Lab 8: Machine Learning 1

Taylor Darby

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.

```
# 'rnorm' provides a random dataset distributed normally, and specifying x and y sets the number of row
tmp <- c(rnorm(30, 3), rnorm(30, -3))

# 'cbind' binds the data in the columns together
data <- cbind(x=tmp, y=rev(tmp))

# We now have a dataset to perform k-means with
data
```

```
##                x          y
##  [1,]  2.7550259 -4.1195588
##  [2,]  3.0633328 -2.4829510
##  [3,]  3.1881915 -4.3939522
##  [4,]  1.1127519 -3.2394942
##  [5,]  3.2874358 -4.7007221
##  [6,]  1.6708457 -1.4849593
##  [7,]  2.3694659 -0.4289242
##  [8,]  2.0173767 -2.1843387
##  [9,]  2.5870592 -2.4793419
## [10,]  1.8960701 -2.1617600
## [11,]  2.2677314 -2.9885094
## [12,]  2.8324203 -3.5932365
## [13,]  3.2959694 -2.0079145
## [14,]  3.8705091 -2.2604250
## [15,]  3.1937913 -2.9653960
## [16,]  2.9117002 -3.6942136
## [17,]  2.7912476 -2.9917906
## [18,]  3.2955767 -4.5235896
## [19,]  2.4762455 -4.1766312
## [20,]  2.6987888 -2.7648218
## [21,]  3.1586320 -1.8469826
## [22,]  2.2219785 -4.3122930
## [23,]  1.0754638 -2.3513653
## [24,]  1.4805525 -3.4124065
## [25,]  3.1304136 -2.2143707
## [26,]  2.4905842 -3.1523270
## [27,]  2.3265662 -2.8597214
## [28,]  4.2469035 -2.6387041
## [29,]  4.7027752 -3.5195426
## [30,]  3.0637949 -1.7861700
## [31,] -1.7861700  3.0637949
## [32,] -3.5195426  4.7027752
## [33,] -2.6387041  4.2469035
## [34,] -2.8597214  2.3265662
## [35,] -3.1523270  2.4905842
## [36,] -2.2143707  3.1304136
## [37,] -3.4124065  1.4805525
## [38,] -2.3513653  1.0754638
## [39,] -4.3122930  2.2219785
## [40,] -1.8469826  3.1586320
## [41,] -2.7648218  2.6987888
## [42,] -4.1766312  2.4762455
## [43,] -4.5235896  3.2955767
## [44,] -2.9917906  2.7912476
## [45,] -3.6942136  2.9117002
## [46,] -2.9653960  3.1937913
## [47,] -2.2604250  3.8705091
## [48,] -2.0079145  3.2959694
## [49,] -3.5932365  2.8324203
## [50,] -2.9885094  2.2677314
## [51,] -2.1617600  1.8960701
## [52,] -2.4793419  2.5870592
## [53,] -2.1843387  2.0173767
## [54,] -0.4289242  2.3694659
## [55,] -1.4849593  1.6708457
## [56,] -4.7007221  3.2874358
## [57,] -3.2394942  1.1127519
## [58,] -4.3939522  3.1881915
## [59,] -2.4829510  3.0633328
## [60,] -4.1195588  2.7550259
```

Run ‘kmeans()’: Set “k”(“centers”) to 2 nstart to 20. The thing with ‘kmeans’ is that you have to tell it how many clusters you want (in this case = 2)

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

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##           x         y
## 1 -2.924547  2.715973
## 2  2.715973 -2.924547
##
## 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
##
## Within cluster sum of squares by cluster:
```

```
## [1] 48.71651 48.71651
##  (between_SS / total_SS =  90.7 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

Q1. How many points are in each cluster?

```
km$size
```

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

Q2. 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
```

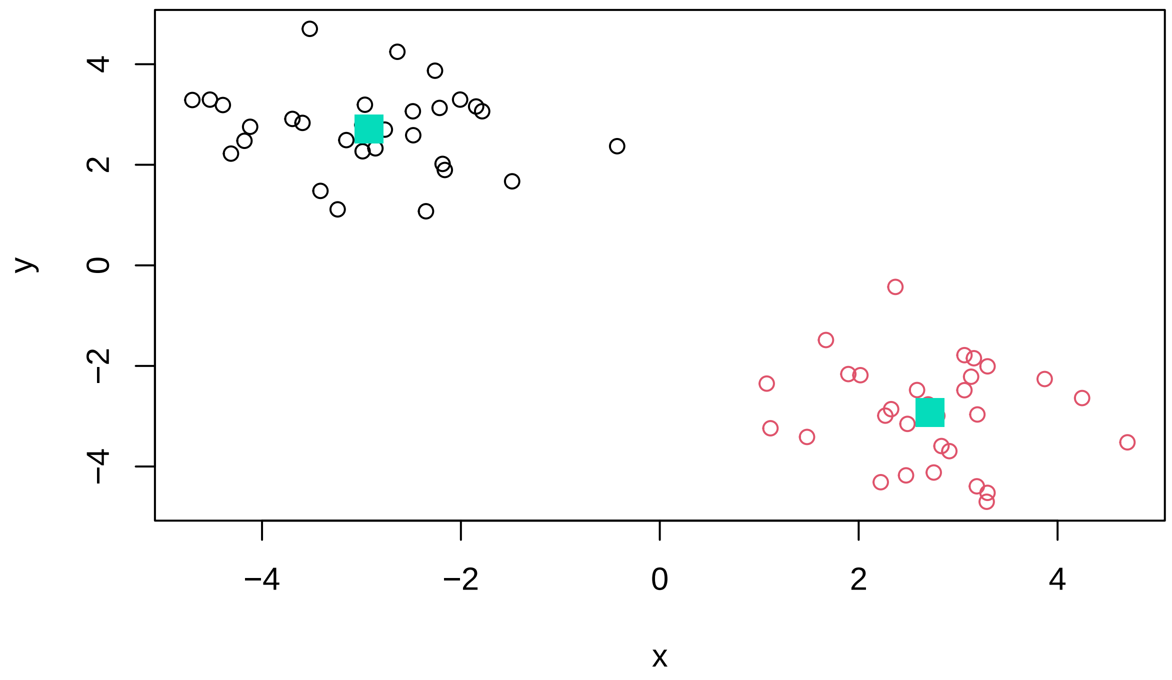
Q3. What 'component' of your result object details cluster center?

```
km$centers
```

```
##           x         y
## 1 -2.924547  2.715973
## 2  2.715973 -2.924547
```

Q4. Plot x colored by the kmeans cluster assignment and add cluster centers as blue points

```
plot(data, col=km$cluster)
points(km$centers, col="#05DCBB", pch=15, cex=2)
```



Hierarchical Clustering

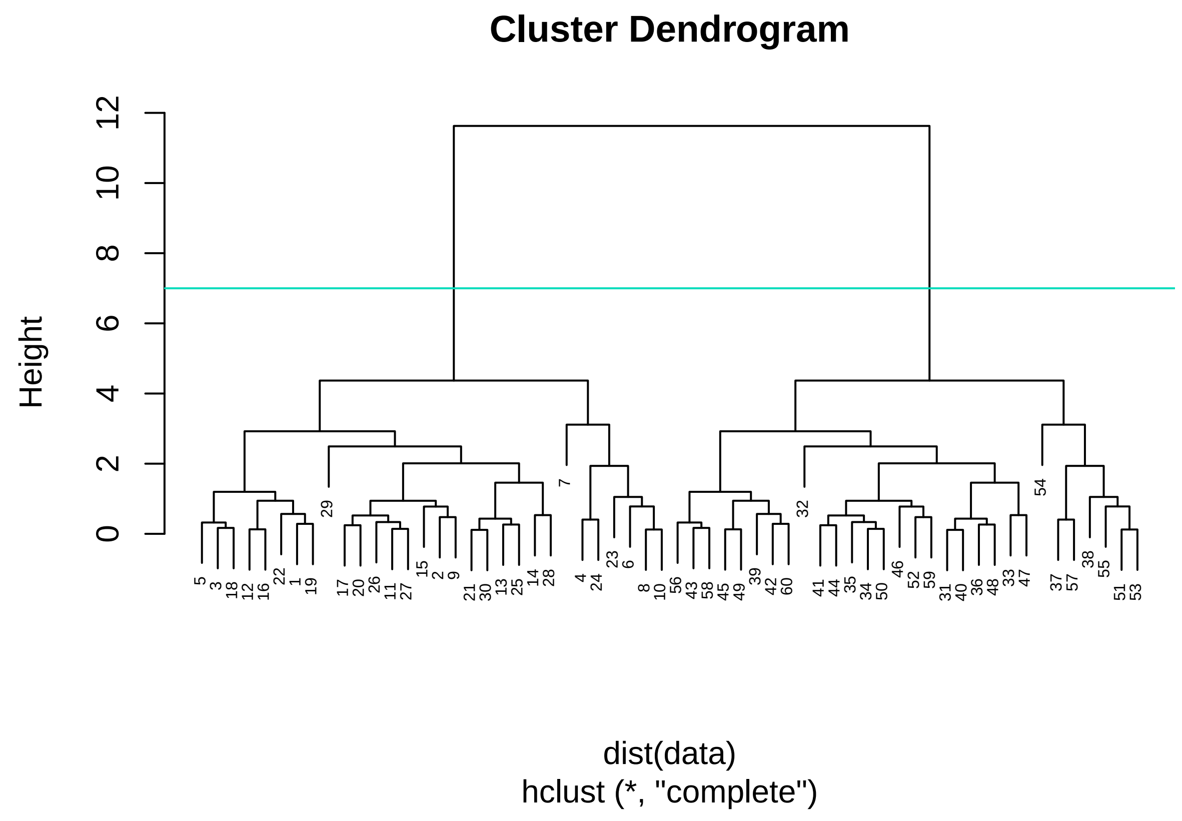
We will use the ‘hclust()’ function on the same data as before and see how this method works.

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

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

‘hclust’ gas a plot method

```
plot(hc, cex=0.5)
abline(h=7, col="#05DCBB")
```



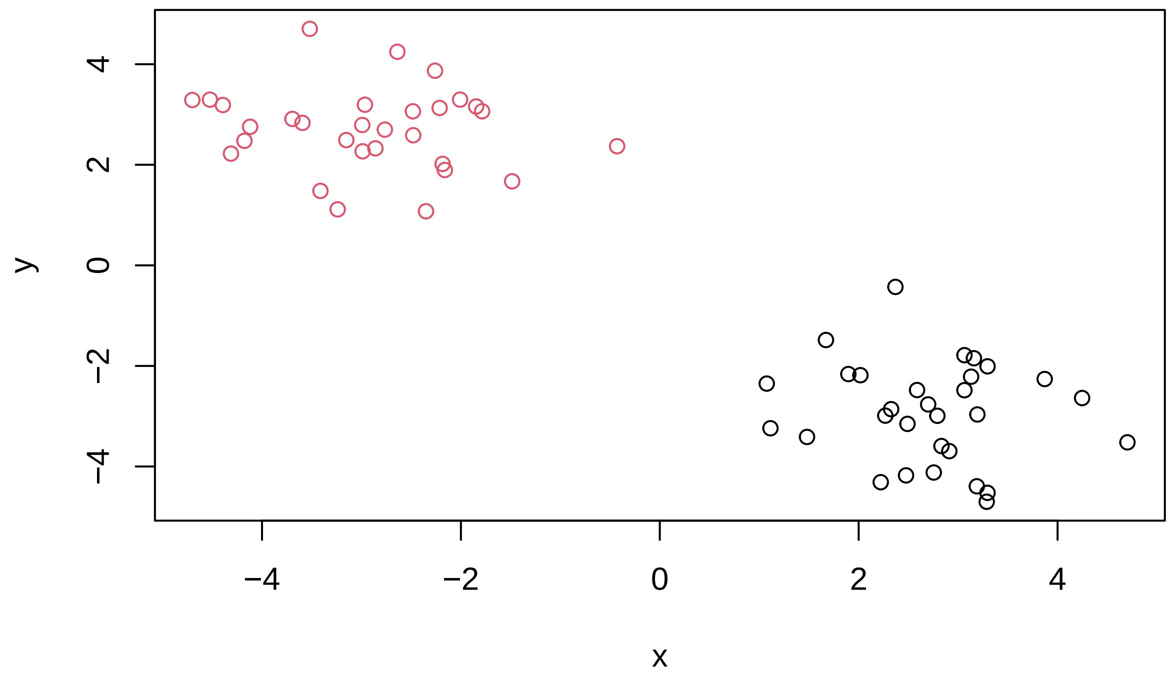
To find our membership vector we need to "cut" the tree and for this we use the 'cutree()' function and tell it the height to cut at.

```
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 2 2
```

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

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

plot(data, col=grps)
```



Principal Component Analysis (PCA)

PCA is useful for visualizing key variance in datasets with high dimensionality.

PCA of UK food data

Import UK food dataset

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

```
##                X England Wales Scotland N.Ireland
## 1         Cheese     105   103      103        66
## 2  Carcass_meat      245   227      242       267
## 3    Other_meat      685   803      750       586
## 4           Fish     147   160      122        93
## 5 Fats_and_oils      193   235      184       209
## 6         Sugars     156   175      147       139
```

> **Q1.** How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?

```
## Complete the following code to find out how many rows and columns are in x?
dim(x)
```

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

```
## Preview the first 6 rows
head(x)
```

```
##                X England Wales Scotland N.Ireland
## 1         Cheese     105   103      103        66
## 2  Carcass_meat      245   227      242       267
## 3    Other_meat      685   803      750       586
## 4           Fish     147   160      122        93
## 5 Fats_and_oils      193   235      184       209
## 6         Sugars     156   175      147       139
```

> **Q2.** Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

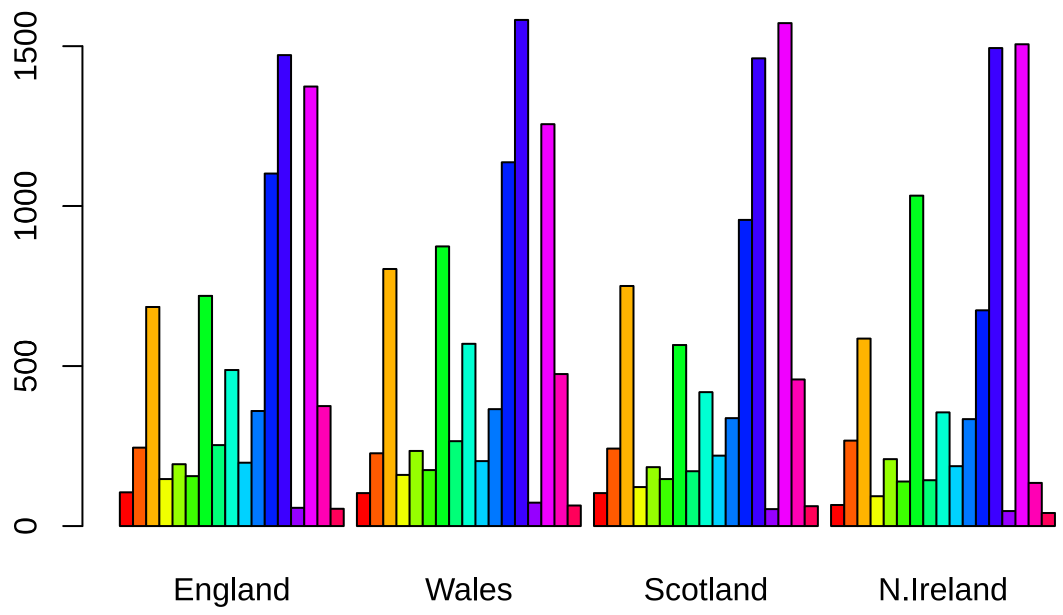
```
# Note how the minus indexing works
# rownames(x) <- x[,1] "This is not a good way to code because you will lose a column every time you ru
# x <- x[,-1]

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

Spotting major differences and trends

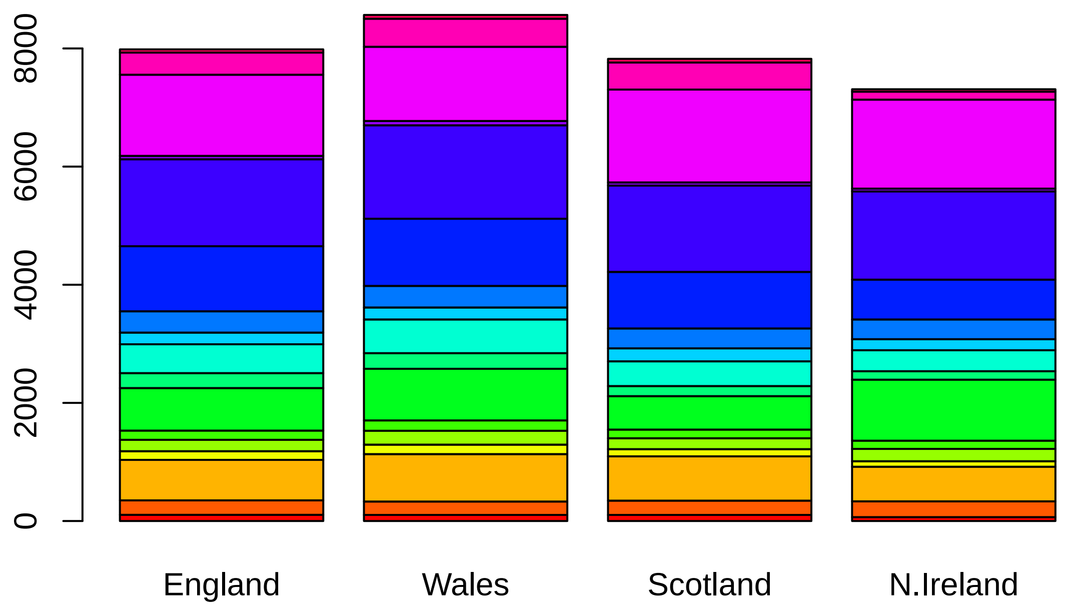
Let's plot the data

```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



Q3: Changing what optional argument in the above barplot() function results in the following plot?

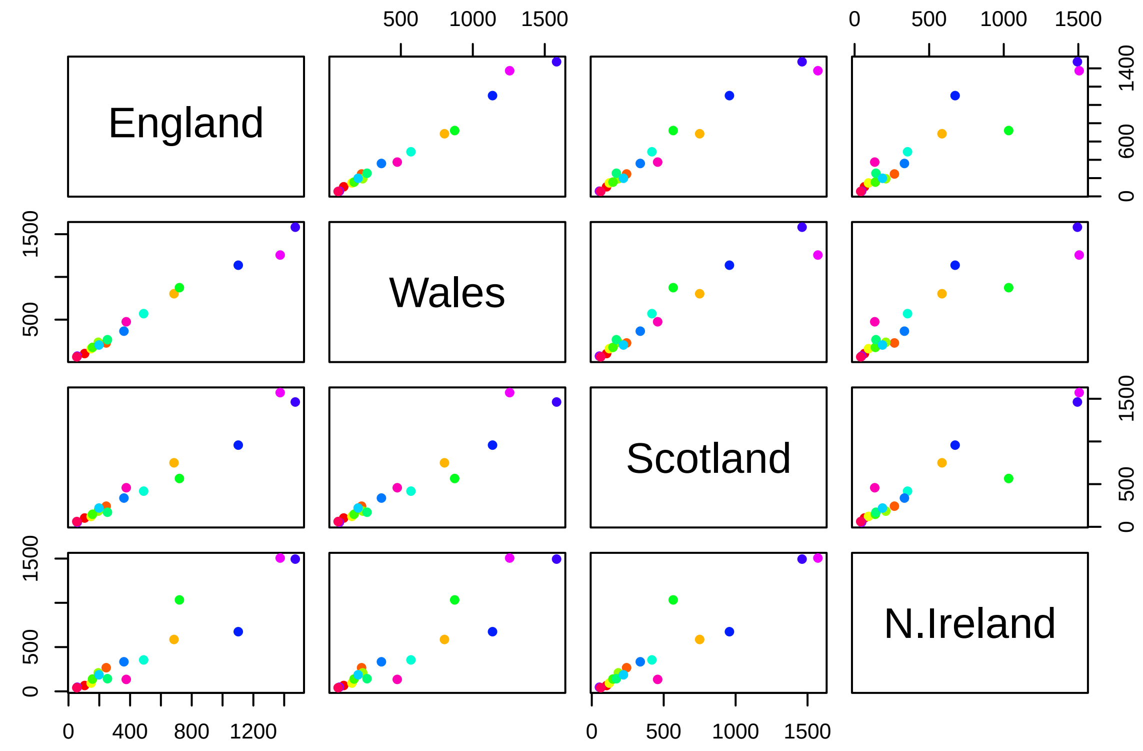
```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



Q5: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

Make a pairwise plot

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



Answer: The axis comparisons change across rows and columns. If the point lies on the diagonal then that food is consumed at the same rate in both countries.

> **Q6.** What is the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

N. Ireland consumes less of one of the values than the rest of the countries.

PCA to the rescue

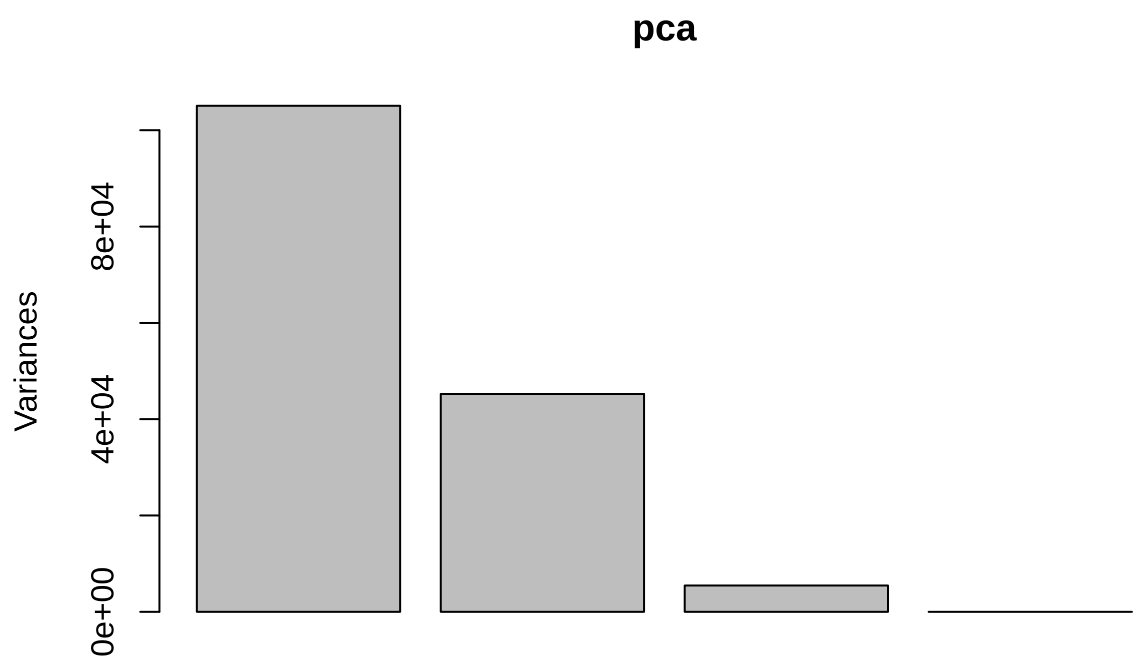
Here we will use the base R function for PCA, which is called 'prcomp()'. Note: This function wants the transpose of our data.

```r
# Use the prcomp() PCA function
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
```

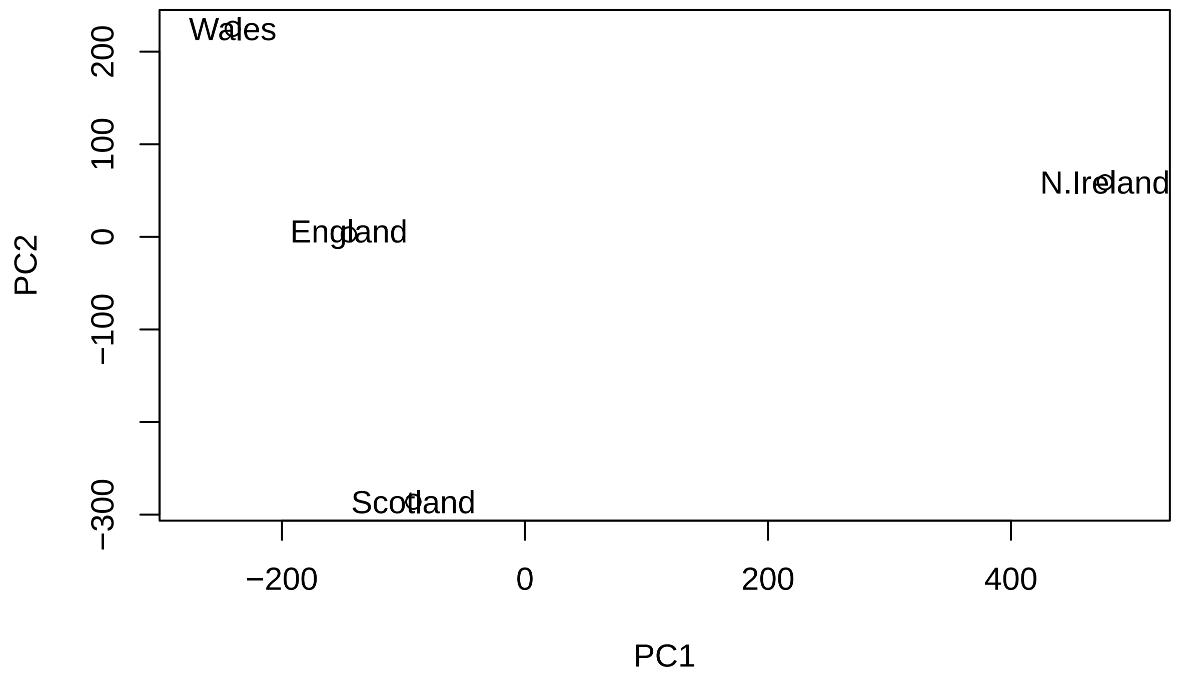
Plot this pca

```
plot(pca)
```



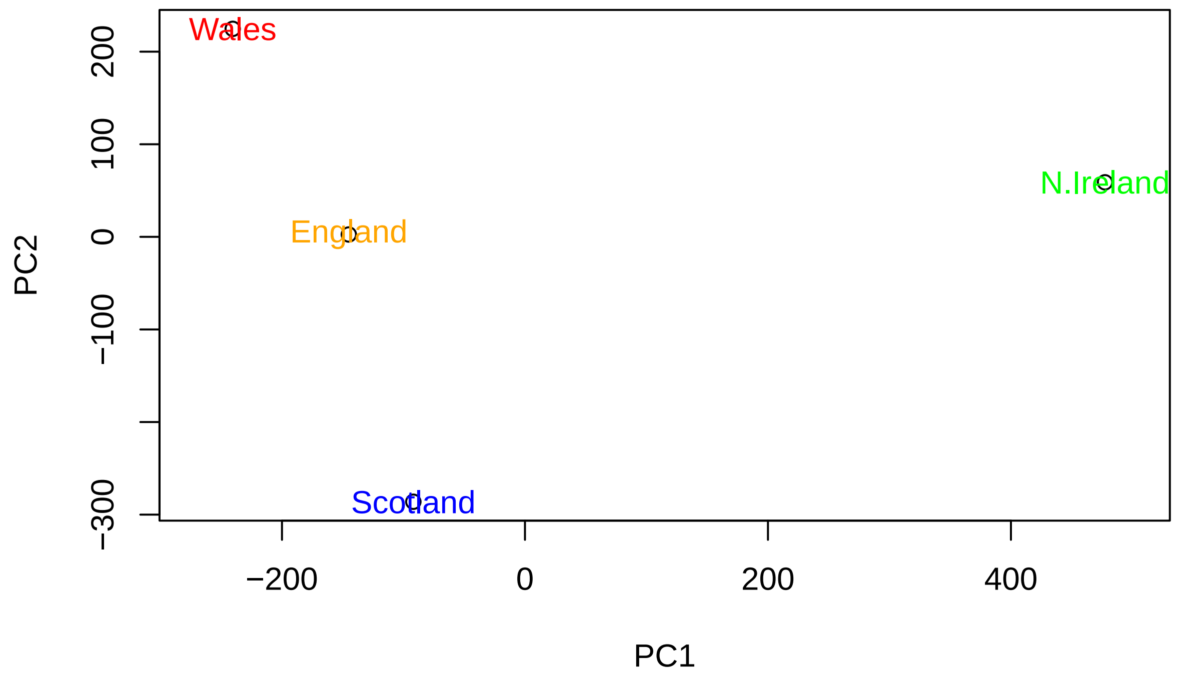
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x))
```



Q8. Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

```r
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], labels = colnames(x), col=c("orange", "red", "blue", "green"))
```



Below we can use the square of pca$sdev , which stands for "standard deviation", to calculate how much variation in the original data each PC accounts for.

```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

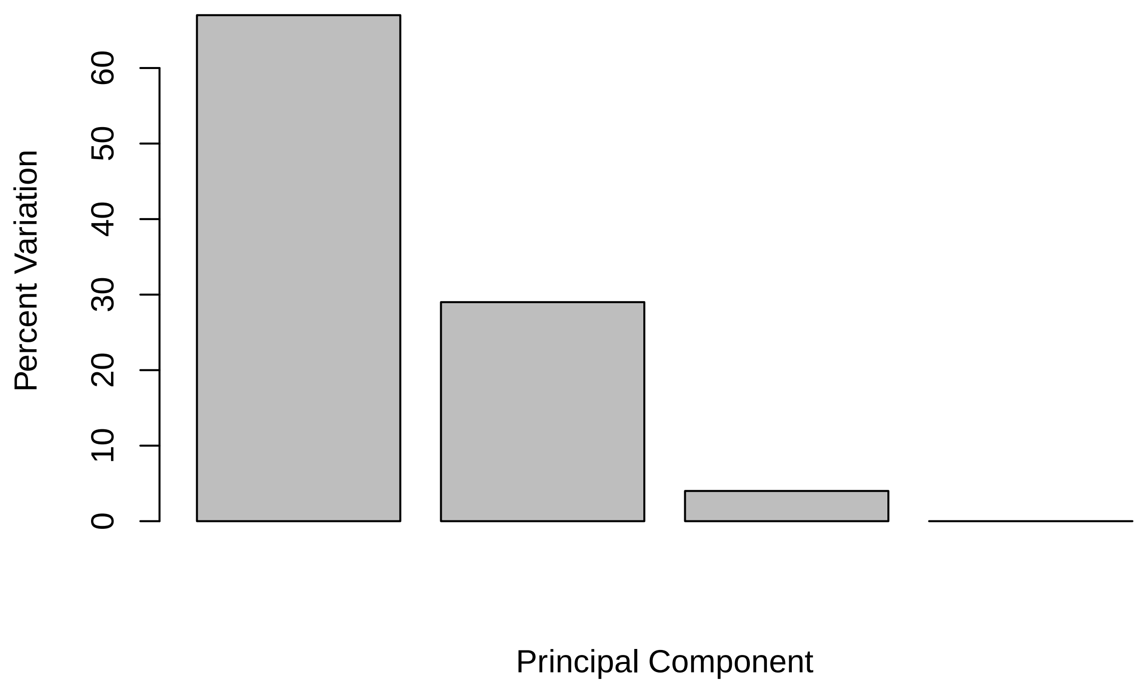
```
## [1] 67 29  4  0
```

```
## or the second row here...
z <- summary(pca)
z$importance
```

```
##                              PC1       PC2      PC3          PC4
## Standard deviation     324.15019 212.74780 73.87622 4.188568e-14
## Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
## Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

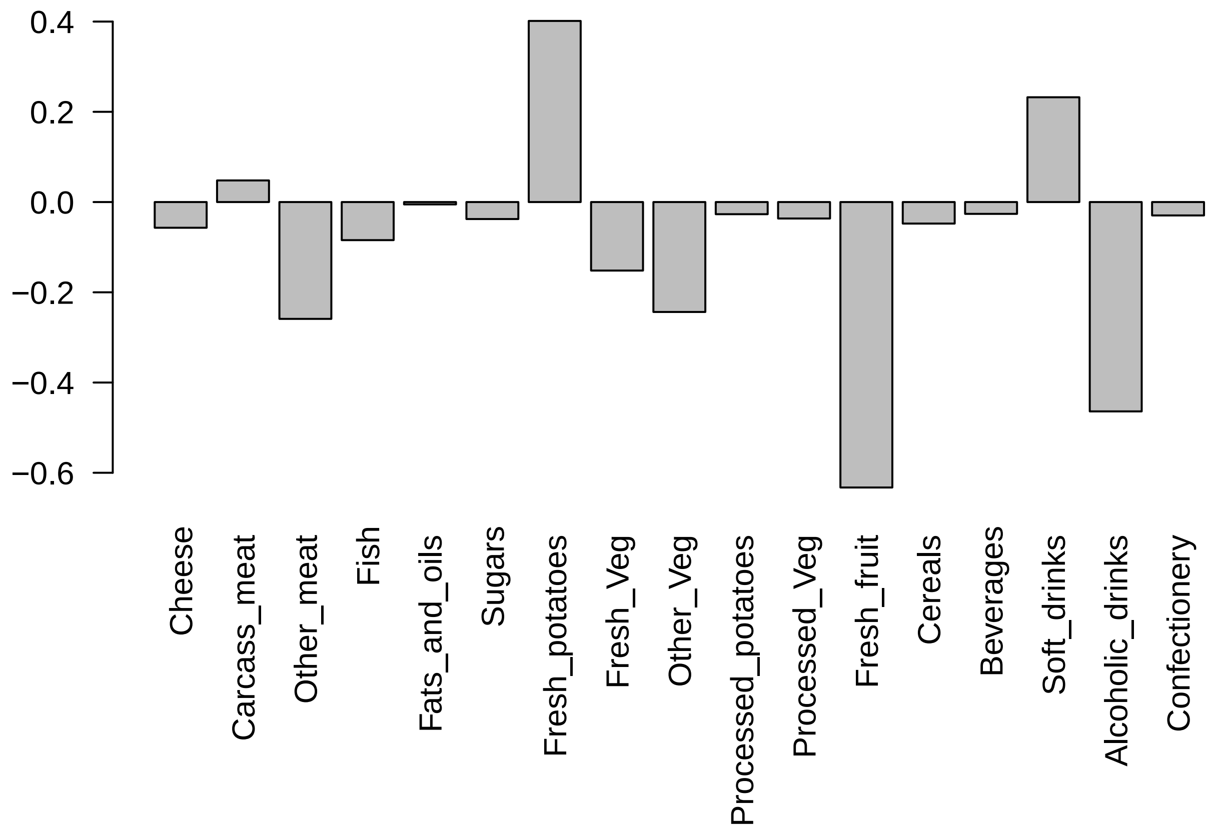
This information can be summarized in a plot of the variances (eigenvalues) with respect to the principal component number (eigenvector number), which is given below.

```r
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```



Digging deeper (variable loadings)

```r
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```



> **Q9:** Generate a similar 'loadings plot' for PC2. What two food groups feature prominantely and what does PC2 maninly tell us about?

One more PCA for today

Import RNAseq data

```
url2 <- "https://tinyurl.com/expression-CSV"
rna.data <- read.csv(url2, row.names=1)
head(rna.data)
```

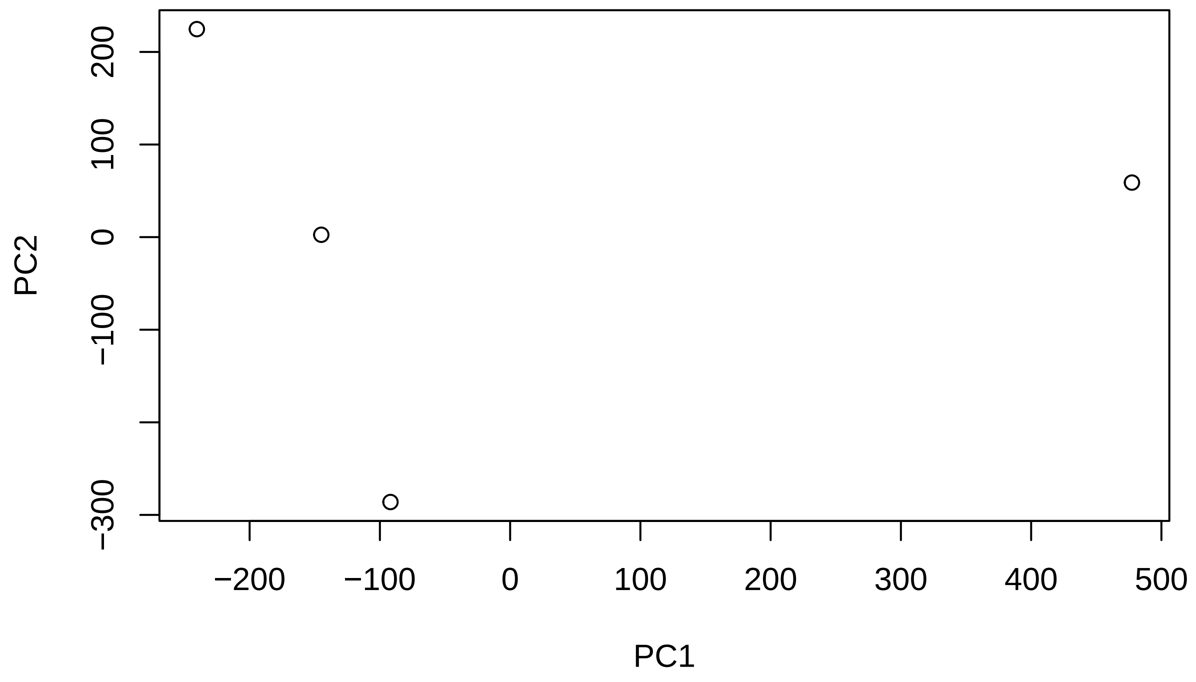
```
##        wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
## gene1  439 458  408  429 420  90  88  86  90  93
## gene2  219 200  204  210 187 427 423 434 433 426
## gene3 1006 989 1030 1017 973 252 237 238 226 210
## gene4  783 792  829  856 760 849 856 835 885 894
## gene5  181 249  204  244 225 277 305 272 270 279
## gene6  460 502  491  491 493 612 594 577 618 638
```

> **Q10:** How many genes and samples are in this data set?

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

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

```r
## Again we have to take the transpose of our data
pca.rna <- prcomp(t(rna.data), scale=TRUE)

## Simple un polished plot of pc1 and pc2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
```

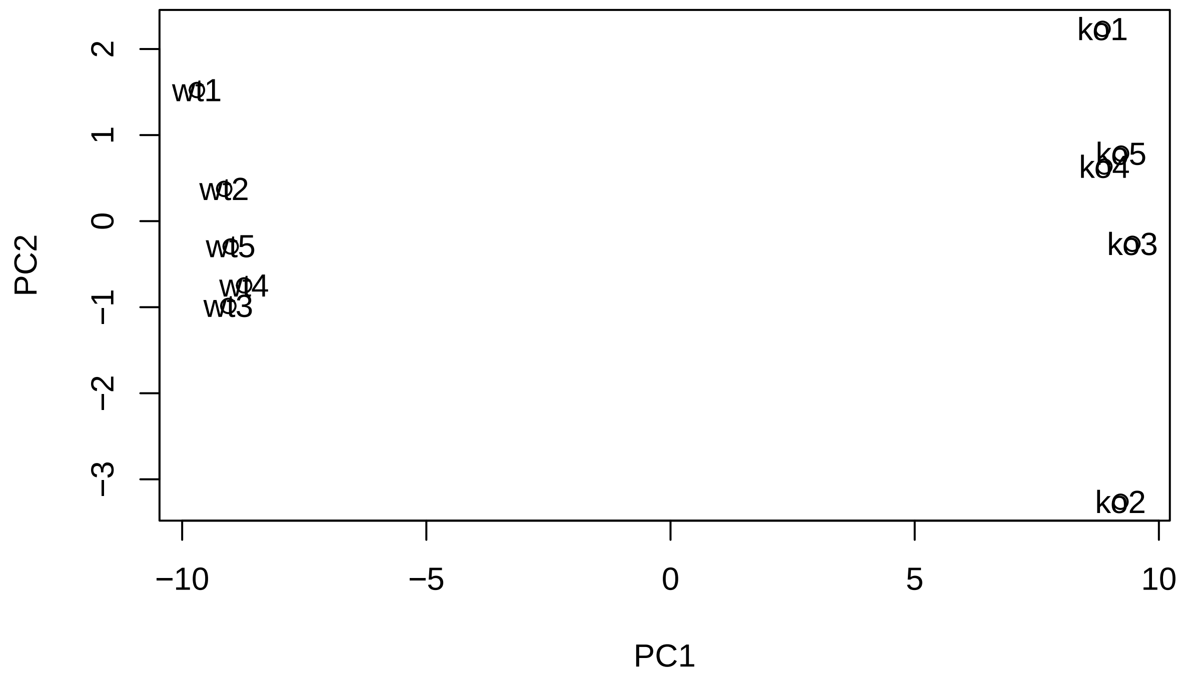


```r
summary(pca.rna)
```

```
## 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
```

Scree plot of RNA data

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



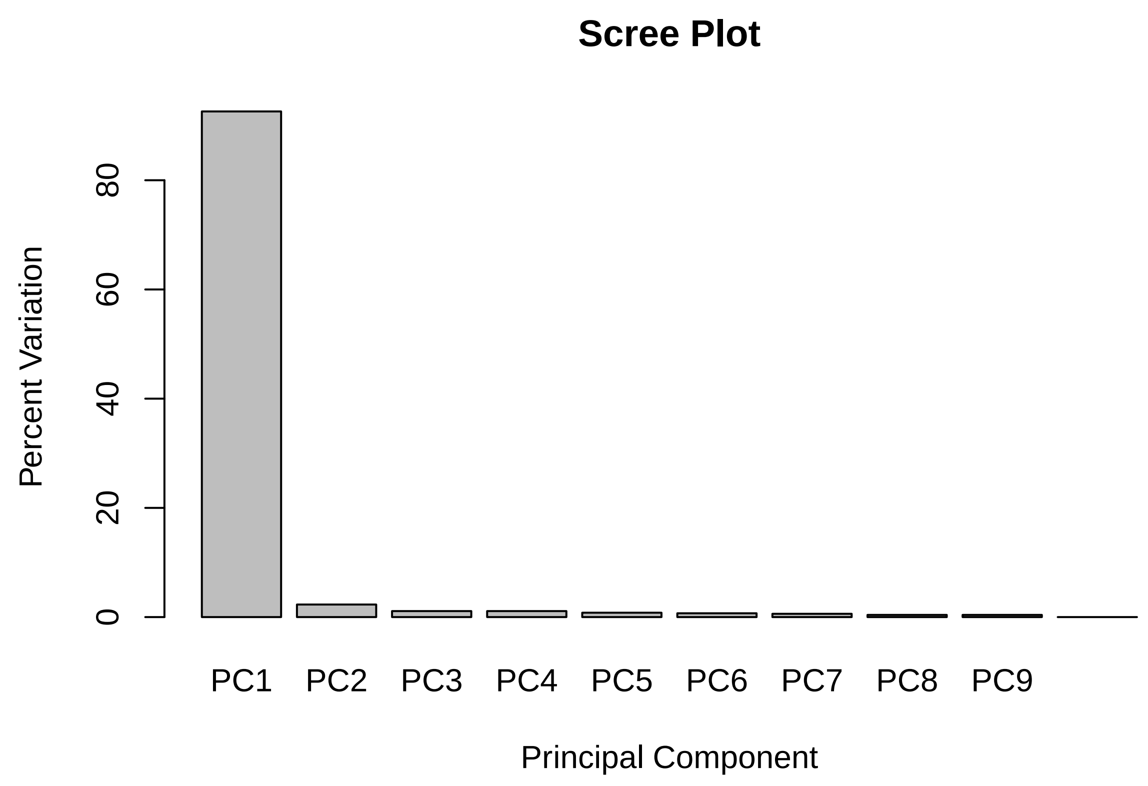
OR Let's make the above scree plot ourselves and in so doing explore the object returned from prcomp() a little further. We can use the square of pca$sdev, which stands for "standard deviation", to calculate how much variation in the original data each PC accounts for:

```
## Variance captured per PC
pca.var <- pca.rna$sdev^2

## Percent variance is often more informative to look at
pca.var.per <- round(pca.var/sum(pca.var)*100, 1)
pca.var.per
```

```
##  [1] 92.6  2.3  1.1  1.1  0.8  0.7  0.6  0.4  0.4  0.0
```

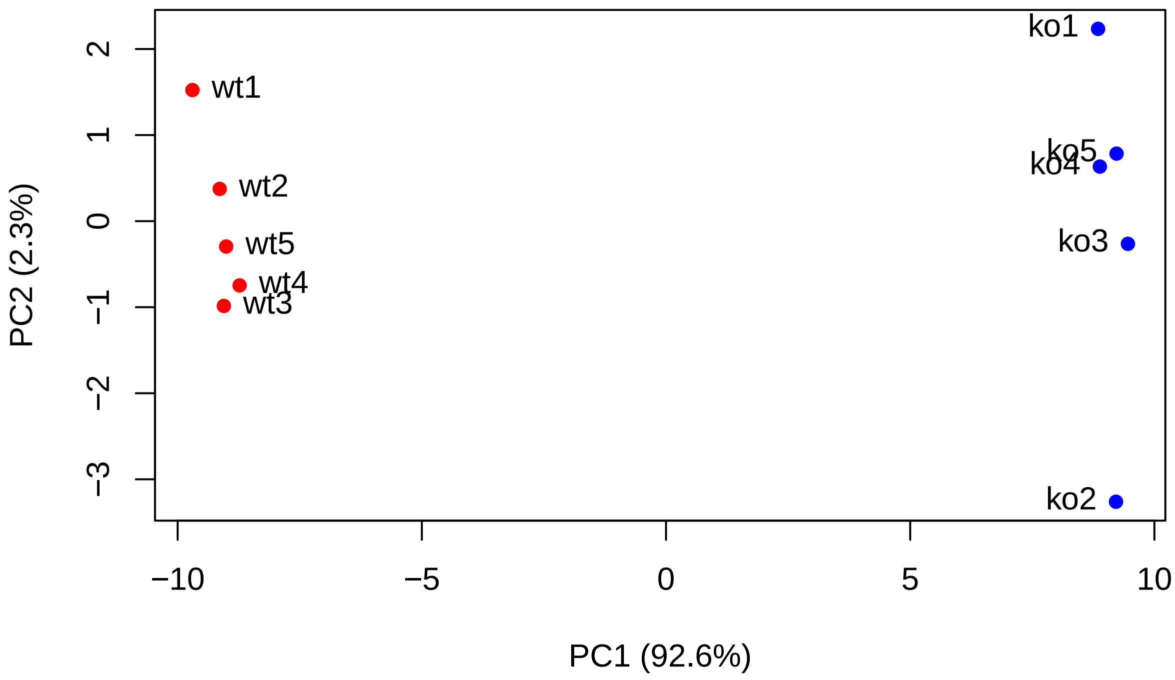
We can use this to generate our own scree-plot like this

```
barplot(pca.var.per, main="Scree Plot",
        names.arg = paste0("PC", 1:10),
        xlab="Principal Component", ylab="Percent Variation")
```



Now lets make our main PCA plot a bit more attractive and useful

```
## A vector of colors for wt and ko samples
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
colvec[grep("ko", colvec)] <- "blue"

plot(pca.rna$x[,1], pca.rna$x[,2], col=colvec, pch=16,
     xlab=paste0("PC1 (", pca.var.per[1], "%)"),
     ylab=paste0("PC2 (", pca.var.per[2], "%)"))

text(pca.rna$x[,1], pca.rna$x[,2], labels = colnames(rna.data), pos=c(rep(4,5), rep(2,5)))
```



... left off on ggplot section