class7: machine learning 1

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#clustering methods

Find groups (a.k.a) clusters in my data

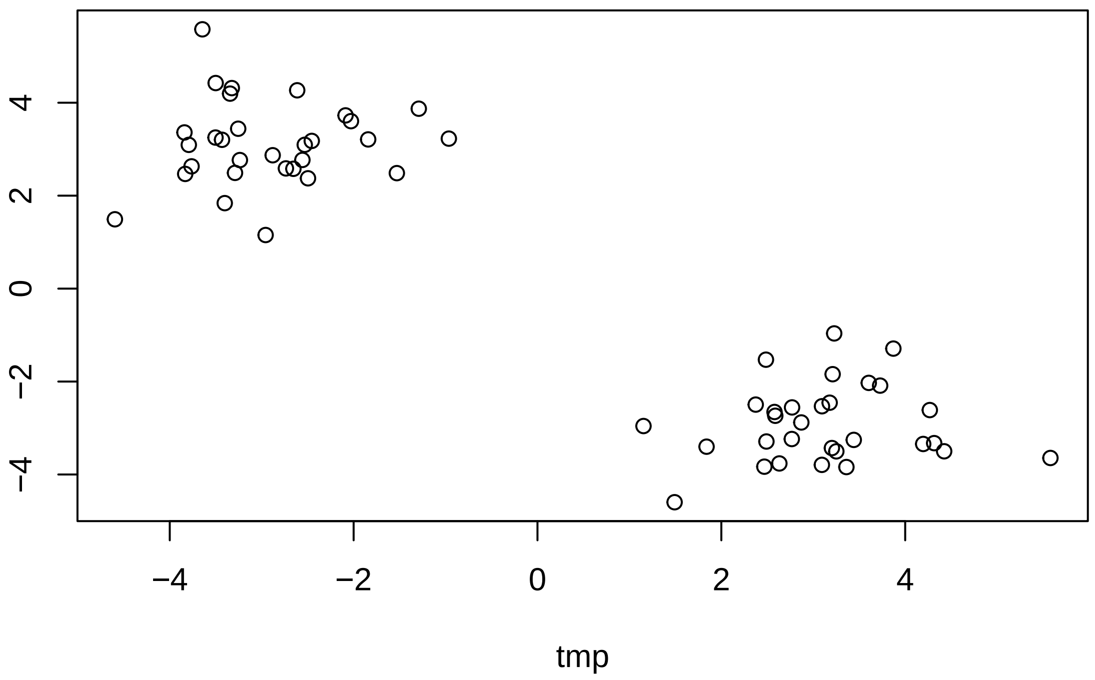
##k-means clustering

Make up some data to test with.

```
#make up some data with 2 clear groups
tmp <- c(rnorm(30, mean= 3), rnorm(30, mean= -3))

x <- cbind(tmp, rev(tmp))

plot(x)
```



The `kmeans()` function does k-means clustering

```r
k <- kmeans(x, centers=4, nstart=20)
k
```

```
## K-means clustering with 4 clusters of sizes 17, 17, 13, 13
##
## Cluster means:
##         tmp
## 1  2.609879 -3.307485
## 2 -3.307485  2.609879
## 3 -2.396884  3.783276
## 4  3.783276 -2.396884
##
## Clustering vector:
##  [1] 4 4 4 4 1 1 1 4 1 1 1 1 1 1 1 4 1 1 1 1 1 4 4 1 4 4 4 1 4 4 3 3 2 3 3 3 2 3
## [39] 3 2 2 2 2 2 3 2 2 2 2 2 2 2 3 2 2 2 3 3 3 3
##
## Within cluster sum of squares by cluster:
## [1] 11.43859 11.43859 16.70071 16.70071
##  (between_SS / total_SS =  95.2 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

We can use the dollar syntax to get at the results (components of the returned list).

> Q1. How many points are in each cluster?

```r
k$size
```

```
## [1] 17 17 13 13
```

> What component of your result object details -Cluster size -Cluster assignment/membership -Cluster center?

```r
k$size
```

```
## [1] 17 17 13 13
```

```r
k$cluster
```

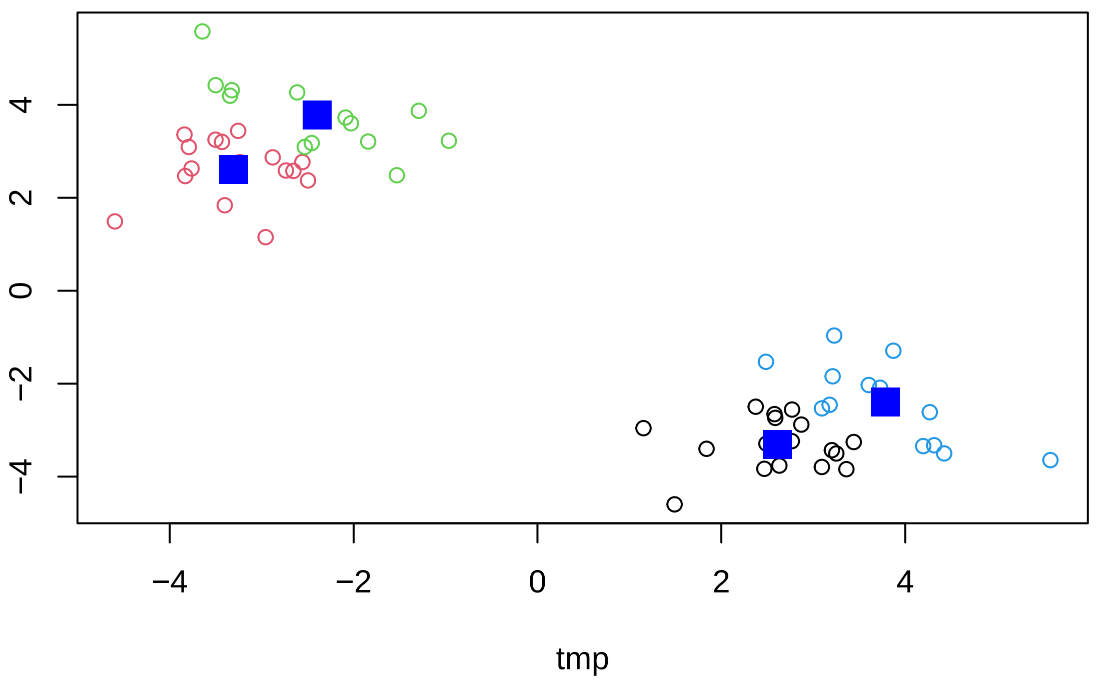
```
##  [1] 4 4 4 4 1 1 1 4 1 1 1 1 1 1 1 4 1 1 1 1 1 4 4 1 4 4 4 1 4 4 3 3 2 3 3 3 2 3
## [39] 3 2 2 2 2 2 3 2 2 2 2 2 2 2 3 2 2 2 3 3 3 3
```

```r
k$centers
```

```
##         tmp
## 1  2.609879 -3.307485
## 2 -3.307485  2.609879
## 3 -2.396884  3.783276
## 4  3.783276 -2.396884
```

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

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



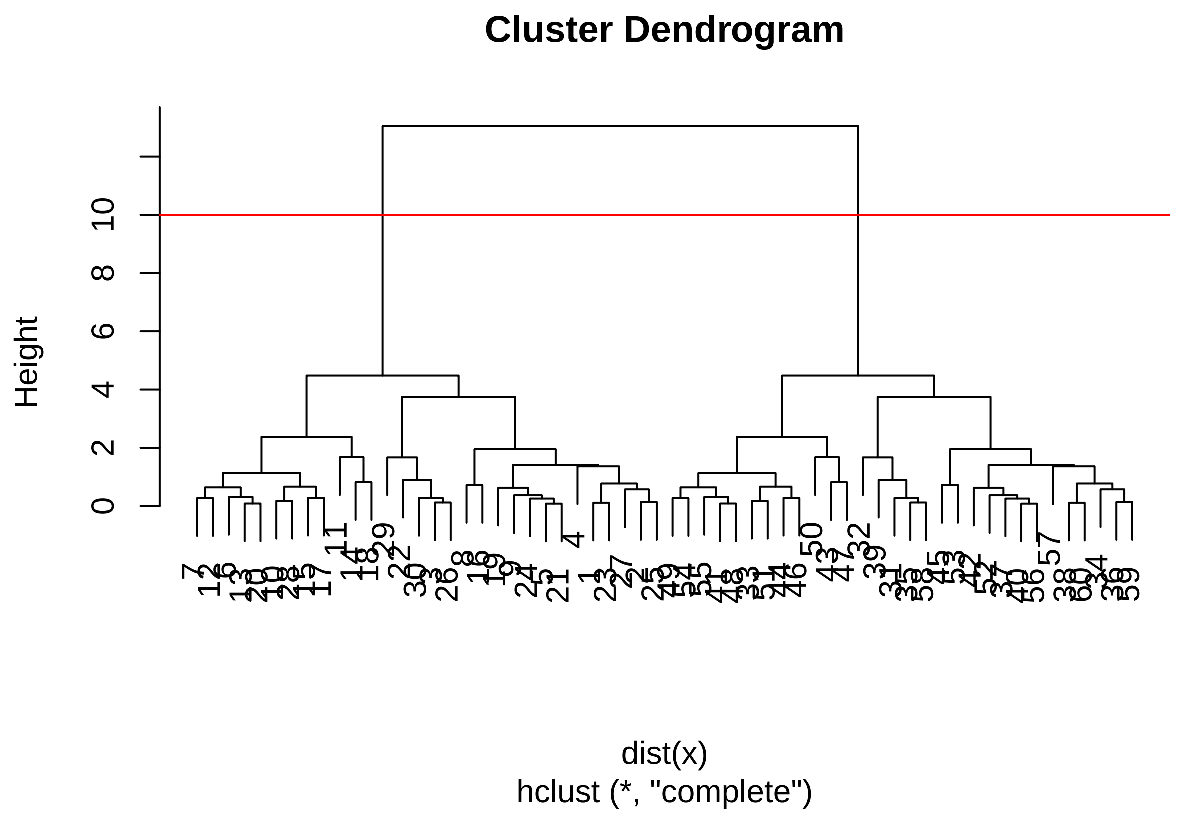
Hierarchical Clustering

The `hclust()` function needs a distance matrix as input not our original data. For this we use the `dist()` function

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

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

```
plot(hc)
abline(h=10, col="red")
```



To get our cluster membership vector we need to cut our tree and for this we use the `cutree()`

```r
cutree(hc, h=10)
```

```
##  [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 2 2
```

You can cut by a given height h= or into a given number of k groups with k=

```r
cutree(hc, k=2)
```

```
##  [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 2 2
```

#Principal Component Analysis

PCA of UK food data

Let's read our data about the weird stuff folks from the UK eat and drink

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

Look at the first bit of the file:

```
head(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
```

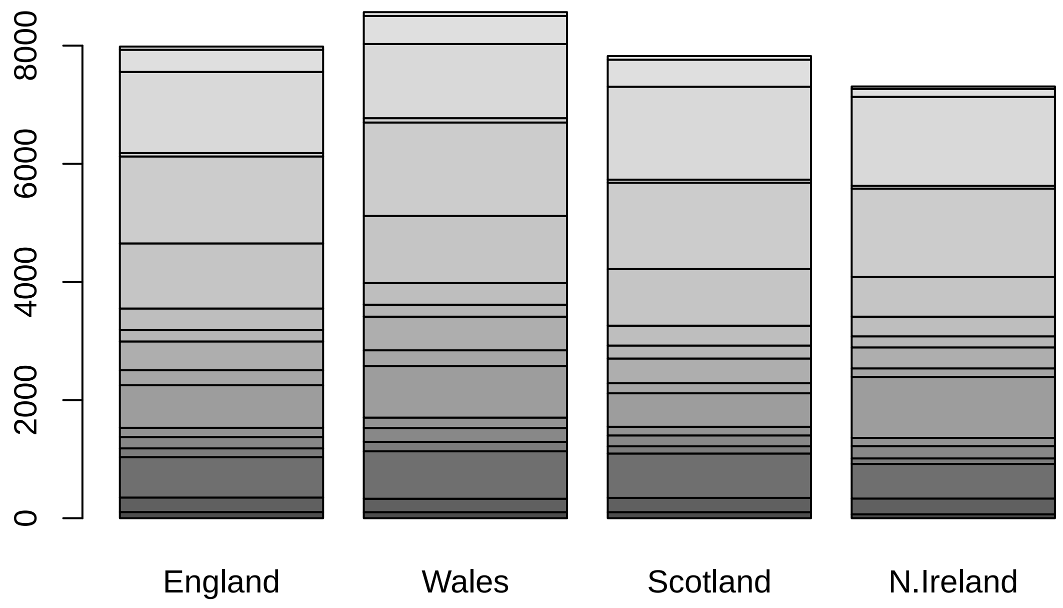
How many columns in this dataset:

```
ncol(x)
```

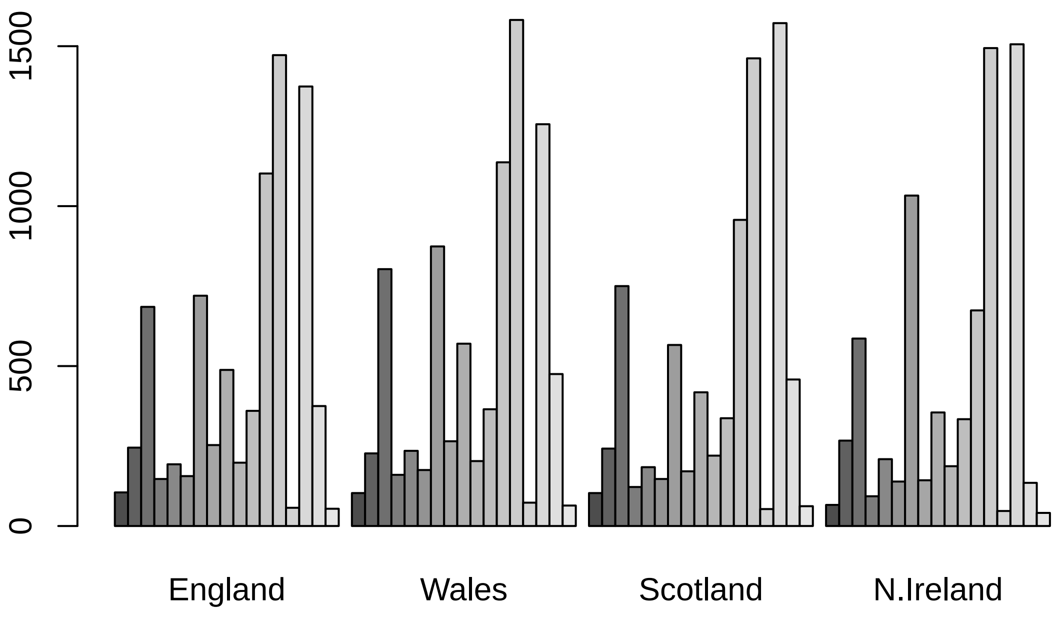
```
## [1] 4
```

We can make some plots to try to understand this data a bit more. For example barplots:

```
barplot(as.matrix(x))
```



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



#PCA to the rescue

The main base R function for PCA is called `prcomp()`. prcomp() expects the observations to be rows and the variables to be columns therefore we need to first transpose our data.frame matrix with the t() transpose function.

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

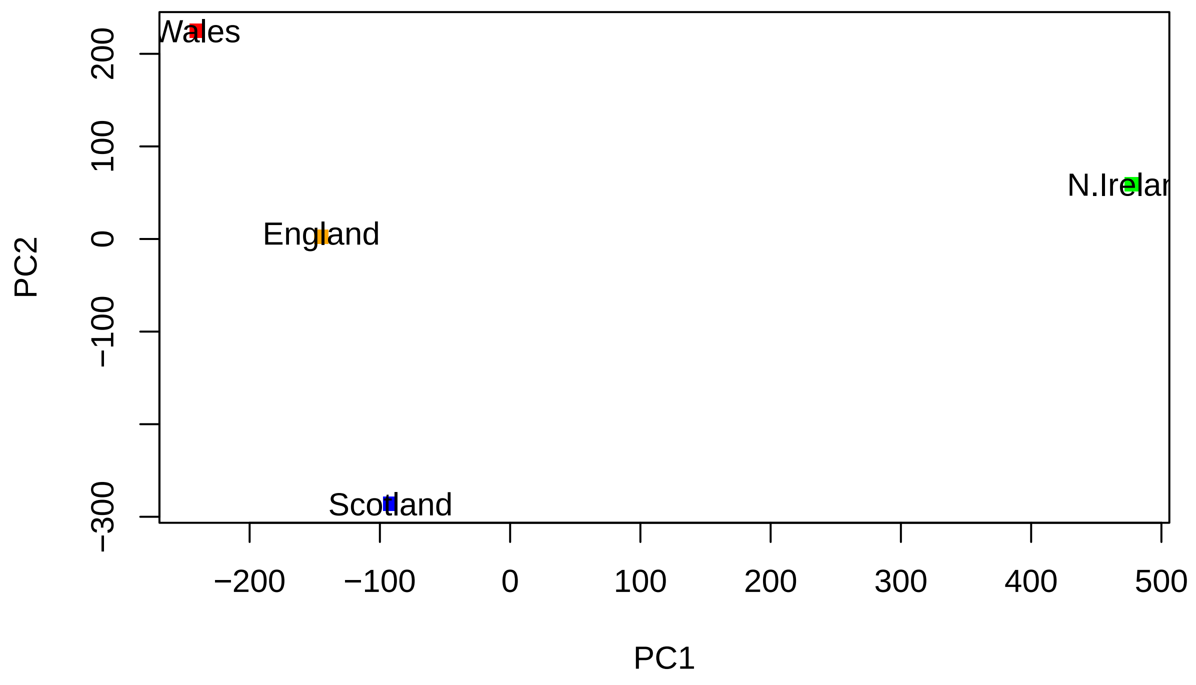
```
## Importance of components:
##                              PC1      PC2      PC3       PC4
## Standard deviation     324.1502 212.7478 73.87622 5.552e-14
## Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
## Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

What is in this returned pca object?

```
attributes(pca)
```

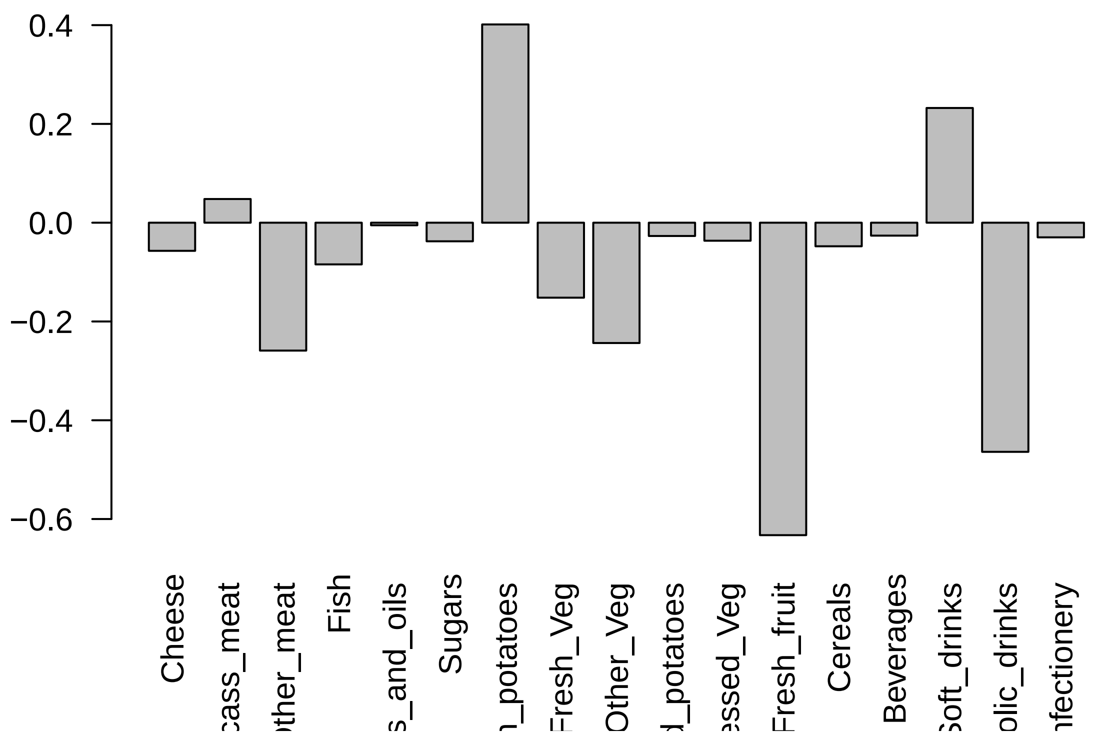
```
## $names
## [1] "sdev"     "rotation" "center"   "scale"    "x"
##
## $class
## [1] "prcomp"
```

```
plot(pca$x[,1:2], col=c("orange", "red", "blue", "green"), pch=15)
text(pca$x[,1], pca$x[,2], labels=colnames(x))
```



We can look at how the variables contribute to our new PCs by examining the `pca$rotation` component of our results

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



#PCA of RNA-Seq Data example…

Read data first:

```
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
```

How many genes(how many rows?)

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

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

How many experiments (columns)?

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

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

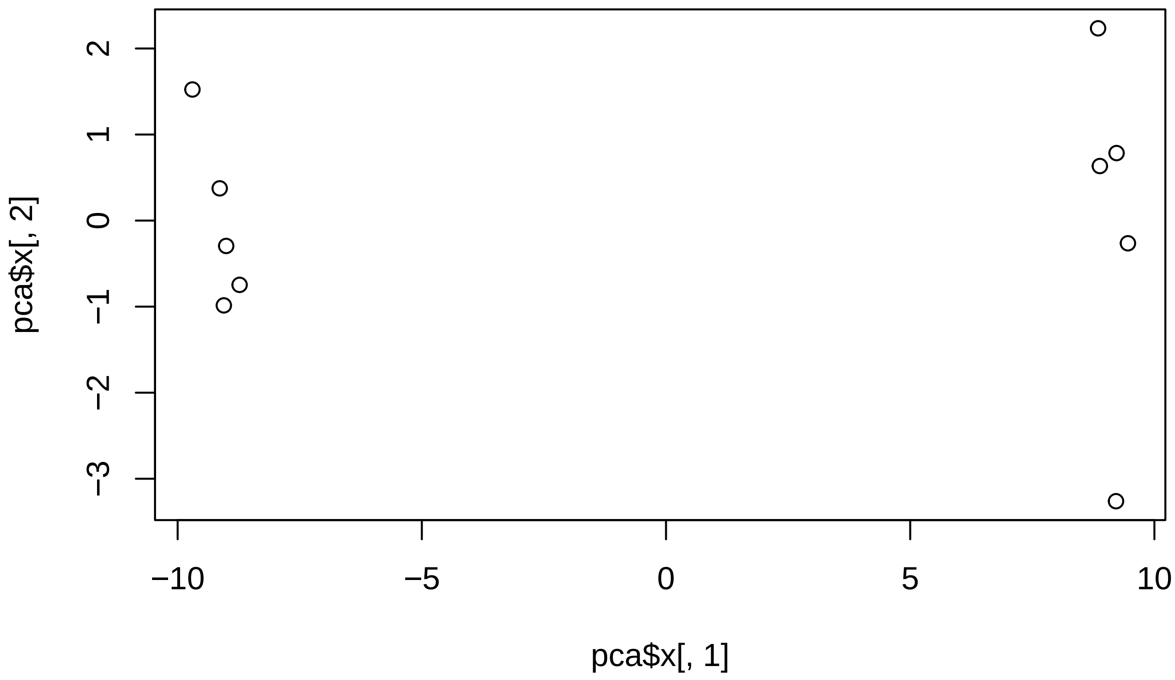
Let's do PCA of this dataset. First take the transpose as that is what the prcomp() function wants…

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

```
## 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
```

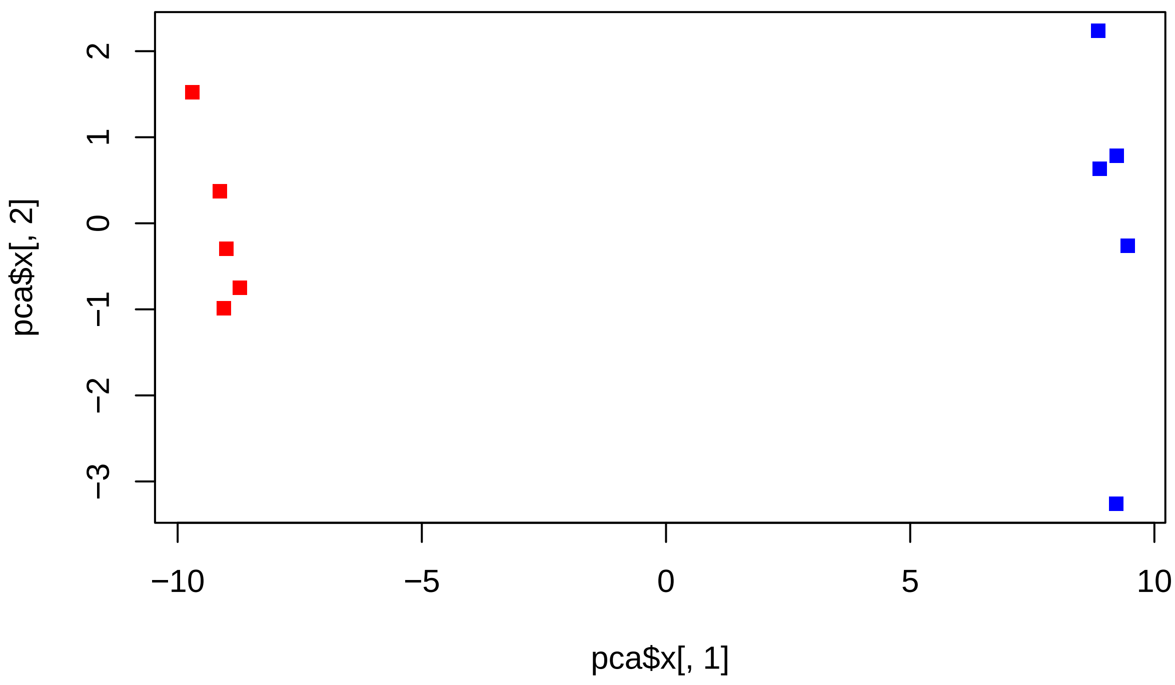
We can make our score plot (a.k.a PCA plot) from the `pca$x` .

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



Make a little color vector to color up our plot by wt and ko

```
colvec <- c(rep("red",5), rep("blue",5))
plot(pca$x[,1], pca$x[,2], col= colvec, pch=15)
```


pca$x[, 2]
pca$x[, 1]