Machine Learning 1

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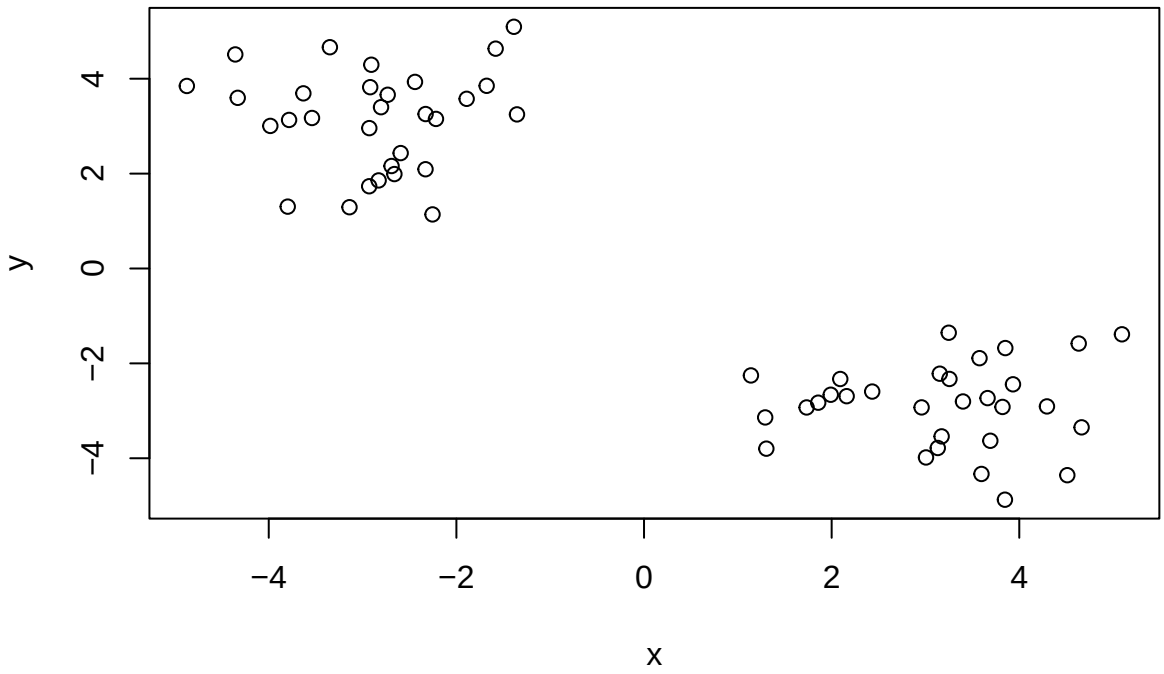
First up is clustering methods

Kmeans clustering

The function in base R to do Kmeans clustering is called `kmeans()`.

First make up some data where we know what the answer should be:

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



Q. Can we use kmeans() to cluster this data setting k 2 and nstart to 20?

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

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##           x         y
## 1 -2.874582  3.149966
## 2  3.149966 -2.874582
##
## 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 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
##
## Within cluster sum of squares by cluster:
## [1] 56.01966 56.01966
##  (between_SS / total_SS =  90.7 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

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 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
```

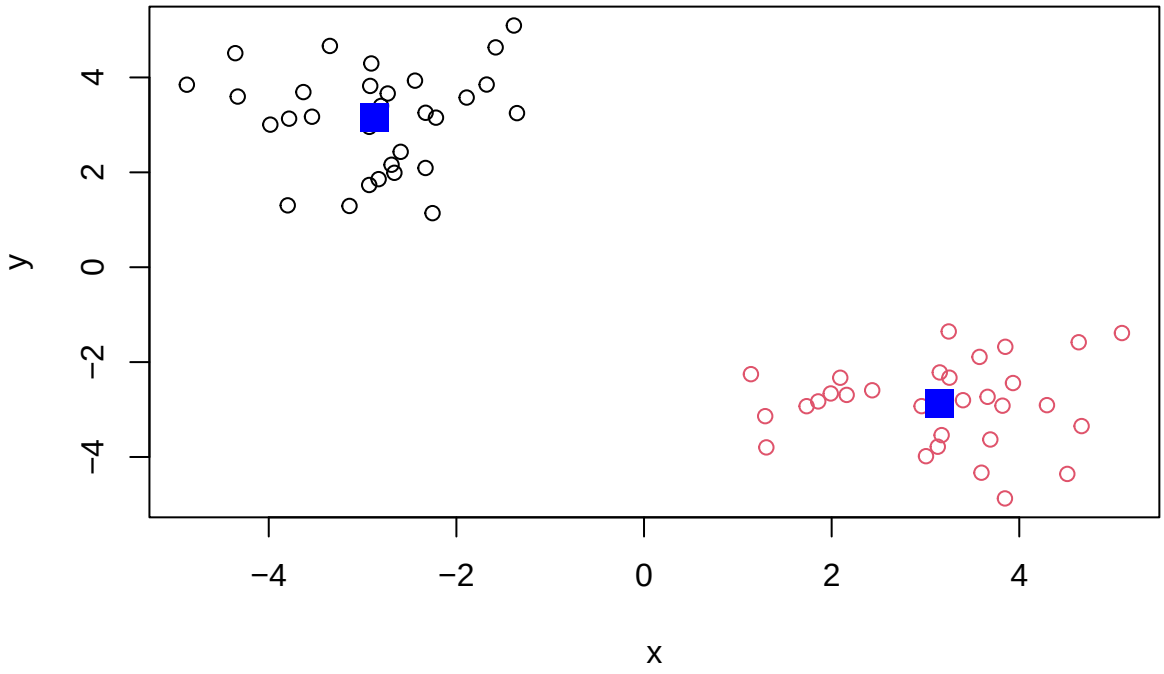
Q. What 'component' of your result object details cluster center?

```
km$centers
```

```
##           x         y
## 1 -2.874582  3.149966
## 2  3.149966 -2.874582
```

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

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



Hierarchical Clustering

A big limitation with k-means is that we have to tell it K (the number of clusters we want).

Analyze this same data with hclust()

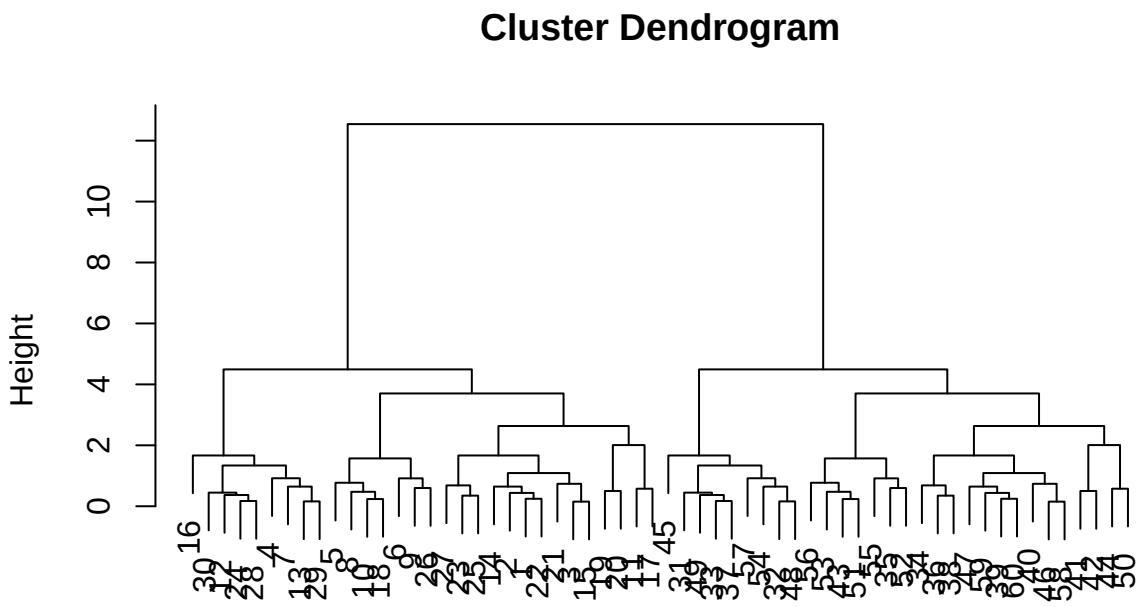
Demonstrate the use of dist(), hclust(), plot(), and cutree() functions to do clustering. Generate dendrograms and return cluster assignment/membership vector...

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

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

There is a plot method for hclust result objects. Let's see it

```
plot(hc)
```



To get our cluster membership vector we have to do a wee bit more work. We have to "cut" the tree where we think it makes sense. For this we use the `cutree()` function.

```
cutree(hc, h=6)
```

```
##  [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
```

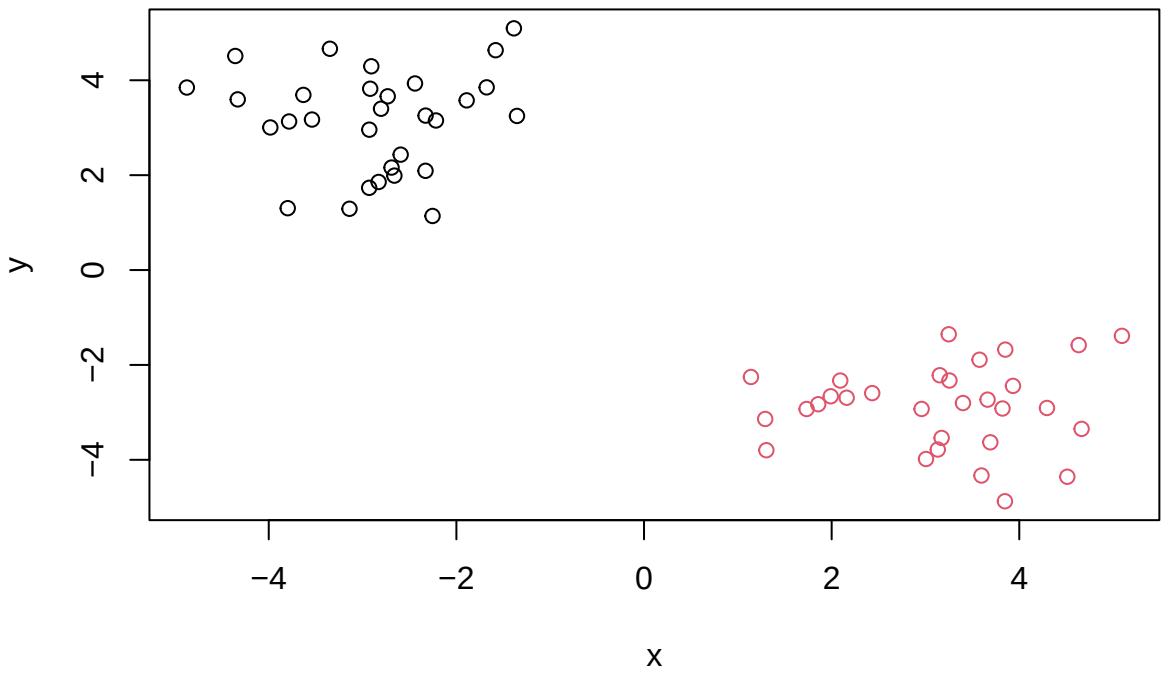
You can also call `cutree()` setting k=the number of groups/clusters you want

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

```
##  [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
```

Make our results plot

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



Principal Component Analysis (PCA)

PCA of UK food data

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

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

```
dim(x)
```

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

Checking the data

```
View(x)
```

Note how the minus indexing works

```
rownames(x) <- x[, 1]
x <- x[, -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
```

Check the dimensions

```
dim(x)
```

```
## [1] 17  4
```

```
x <- read.csv(url, row.names=1)
head(x)
```

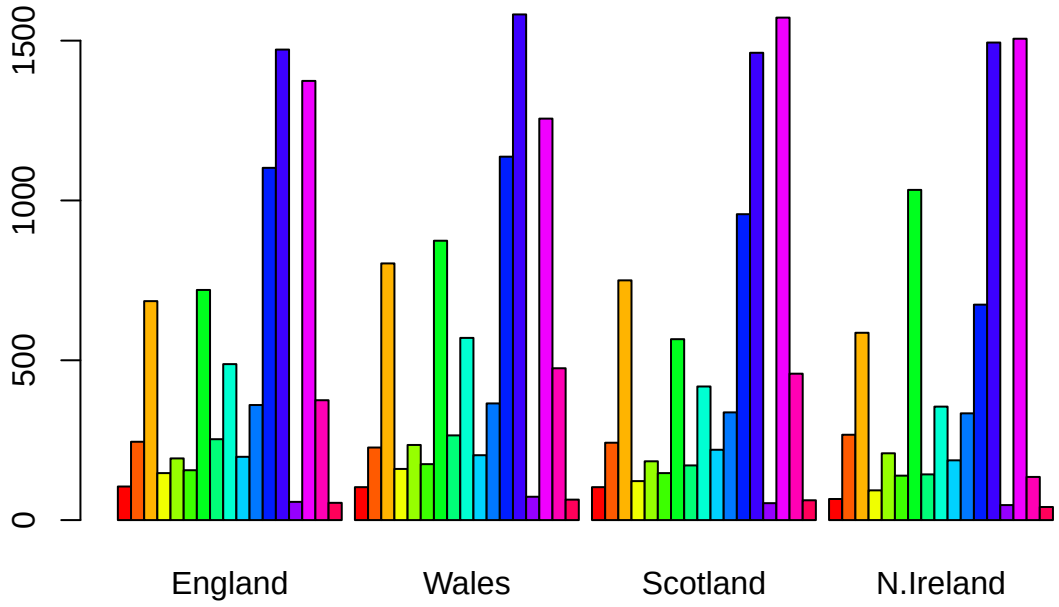
```
##                England Wales Scotland N.Ireland
## Cheese             105   103      103        66
## Carcass_meat       245   227      242       267
## Other_meat         685   803      750       586
## Fish               147   160      122        93
## Fats_and_oils      193   235      184 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

> 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 the second approach because as you run the code block x <- x[, -1] over and over again, the next column on the right will become the first column and the left-most column will be removed. Once you run the code block enough times, you'll receive an error message. Yes, the second approach is more robust because it resets the first column to be the rows and once it does that, running the code block multiple times won't change that and you won't eventually receive an error message, unlike the first approach.

Now we have the data looking good, we want to explore it. We will use some conventional plots (barplots and pair plots).

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



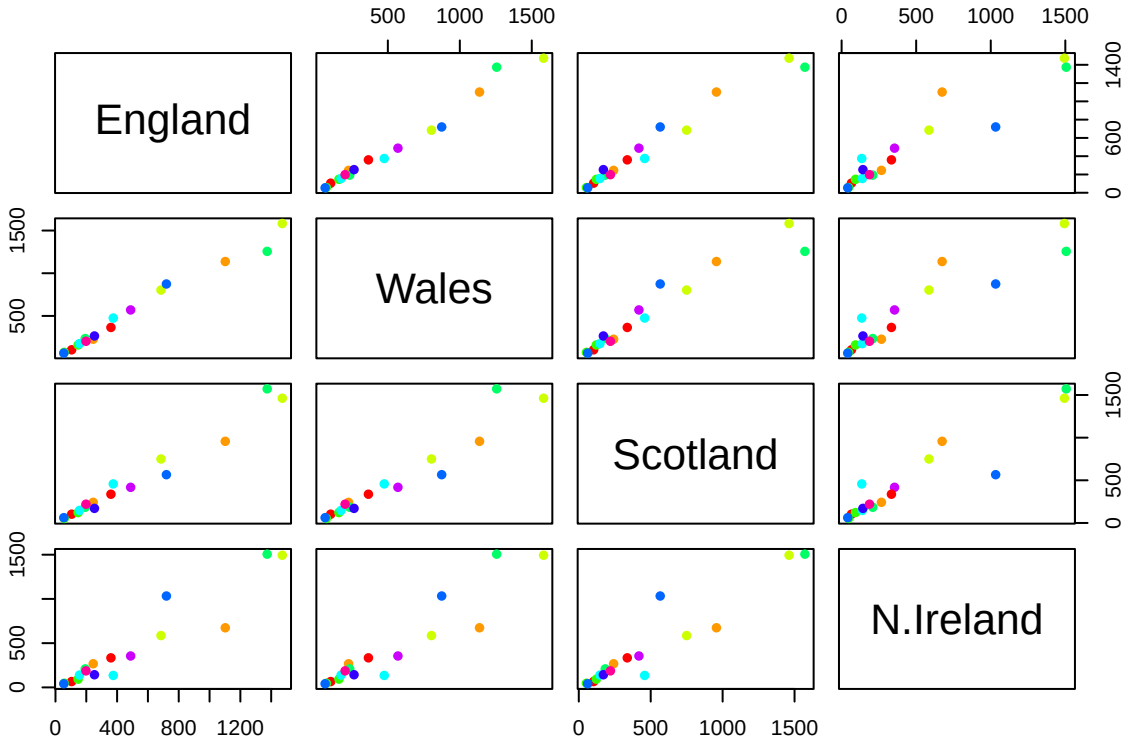
Q3: Changing what optional argument in the above barplot() function results in the following plot?

Changing the argument beside=FALSE in the barplot() function will result in a barplot with stacked bars instead of juxtaposed bars.

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?

If a point lies on the diagonal, this indicates that the quantity of food eaten, whichever one it may be, is the same in the two countries being measured on the x-axis and y-axis.

```
pairs(x, col=rainbow(10), pch=16)
```



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

One of the main differences is that N. Ireland consumes less fresh fruit, alcoholic drinks, other meat, and other vegetables, but more fresh potatoes than the other countries in the data-set.

PCA to the rescue!

The main function in base R for PCA is `prcomp()` This wants the transpose of our data

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
```

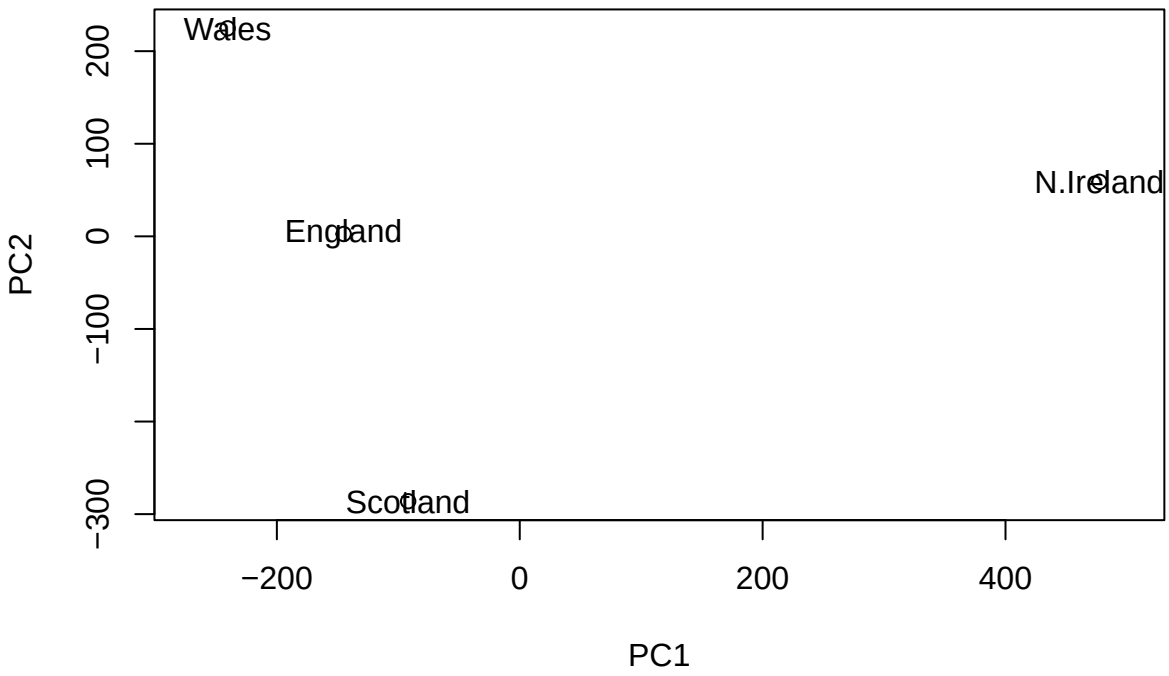
```
pca
```

```
## Standard deviations (1, .., p=4):
## [1] 3.241502e+02 2.127478e+02 7.387622e+01 4.188568e-14
##
## Rotation (n x k) = (17 x 4):
##                             PC1          PC2         PC3          PC4
## Cheese              -0.056955380 -0.016012850 -0.02394295 -0.691718038
## Carcass_meat         0.047927628 -0.013915823 -0.06367111  0.635384915
## Other_meat          -0.258916658  0.015331138  0.55384854  0.198175921
## Fish                -0.084414983  0.050754947 -0.03906481 -0.015824630
## Fats_and_oils       -0.005193623  0.095388656  0.12522257  0.052347444
## Sugars              -0.037620983  0.043021699  0.03605745  0.014481347
## Fresh_potatoes       0.401402060  0.715017078  0.20668248 -0.151706089
## Fresh_Veg           -0.151849942  0.144900268 -0.21382237  0.056182433
## Other_Veg           -0.243593729  0.225450923  0.05332841 -0.080722623
## Processed_potatoes  -0.026886233 -0.042850761  0.07364902 -0.022618707
## Processed_Veg       -0.036488269  0.045451802 -0.05289191  0.009235001
## Fresh_fruit         -0.632640898  0.177740743 -0.40012865 -0.021899087
## Cereals             -0.047702858  0.212599678  0.35884921  0.084667257
## Beverages           -0.026187756  0.030560542  0.04135860 -0.011880823
## Soft_drinks          0.232244140 -0.555124311  0.16942648 -0.144367046
## Alcoholic_drinks    -0.463968168 -0.113536523  0.49858320 -0.115797605
## Confectionery       -0.029650201 -0.005949921  0.05232164 -0.003695024
```

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

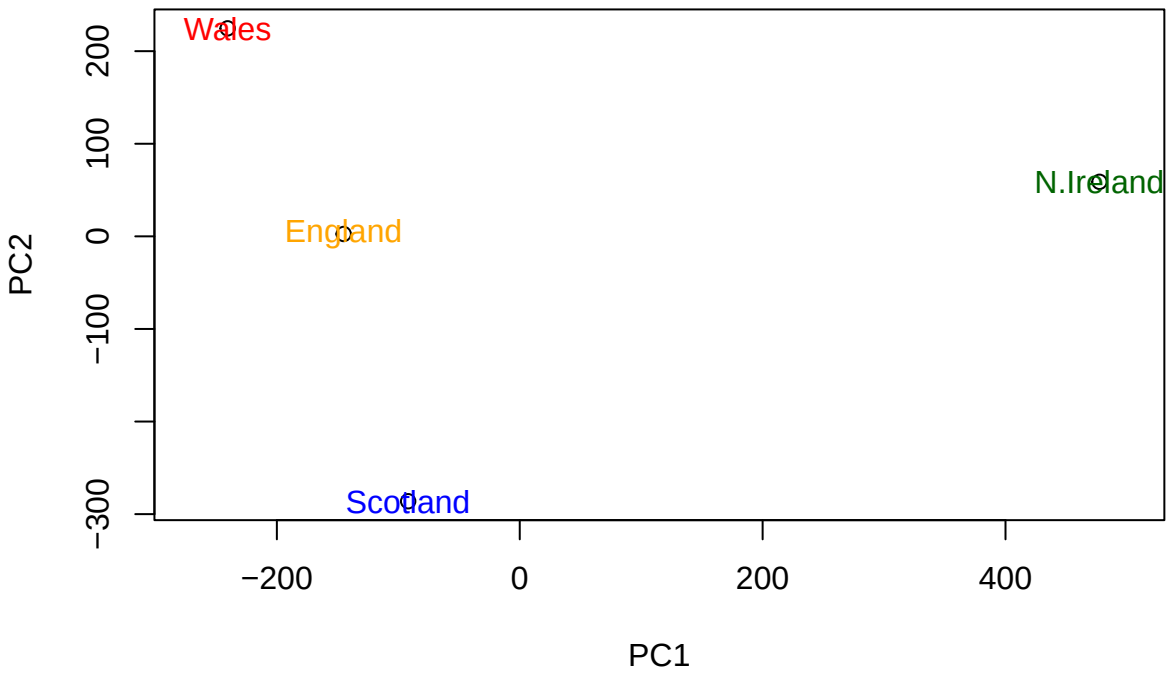
Plot PC1 vs PC2

```
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.

```
country_cols <- c("orange", "red", "blue", "dark green")
plot(pca$x[, 1], pca$x[, 2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[, 1], pca$x[, 2], colnames(x), col=country_cols)
```



How much variation in the original data does each PC account for?

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

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

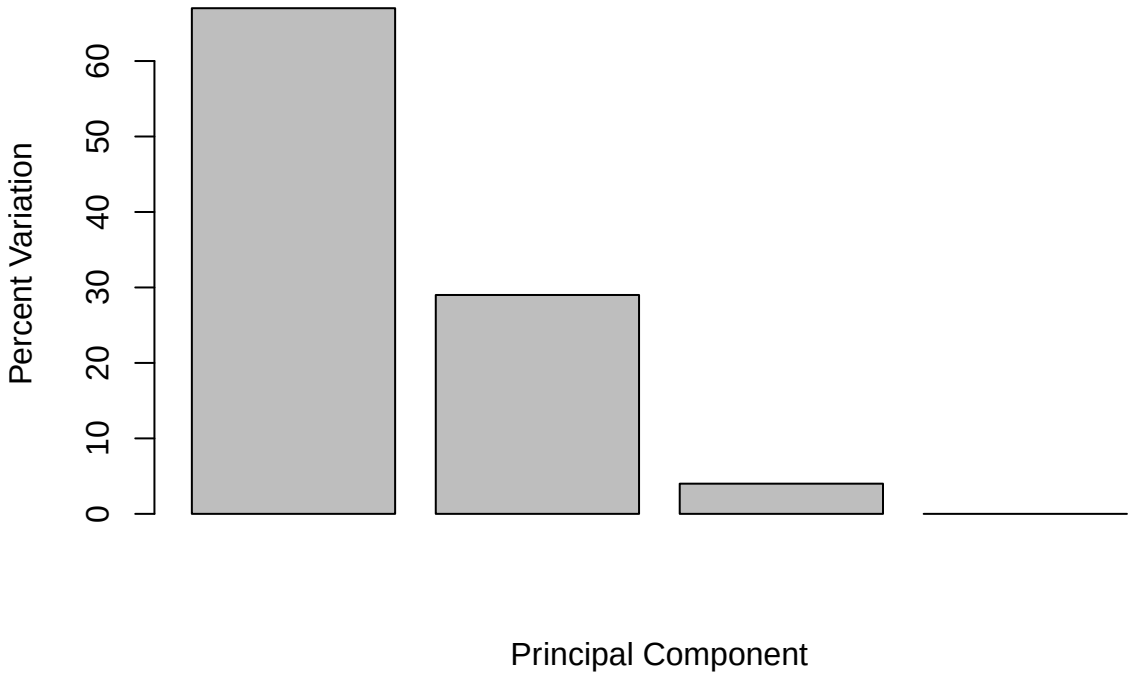
or the second row here...

```
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
```

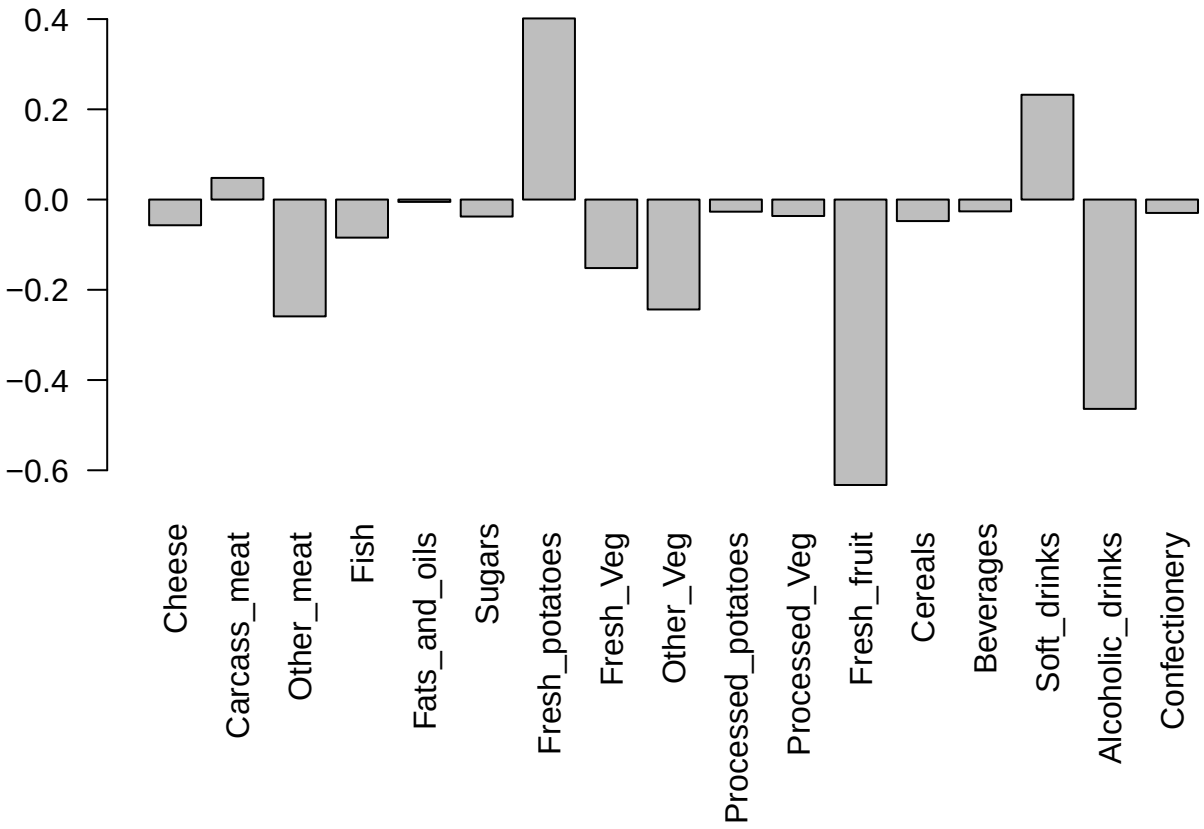
Plot of variances

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



Let's focus on PC1 as it accounts for >90% of variance

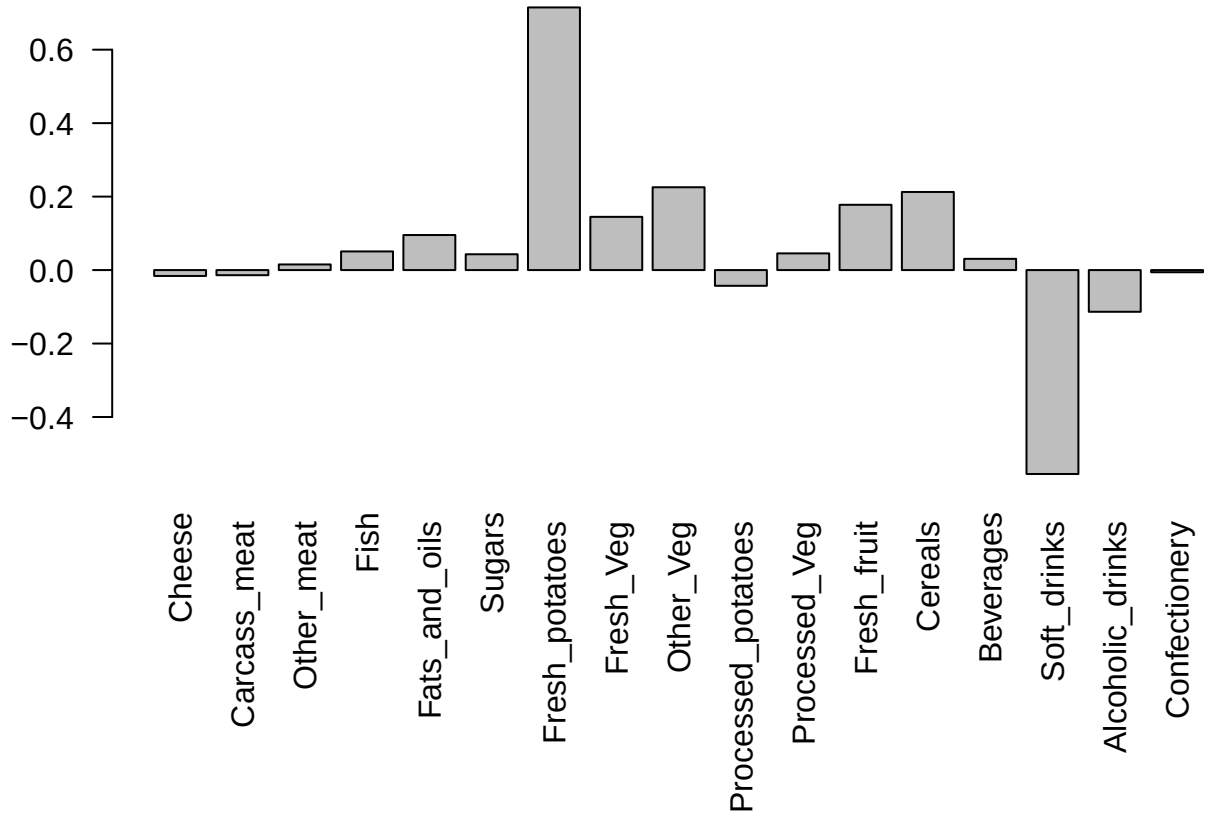
```
par(mar=c(10, 3, 0.35, 0))
barplot(pca$rotation[, 1], las=2)
```



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

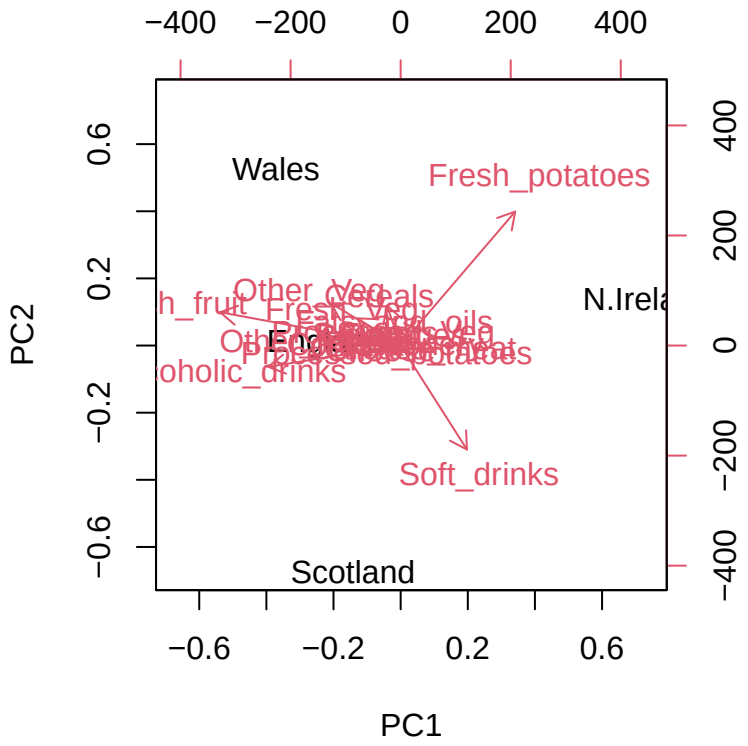
Fresh potatoes and soft drinks are the most prominent food groups that constitute variance in PC2. PC2 tells us that it captures approximately 29% of the variance in the original data-set and of that 29%, the majority of the variance comes from fresh potatoes and soft drinks.

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



The inbuilt biplot() can be useful for small datasets

```
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?

```
dim(rna.data)
```

```
## [1] 100  10
```

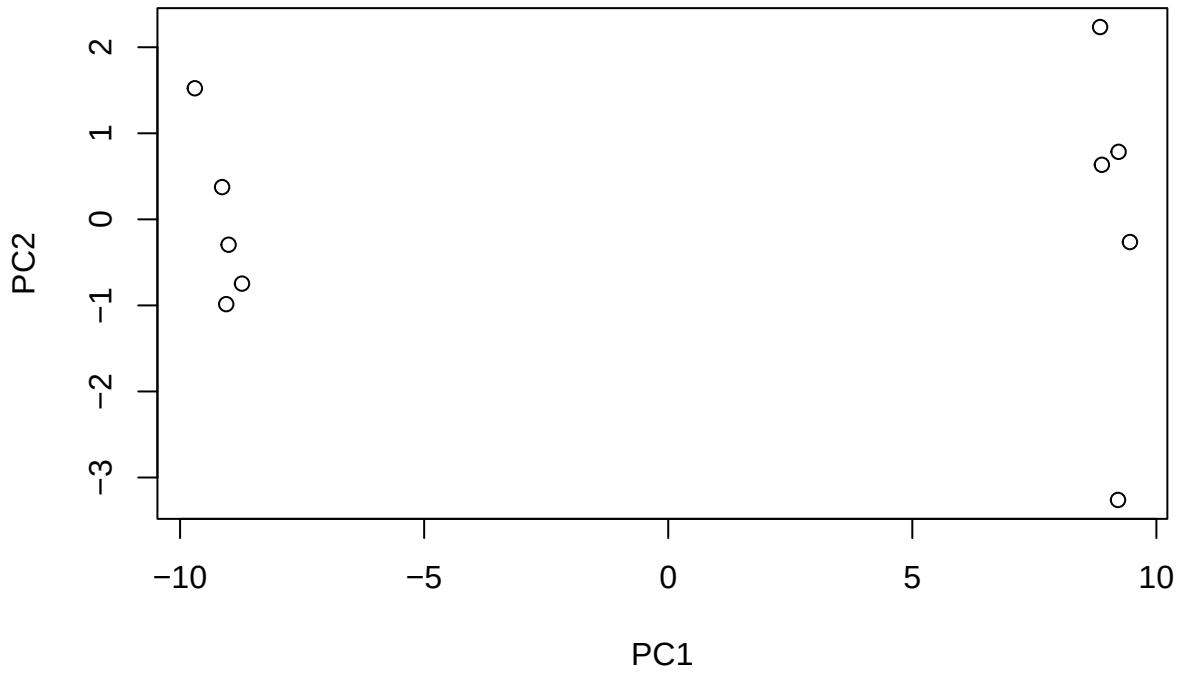
There are 100 genes and 10 samples.

Again we have to take the transpose of our data

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

Simple unpolished plot of pc1 and pc2

```
plot(pca$x[, 1], pca$x[, 2], xlab="PC1", ylab="PC2")
```



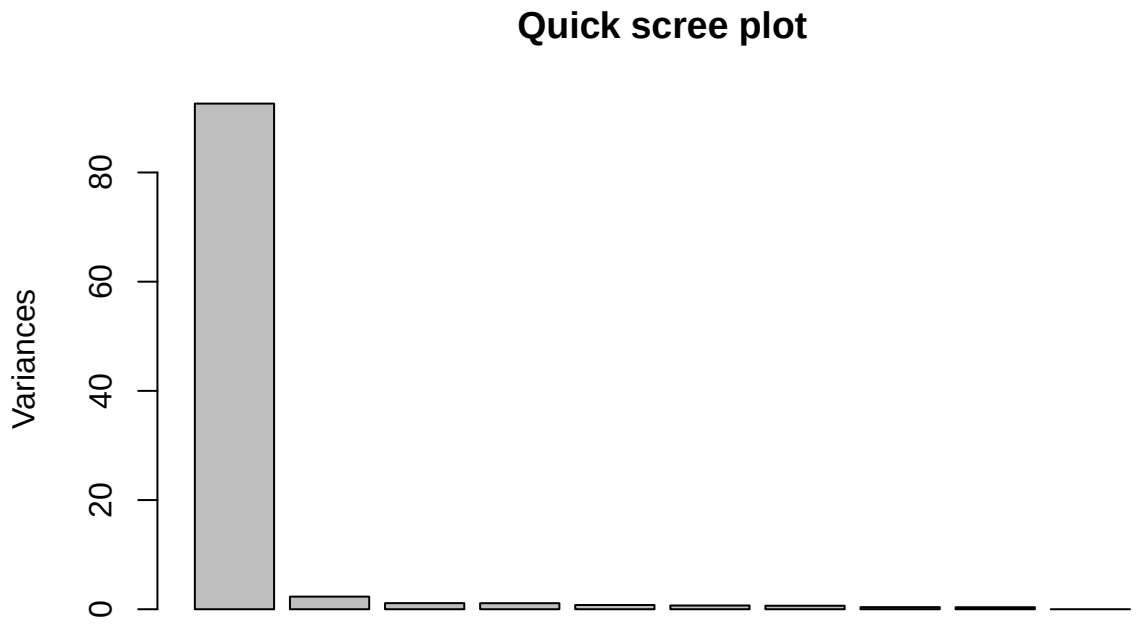
How much variation does each PC account for?

```
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 3.348e-15
## Proportion of Variance 0.00385 0.00364 0.000e+00
## Cumulative Proportion  0.99636 1.00000 1.000e+00
```

Let's make a quick barplot summary

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



Variance captured per PC

```
pca.var <- pca$sdev^2
```

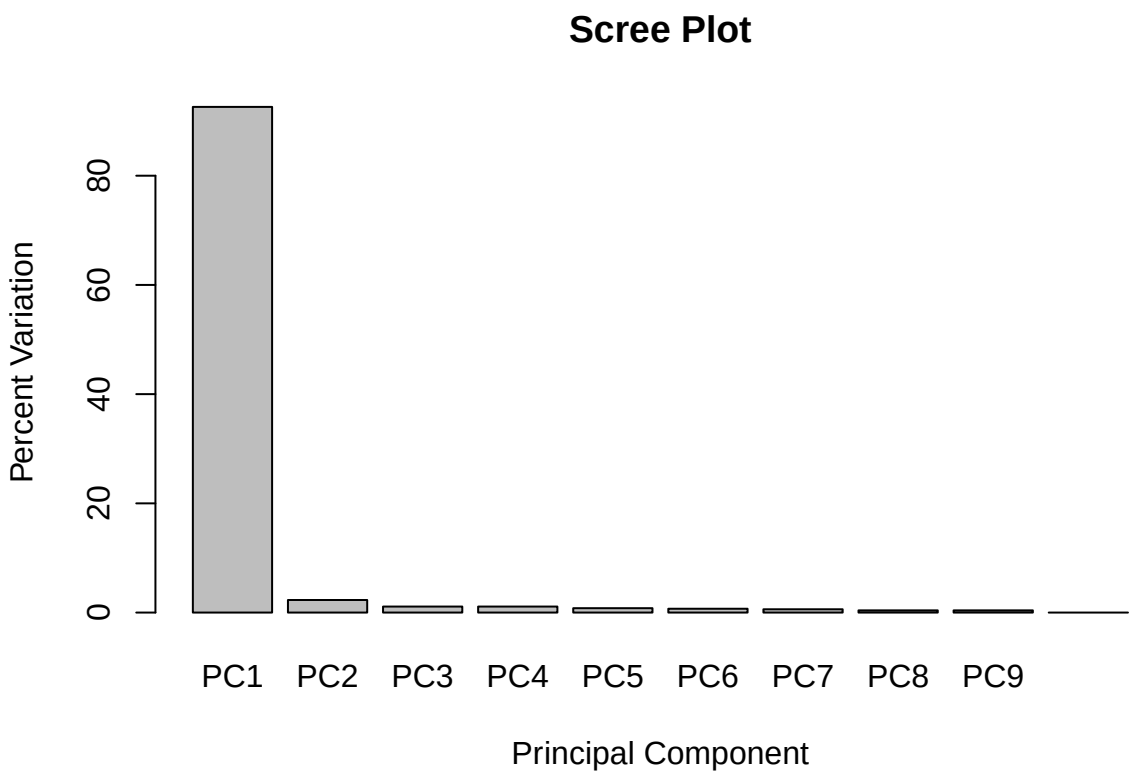
Percent variance is often more informative to look at

```
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
```

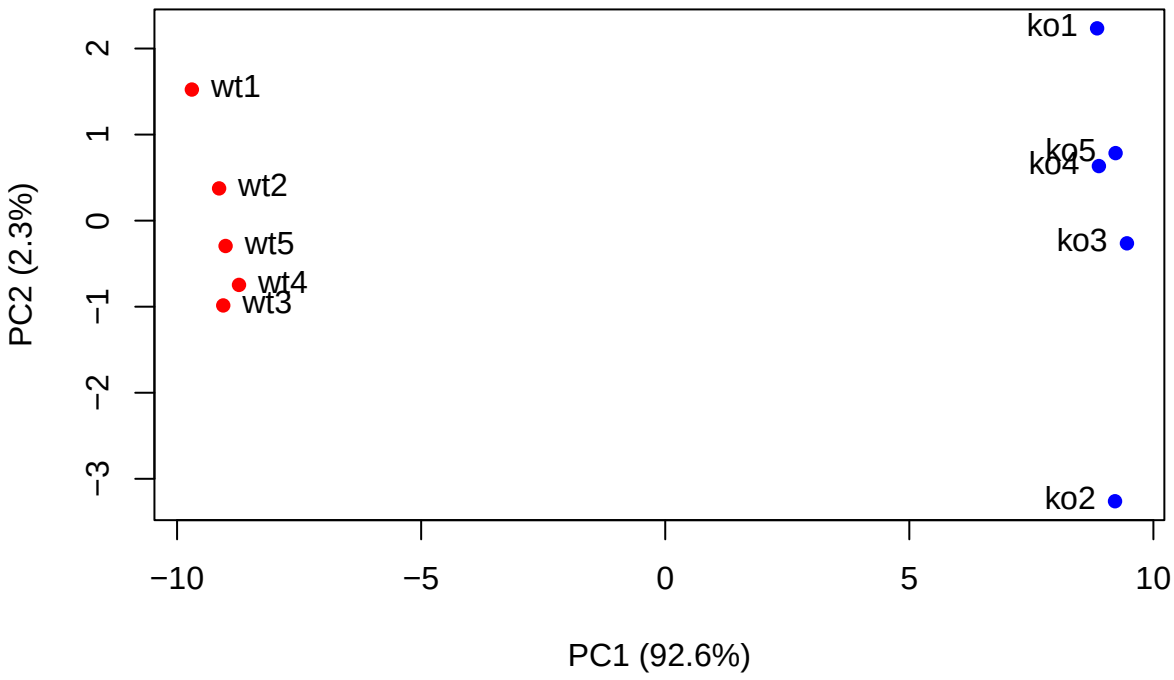
Generating our own scree plot

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



A vector of colors for wt and ko samples

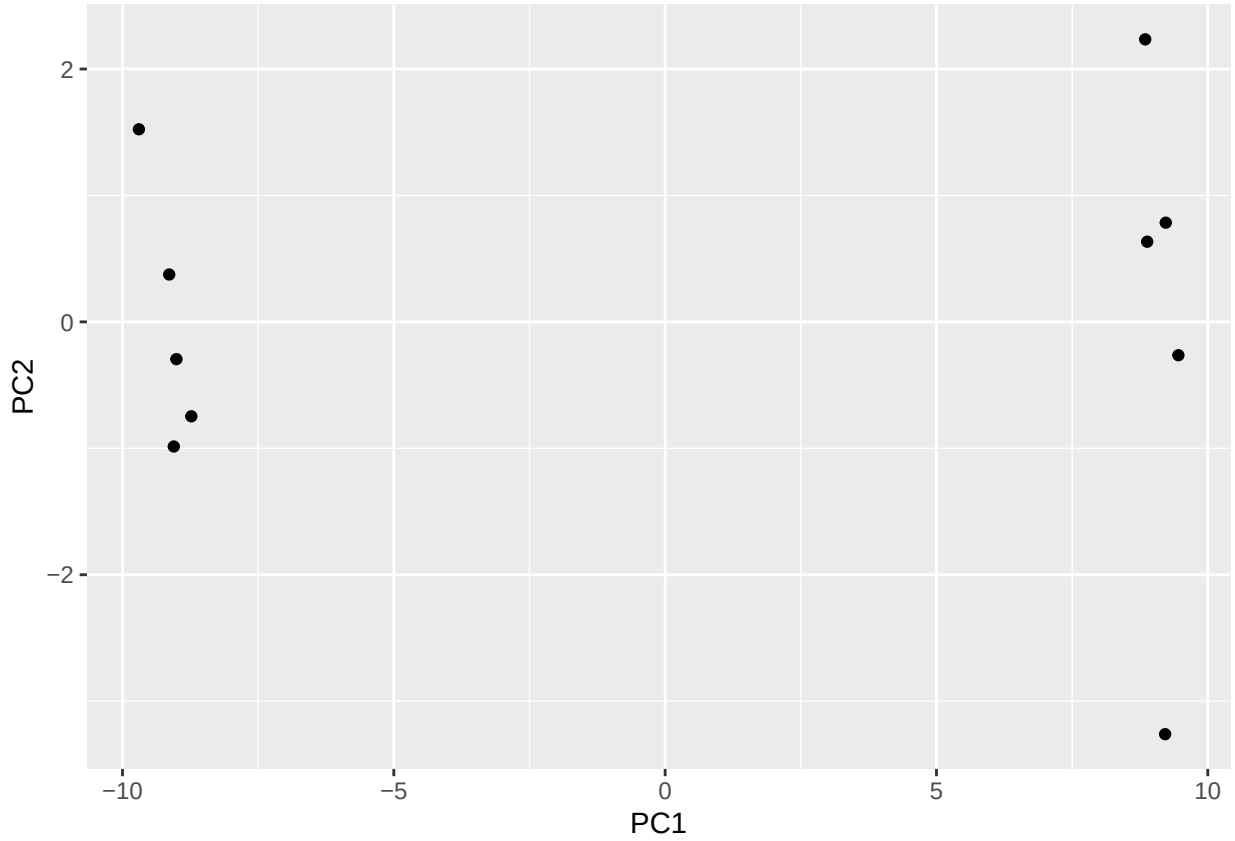
```
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
colvec[grep("ko", colvec)] <- "blue"

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

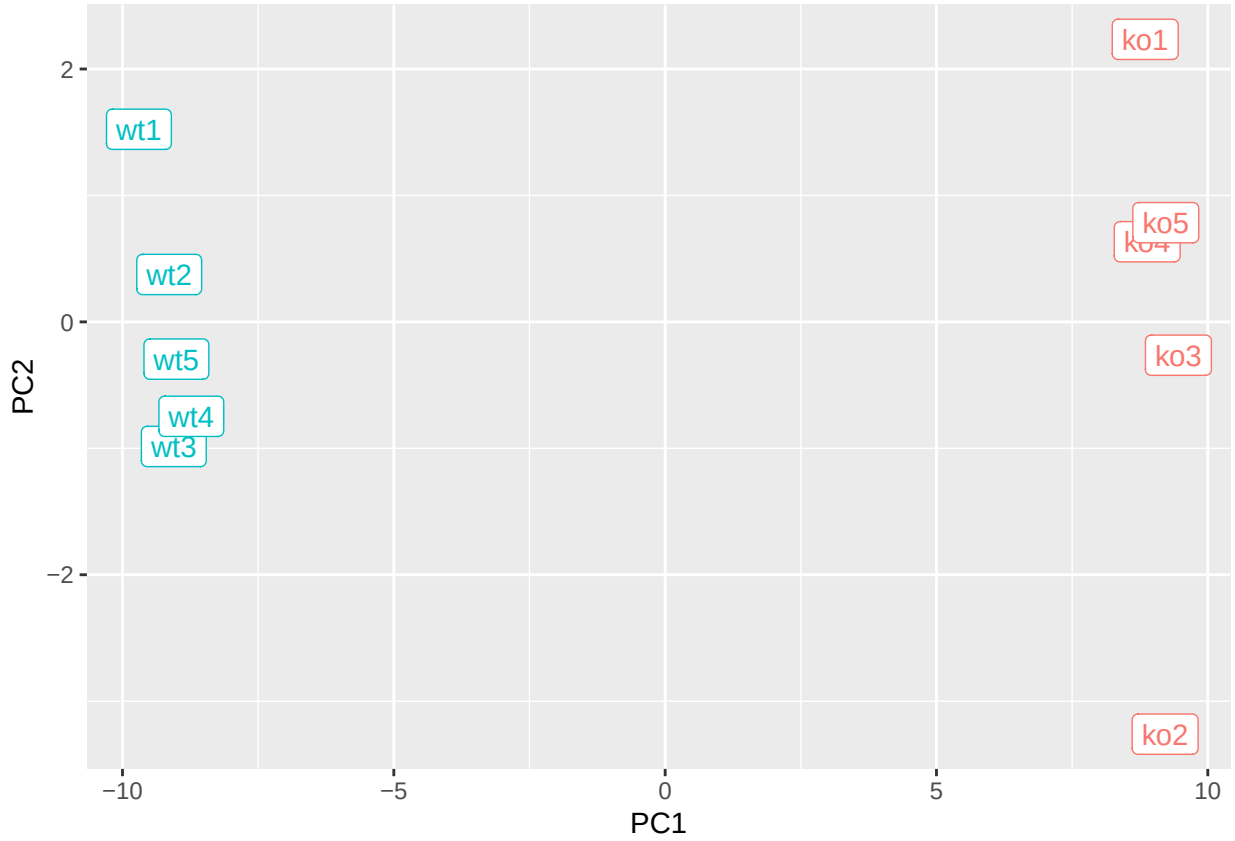
Our first basic plot

```
ggplot(df) +
  aes(PC1, PC2) +
  geom_point()
```

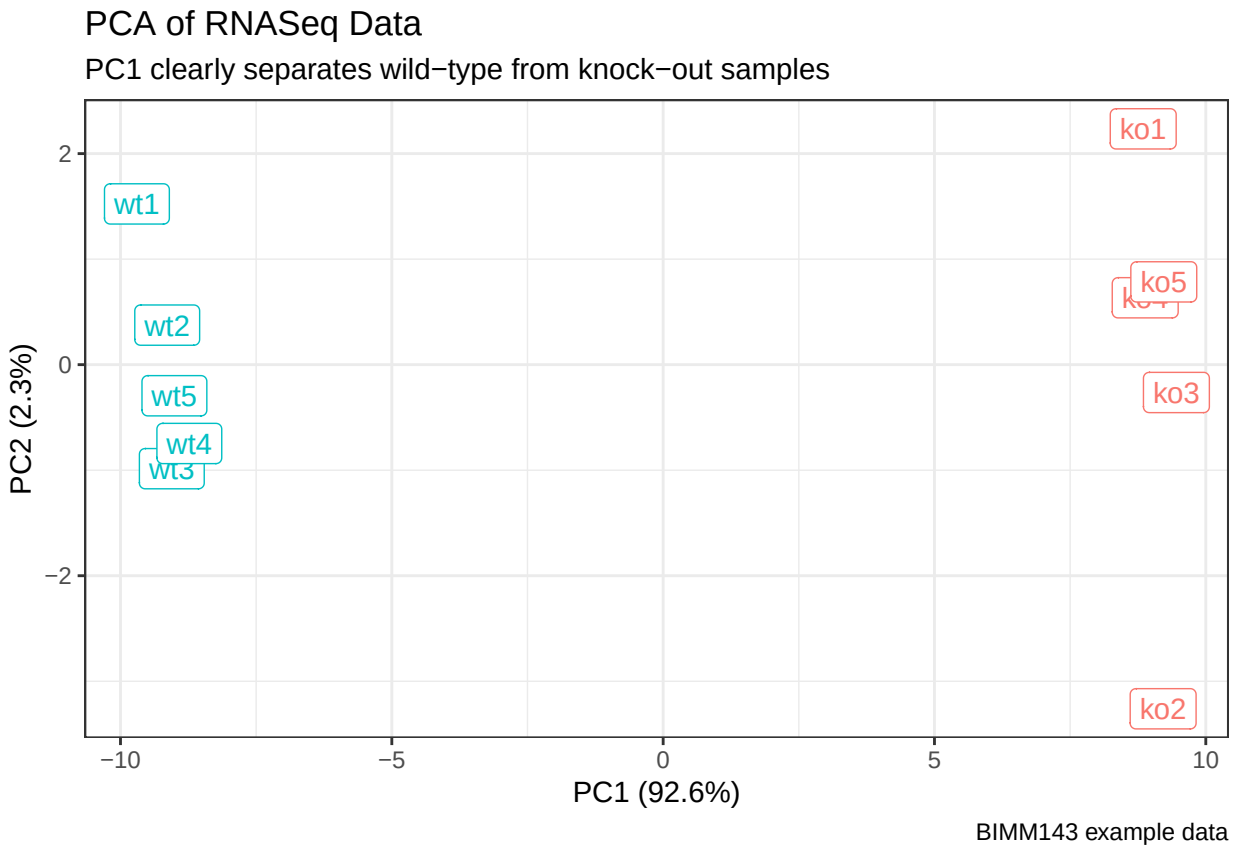


Add a ‘wt’ and ‘ko’ “condition” column

```
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
```




```
p + labs(title="PCA of RNASeq Data",
       subtitle = "PC1 clearly separates wild-type from knock-out samples",
       x=paste0("PC1 (", pca.var.per[1], "%)"),
       y=paste0("PC2 (", pca.var.per[2], "%)"),
       caption="BIMM143 example data") +
     theme_bw()
```




```
loading_scores <- pca$rotation[,1]
```

Find the top 10 measurements (genes) that contribute most to PC1 in either direction (+ or -)

```
gene_scores <- abs(loading_scores)
gene_score_ranked <- sort(gene_scores, decreasing=TRUE)
```

Show the names of the top 10 genes

```
top_10_genes <- names(gene_score_ranked[1:10])
top_10_genes
```

```
##  [1] "gene100" "gene66"  "gene45"  "gene68"  "gene98"  "gene60"  "gene21"
##  [8] "gene56"  "gene10"  "gene90"
```