Machine Learning 1

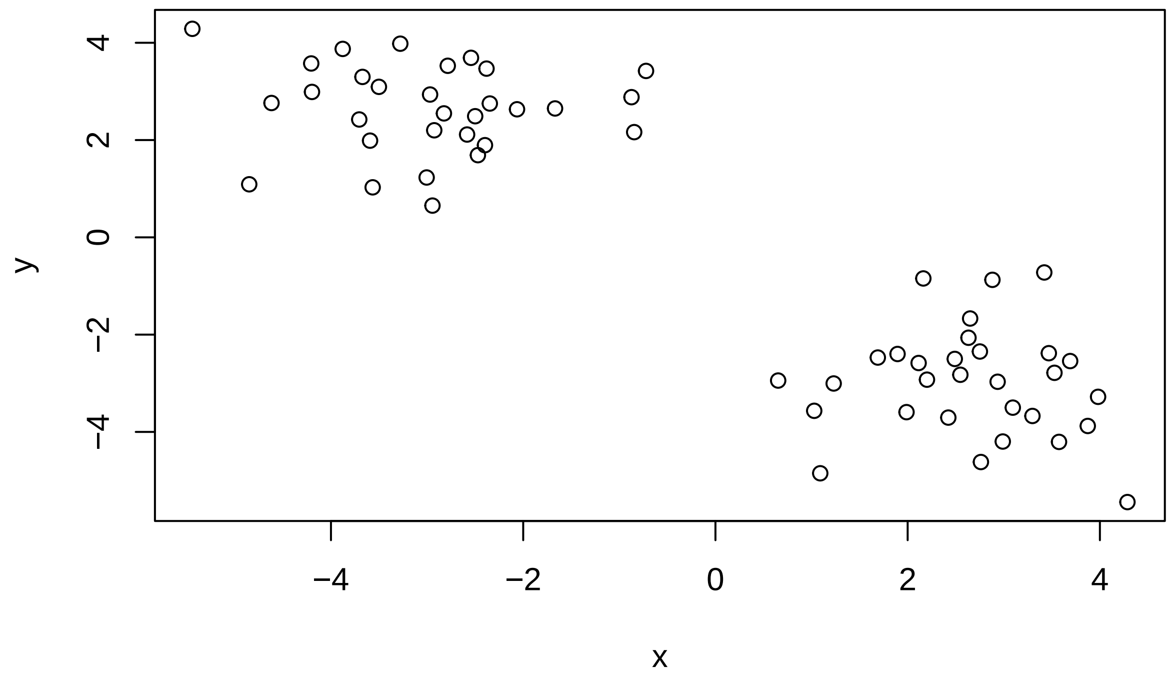
Angela Abraham

2025-10-21

First up kmeans()

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

```r
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

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

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##           x         y
## 1  2.644404 -2.978722
## 2 -2.978722  2.644404
##
## 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] 61.40128 61.40128
##  (between_SS / total_SS =  88.5 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

Q. How many points are in each cluster

```
k$size
```

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

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

```
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
```

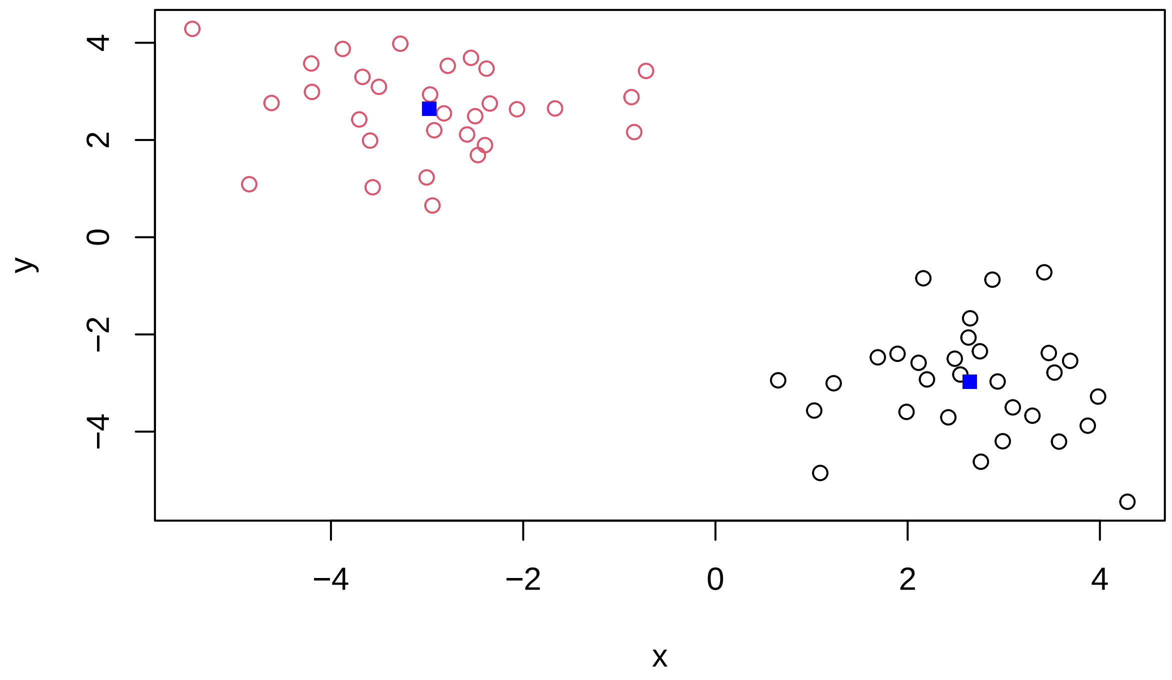
Q. What about cluster centers?

```
k$centers
```

```
##           x         y
## 1  2.644404 -2.978722
## 2 -2.978722  2.644404
```

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

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



Now for Hierarchical Clustering

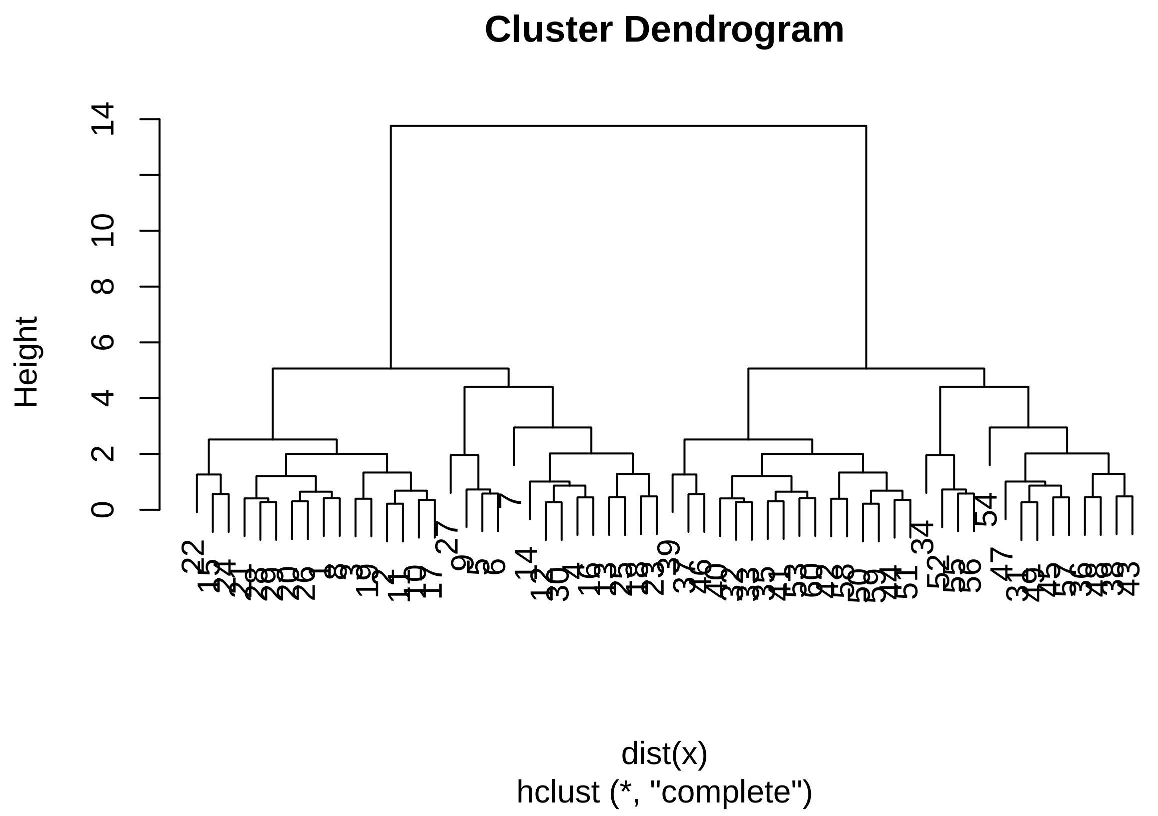
We will cluster the same data 'x' with the 'hclust()'. In this case 'hclust()' requires a distance matrix as input.

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

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

Let's plot our hclist result

```r
plot(hc)
```



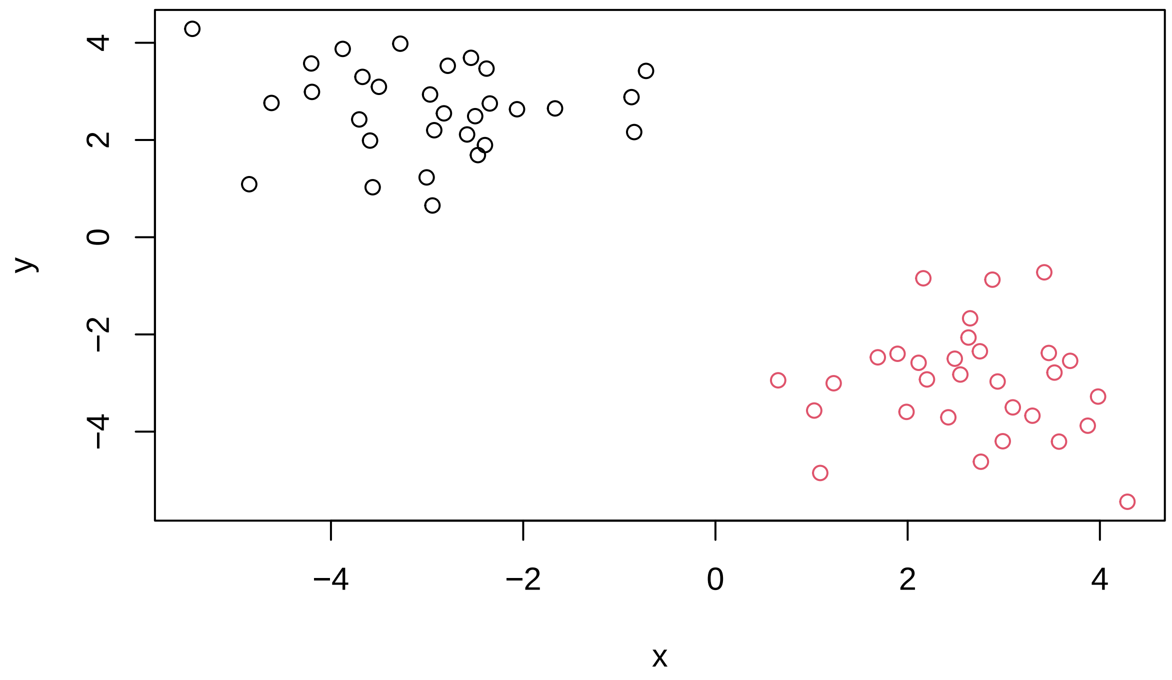
To get our cluster membership vector we need to “cut” the tree with the ‘cutree()’

```
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
```

Now plot our data with the hclust() results.

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



#Principal Component Analysis (PCA)

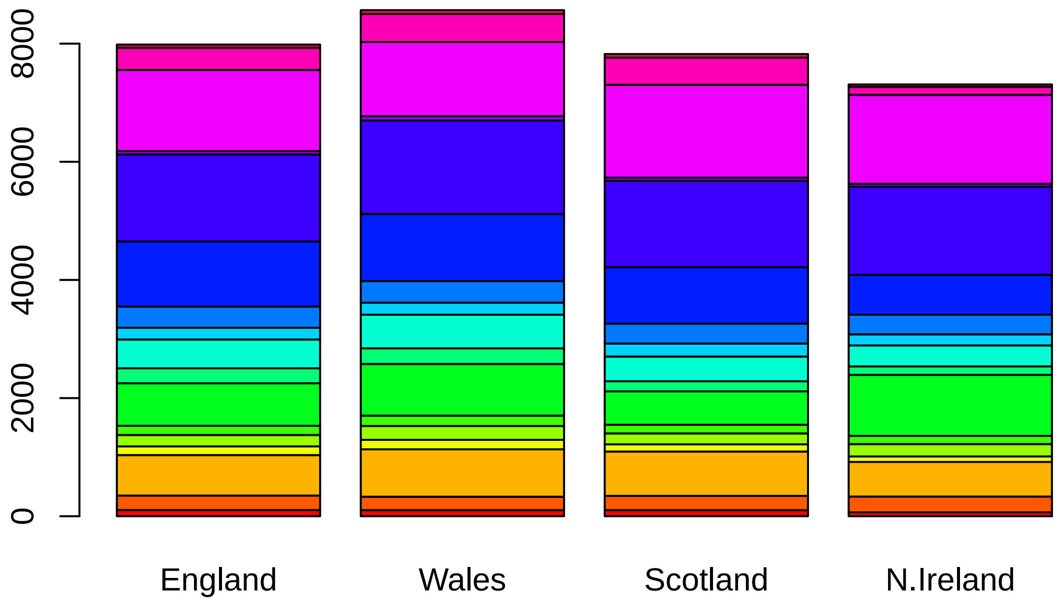
PCA of UK food data

Read data from website and try a few visualizations.

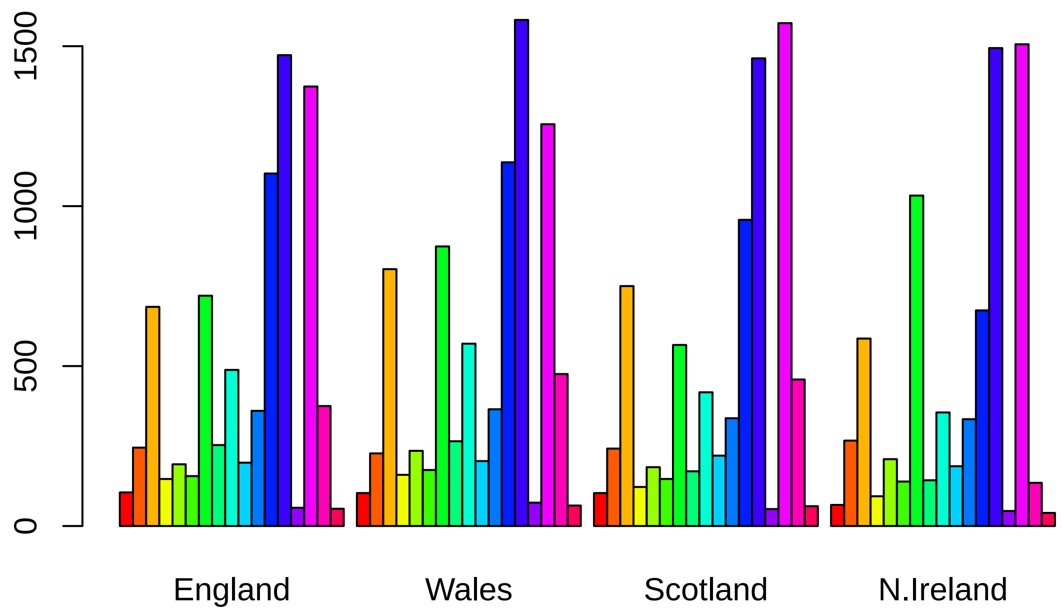
```r
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names=1)
x
```

```
##                     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
```

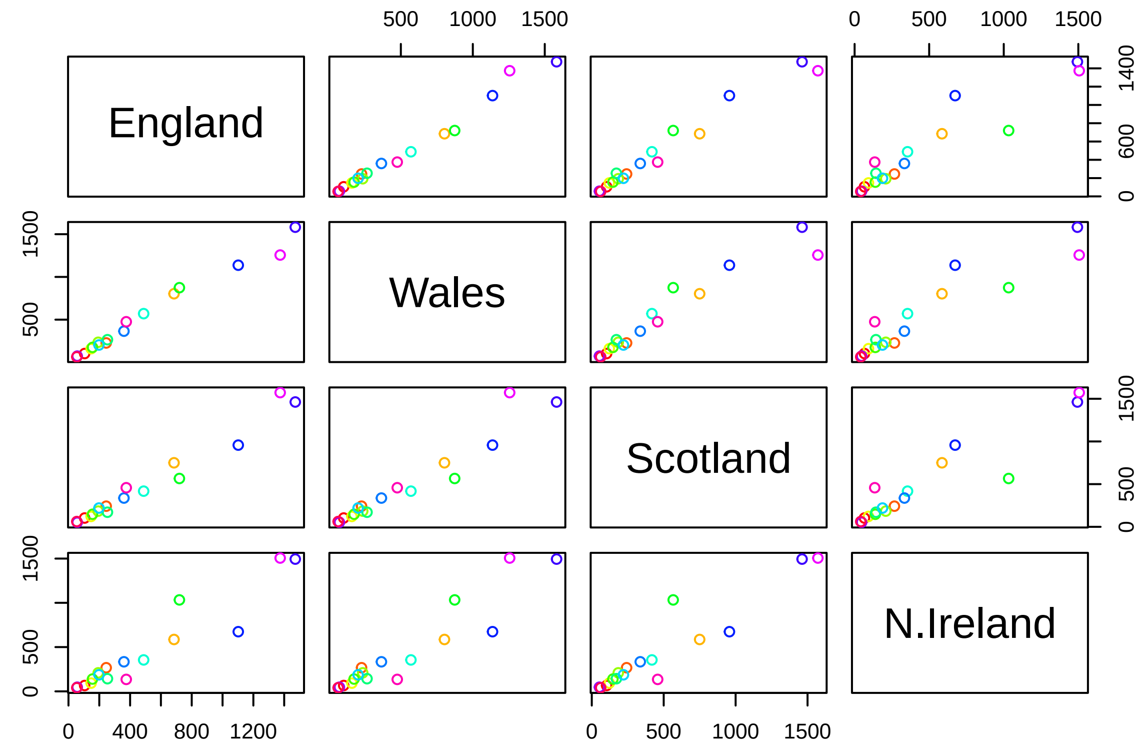
```
cols<-rainbow(nrow(x))
barplot(as.matrix(x), col=cols )
```



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



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



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

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

There is a nice summary of how well PCA is doing

```r
summary(pca)
```

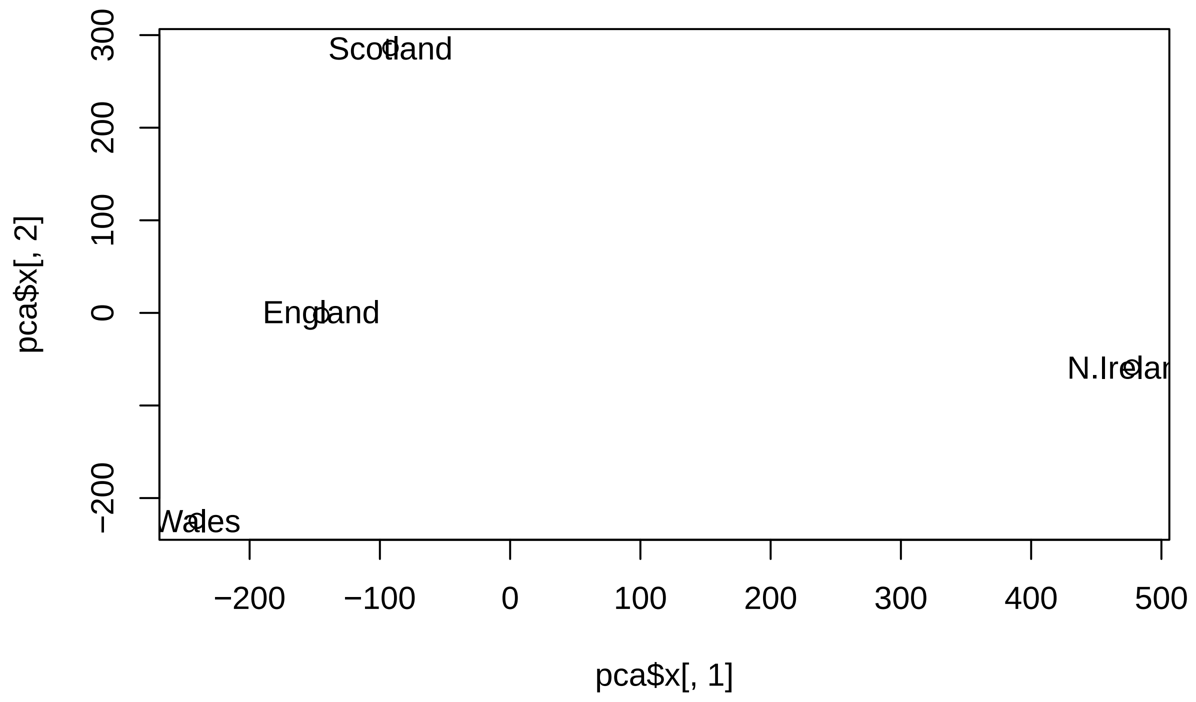
```
## Importance of components:
##                             PC1      PC2      PC3       PC4
## Standard deviation     324.1502 212.7478 73.87622 3.176e-14
## Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
## Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```r
attributes(pca)
```

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

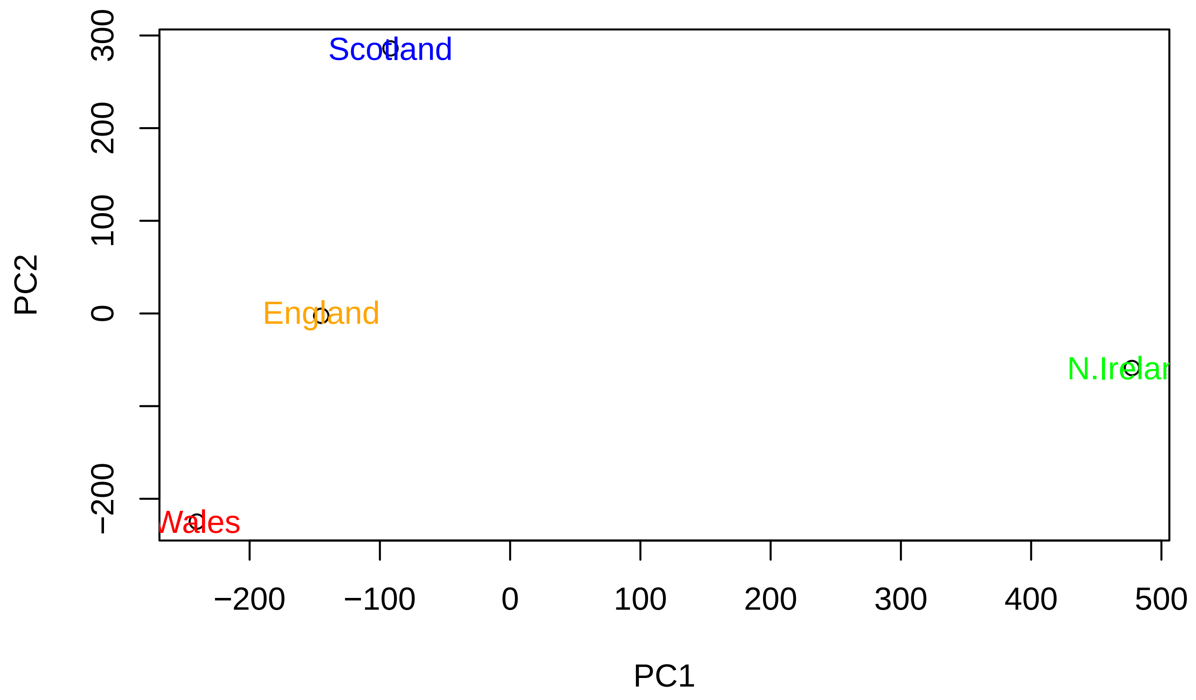
To make our new PCA plot (a.k.a PCA score plot) we access 'pca$x'

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



color up the plot

```
country_cols<- c("orange", "red", "blue", "green")
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
text(pca$x[,1], pca$x[,2], colnames(x), col=country_cols)
```



PCA of RNA-Seq data

Read in data from website

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

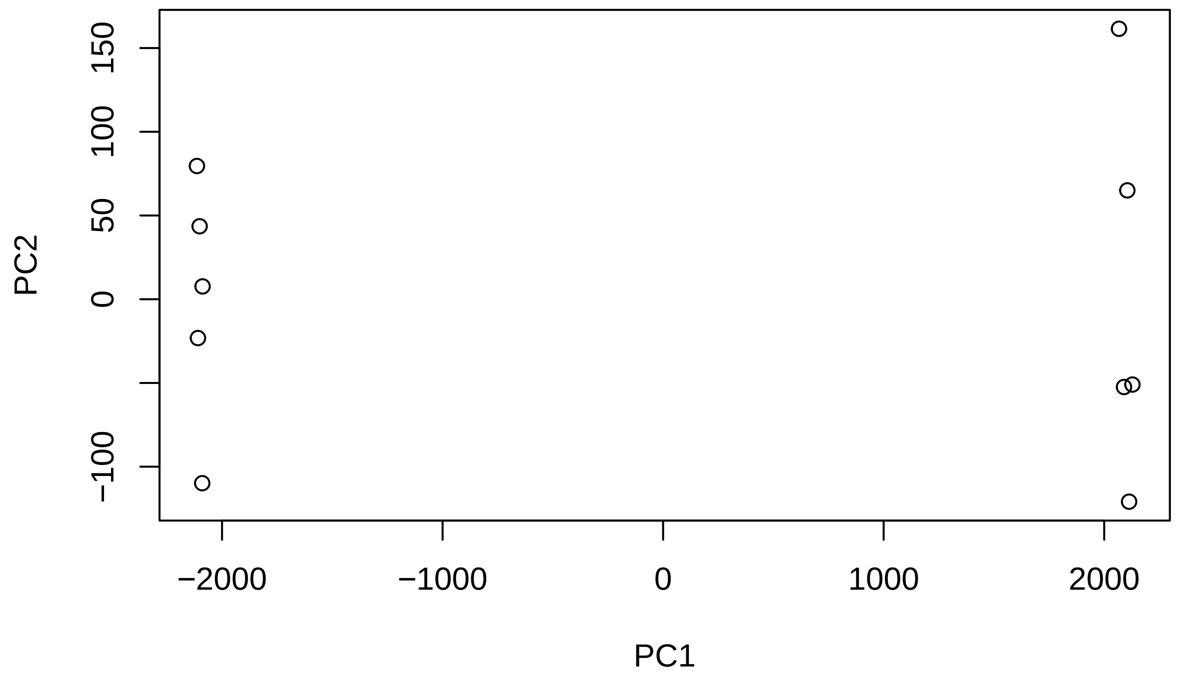
```
##        wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
## gene1  439 458  408  429 420  90  88  86  90  93
## gene2  219 200  204  210 187 427 423 434 433 426
## gene3 1006 989 1030 1017 973 252 237 238 226 210
## gene4  783 792  829  856 760 849 856 835 885 894
## gene5  181 249  204  244 225 277 305 272 270 279
## gene6  460 502  491  491 493 612 594 577 618 638
```

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

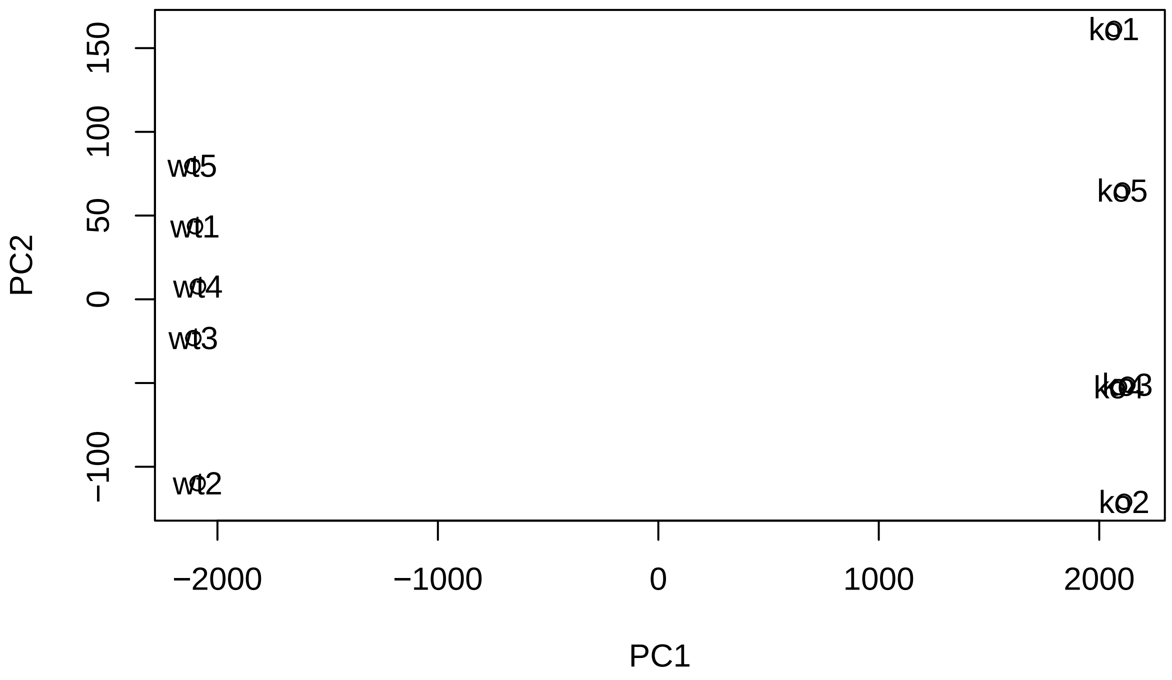
```
## Importance of components:
##                              PC1     PC2      PC3      PC4      PC5      PC6
## Standard deviation     2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
## Proportion of Variance    0.9917  0.0016  0.00144  0.00122  0.00098  0.00093
## Cumulative Proportion     0.9917  0.9933  0.99471  0.99593  0.99691  0.99784
##                               PC7      PC8      PC9      PC10
## Standard deviation     65.29428 59.90981 53.20803 2.684e-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

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



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


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