Machine Learning 1

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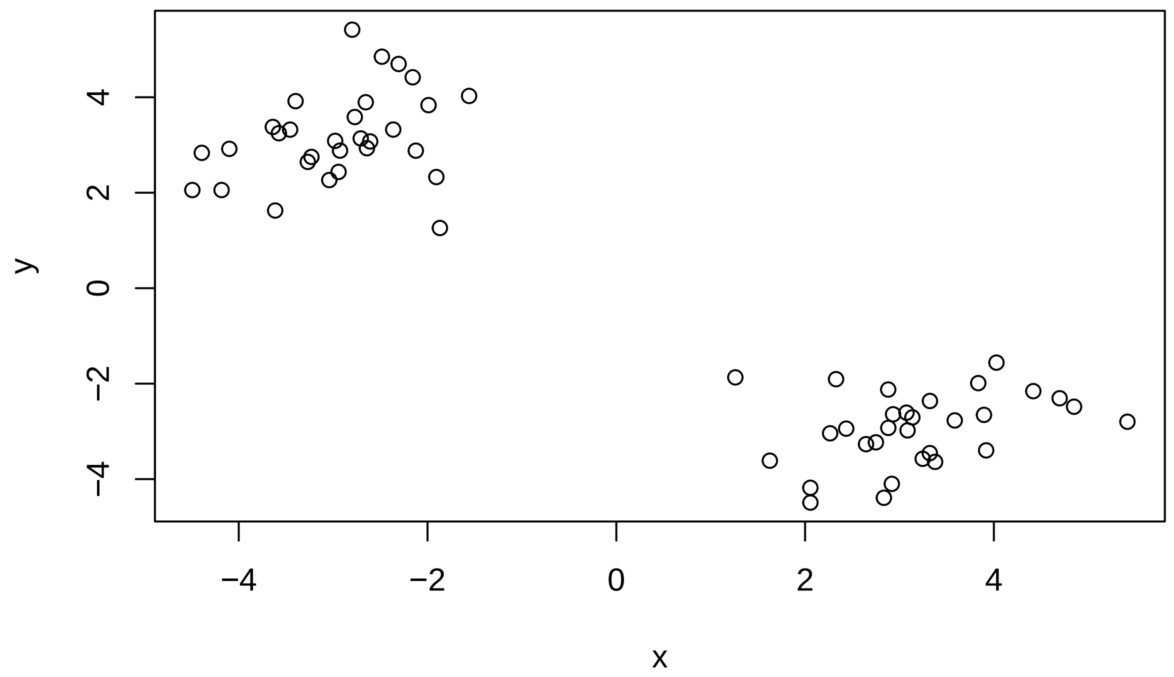
10/22/2021

Clustering methods

Kmeans clustering in R is done with the `kmeans()` function. Here we makeup some data to test and learn with.

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



Run `kmeans()` set k (centers) to 2 (i.e. the number of clusters we want) nstart 20 (to tun multiple times). The thing with Kmeans is you have to tell it how many clusters you want.

```
km <- kmeans(data, centers = 2, nstart=20)
km
```

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##           x         y
## 1 -2.939075  3.169263
## 2  3.169263 -2.939075
##
## 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 1 1
##
## Within cluster sum of squares by cluster:
## [1] 42.78048 42.78048
##  (between_SS / total_SS =  92.9 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

Q. How many points are in each cluster?

```
km$size
```

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

Q. What 'component' of your result object details cluster assignment/membership?

```
km$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 1 1
```

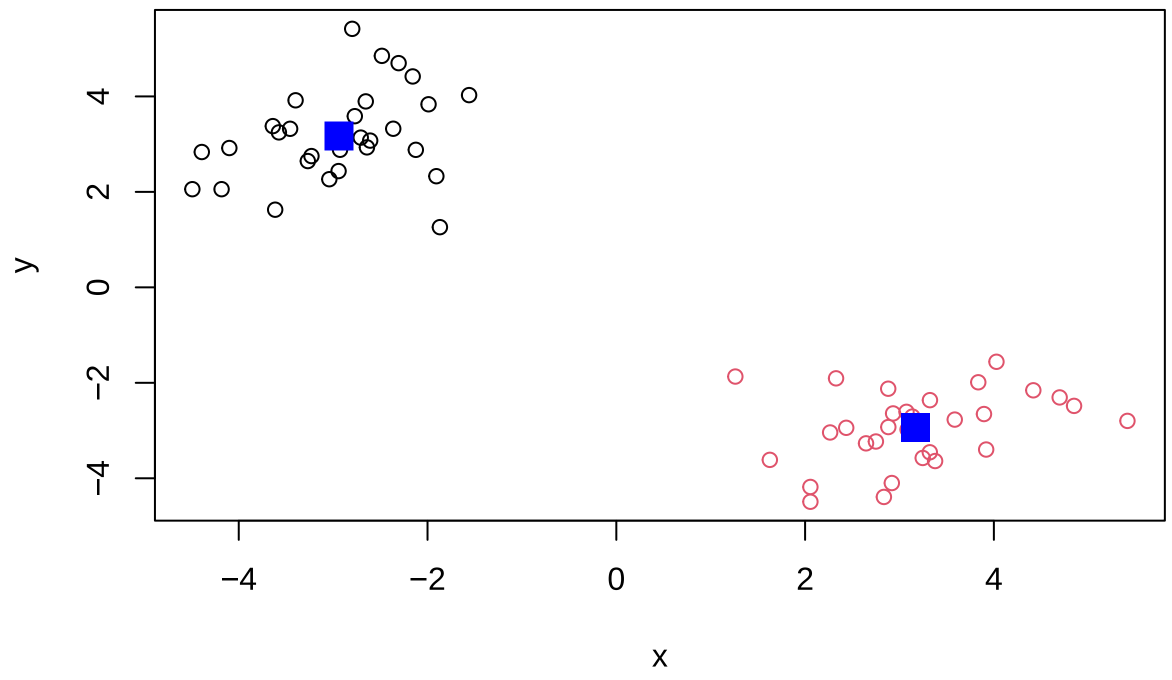
Q. What 'component' of your result object details cluster center?

```
km$centers
```

```
##           x         y
## 1 -2.939075  3.169263
## 2  3.169263 -2.939075
```

Q. Plot x colored by the kmeans cluster assignment and add cluster centers as blue points

```
plot(data, col=km$cluster)
points(km$centers, col="blue", pch=15, cex=2)
```



Hierarchical Clustering

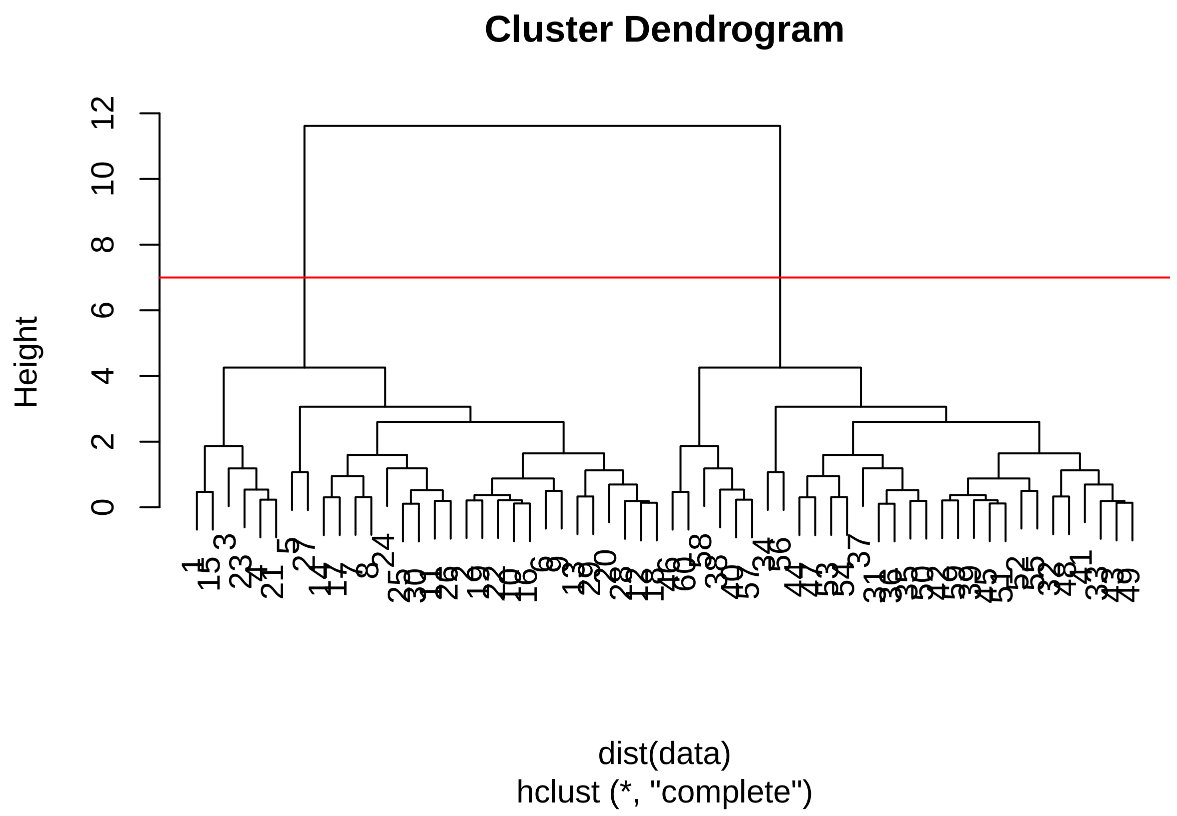
We will use the `hclust()` function on the same data as before and see how this method works.

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

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

hclust has a plot method

```
plot(hc)
abline(h=7, col="red")
```



To find our membership vector we need to "cut" the tree and for this we use the `cutree()` function and tell it the height to cut at.

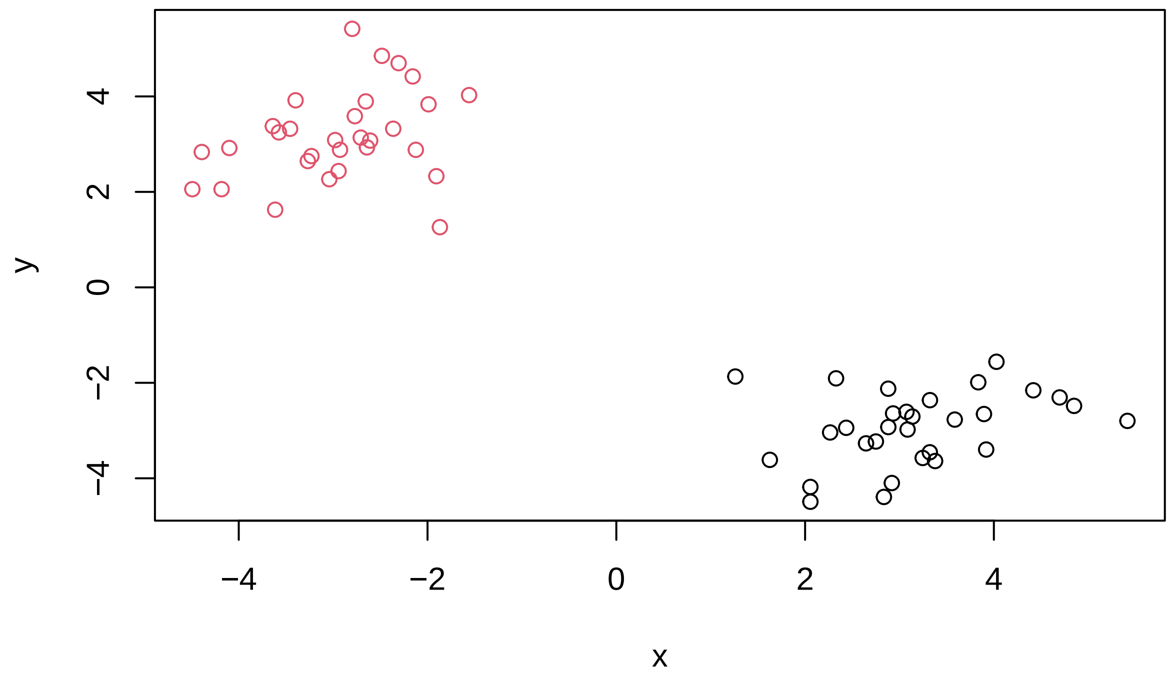
```
cutree(hc, h=7)
```

```
##  [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
```

We can also use `cutree()` and sate the number of k clusters we want. . .

```
grps <- cutree(hc, k=2)
```

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



Principal Component Analysis (PCA)

PCA is a super useful analysis method when you have lots of dimensions in your data…

PCA of UK food data

Import the data from a CSV file

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
```

How many rows and cols?

```
dim(x)
```

```
## [1] 17  5
```

```
x[,-1]
```

```
##    England Wales Scotland N.Ireland
## 1      105   103      103        66
## 2      245   227      242       267
## 3      685   803      750       586
## 4      147   160      122        93
## 5      193   235      184       209
## 6      156   175      147       139
## 7      720   874      566      1033
## 8      253   265      171       143
## 9      488   570      418       355
## 10     198   203      220       187
## 11     360   365      337       334
## 12    1102  1137      957       674
## 13    1472  1582     1462      1494
## 14      57    73       53        47
## 15    1374  1256     1572      1506
## 16     375   475      458       135
## 17      54    64       62        41
```

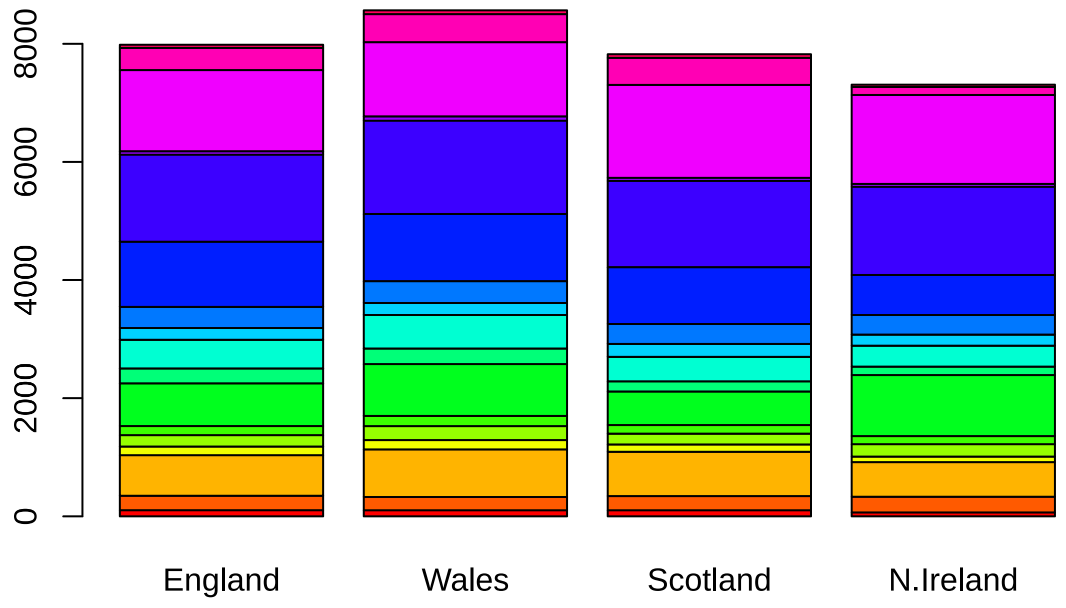
```
rownames(x) <- x[,1]
x <- x[,-1]
x
```

```
##                     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
```

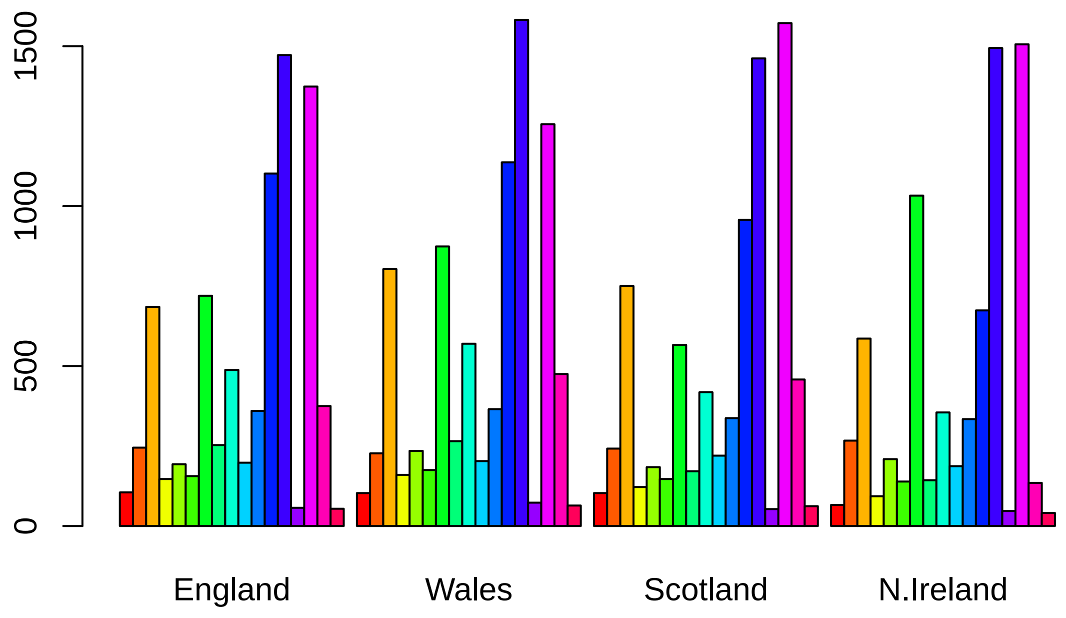
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names=1)
x
```

```
##                     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
```

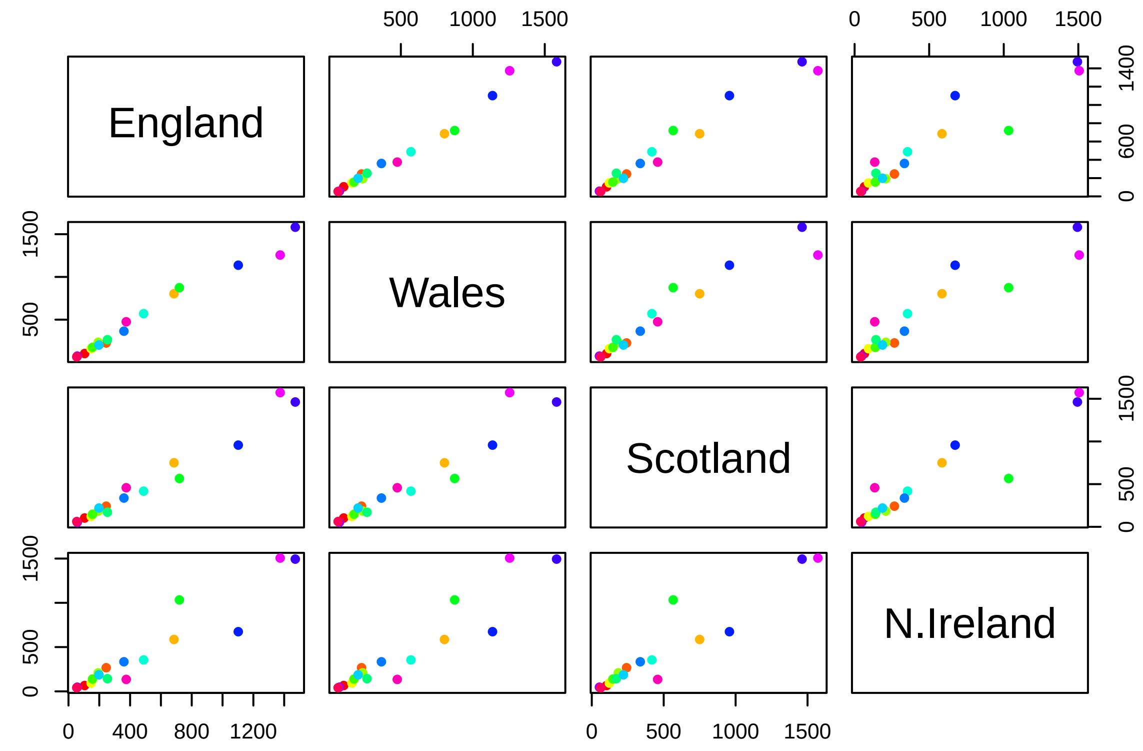
```
barplot( as.matrix(x), col=rainbow(17) )
```



```
barplot( as.matrix(x), col=rainbow(17), beside=TRUE )
```



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



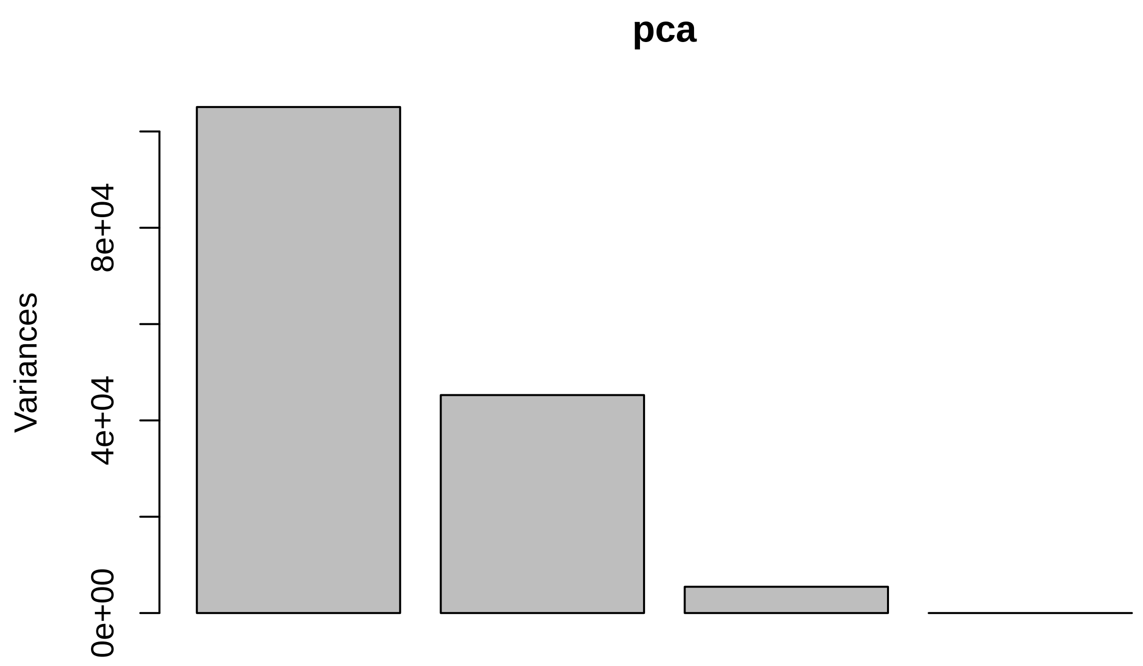
PCA to the rescue!

Here we will use the base R function for PCA, which is called `prcomp()`. This function wants the transpose of of data.

```
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
```

```
plot(pca)
```



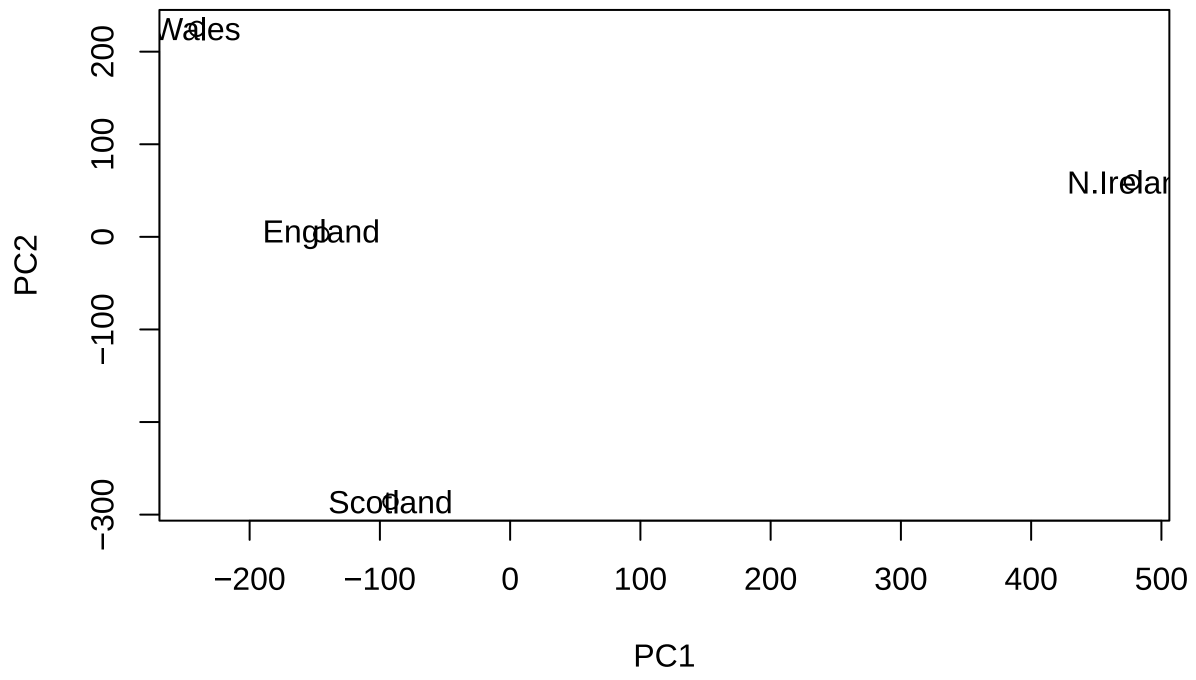
We want score plot (a.k.a. PCA plot). Basically of PC1 vs PC2

```
attributes(pca)
```

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

We are after the pca$x component for this plot…

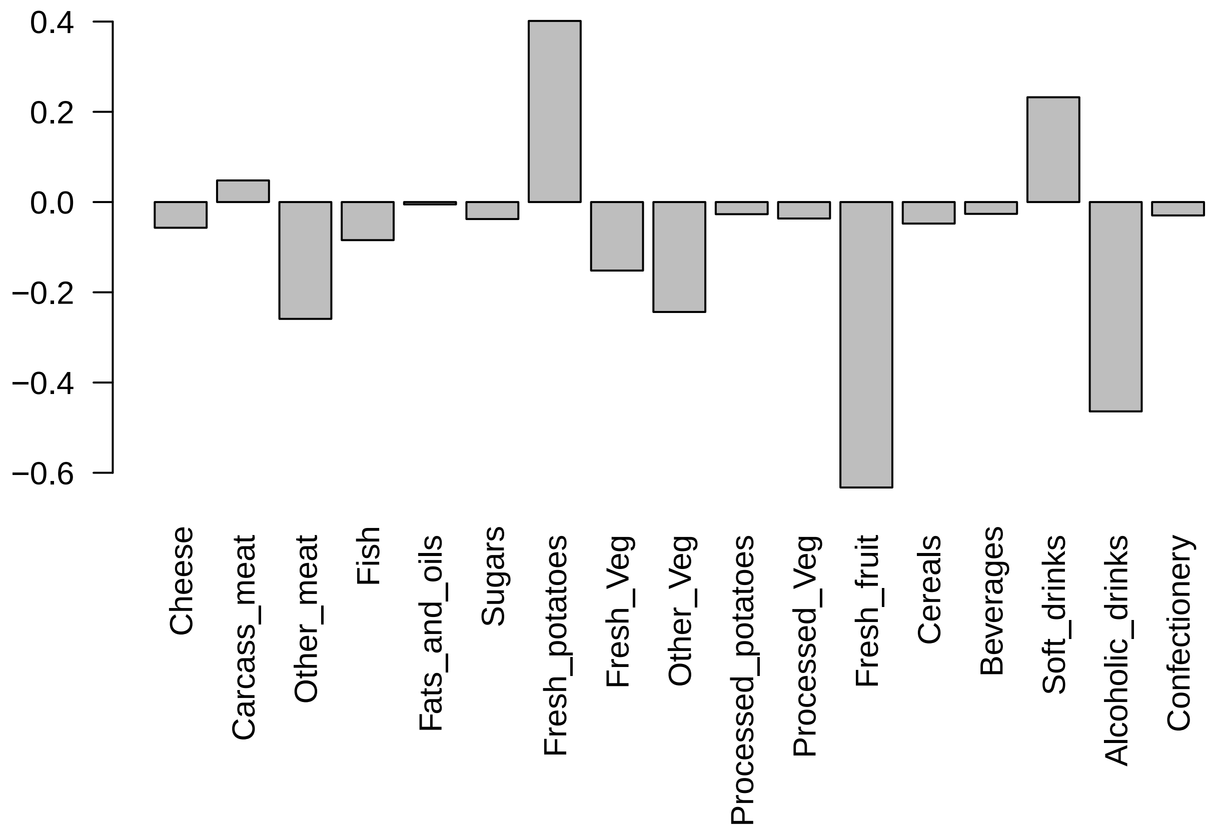
```
plot(pca$x[,1:2])
text(pca$x[,1:2], labels = colnames(x))
```



We can also examine the PCA "loadings", which tell us how much the original variables contribute to each new PC...

```r
par(mar=c(10, 3, 0.35, 0))

barplot(pca$rotation[,1], las=2)
```



One more PCA for today

```
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
```

```
nrow(rna.data)
```

```
## [1] 100
```

```
ncol(rna.data)
```

```
## [1] 10
```

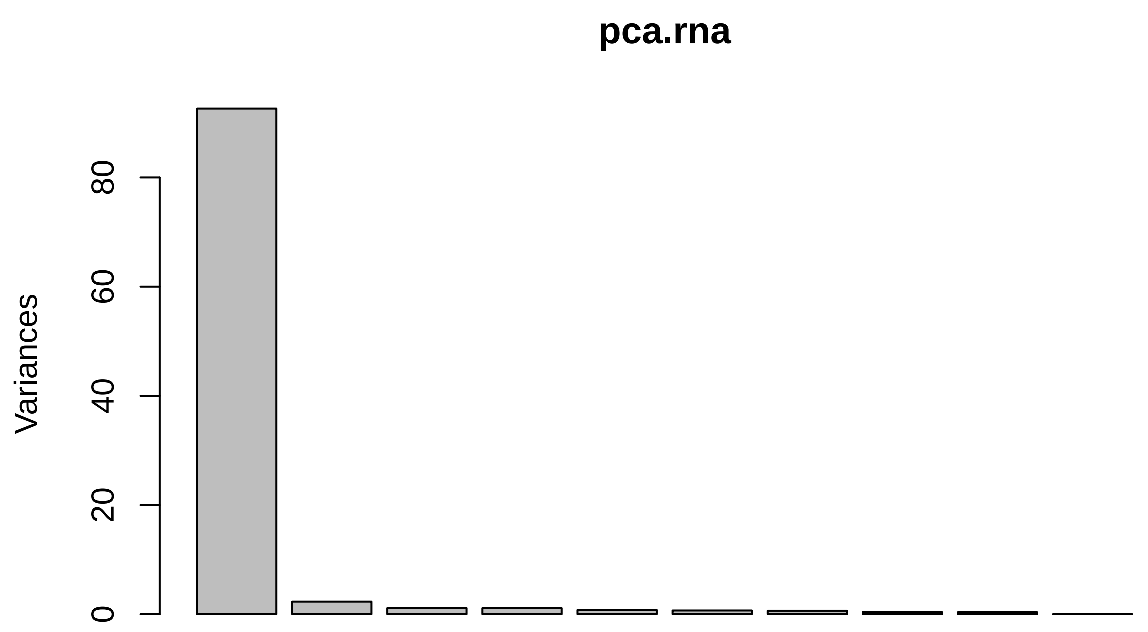
```
colnames(rna.data)
```

```
##  [1] "wt1" "wt2" "wt3" "wt4" "wt5" "ko1" "ko2" "ko3" "ko4" "ko5"
```

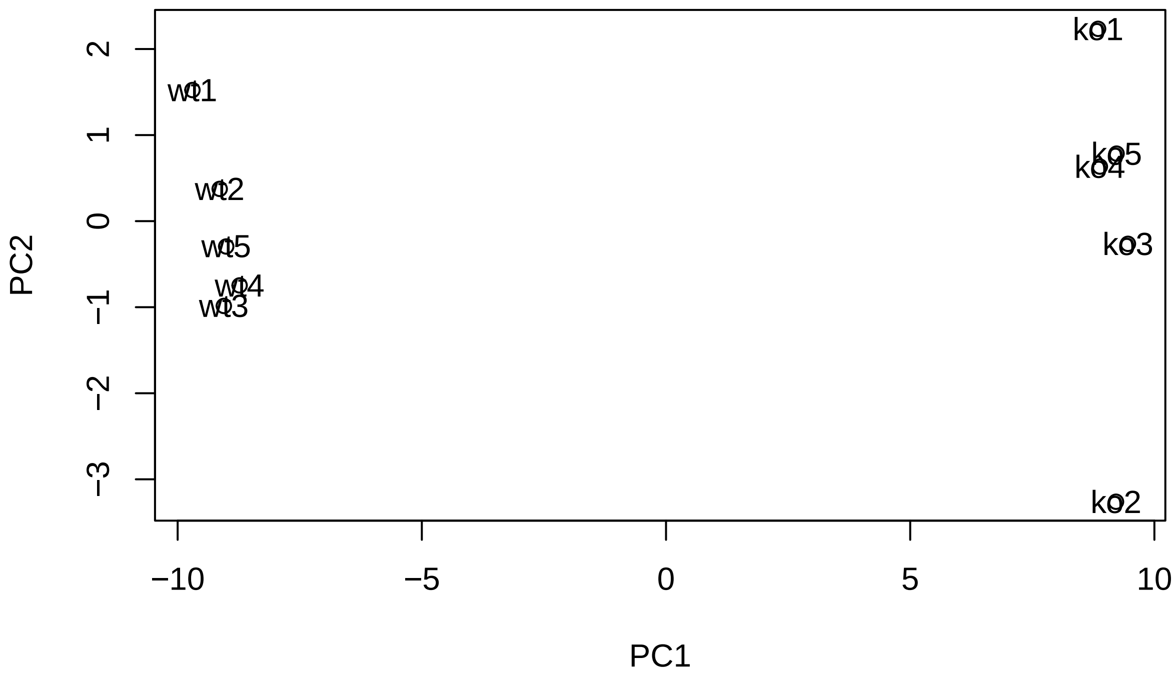
```
pca.rna <- prcomp( t(rna.data), scale=TRUE )
summary(pca.rna)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     9.6237 1.5198 1.05787 1.05203 0.88062 0.82545 0.80111
## Proportion of Variance 0.9262 0.0231 0.01119 0.01107 0.00775 0.00681 0.00642
## Cumulative Proportion  0.9262 0.9493 0.96045 0.97152 0.97928 0.98609 0.99251
##                            PC8     PC9      PC10
## Standard deviation     0.62065 0.60342 3.327e-15
## Proportion of Variance 0.00385 0.00364 0.000e+00
## Cumulative Proportion  0.99636 1.00000 1.000e+00
```

```
plot(pca.rna)
```



```
plot(pca.rna$x[,1:2])
text(pca.rna$x[,1:2], labels = colnames(rna.data))
```



Let's Knit to PDF and also github_document then push to github.