Machine Learning 1

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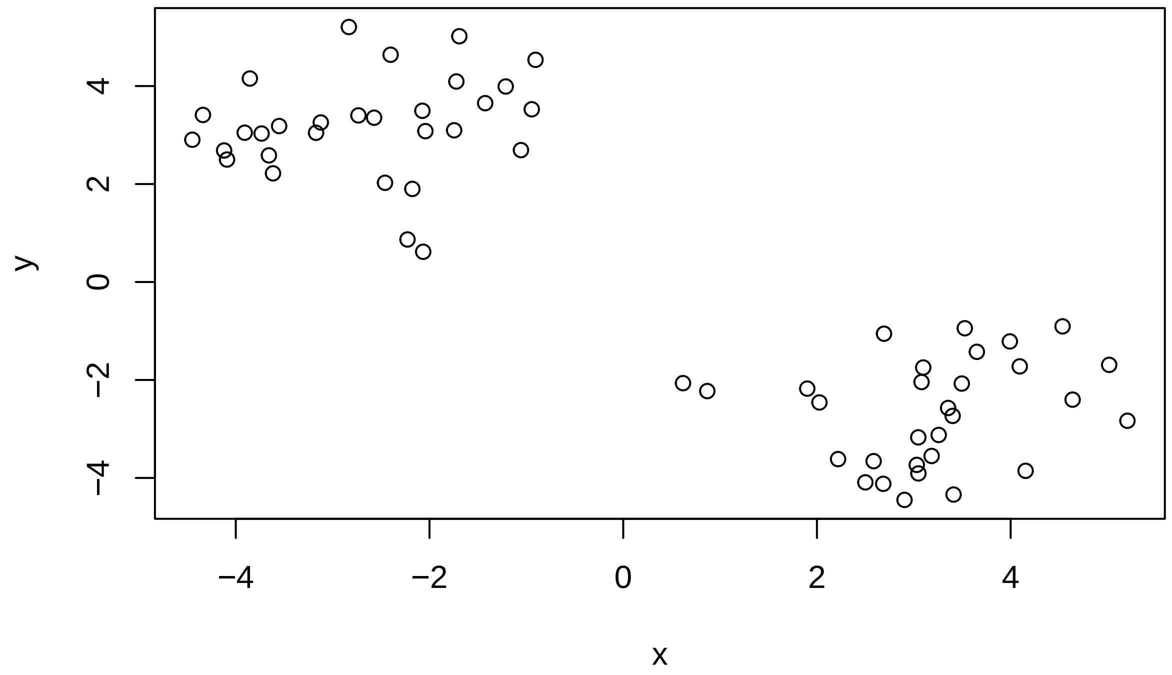
Clustering methods

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

rev reverses order of vector cbind concatenates the two vectors in tmp

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



Run 'kmeans()' set k to 2, nstart to 20. Have to tell it how many clusters you want.

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

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##           x         y
## 1  3.173994 -2.663504
## 2 -2.663504  3.173994
##
## 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 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] 65.76392 65.76392
##  (between_SS / total_SS =  88.6 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

Q. How many points are in each cluster?

```r
km$size
```

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

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

```r
km$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 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
```

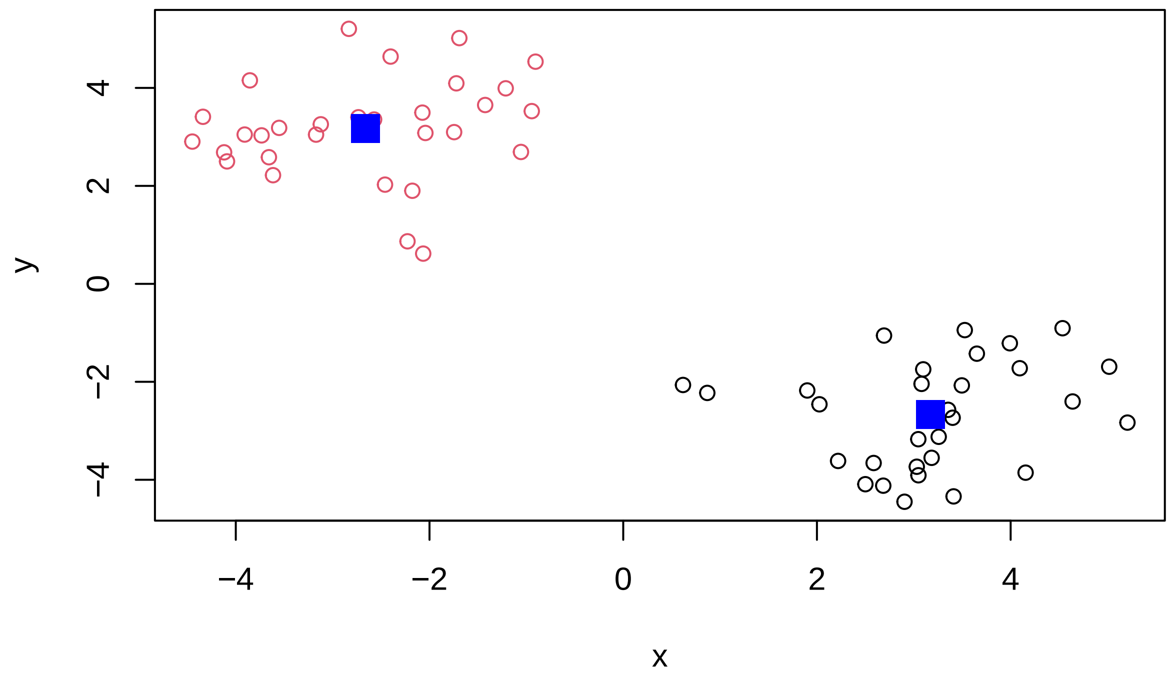
Q. What 'component' of your result object details cluster center?

```r
km$centers
```

```
##           x         y
## 1  3.173994 -2.663504
## 2 -2.663504  3.173994
```

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

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



Hierarchical Clustering

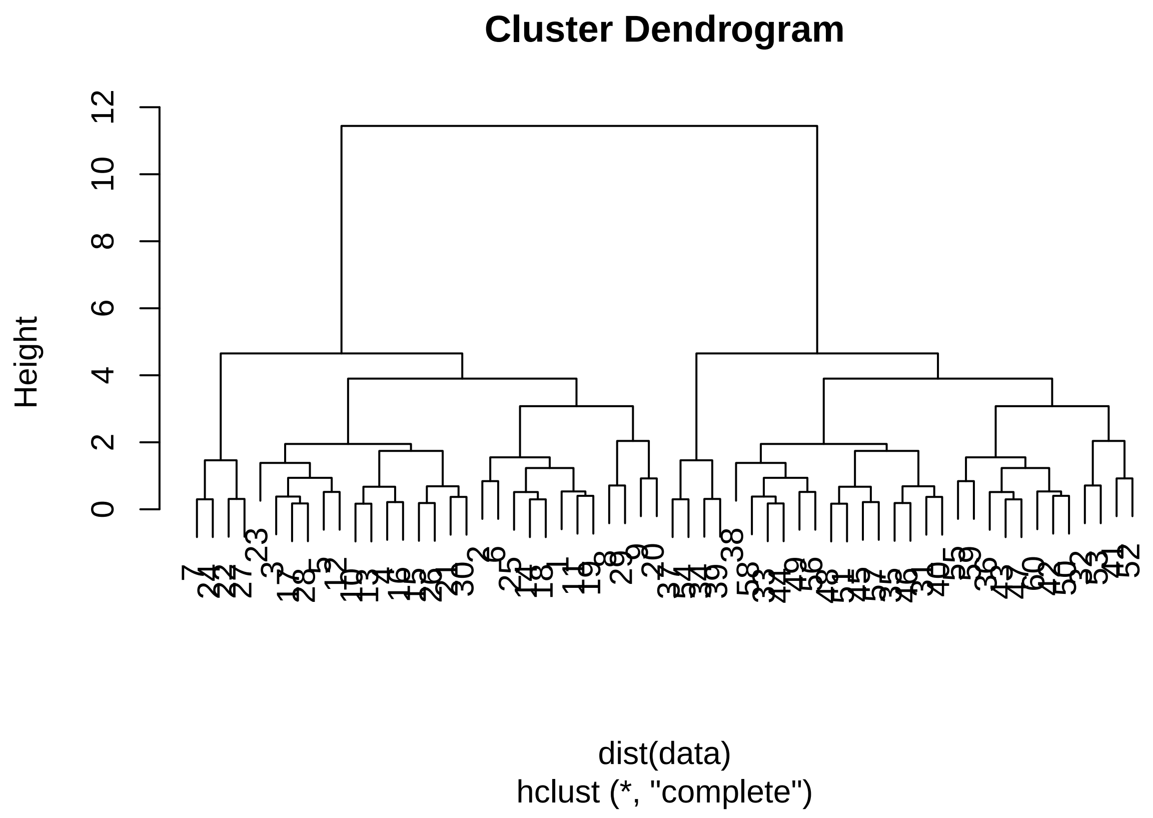
Use the 'hclust()' function on the same data as before

```
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)
```



To find membership vector, need to 'cut' the tree by using 'cutree' function and tell it the height to cut at

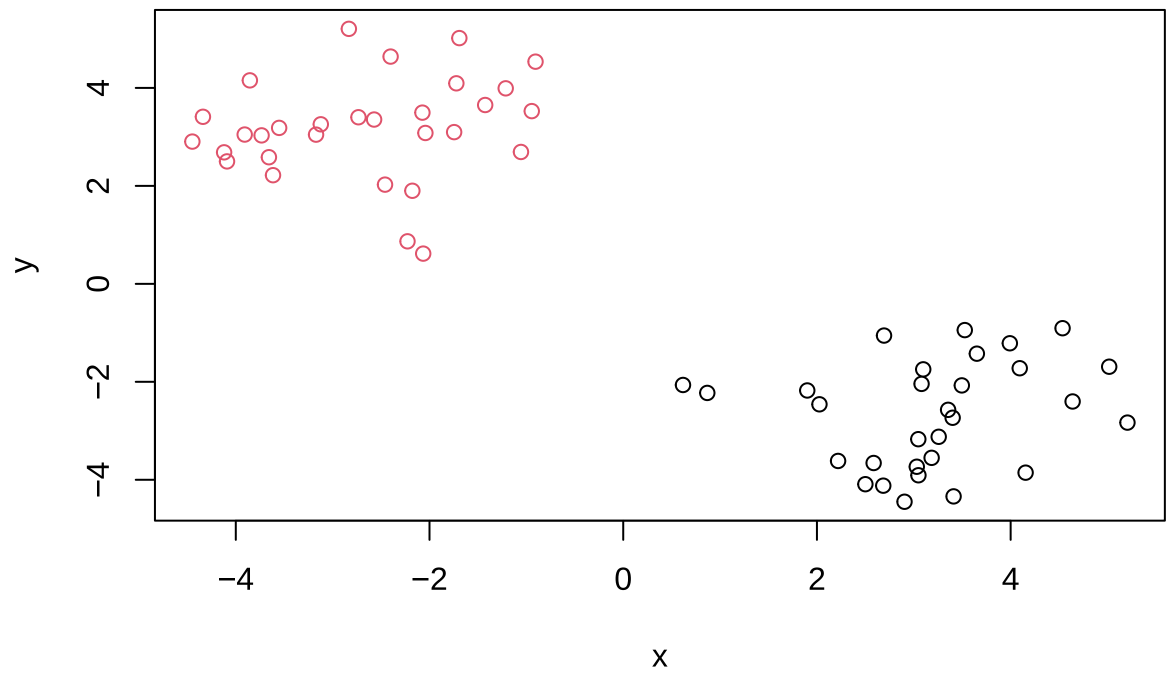
```r
cutree(hc, h = 7)
```

```
##  [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
```

Use 'cutree()' and sate the number of k clusters we want

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

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



Principal Component Analysis (PCA)

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

How many rows and cols?

```r
dim(x)
```

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

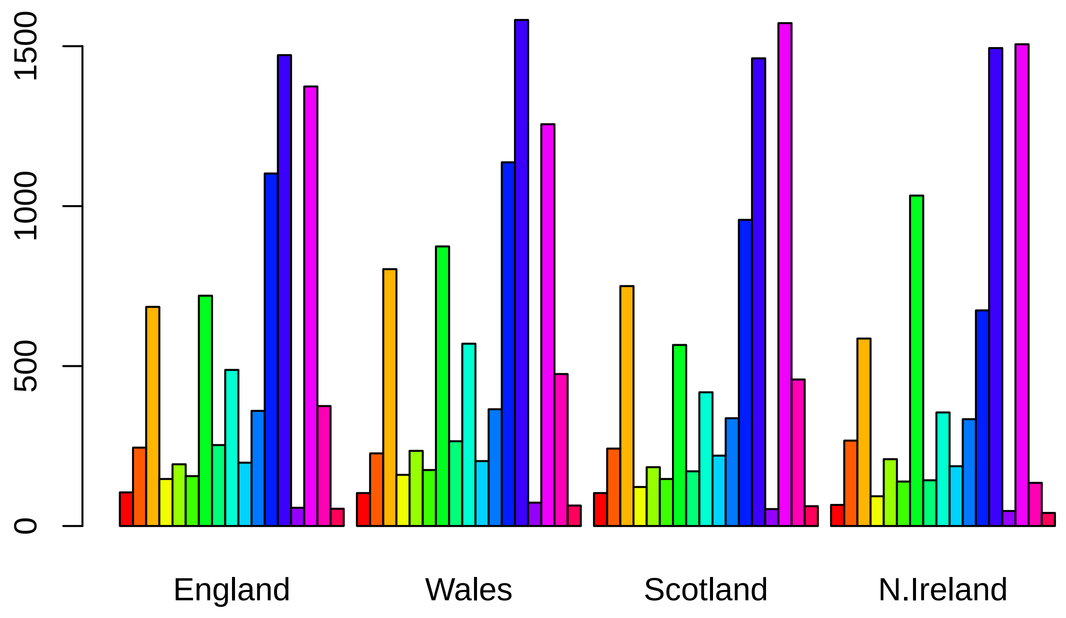
```r
x[,-1]
```

```
##    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
```

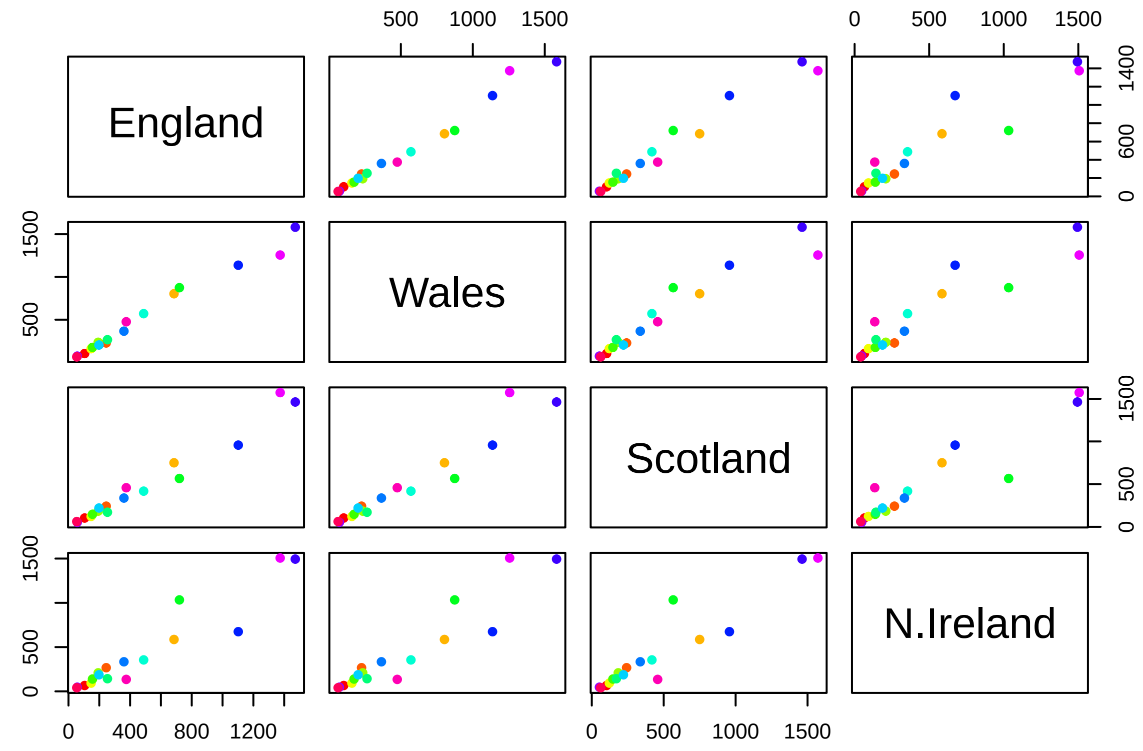
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
x
```

```
##                     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), beside = TRUE)
```



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



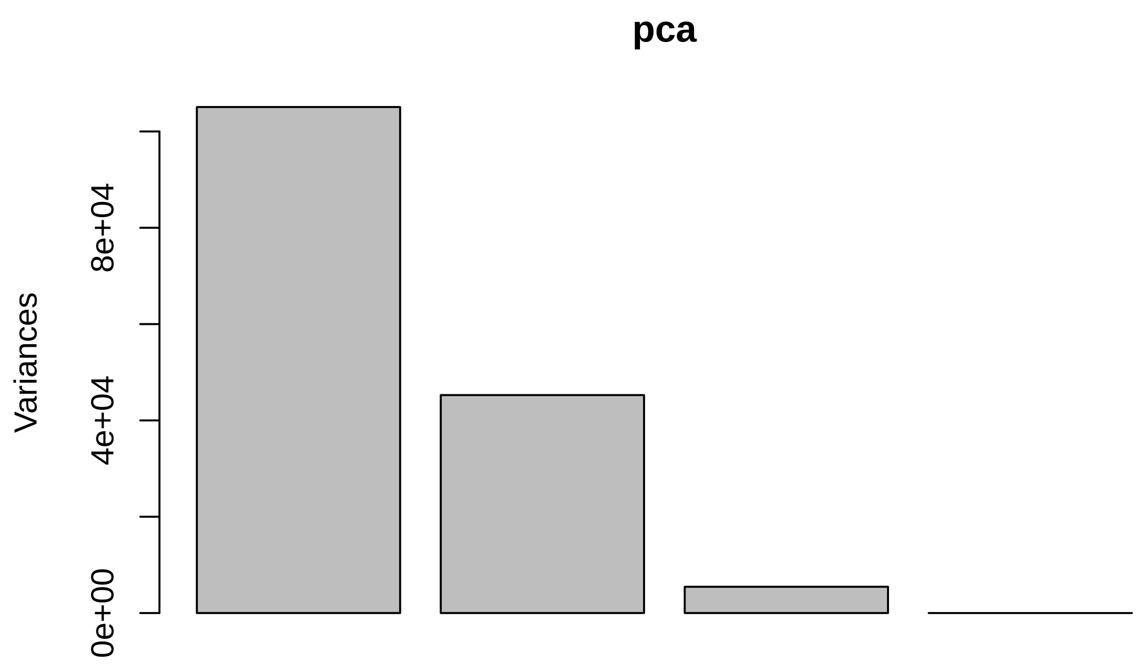
PCA to the rescue!

Use base R function for PCA, which is called 'prcomp()'. This function wants the transpose of our data.

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

```
## Importance of components:
##                              PC1      PC2      PC3       PC4
## Standard deviation     324.1502 212.7478 73.87622 4.189e-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)
```



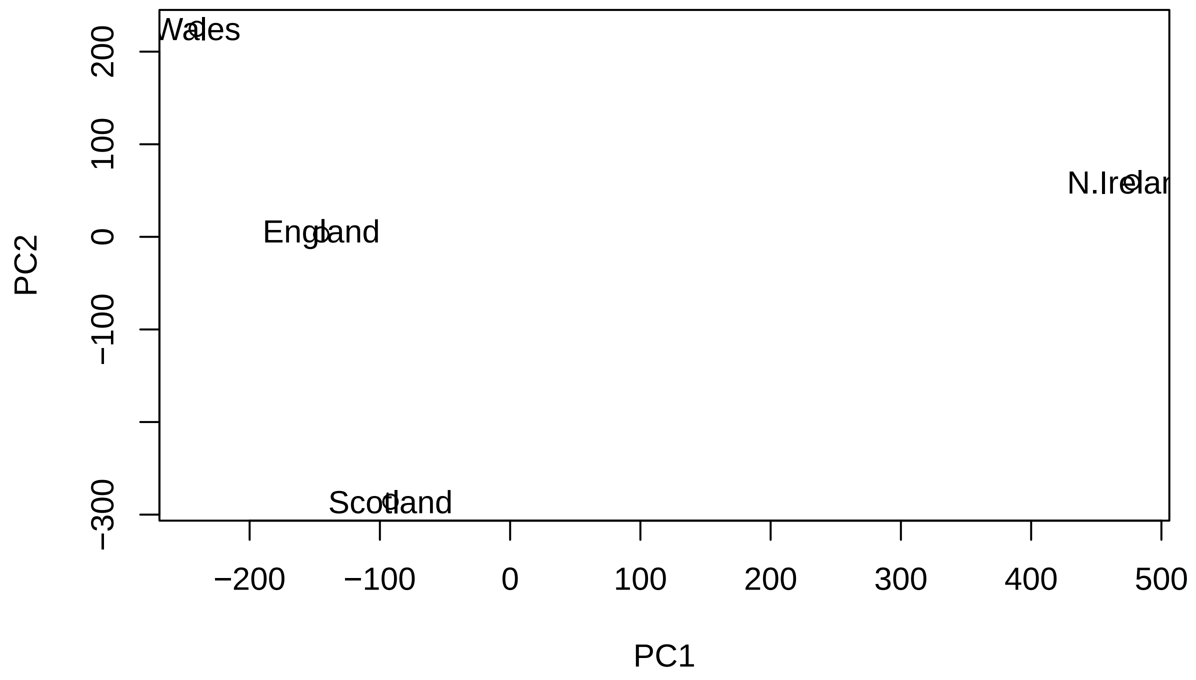
We want score plot (aka PCA plot). Basically of PC1 vs PC2

```
attributes(pca)
```

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

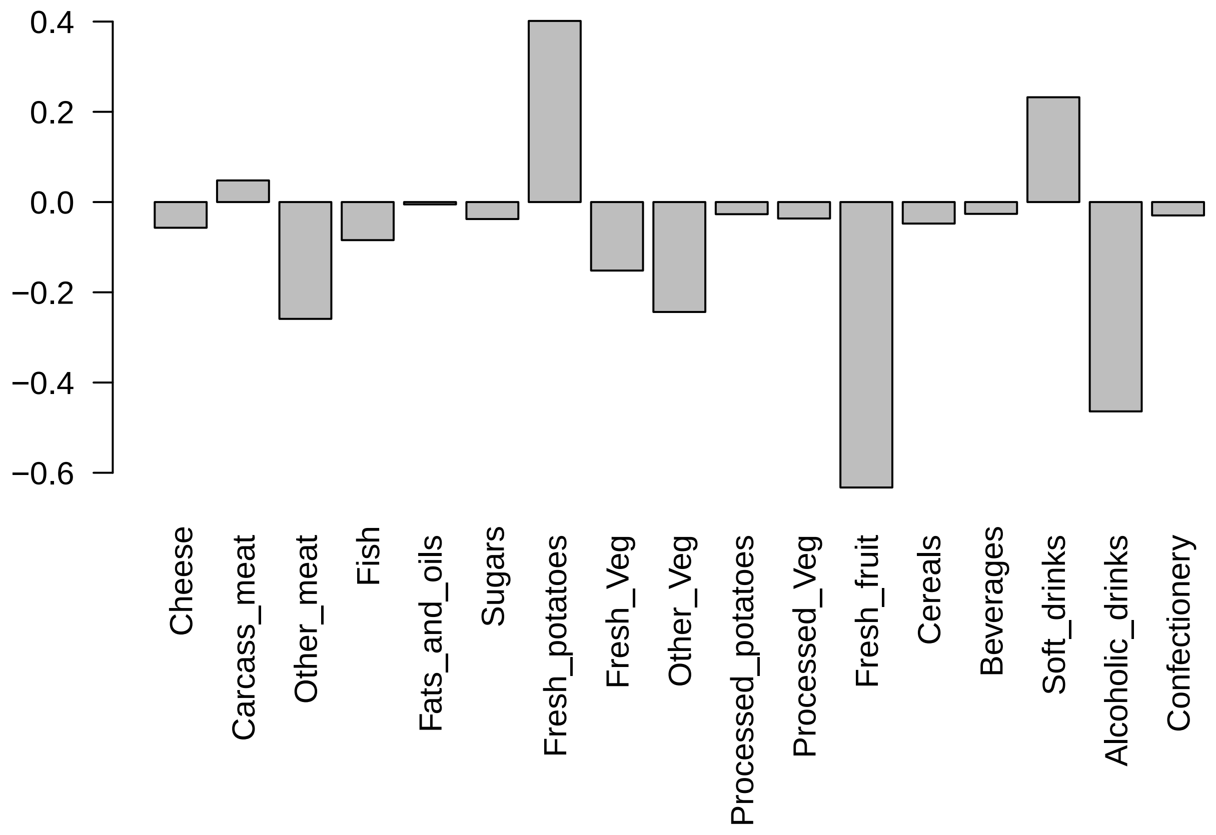
We are after the pca$x component for this plot

```
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 PC

```
par(mar=c(10, 3, 0.35, 0))
barplot(pca$rotation[,1], las = 2)
```



One more PCA for today

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

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

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

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

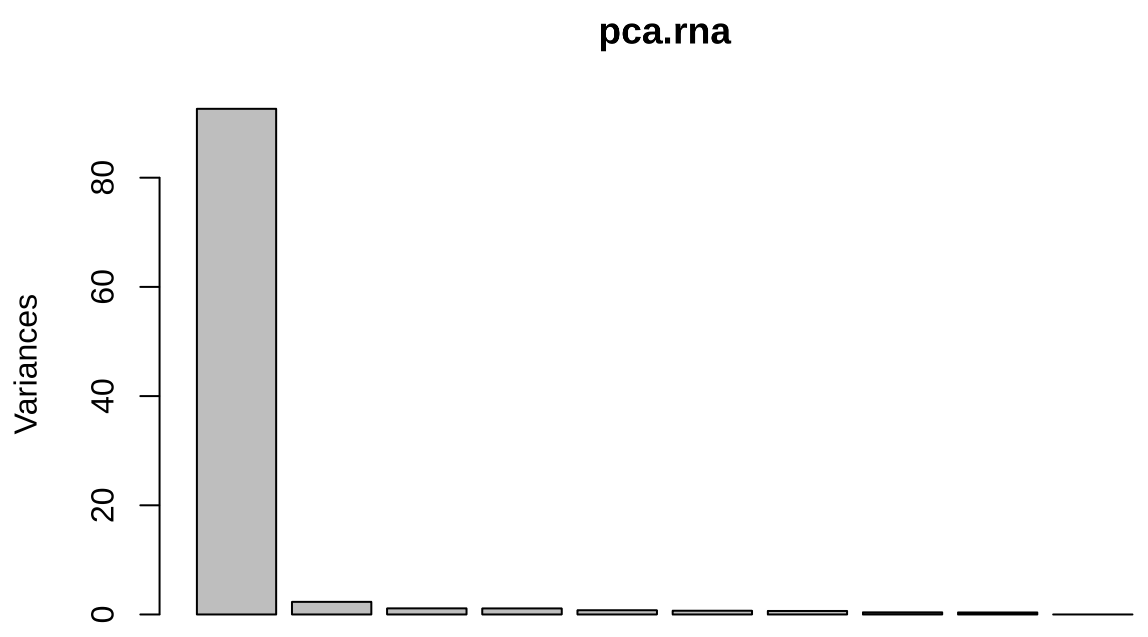
```
colnames(rna.data)
```

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

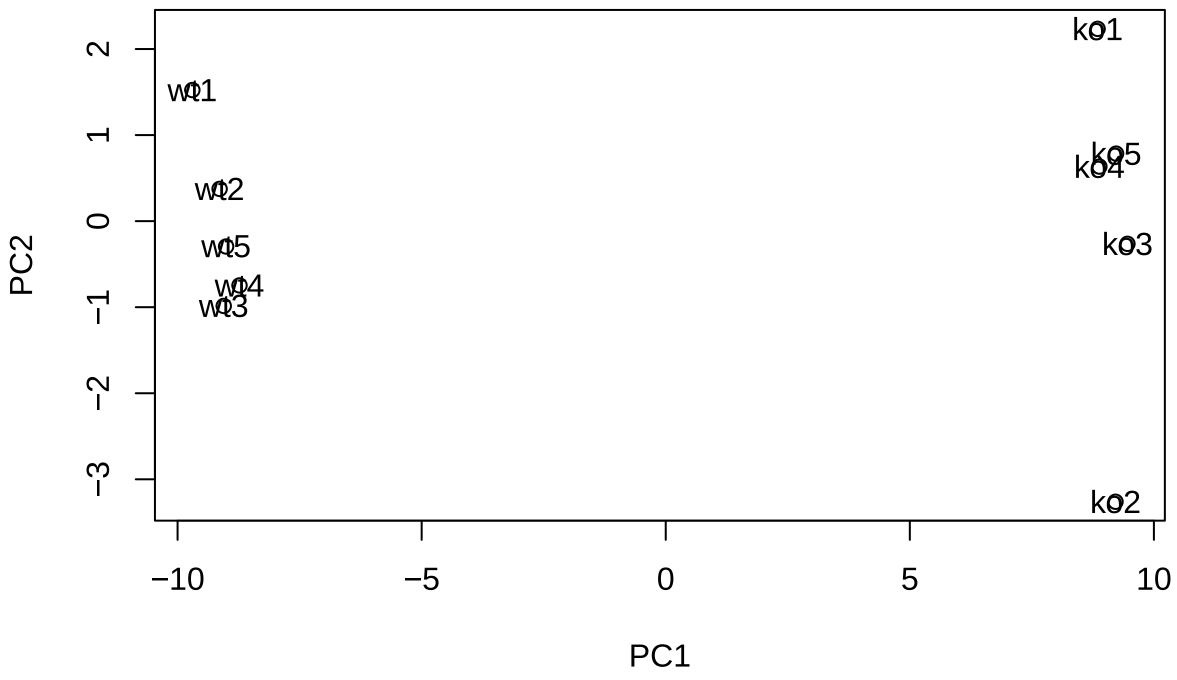
```
pca.rna <- prcomp(t(rna.data), scale = TRUE)
summary(pca.rna)
```

```
## 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 3.348e-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))
```



PC2
PC1
2
1
0
−1
−2
−3
−10
−5
0
5
10
wt1
wt2
wt5
wt4
wt3
ko1
ko5
ko4
ko3
ko2