Class 7: Machine Learning 1

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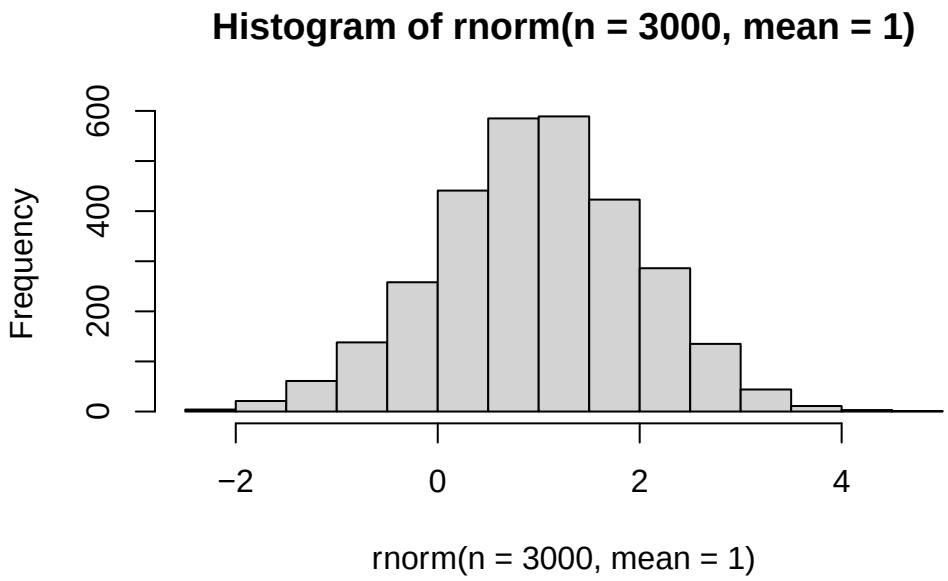
Today we will explore unsupervised machine learning methods, including clustering and dimensionallity reduction methods.

Let's start by making up some data (where we know there are clear groups) that we can use to test out different clustering methods.

We can use the `rnorm()` function to help us here:

```
hist(rnorm(n = 3000, mean = 1))
```

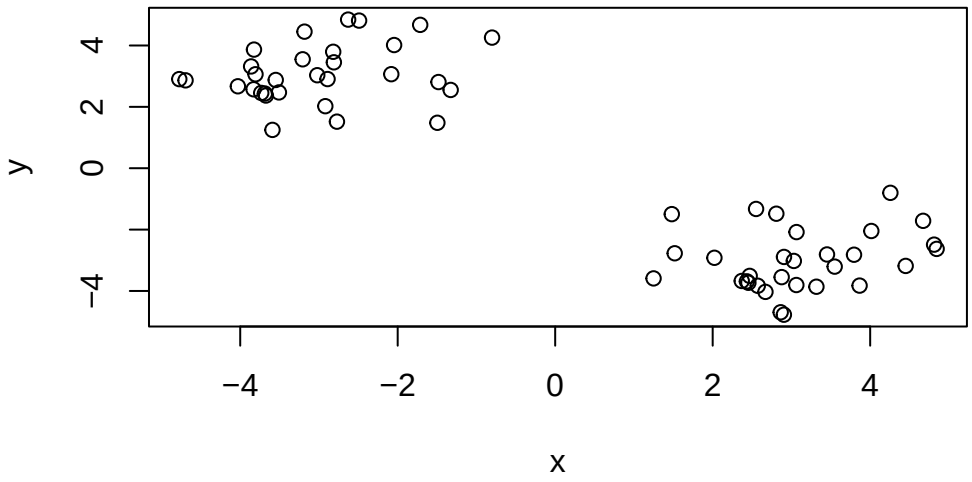


Make data `z` with two "clusters"

```r
x <- c( rnorm(30, mean = -3), rnorm(30, mean = 3) )

z <- cbind(x=x, y=rev(x))
head(z)
```

```
             x        y
[1,] -3.183680 4.450886
[2,] -3.548759 2.876119
[3,] -2.890676 2.905432
[4,] -3.686936 2.434117
[5,] -4.694051 2.863518
[6,] -2.810581 3.451711
```

```r
plot(z)
```



K-means clustering

The main function in "base" R for K-means clustering is called `kmeans()`

```r
k <- kmeans(z, centers = 2)
k
```

```
K-means clustering with 2 clusters of sizes 30, 30

Cluster means:
          x         y
1  3.077765 -3.008406
2 -3.008406  3.077765

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 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] 54.83824 54.83824
 (between_SS / total_SS =  91.0 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

```r
attributes(k)
```

```
$names
[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"

$class
[1] "kmeans"
```

Q. How many points lie in each cluster?

```r
k$size
```

```
[1] 30 30
```

Q. What component of our results tells us about the cluster membership (i.e. which point lies in which cluster)?

```
k$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 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
```

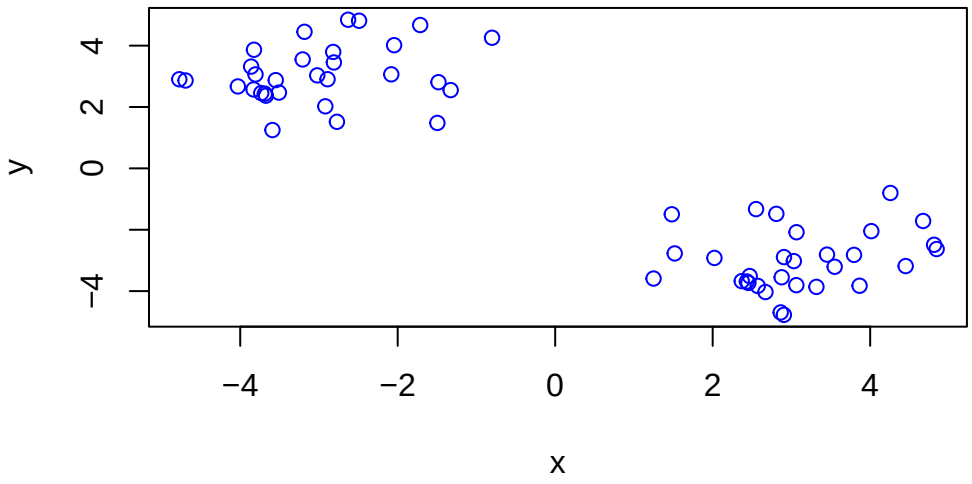
Q. Center of each cluster?

```
k$centers
```

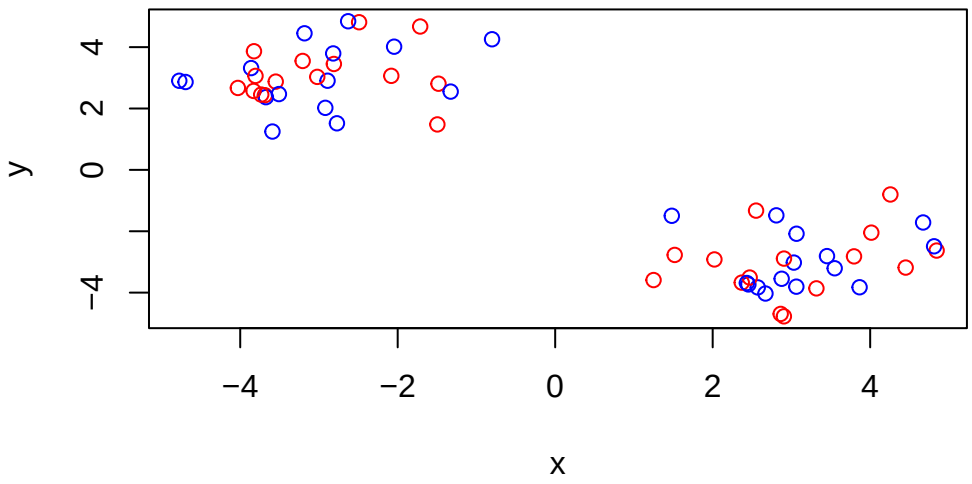
```
          x         y
1  3.077765 -3.008406
2 -3.008406  3.077765
```

Q. Put this result info together and make a little "base R" plot of our clustering result. Also, add the cluster center points to this plot.

```
plot(z, col = "blue")
```

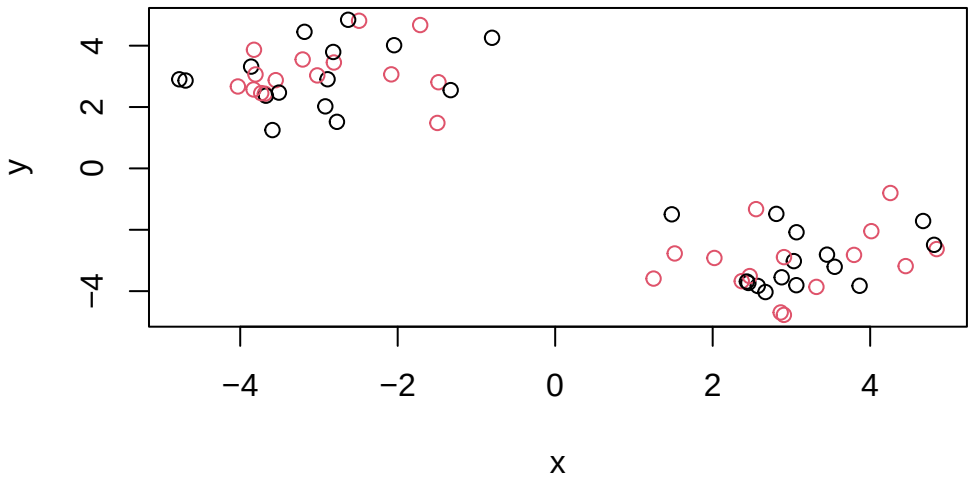



```
plot(z, col = c("blue","red"))
```



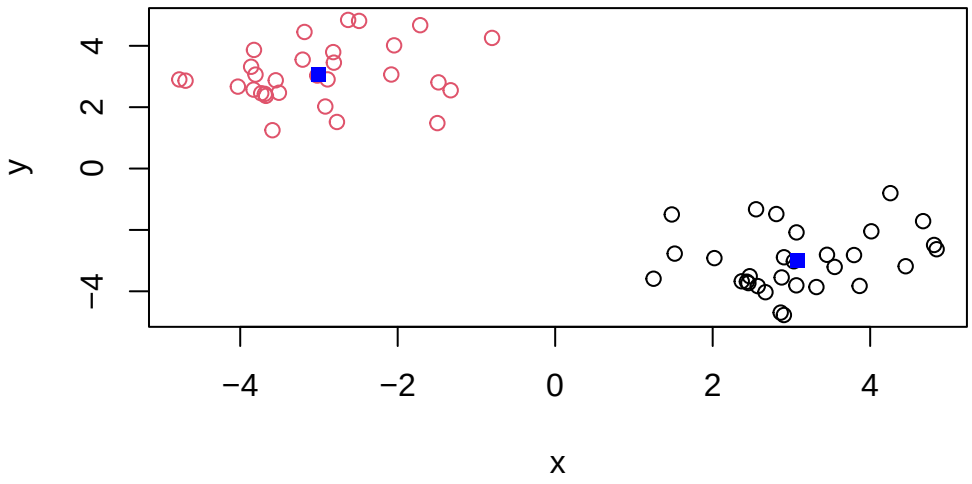
You can color by number.

```
plot(z, col = c(1, 2))
```



Plot colored by cluster membership:

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



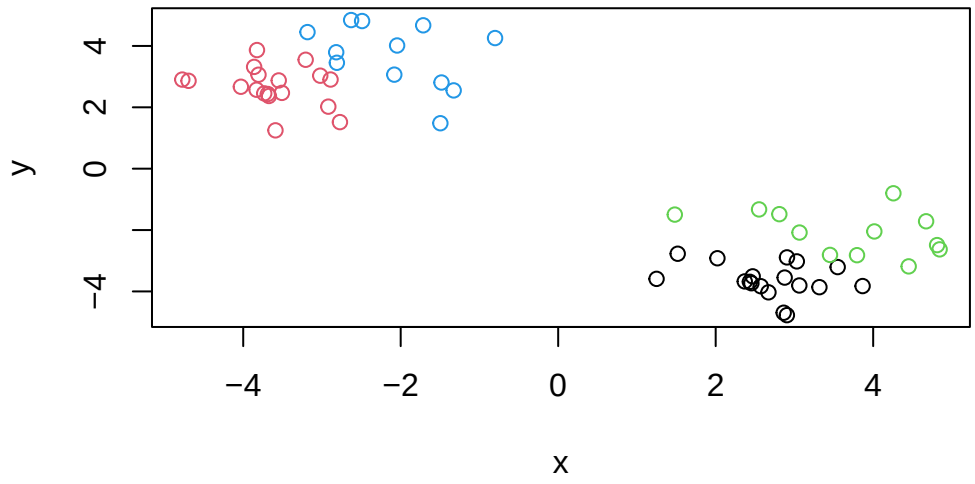
Q. Run kmeans on our input `z` and define 4 clusters, making the same result visualization plot as above (pot of z colored by cluster membership)

```
k4 <- kmeans(z, centers = 4)
k4
```

```
K-means clustering with 4 clusters of sizes 18, 18, 12, 12

Cluster means:
          x         y
1  2.673991 -3.631733
2 -3.631733  2.673991
3  3.683427 -2.073414
4 -2.073414  3.683427

Clustering vector:
 [1] 4 2 2 2 2 4 2 2 2 4 2 2 4 2 2 2 2 4 4 2 2 4 4 4 4 2 2 4 4 2 1 3 3 1 1 3 3 3
```

```
[39] 3 1 1 3 3 1 1 1 1 3 1 1 3 1 1 1 3 1 1 1 1 3

Within cluster sum of squares by cluster:
[1] 12.24313 12.24313 17.77443 17.77443
 (between_SS / total_SS =  95.1 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

```
plot(z, col = k4$cluster)
```




```
k4$totss
```

```
[1] 1220.921
```

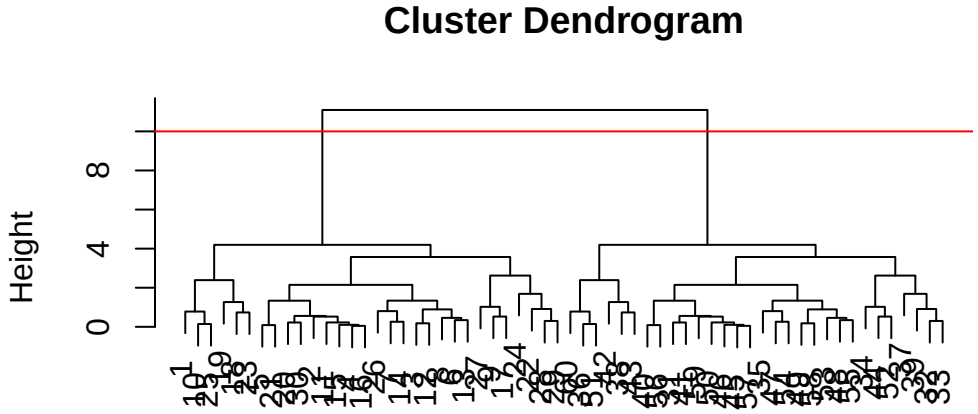
Hierarchical Clustering

The main function in base R for this is called `hclust()`. It will take as input a distance matrix (key point is that you can't just give your "raw" data as input - you have to first calculate a distance matrix from your data).

```r
d <- dist(z)
hc <- hclust(d)
hc
```

```
Call:
hclust(d = d)

Cluster method   : complete
Distance         : euclidean
Number of objects: 60
```

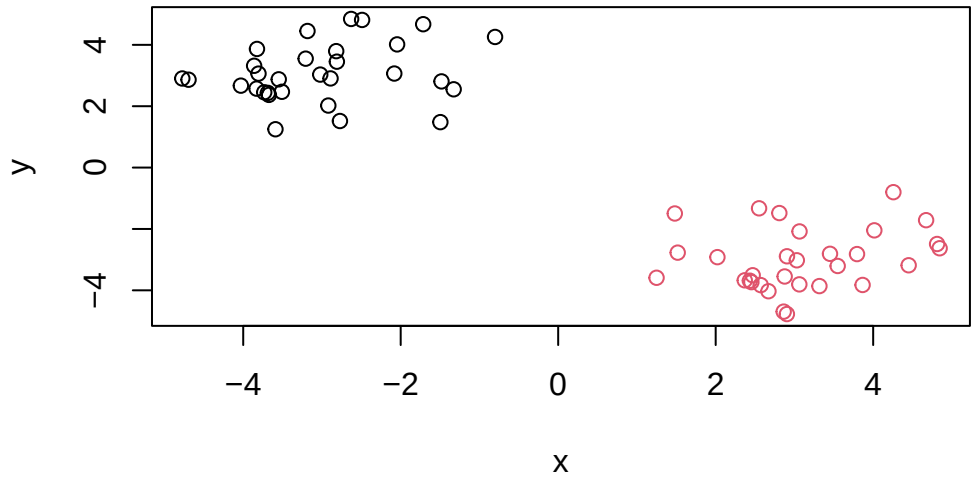
```r
plot(hc)
abline(h = 10, col = "red")
```



Once I inspect the "tree" I can "cut" the tree to yield my groupings or clusters. The function to do this is called `cutree()`.

```r
grps <- cutree(hc, h = 10)
```

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



Hands on with Principal Component Analysis (PCA)

Let's examine some silly 17-dimensional data detailing food consumption in the UK.

Data import

```
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
```

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

```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

```
[1] 4
```

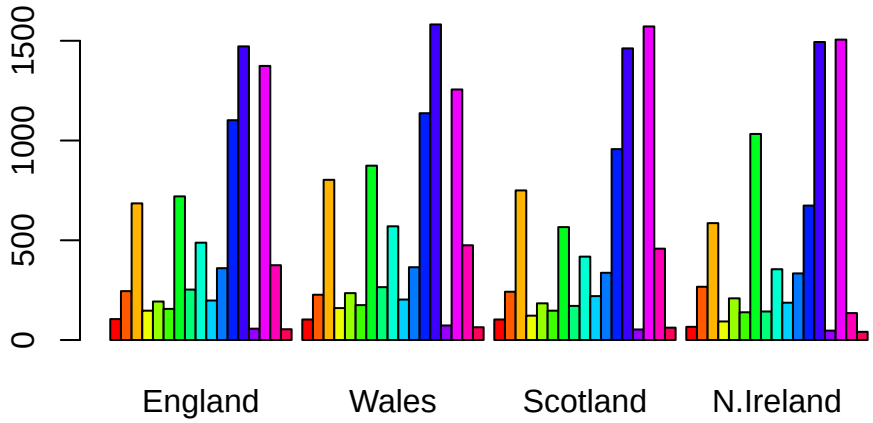
```
dim(x)
```

```
[1] 17  4
```

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?

I prefer editing the data import code because it's more simple than the other option. The other option adds more lines of code overall.

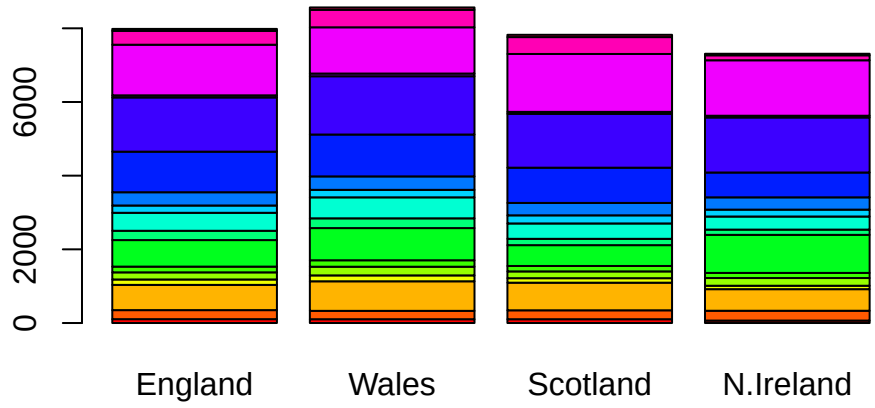
```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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

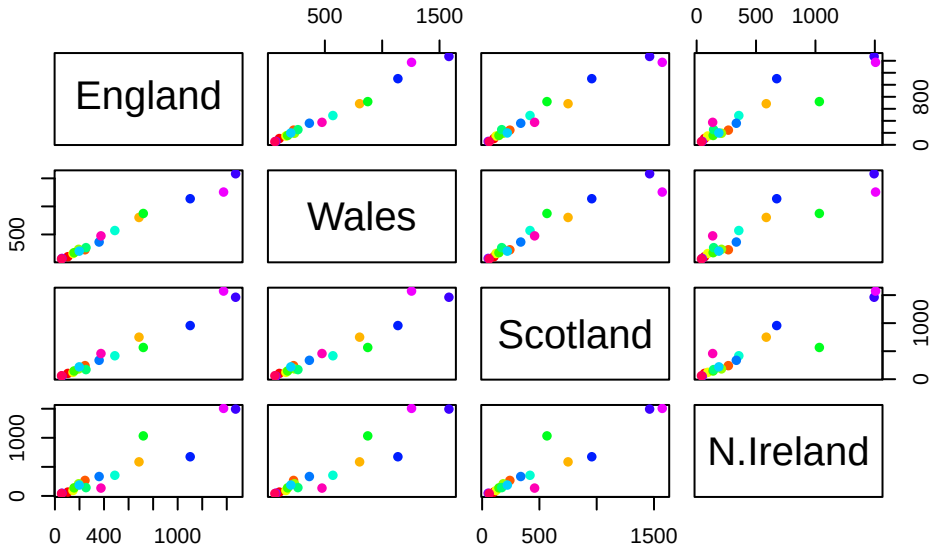
This plot is a result of setting the beside argument to F, where the different foods are stacked on top of each other.

```
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?

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



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

Compared to other countries in the UK, people in N. Ireland eat more potatoes and less fresh fruit.

Looking at these types of "pairwise plots" can be helpful but it does not scale well and kind of sucks! There must be a better way…

PCA to the rescue!

The main function for PCA in base R is called `prcomp()`. This function wants the transpose of our input data - i.e. the important foods in as columns and the countries as rows.

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

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 2.921e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

Let's see what is in our PCA result object `pca`

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

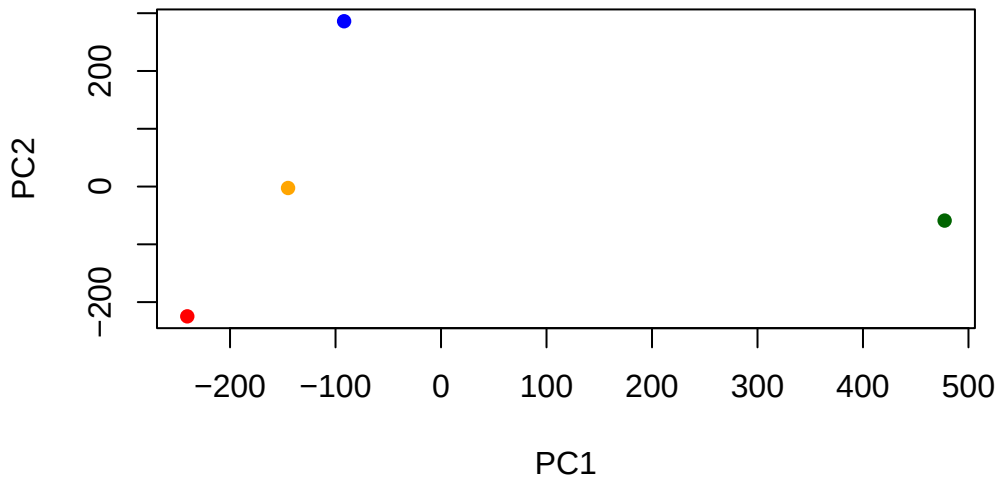
The `pca$x` result object is where we will focus first as this details how the countries are related to eachother in terms of our new "axis" (aka "PCs", "eigenvectors", etc)

```
head(pca$x)
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -9.152022e-15
Wales     -240.52915 -224.646925 -56.475555  5.560040e-13
Scotland   -91.86934  286.081786 -44.415495 -6.638419e-13
N.Ireland  477.39164  -58.901862  -4.877895  1.329771e-13
```

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

```
plot(pca$x[,1], pca$x[,2], pch=16, col = c("orange","red","blue","darkgreen"), xlab="PC1", yl
```



We can look at the so-called PC "loadings" result object to see how the original foods contribute to our new PCs (i.e. how the original variables contribute to our new, better PC variables).

```
pca$rotation[,1]
```

```
          Cheese       Carcass_meat         Other_meat                Fish
     -0.056955380         0.047927628       -0.258916658       -0.084414983
   Fats_and_oils              Sugars     Fresh_potatoes          Fresh_Veg
     -0.005193623       -0.037620983        0.401402060       -0.151849942
     Other_Veg  Processed_potatoes      Processed_Veg         Fresh_fruit
     -0.243593729       -0.026886233       -0.036488269       -0.632640898
        Cereals          Beverages       Soft_drinks    Alcoholic_drinks
     -0.047702858       -0.026187756        0.232244140       -0.463968168
   Confectionery
     -0.029650201
```

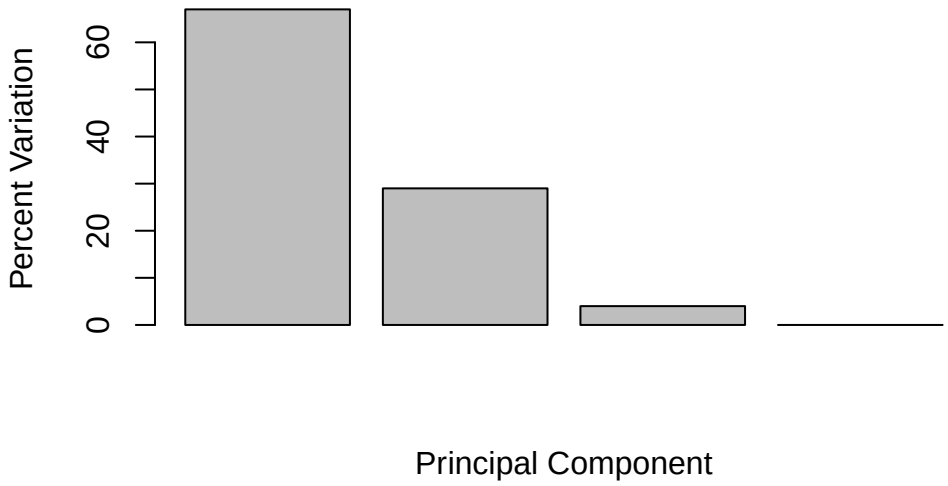
```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

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

```
z <- summary(pca)
z$importance
```

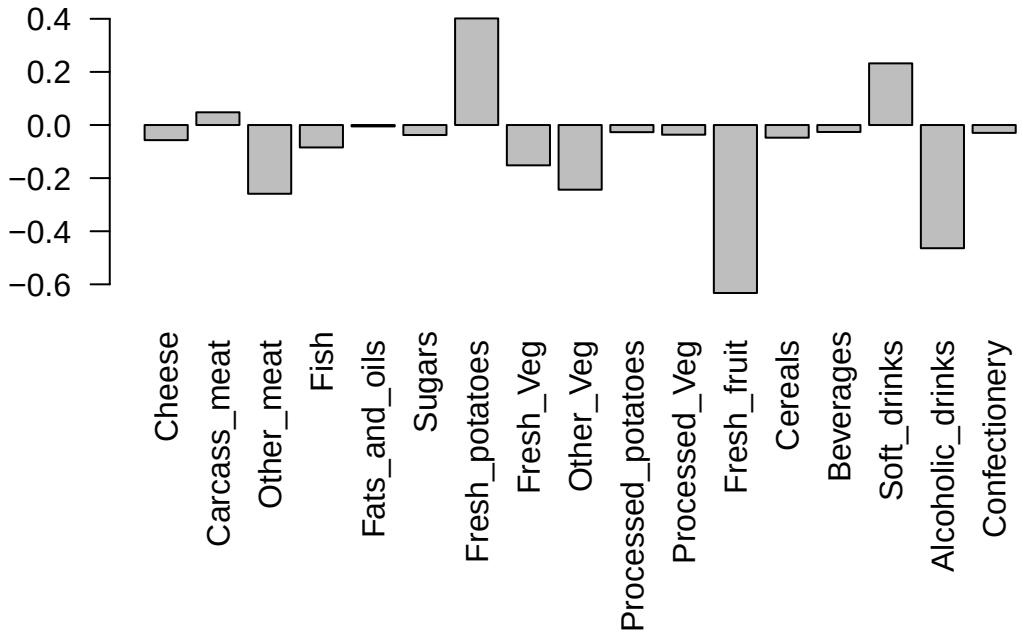
```
                            PC1       PC2      PC3           PC4
Standard deviation     324.15019 212.74780 73.87622 2.921348e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

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



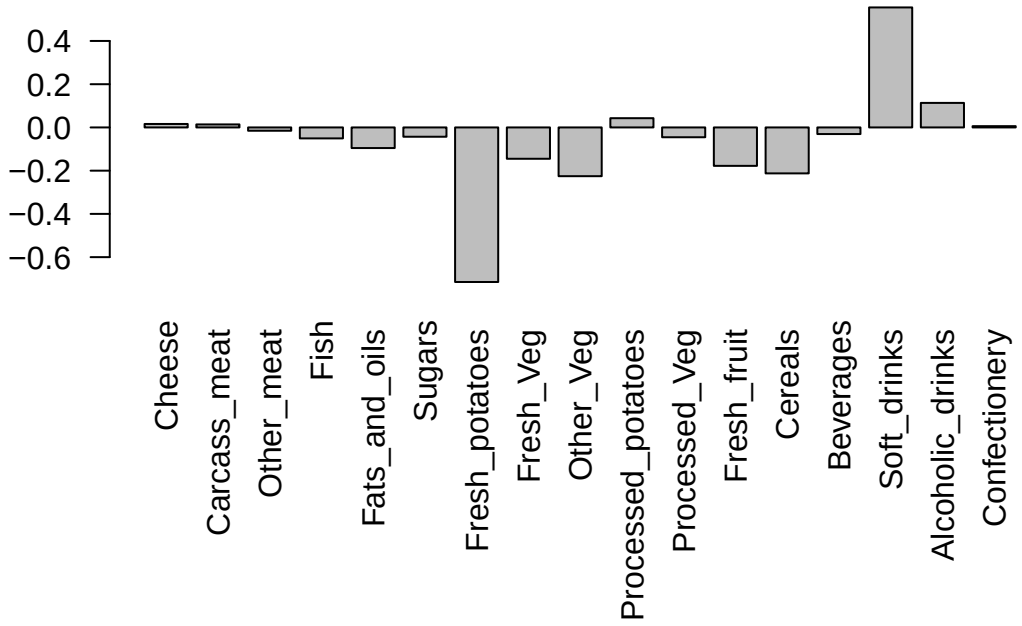
Digging deeper (variable loadings)

```
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 mainly tell us about?

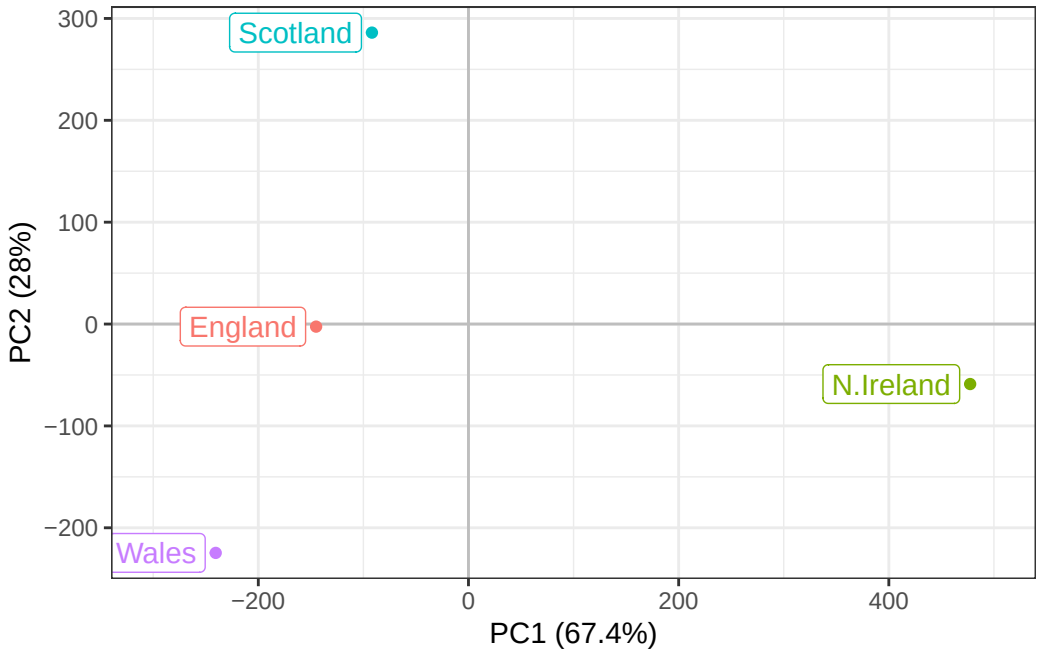
```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```



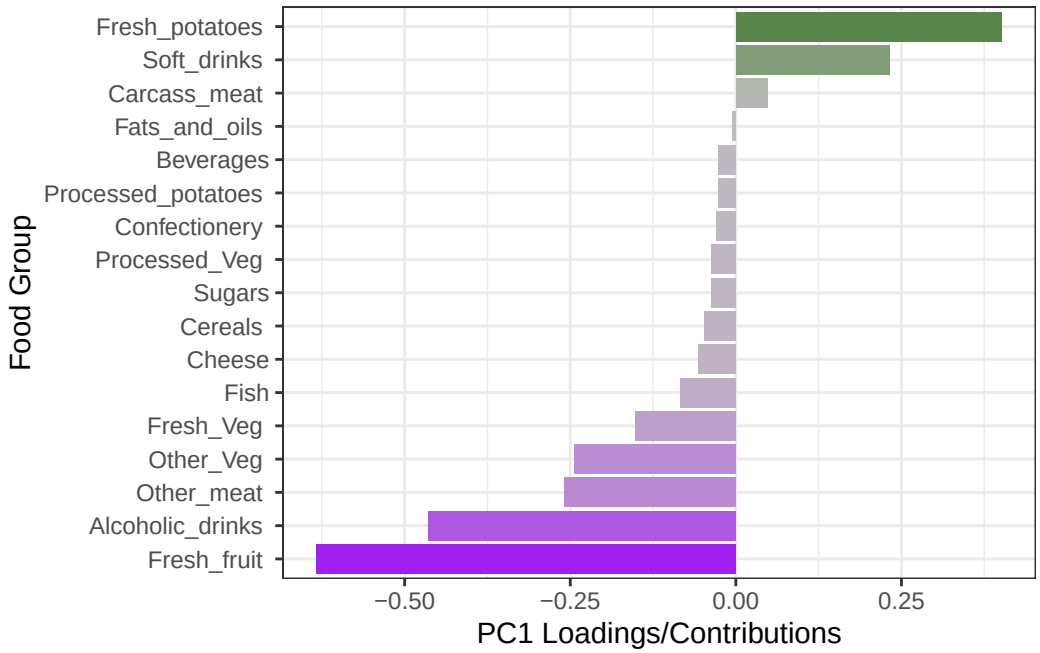
PC2 is mainly influenced by the soft drinks and fresh potatoes food groups.There are higher PC2 scores with soft drinks and lower PC2 scores with fresh potatoes. PC2 provides us with information from an additional 29% of the data that contribute to N. Ireland's position on the PCA plot.

Using ggplot for these figures

```
library(ggplot2)

df <- as.data.frame(pca$x)
df_lab <- tibble::rownames_to_column(df, "Country")

ggplot(df_lab) +
  aes(PC1, PC2, col=Country, label=Country) +
  geom_hline(yintercept = 0, col="gray") +
  geom_vline(xintercept = 0, col="gray") +
  geom_point(show.legend = FALSE) +
  geom_label(hjust=1, nudge_x = -10, show.legend = FALSE) +
  expand_limits(x = c(-300,500)) +
  xlab("PC1 (67.4%)") +
  ylab("PC2 (28%)") +
  theme_bw()
```

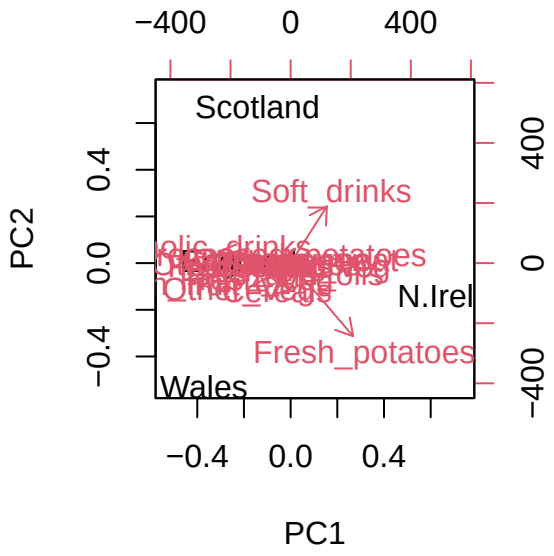



```
ld <- as.data.frame(pca$rotation)
ld_lab <- tibble::rownames_to_column(ld, "Food")

ggplot(ld_lab) +
  aes(PC1, reorder(Food, PC1), bg=PC1) +
  geom_col() +
  xlab("PC1 Loadings/Contributions") +
  ylab("Food Group") +
  scale_fill_gradient2(low="purple", mid = "gray", high = "darkgreen", guide = NULL) +
  theme_bw()
```



Biplots

```
biplot(pca)
```



PCA of RNA-seq 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?

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

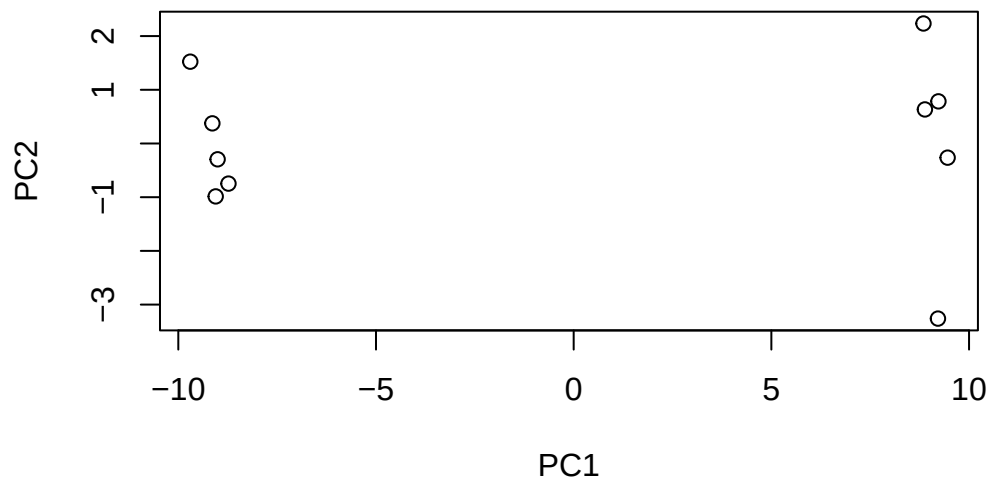
```
[1] 10
```

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

```
[1] 100
```

In this data set, there are 100 genes, # of rows, and 10 samples, # of columns.

```
## Take the transpose of our data
pca <- prcomp(t(rna.data), scale=TRUE)

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

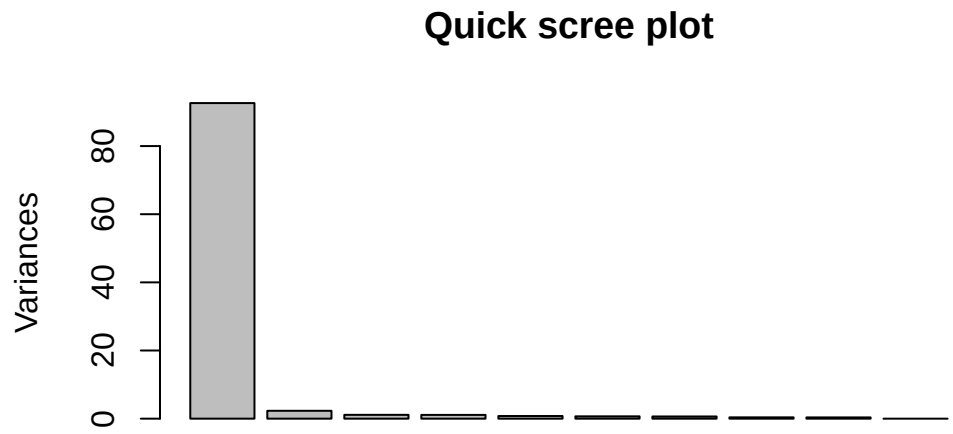



```
summary(pca)
```

```
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 3.345e-15
```

```
Proportion of Variance 0.00385 0.00364 0.000e+00
Cumulative Proportion  0.99636 1.00000 1.000e+00
```

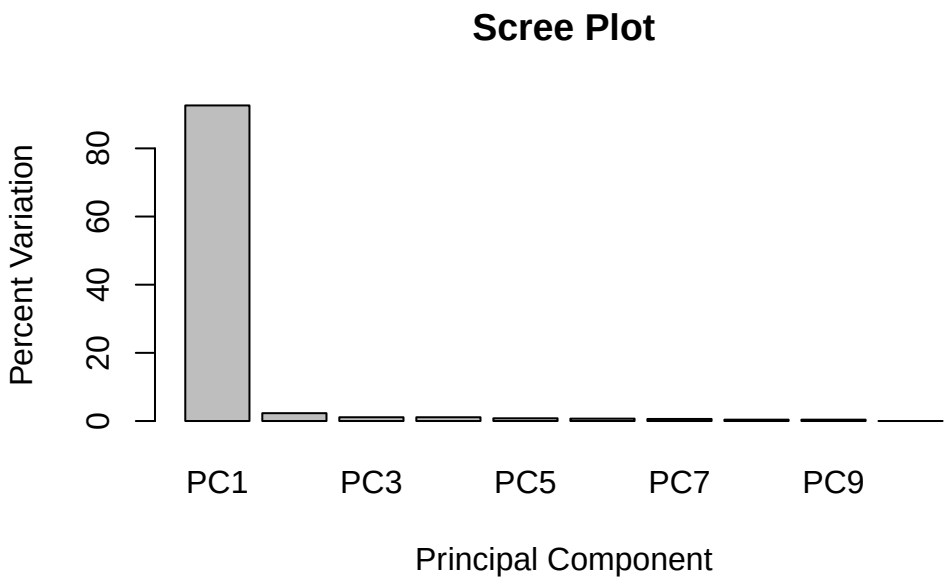
```r
plot(pca, main = "Quick scree plot")
```



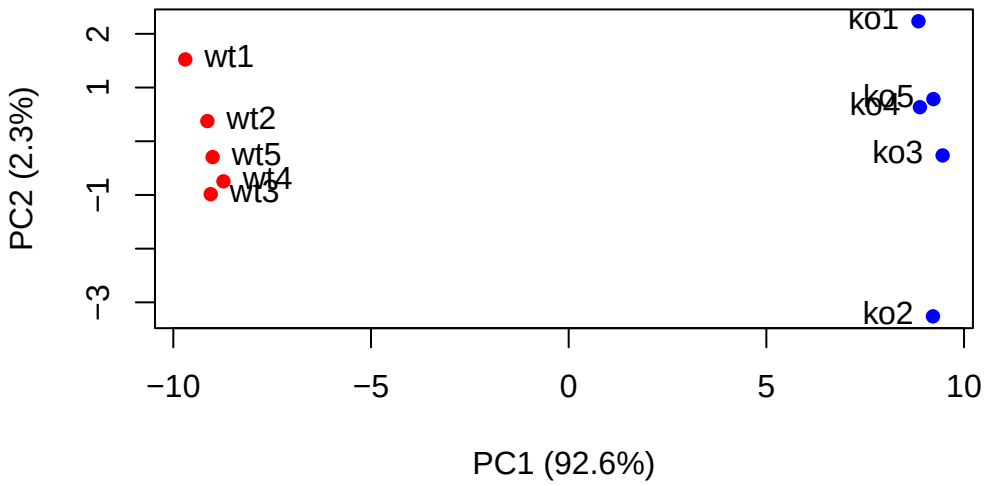

```r
## Variance per PC
pca.var <- pca$sdev^2

## Percent variance
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
```

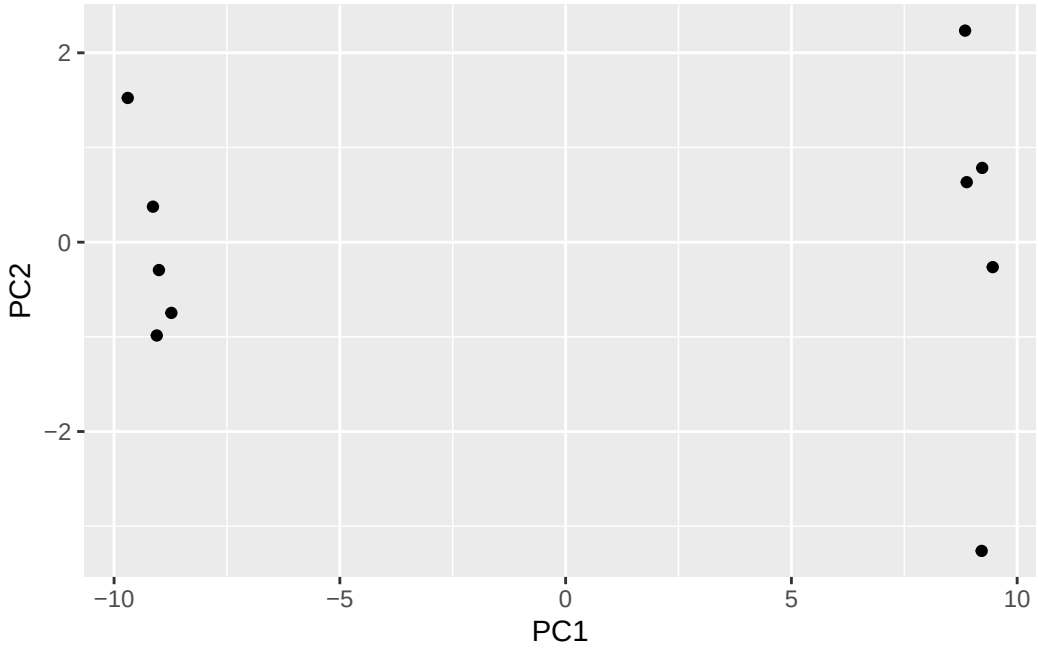
```r
barplot(pca.var.per, main="Scree Plot",
        names.arg = paste0("PC", 1:10),
        xlab="Principal Component", ylab="Percent Variation")
```



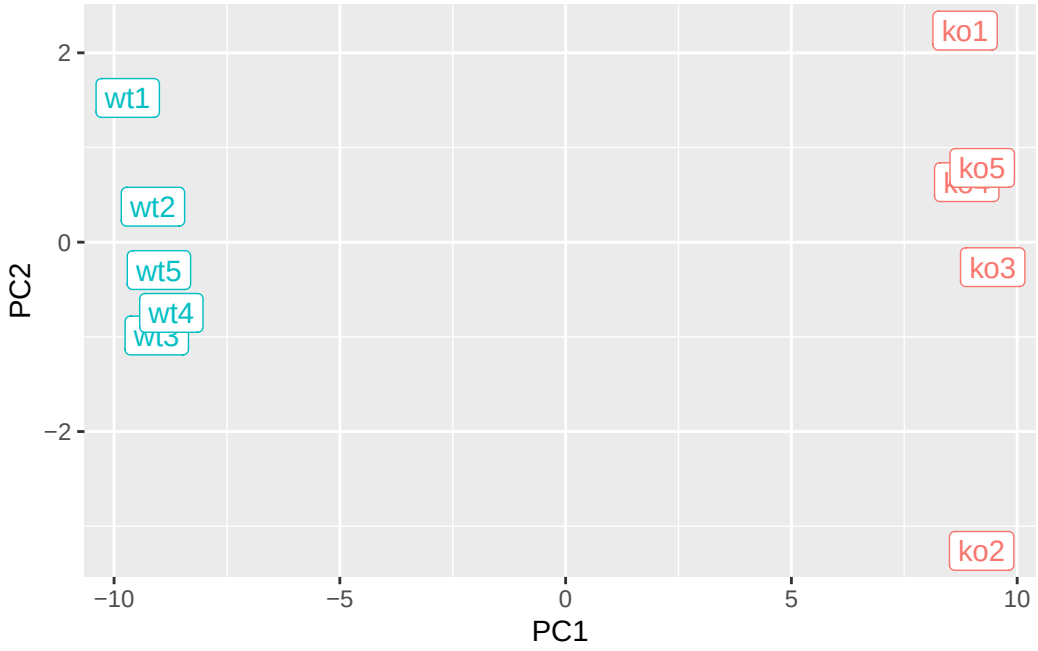

```
## Wt and ko samples - vector for colors
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
colvec[grep("ko", colvec)] <- "blue"

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

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



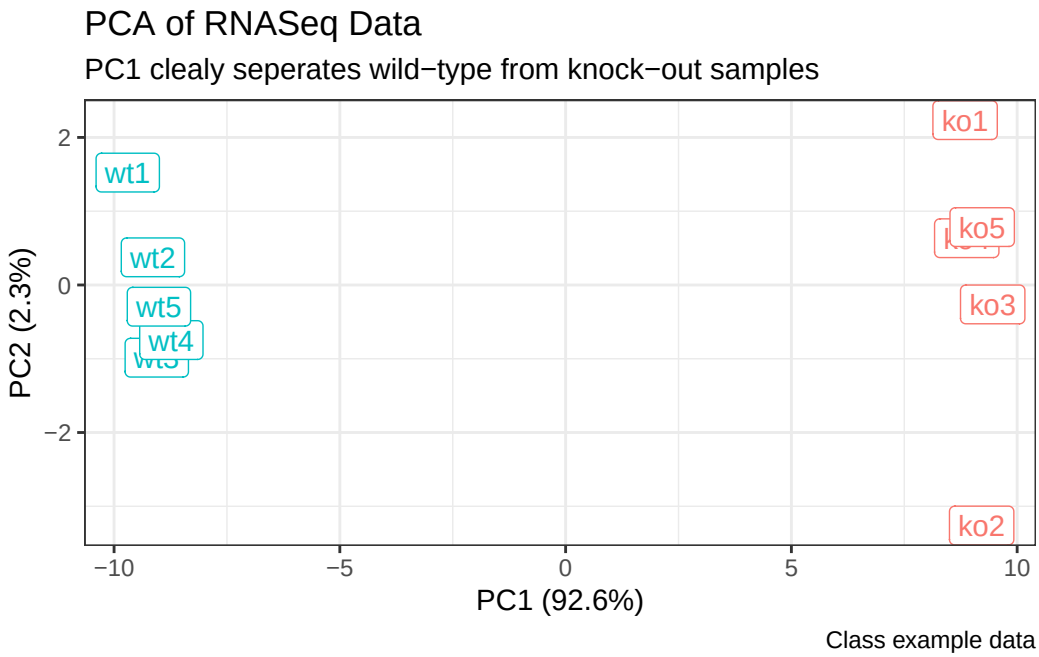

```
library(ggplot2)

df <- as.data.frame(pca$x)

# First basic plot
ggplot(df) +
  aes(PC1, PC2) +
  geom_point()
```




```
# Add a column for 'wt' and 'ko' "condition"
df$samples <- colnames(rna.data)
df$condition <- substr(colnames(rna.data),1,2)

p <- ggplot(df) +
        aes(PC1, PC2, label = samples, col = condition) +
        geom_label(show.legend = FALSE)
p
```




```
# 'Polishing' the graph
p + labs(title = "PCA of RNASeq Data",
       subtitle = "PC1 clealy seperates wild-type from knock-out samples",
       x = paste0("PC1 (", pca.var.per[1], "%)"),
       y = paste0("PC2 (", pca.var.per[2], "%)"),
       caption = "Class example data") +
     theme_bw()
```


PCA of RNASeq Data
PC1 clealy seperates wild−type from knock−out samples
ko1
wt1
ko5
wt2
ko3
wt5
wt4
ko2
2
0
−2
PC2 (2.3%)
−10
−5
0
5
10
PC1 (92.6%)
Class example data