Machine Learning 1

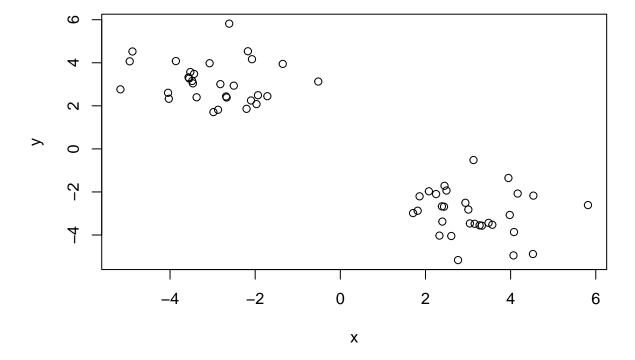
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2/8/2022

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)</pre>
```



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</pre>
```

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##
## 1 3.120216 -2.985689
## 2 -2.985689 3.120216
##
## Clustering vector:
## Within cluster sum of squares by cluster:
## [1] 59.50783 59.50783
## (between_SS / total_SS = 90.4 %)
## 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

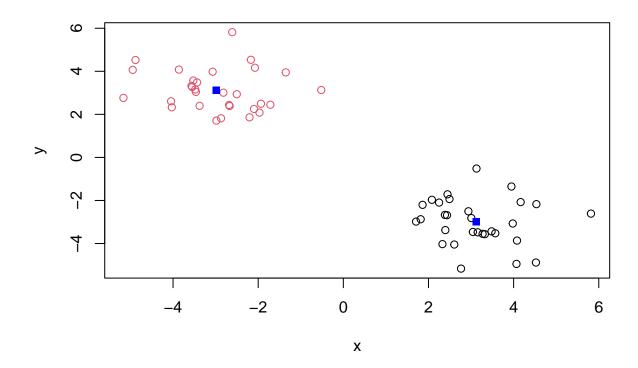
Q. What about cluster centers?

k\$centers

```
## x y
## 1 3.120216 -2.985689
## 2 -2.985689 3.120216
```

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

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



Now for hclust()

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

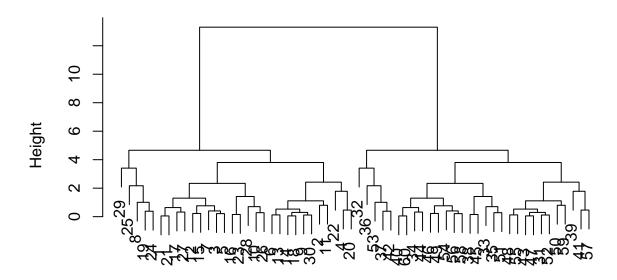
```
hc <- hclust(dist(x))
hc

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

Let's plot our hclust result

plot(hc)</pre>
```

Cluster Dendrogram



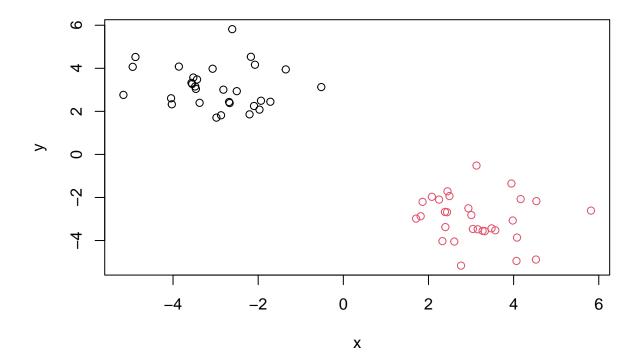
dist(x) hclust (*, "complete")

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

```
grps <- cutree(hc, h=8)
grps</pre>
```

Now plot our data with the hclust() results.

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



Principal Component Analysis (PCA)

PCA of UK food data

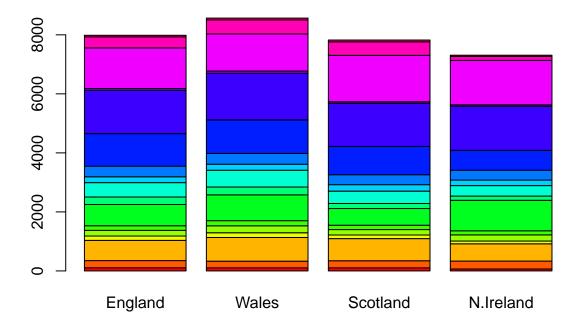
Read data from website and try a few visualizations.

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

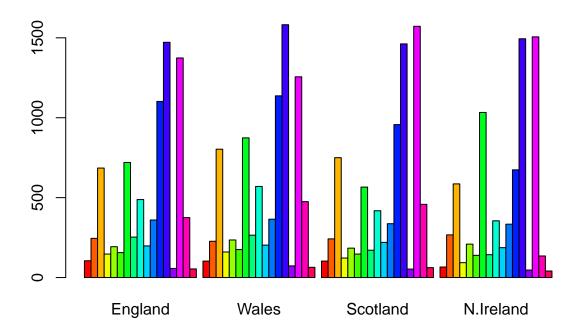
##		England	Wales	Scotland	N.Ireland
##	Cheese	105	103	103	66
##	Carcass_meat	245	227	242	267
##	Other_meat	685	803	750	586
##	Fish	147	160	122	93
##	Fats_and_oils	193	235	184	209
##	Sugars	156	175	147	139
##	Fresh_potatoes	720	874	566	1033
##	Fresh_Veg	253	265	171	143
##	Other_Veg	488	570	418	355
##	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
                                 475
                                          458
                                                    135
                           375
## Confectionery
                            54
                                  64
                                           62
                                                     41
```

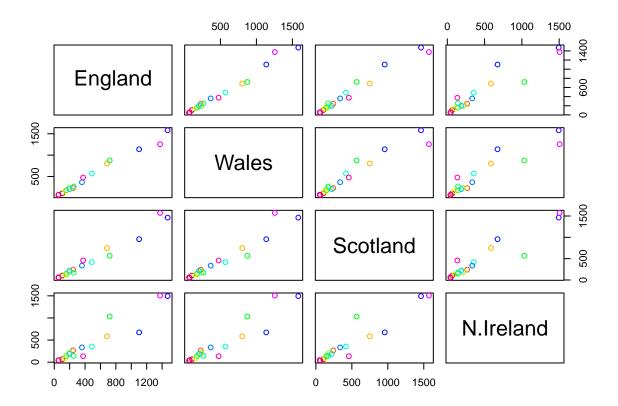
```
cols <- rainbow(nrow(x))
barplot(as.matrix(x), col=cols)</pre>
```



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!

```
pca <- prcomp(t(x))</pre>
```

There is a nice summary of how well PCA is doing

```
summary(pca)
```

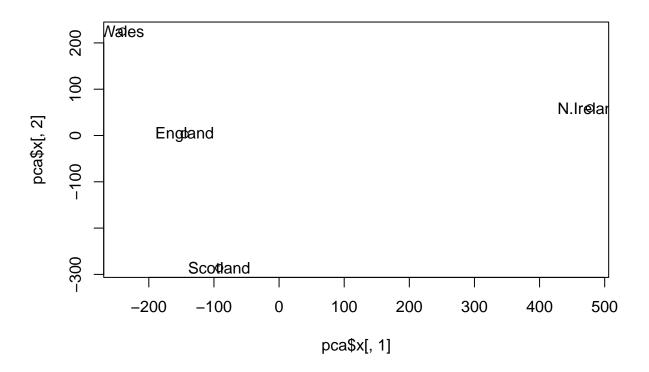
##

\$class ## [1] "prcomp"

```
## Importance of components:
##
                                PC1
                                         PC2
                                                  PC3
                                                             PC4
## Standard deviation
                           324.1502 212.7478 73.87622 4.189e-14
## Proportion of Variance
                                      0.2905
                                              0.03503 0.000e+00
                             0.6744
## Cumulative Proportion
                             0.6744
                                      0.9650
                                              1.00000 1.000e+00
attributes(pca)
## $names
## [1] "sdev"
                   "rotation" "center"
                                                     "x"
                                         "scale"
```

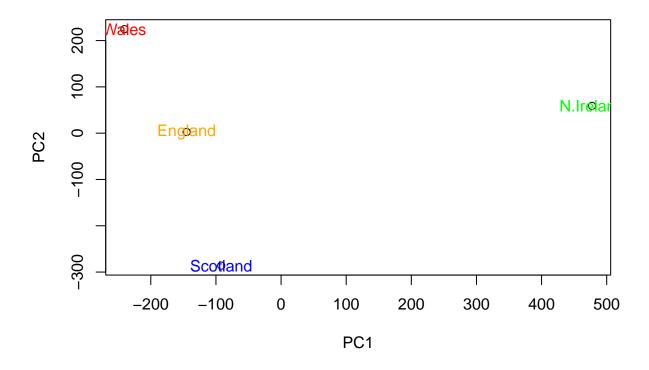
To make our new PCA plot(a.k.a PCA score plot) we access pca\$x

```
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)</pre>
```



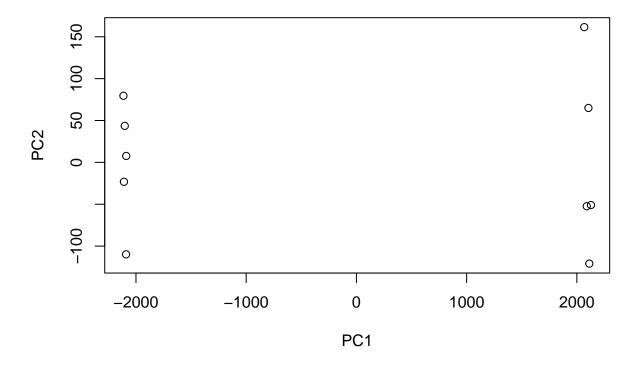
PCA of RNA-Seq data

Read in data from website

```
url2 <- "https://tinyurl.com/expression-CSV"</pre>
rna.data <- read.csv(url2, row.names=1)</pre>
head(rna.data)
##
          wt1 wt2
                   wt3
                         wt4 wt5 ko1 ko2 ko3 ko4 ko5
## gene1
          439 458
                    408
                         429 420
                                  90
                                      88
## gene2
          219 200
                    204
                         210 187 427 423 434 433 426
                  1030 1017 973 252 237 238 226 210
## gene3 1006 989
## 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
pca <- prcomp(t(rna.data))</pre>
summary(pca)
## Importance of components:
##
                                 PC1
                                          PC2
                                                   PC3
                                                             PC4
                                                                      PC5
                                                                                PC6
                           2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
## Standard deviation
## Proportion of Variance
                              0.9917
                                      0.0016 0.00144 0.00122
                                                                 0.00098
                                      0.9933 0.99471 0.99593
## Cumulative Proportion
                              0.9917
                                                                 0.99691 0.99784
```

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))
```

