machine learning 1

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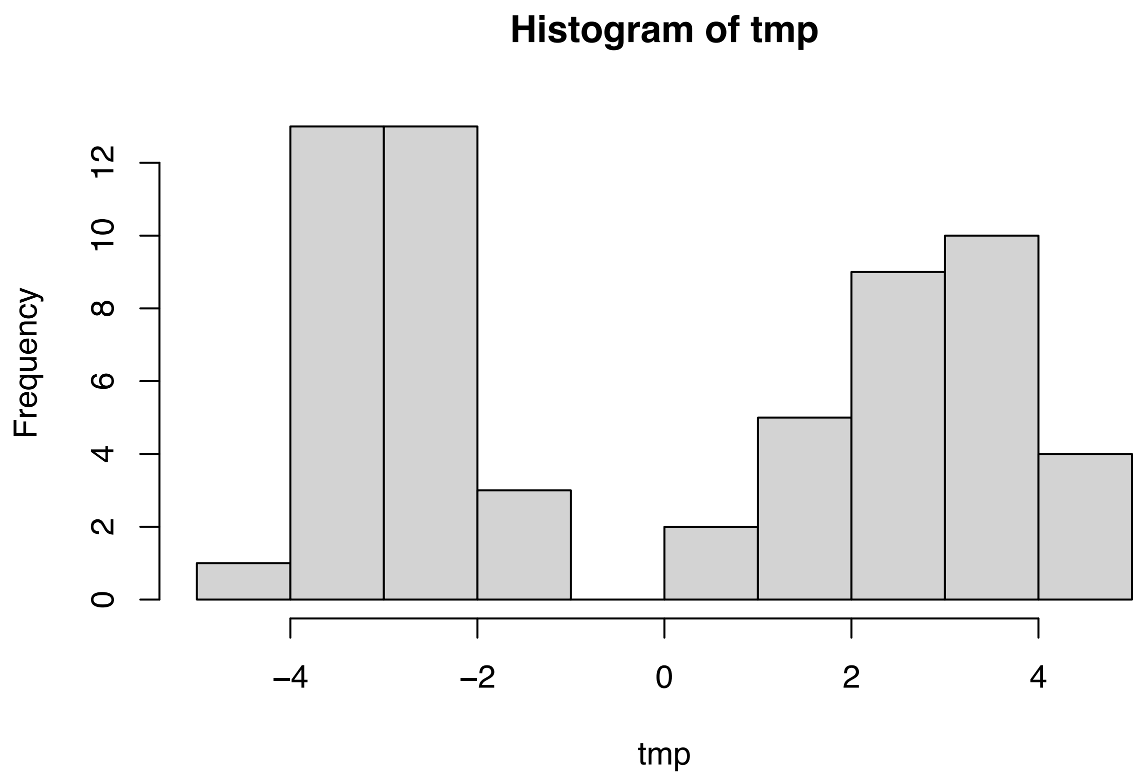
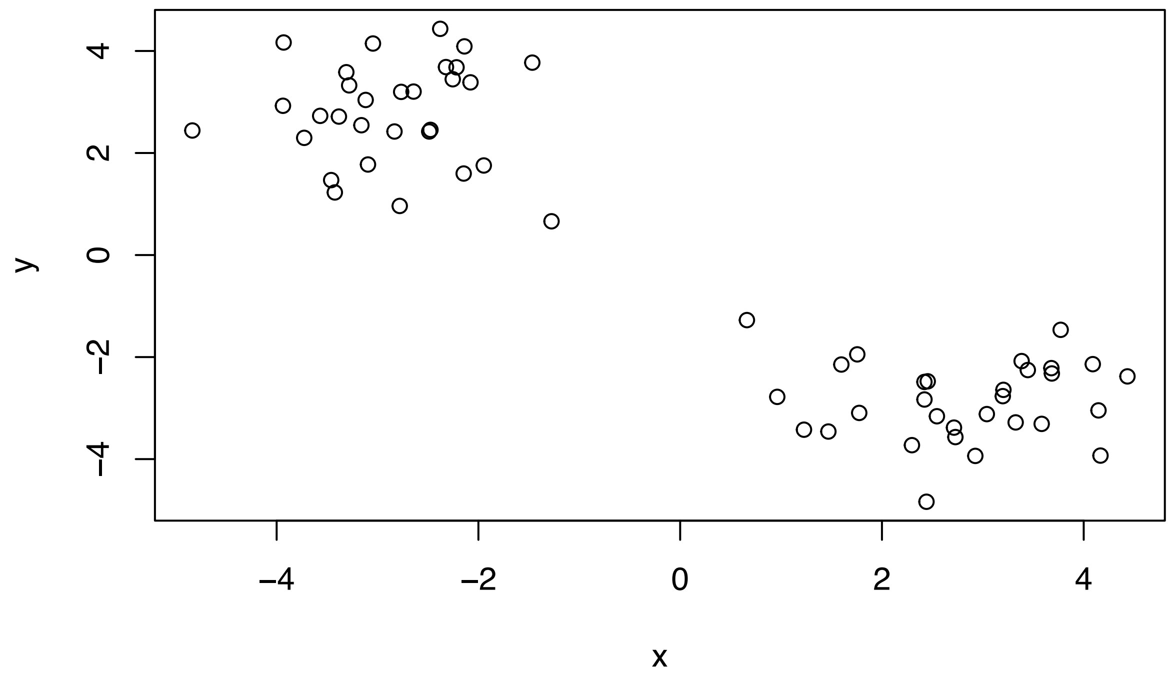
Clustering methods

kmeans clustering in R is done with `kmeans()` function. here we make up some data to test and learn with.

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



```r
plot(data)
```



run `kmeans()` set k (centers) to 2 nstart (numner of iteration) 20. the thing with kmeans is you have to tell it how many clusters you want.

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

> 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] 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
```

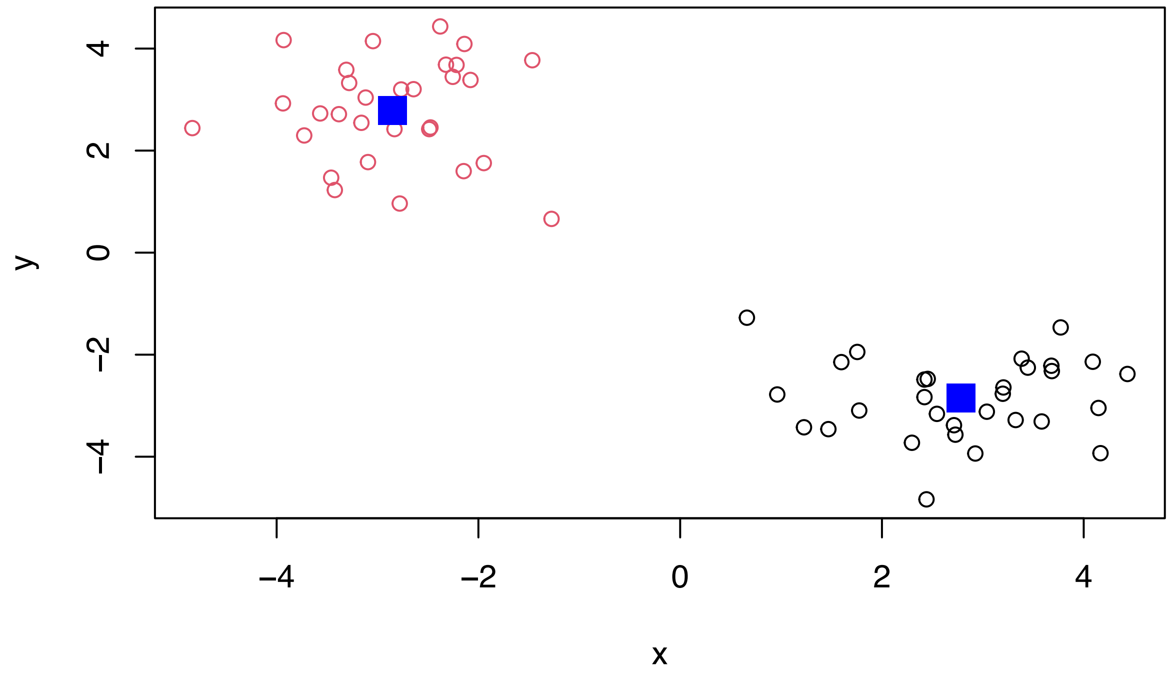
> Q. what 'component' of your result object details cluster center?

```
km$centers
```

```
##           x         y
## 1  2.784966 -2.849169
## 2 -2.849169  2.784966
```

Q. plot x colored by the kmeans assifnment and add cluster centers as blue points.

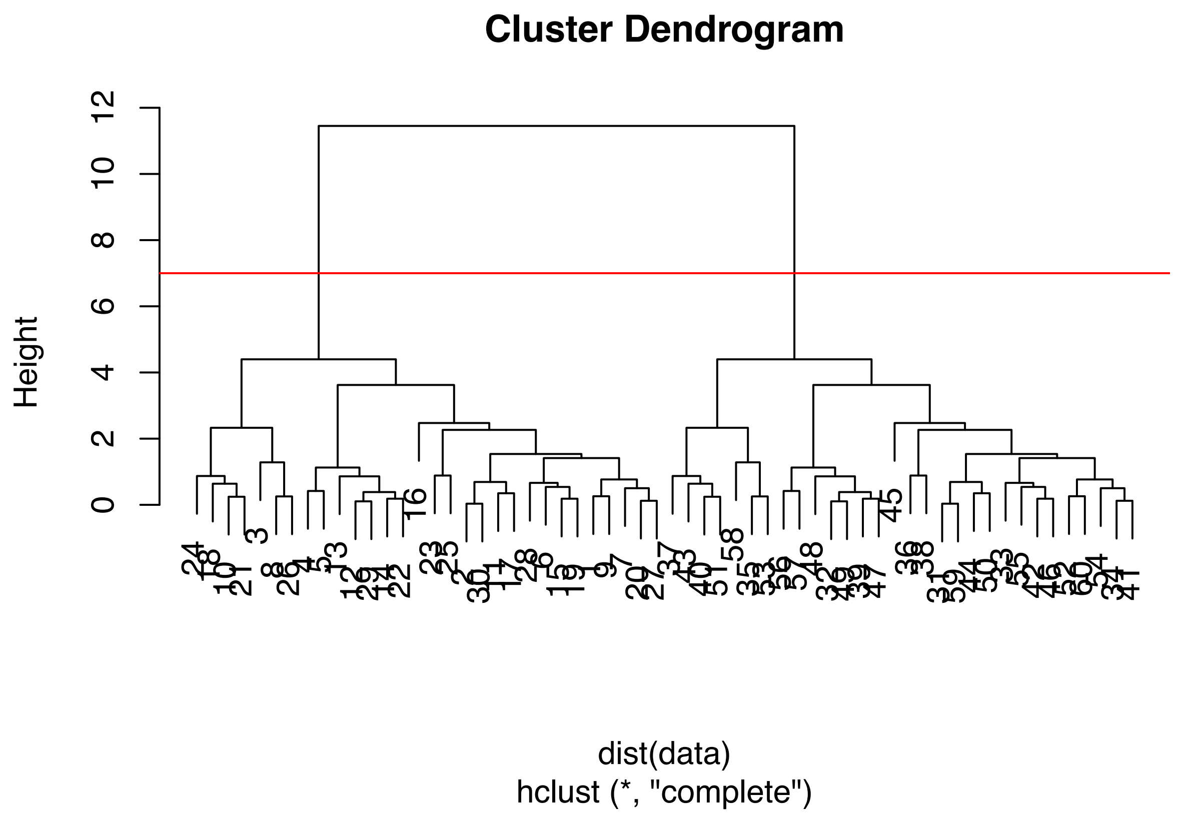
```
plot(data, col = km$cluster)
points(km$centers, col="blue", pch=15, cex=2)
```



Hierarchical clustering

we will use the `hclust()` function on the same data as before and see how this will work

```
hc  = hclust(d = dist(data))
plot(hc)
abline(h=7, col="red")
```



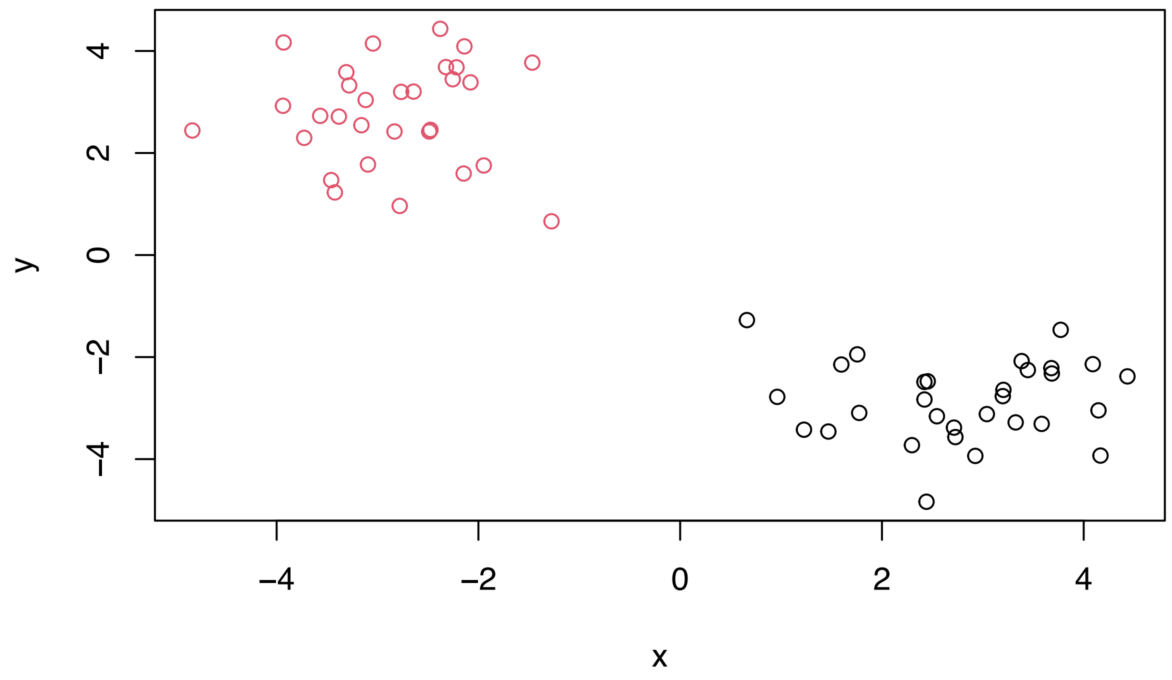
to find our membership vector we need to "cut" the tree and for this we use the `cutree()` method and tell it the height to cut at.

```
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 state the number of k clusters we want

```
groups = cutree(hc, k=2)
plot(data, col = groups)
```



PCA principal component analysis

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 cold?
dim(x)
```

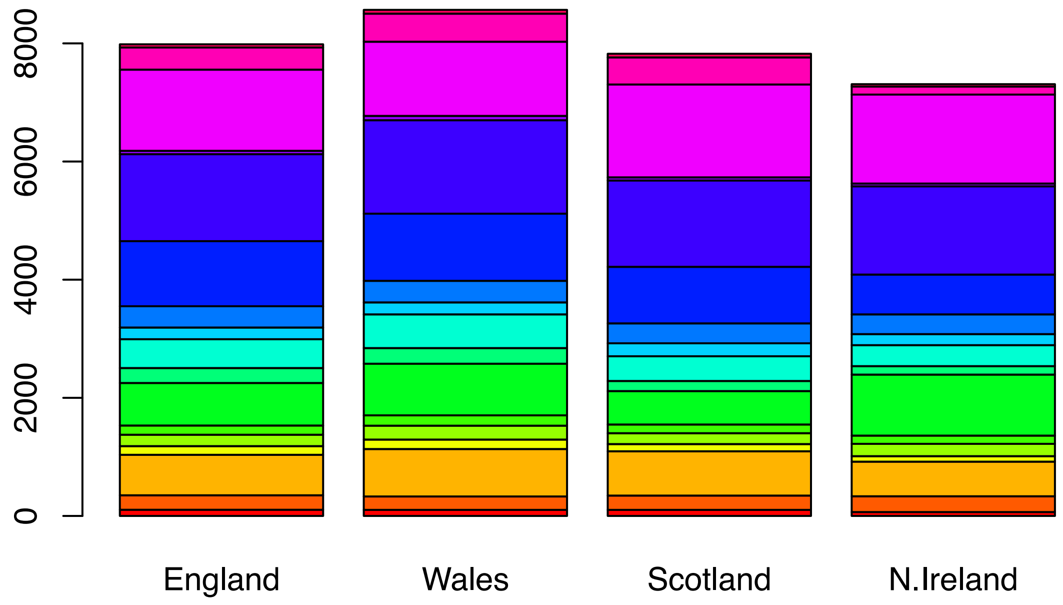
```
## [1] 17  5
```

```
# not good, cuz every time you run it you lost a col
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
```

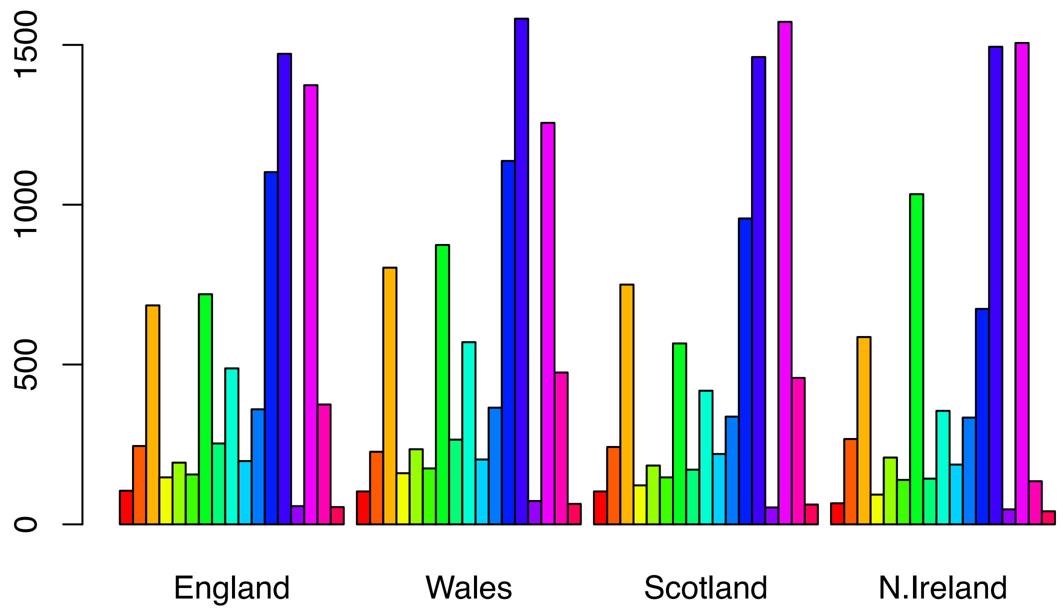
```
# so do this:
x <- read.csv(url, row.names = 1)
```

```
barplot(as.matrix(x), col=rainbow(17)) # number of color in the rainbow
```

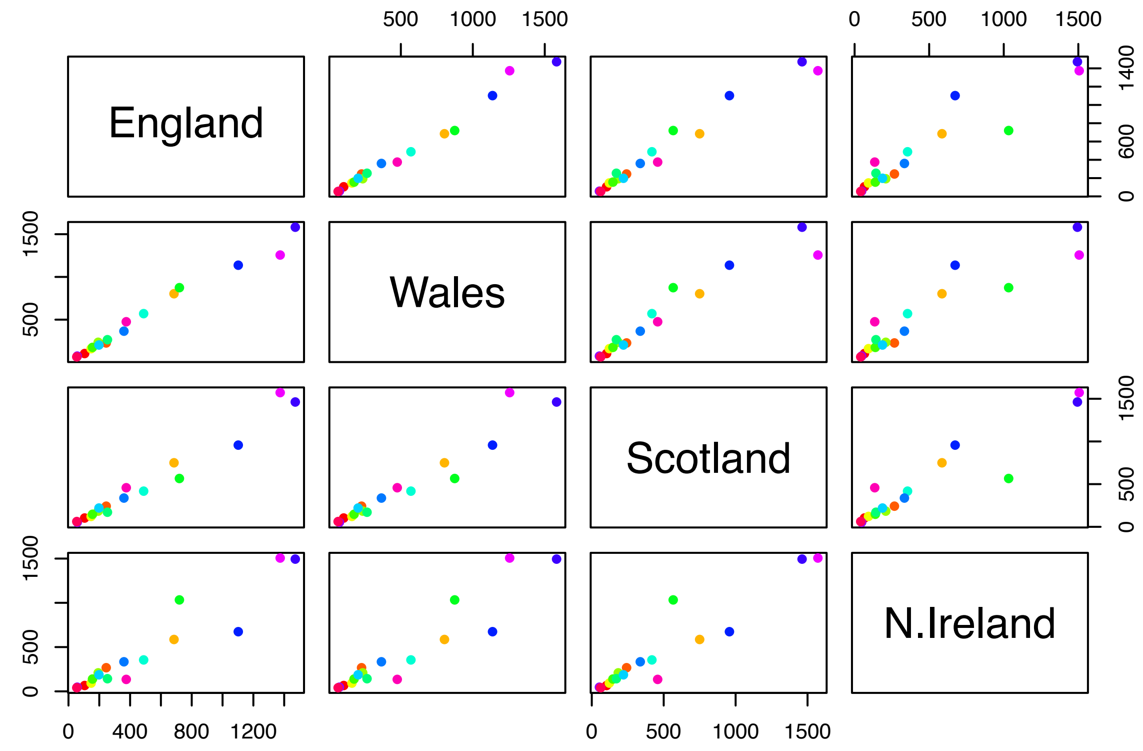


```
mycol=rainbow(nrow(x))
```

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



```
pairs(x, col=mycol, pch=16)
```



## PCA to the rescue here we will use the base R function for PCA, which is call `prcomp()`. this function wants the transpose of data

```
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
```

```
# wants countries in the rows and things in the col
pca = prcomp(t(x))
summary(pca)
```

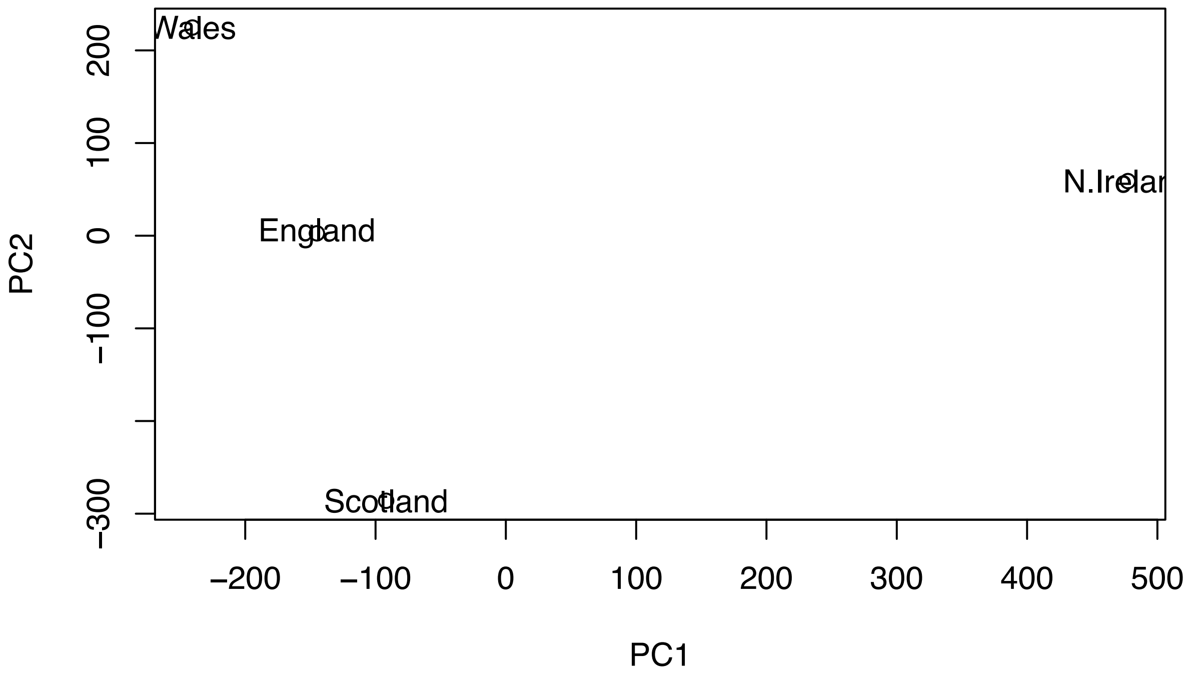
```
## Importance of components:
##                              PC1      PC2      PC3       PC4
## Standard deviation     324.1502 212.7478 73.87622 4.189e-14
## Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
## Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

we want score plot(aka pca plot). basically pc1 vs pc2

```
attributes(pca)
```

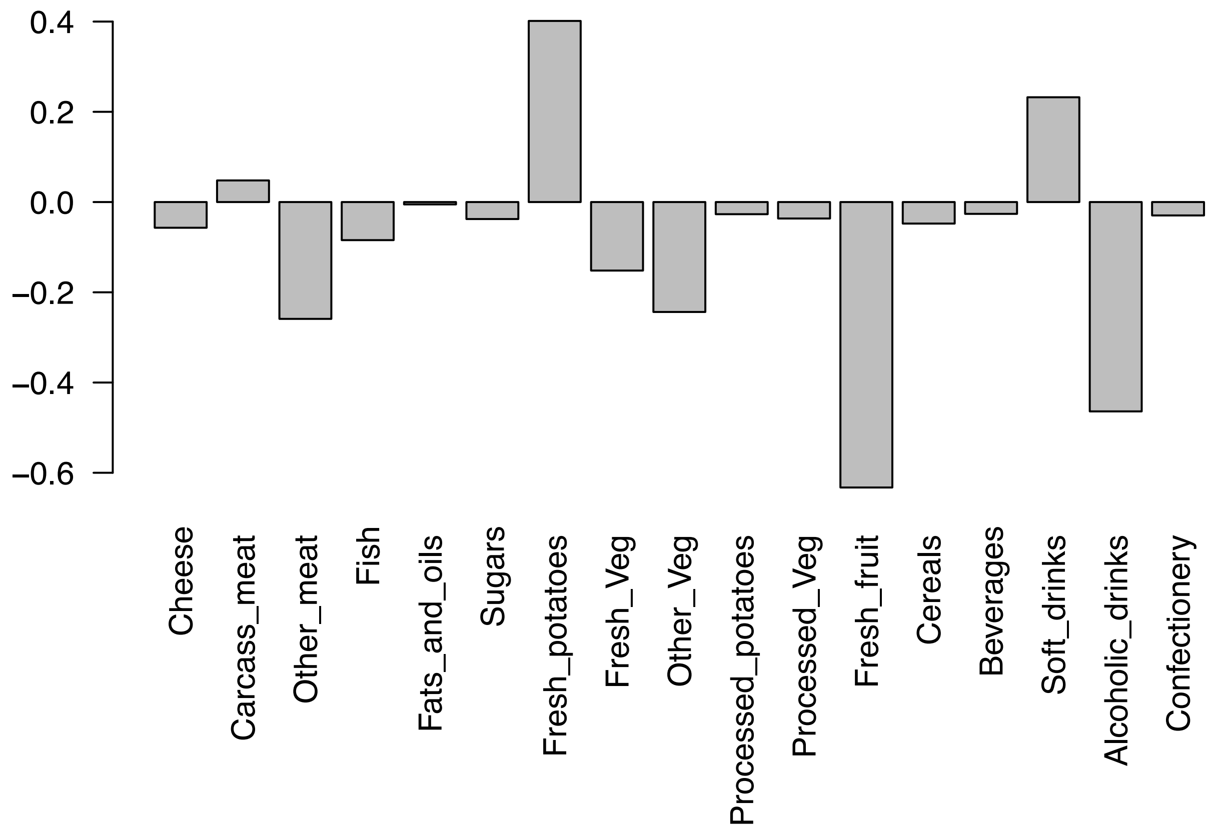
```
## $names
## [1] "sdev"     "rotation" "center"   "scale"    "x"
##
## $class
## [1] "prcomp"
```

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



we can also examine the PCA "loadings" which tells us how much the original variables contribute to each new pc

```
# mar = A numerical vector of the form c(bottom, left, top, right) which gives the number of lines of m
par (mar = c(10,3,0.35,0))
barplot(pca$rotation[,1], las=2)
```



One more PCA stuff

```
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
```

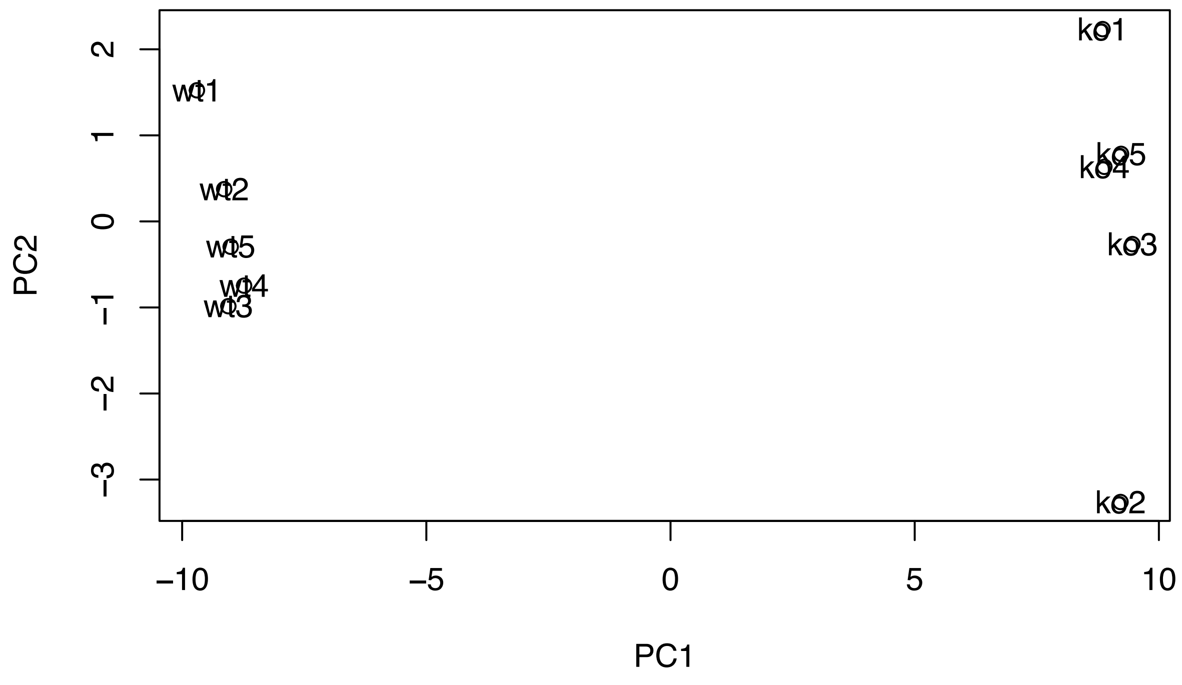
```r
colnames(rna.data)
```

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

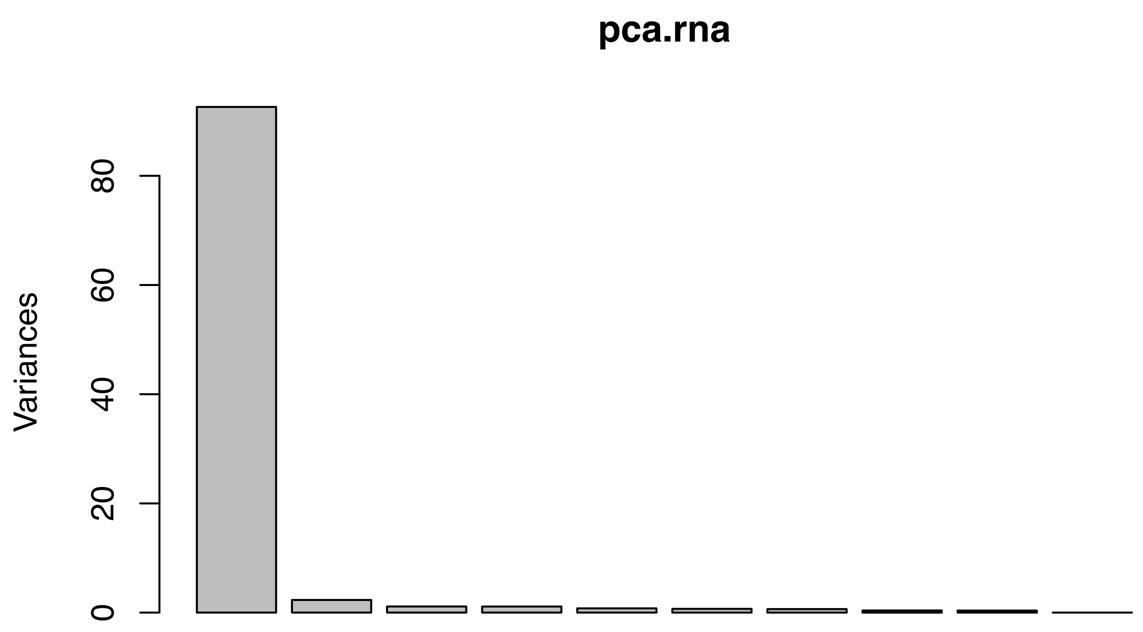
```r
pca.rna = prcomp(t(rna.data), scale = TRUE)
summary(pca.rna)
```

```
## 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
```

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



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


pca.rna
Variances
0
20
40
60
80