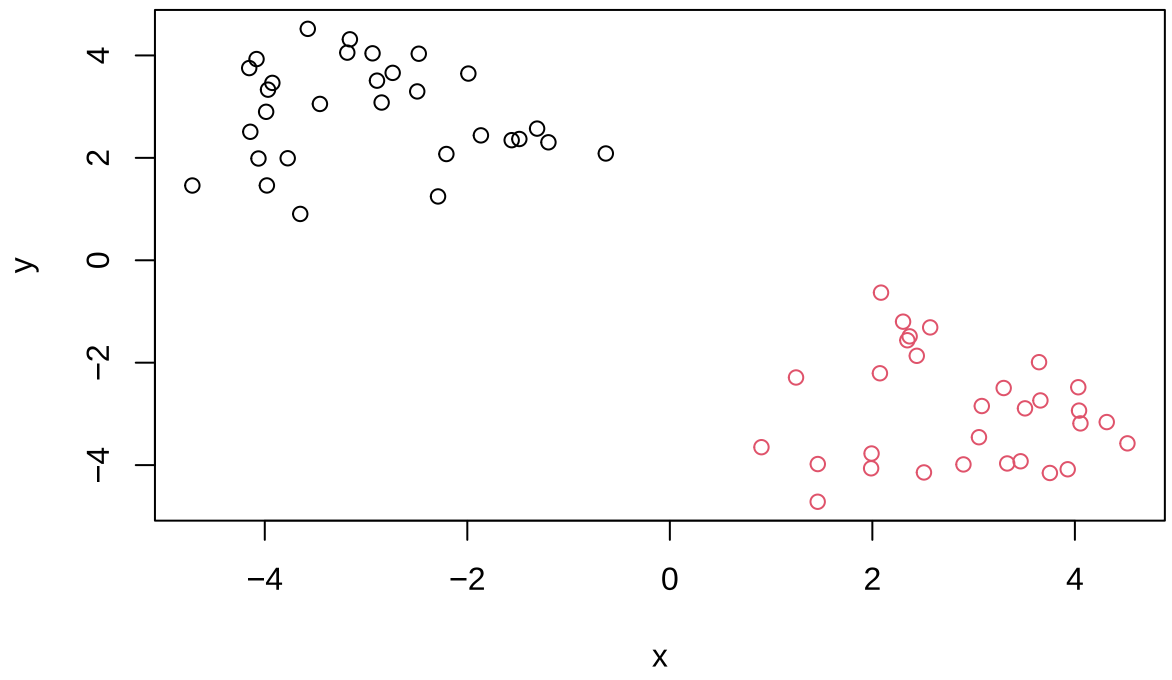
To get our cluster membership vector we need to "cut" the tree with the `cutree()`

```
grps <- cutree(hc, h = 8)
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 2 2
```

Now plot our data with the hclust() results.

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



Principal Component Analysis (PCA)

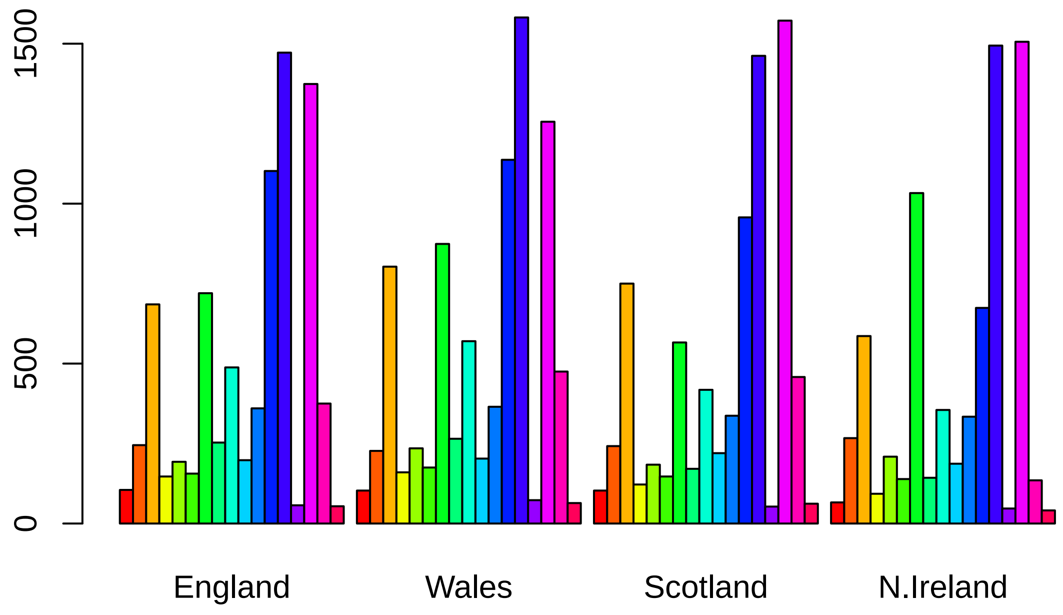
PCA of UK food data

Read data from webstie and try a few visualizations.

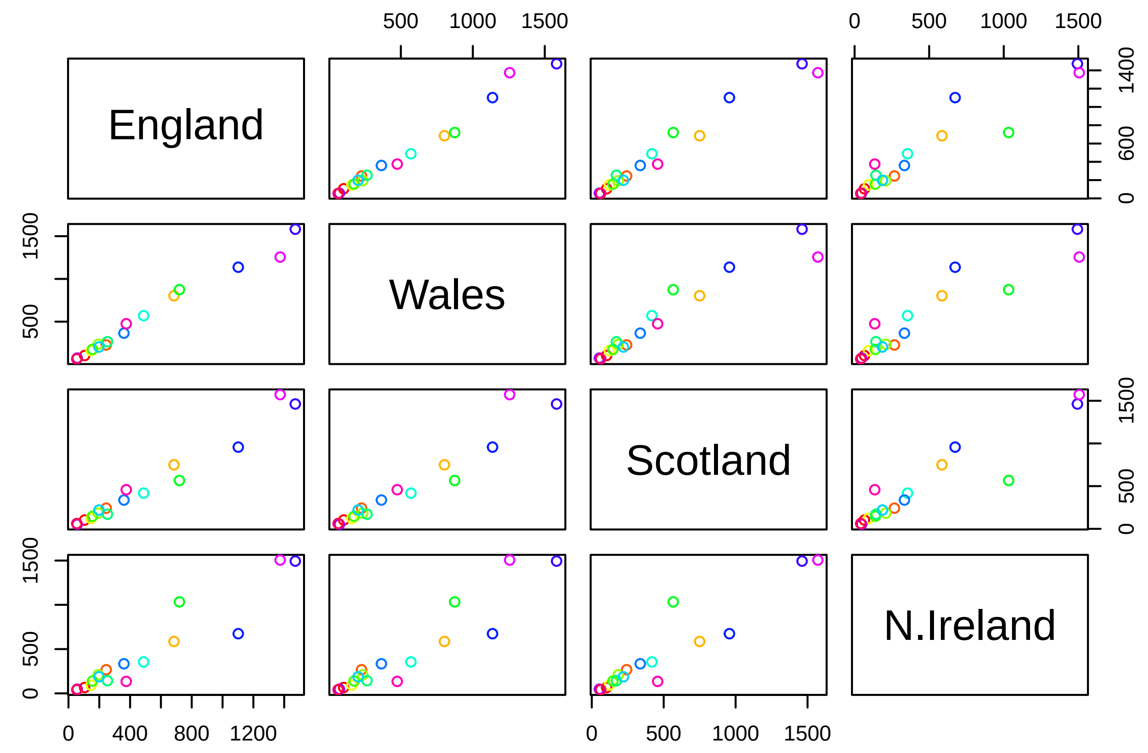
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
x
```

```
##                     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
## Fresh_potatoes          720   874      566      1033
## Fresh_Veg               253   265      171       143
## Other_Veg               488   570      418       355
## Processed_potatoes      198   203      220       187
## Processed_Veg           360   365      337       334
## Fresh_fruit            1102  1137      957       674
## Cereals                1472  1582     1462      1494
## Beverages                57    73       53        47
## Soft_drinks            1374  1256     1572      1506
## Alcoholic_drinks         375   475       458        135
## Confectionery             54    64        62         41
```

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



```
pairs(x, col = cols)
```



PCA to the rescue!!

The main base R PCA function is called `prcomp()` and we will need to give it the transpose of our input data!

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

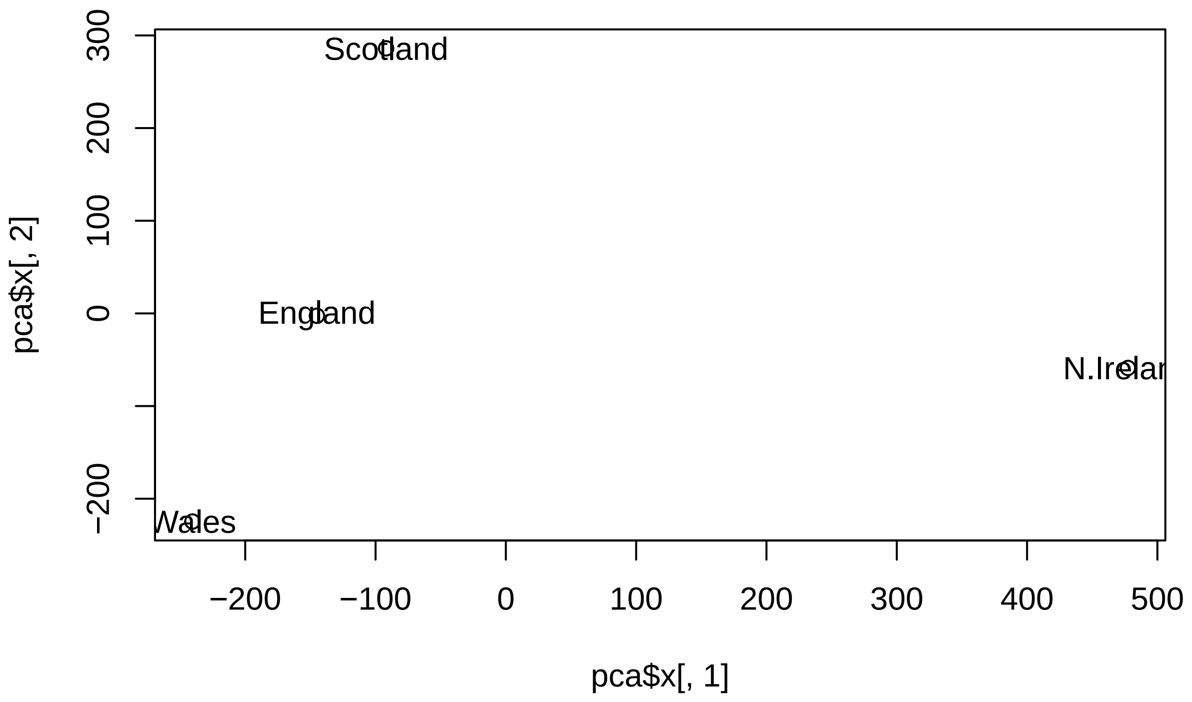
```
## Standard deviations (1, .., p=4):
## [1] 3.241502e+02 2.127478e+02 7.387622e+01 2.921348e-14
##
## Rotation (n x k) = (17 x 4):
##                             PC1          PC2         PC3          PC4
## Cheese              -0.056955380  0.016012850  0.02394295 -0.409382587
## Carcass_meat         0.047927628  0.013915823  0.06367111  0.729481922
## Other_meat          -0.258916658 -0.015331138 -0.55384854  0.331001134
## Fish                -0.084414983 -0.050754947  0.03906481  0.022375878
## Fats_and_oils       -0.005193623 -0.095388656 -0.12522257  0.034512161
## Sugars              -0.037620983 -0.043021699 -0.03605745  0.024943337
## Fresh_potatoes       0.401402060 -0.715017078 -0.20668248  0.021396007
## Fresh_Veg           -0.151849942 -0.144900268  0.21382237  0.001606882
## Other_Veg           -0.243593729 -0.225450923 -0.05332841  0.031153231
## Processed_potatoes  -0.026886233  0.042850761 -0.07364902 -0.017379680
## Processed_Veg       -0.036488269 -0.045451802  0.05289191  0.021250980
## Fresh_fruit         -0.632640898 -0.177740743  0.40012865  0.227657348
## Cereals             -0.047702858 -0.212599678 -0.35884921  0.100043319
## Beverages           -0.026187756 -0.030560542 -0.04135860 -0.018382072
## Soft_drinks          0.232244140  0.555124311 -0.16942648  0.222319484
## Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.273126013
## Confectionery       -0.029650201  0.005949921 -0.05232164  0.001890737
```

```r
attributes(pca)
```

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

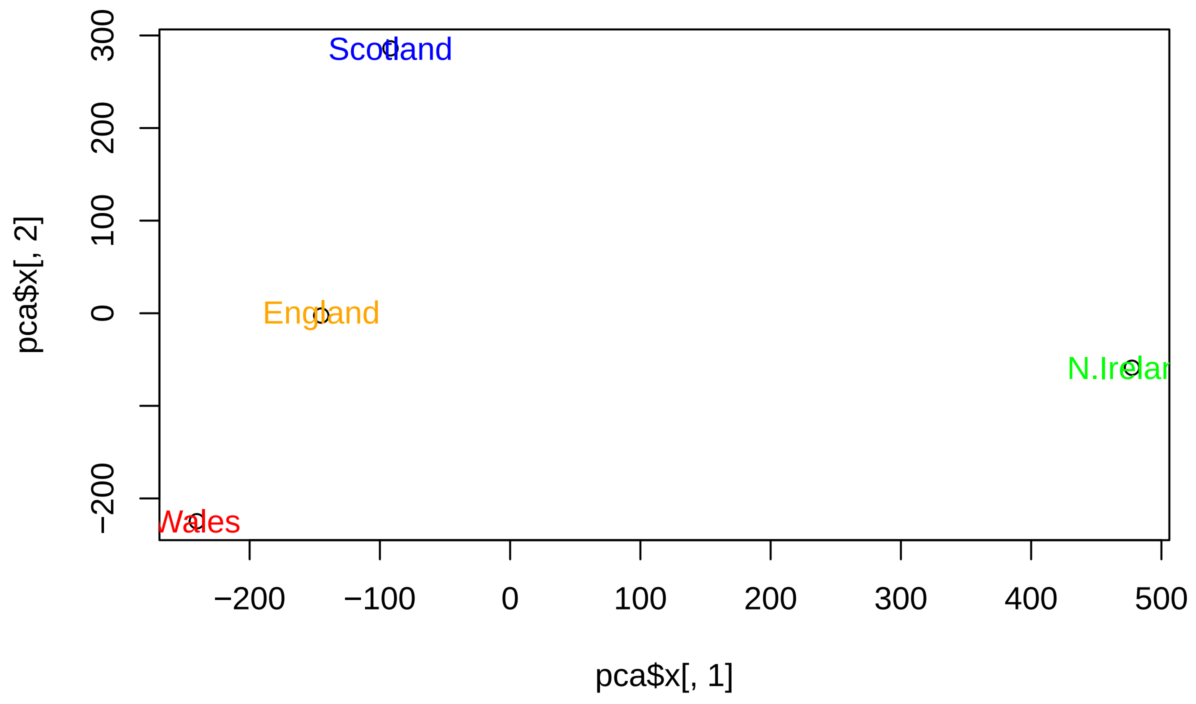
To make our new PCA plot (a.k.a. PCA score plot) we access `pca$x`

```r
plot(pca$x[,1], pca$x[,2])
text(pca$x[,1], pca$x[,2], colnames(x))
```



color up the plot

```r
country_cols <- c("orange", "red", "blue", "green")
plot(pca$x[,1], pca$x[,2])
text(pca$x[,1], pca$x[,2], colnames(x), col = country_cols)
```



PCA of RNA-seq data:

Read in data from website:

```
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
```

Q.10: How many genes and samples are in this data set?

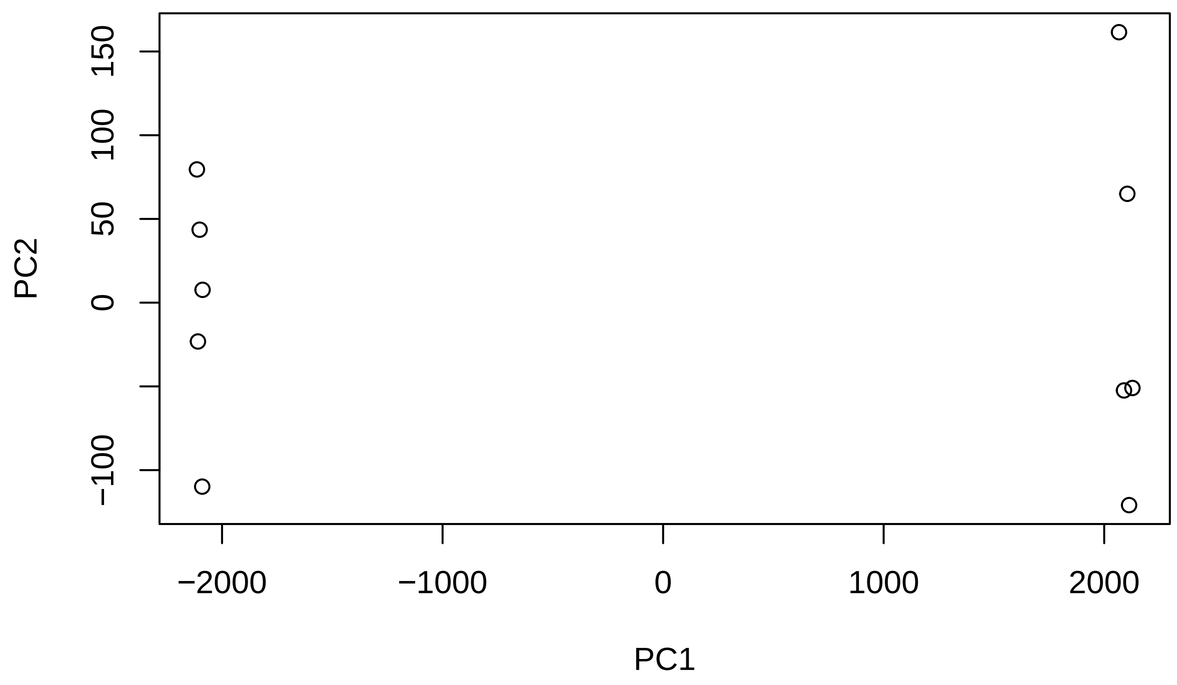
```
pca <-prcomp(t(rna.data))

# There is a nice summary of how well PCA is doing
summary(pca)
```

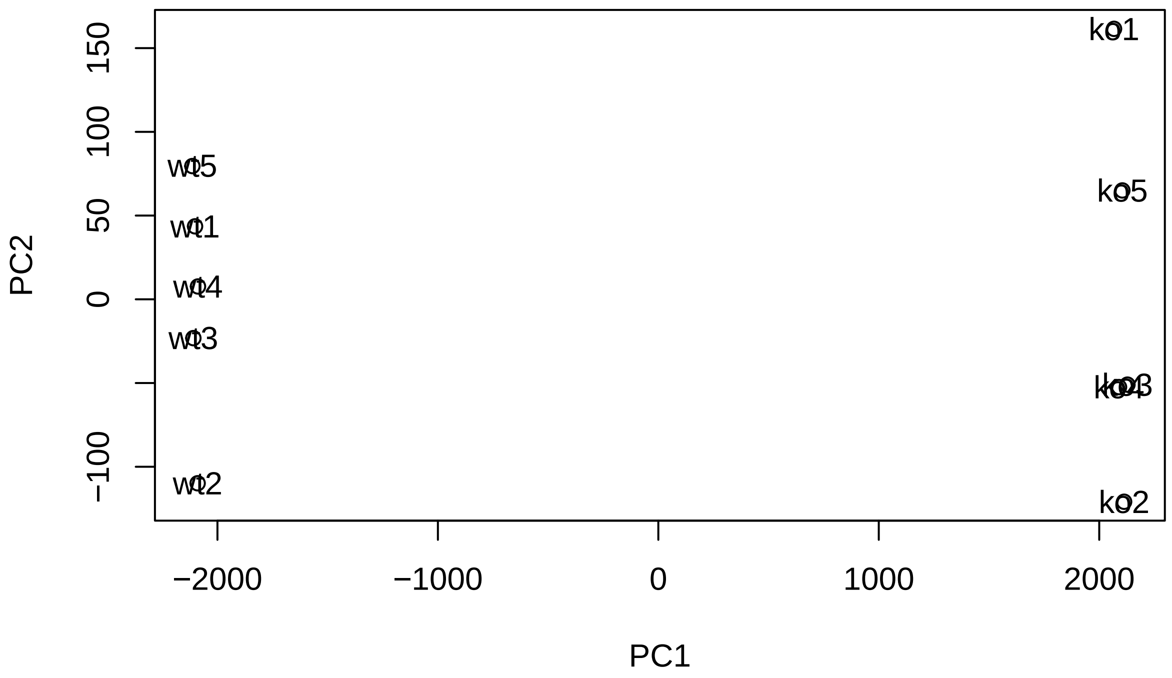
```
## Importance of components:
##                              PC1     PC2      PC3      PC4      PC5      PC6
## Standard deviation     2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
## Proportion of Variance    0.9917  0.0016  0.00144  0.00122  0.00098  0.00093
## Cumulative Proportion     0.9917  0.9933  0.99471  0.99593  0.99691  0.99784
##                              PC7      PC8      PC9      PC10
## Standard deviation     65.29428 59.90981 53.20803 2.662e-13
## Proportion of Variance  0.00086  0.00073  0.00057 0.000e+00
## Cumulative Proportion   0.99870  0.99943  1.00000 1.000e+00
```

Do our PCA plot of this RNA-Seq data

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



```r
plot(pca$x[,1], pca$x[,2], xlab = "PC1", ylab = "PC2")
text(pca$x[,1], pca$x[,2], colnames(rna.data))
```



ko1
wt5
ko5
wt1
wt4
wt3
ko3
ko4
wt2
ko2
150
100
50
0
−100
−2000
−1000
0
1000
2000
PC1
PC2