Machine Learning 1/PCA

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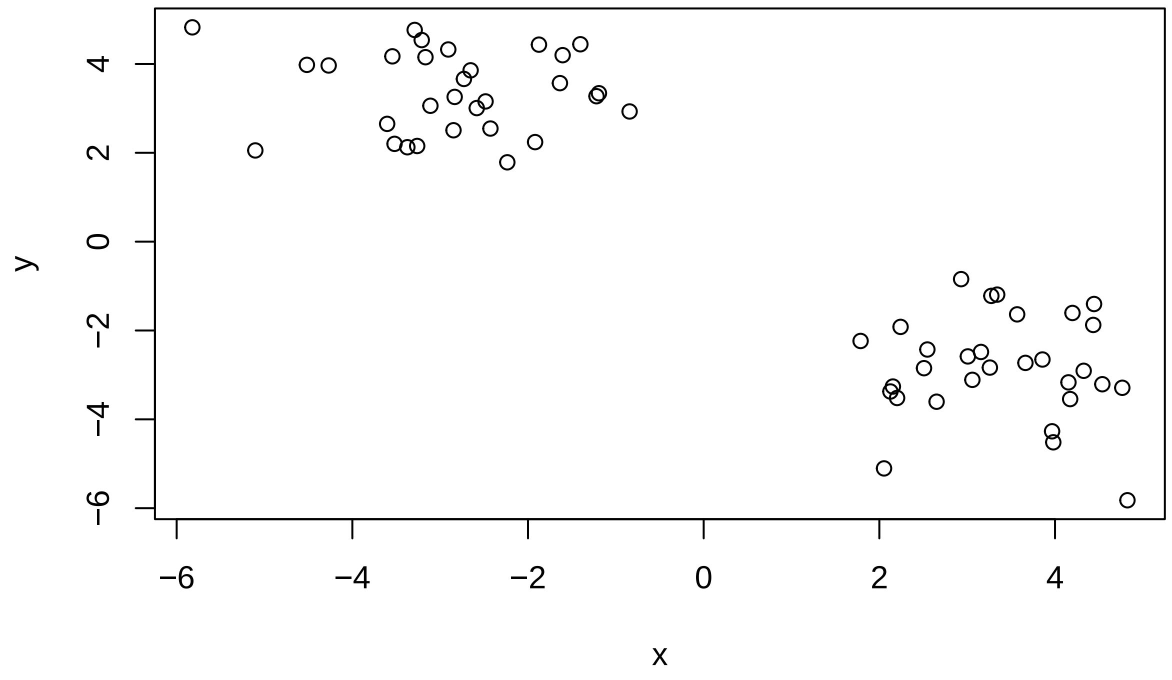
First up is clustering methods

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:

```
# rnorm makes up values that center around mean of -3 with normal distribution
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 to 2 and nstart to 20?

```
# Cluster into 2 and do 20 times
km <- kmeans(x, centers = 2, nstart = 20)
km
```

```
## K-means clustering with 2 clusters of sizes 30, 30
##
## Cluster means:
##           x         y
## 1 -2.839876  3.373186
## 2  3.373186 -2.839876
##
## 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 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
##
## Within cluster sum of squares by cluster:
## [1] 62.31597 62.31597
##  (between_SS / total_SS =  90.3 %)
##
## 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 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
```

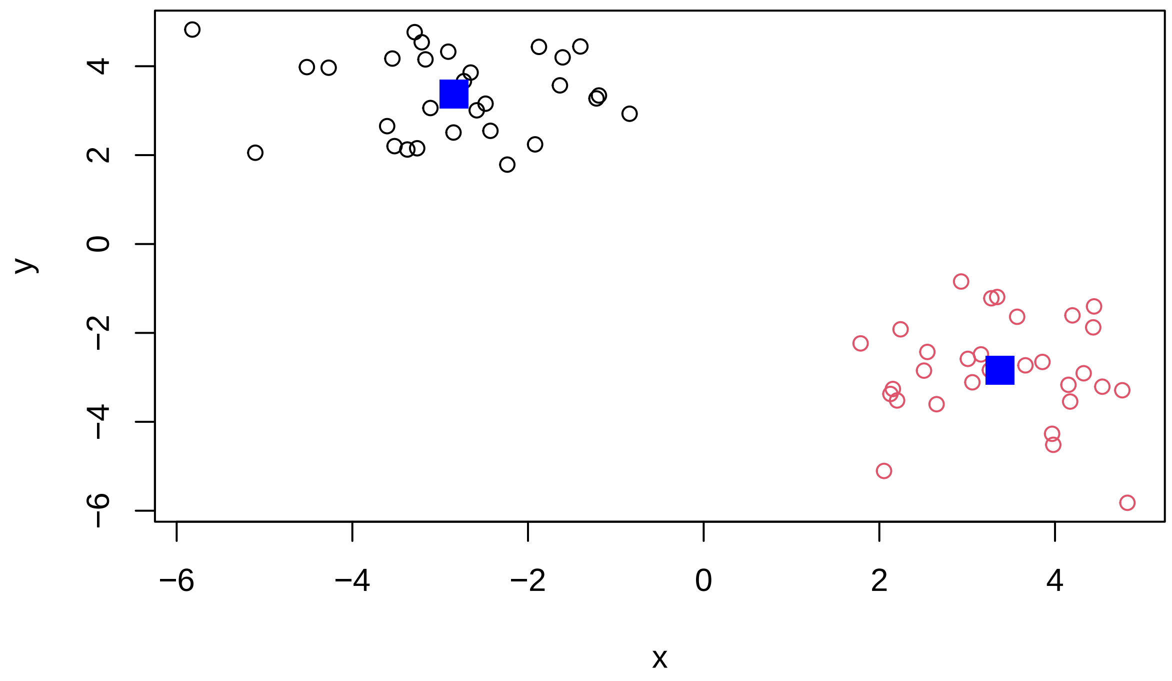
Q. What ‘component’ of your result object details cluster center?

```
km$centers
```

```
##           x         y
## 1 -2.839876  3.373186
## 2  3.373186 -2.839876
```

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().

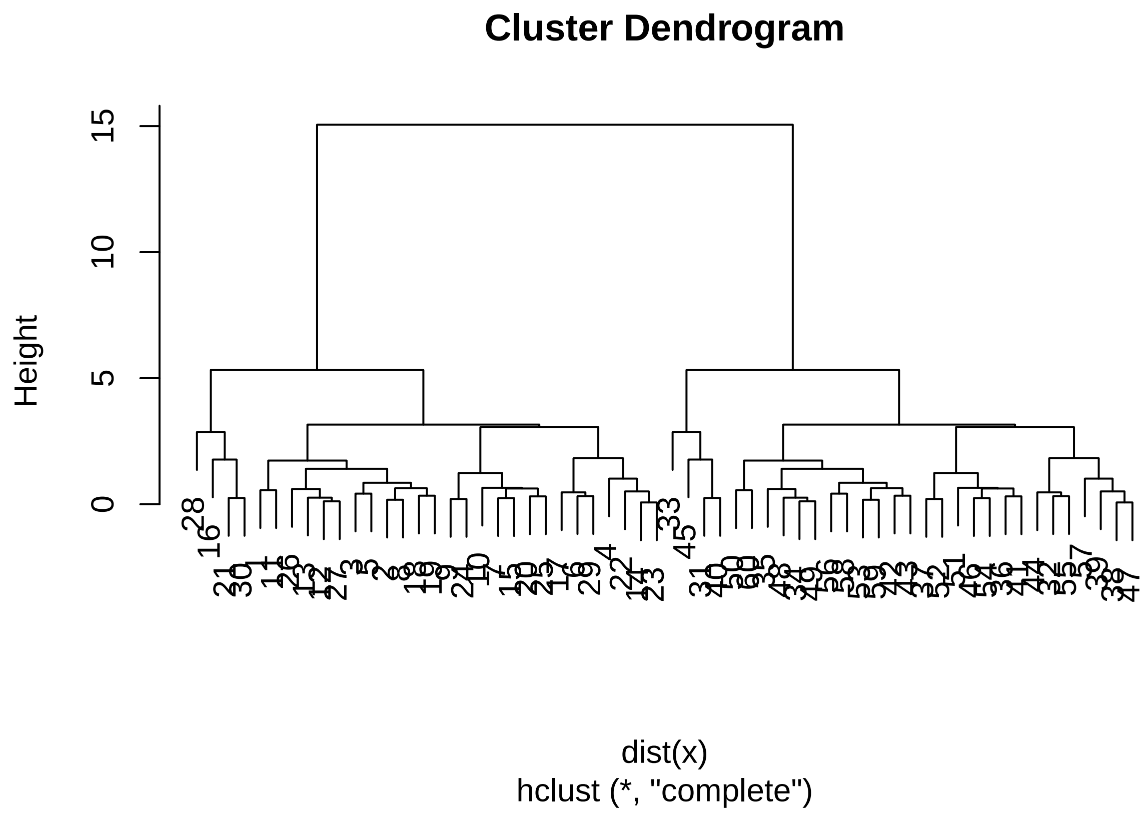
Demonstrate the use of dist(), hclust(), plot(), and cutree() functions to do clustering. Generate dendrograms and return cluster assignment/membership vector…

```
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)
```

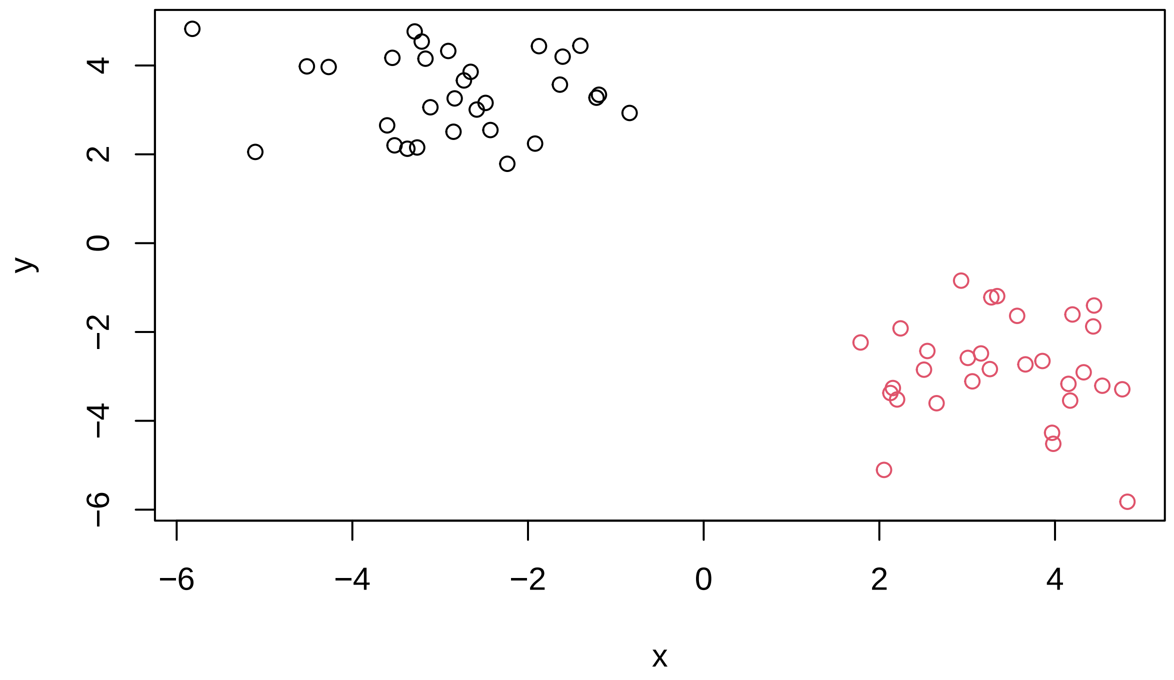
```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
## [39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

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

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

Make our results plot.

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



Principal Component Analysis

Lab 8 Questions:

Checking your data

```r
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 question?

```r
dim(x)
```

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

Answer: There are 17 rows and 15 columns. I can use dim() to answer this question.

```r
# 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
```

```r
# Fix data (method 1)
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
```

```r
# Fix data (method 2)
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
```

```r
# Check data again
dim(x)
```

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

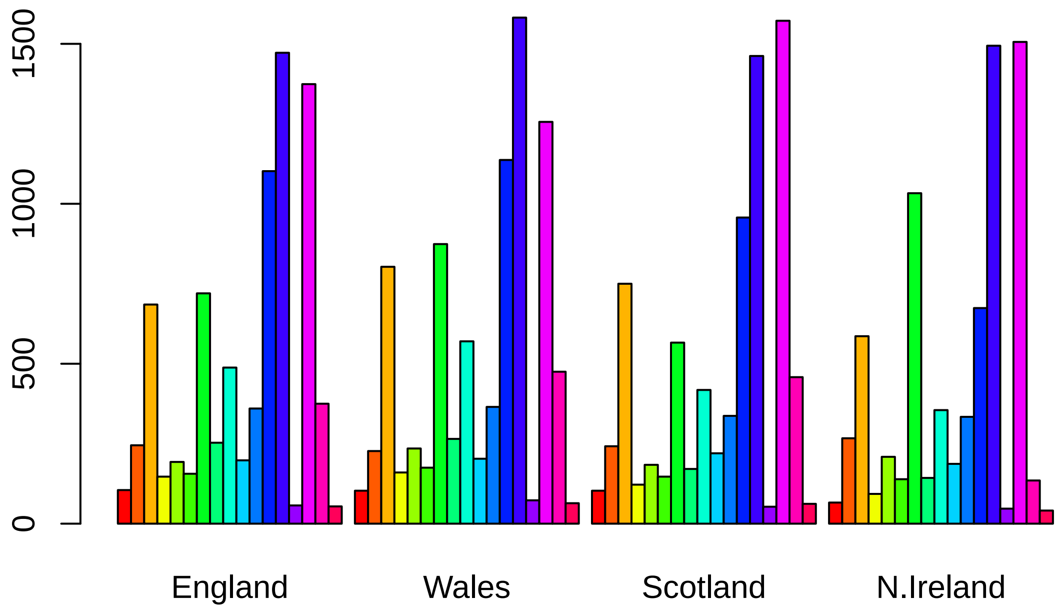
Answer: There are 17 rows and 4 columns in the fixed data.

> **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?

Answer: The second approach above is preferred. Every time the code in the first approach is re-run, a column will be removed, eventually leading to the deletion of all data after multiple re-runs. Thus, the second approach is more robust and avoids data loss.

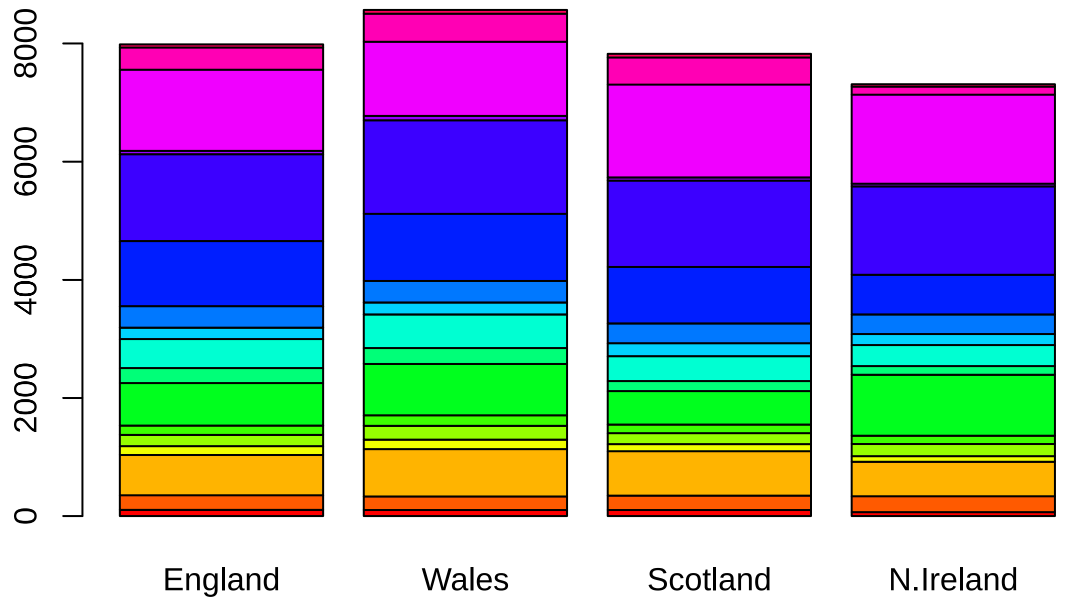
Spotting major differences and trends

```
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)))
```

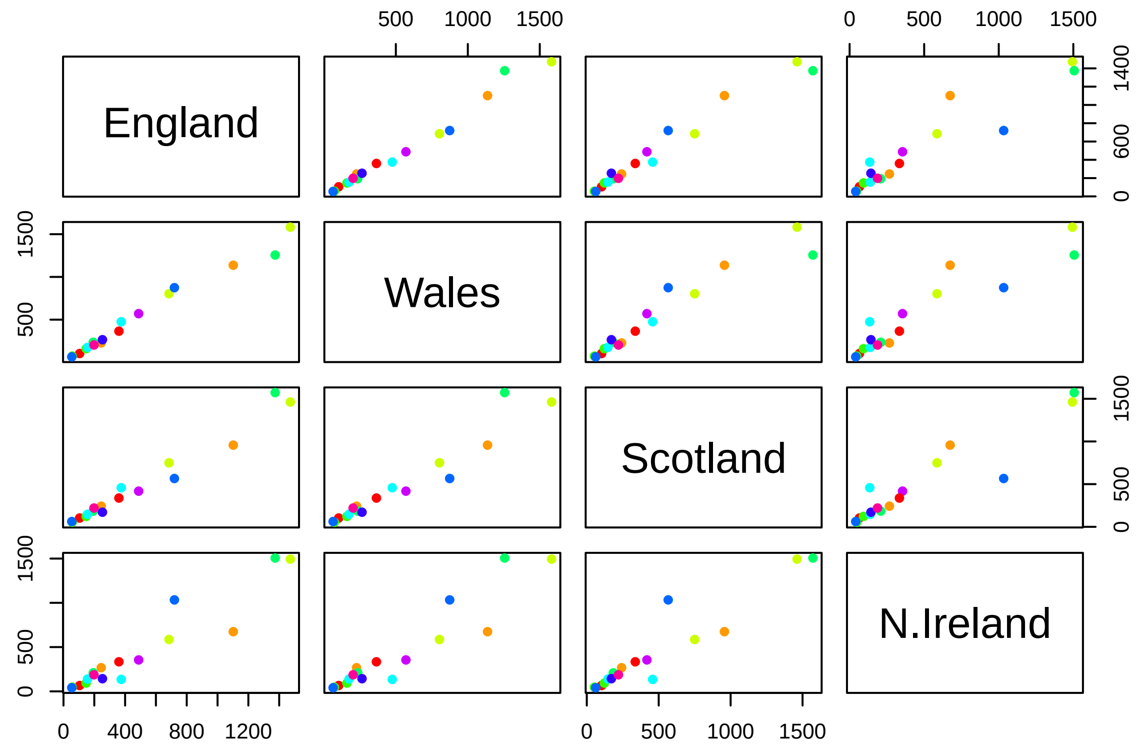


Answer: Changing the beside argument from TRUE to FALSE results in the plot.

Q4. Missing from lab handout.

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(10), pch=16)
```



Answer: Yes, I can make sense of the following code and resulting figure. When a given point lies on the diagonal for a given plot, it means that the expected trend is being followed (similarity between compared countries) and that there is little to no variance.

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

Answer: The points plotted for N. Ireland compared to all the other countries of the UK were more off the diagonal, indicating greater variance and dissimilarity in terms of consumption of food types.

PCA to the rescue!

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

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

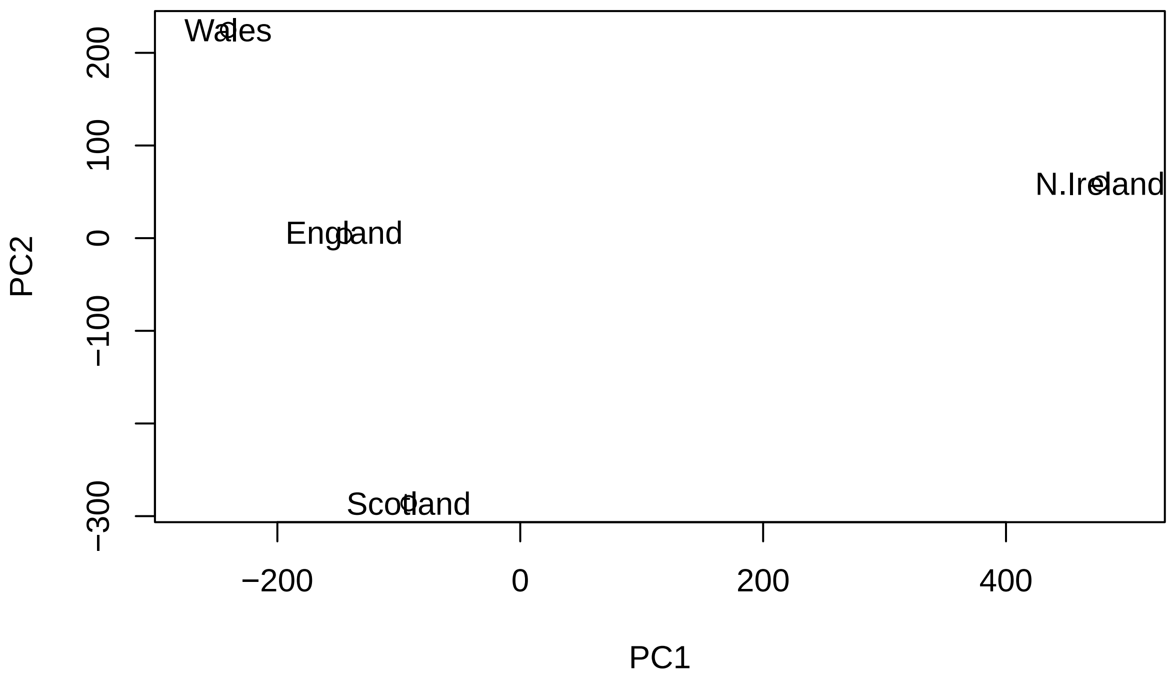
```
## Importance of components:
##                              PC1      PC2      PC3       PC4
## Standard deviation      324.1502 212.7478 73.87622 4.189e-14
## Proportion of Variance    0.6744   0.2905  0.03503 0.000e+00
## Cumulative Proportion     0.6744   0.9650  1.00000 1.000e+00
```

```
attributes(pca)
```

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

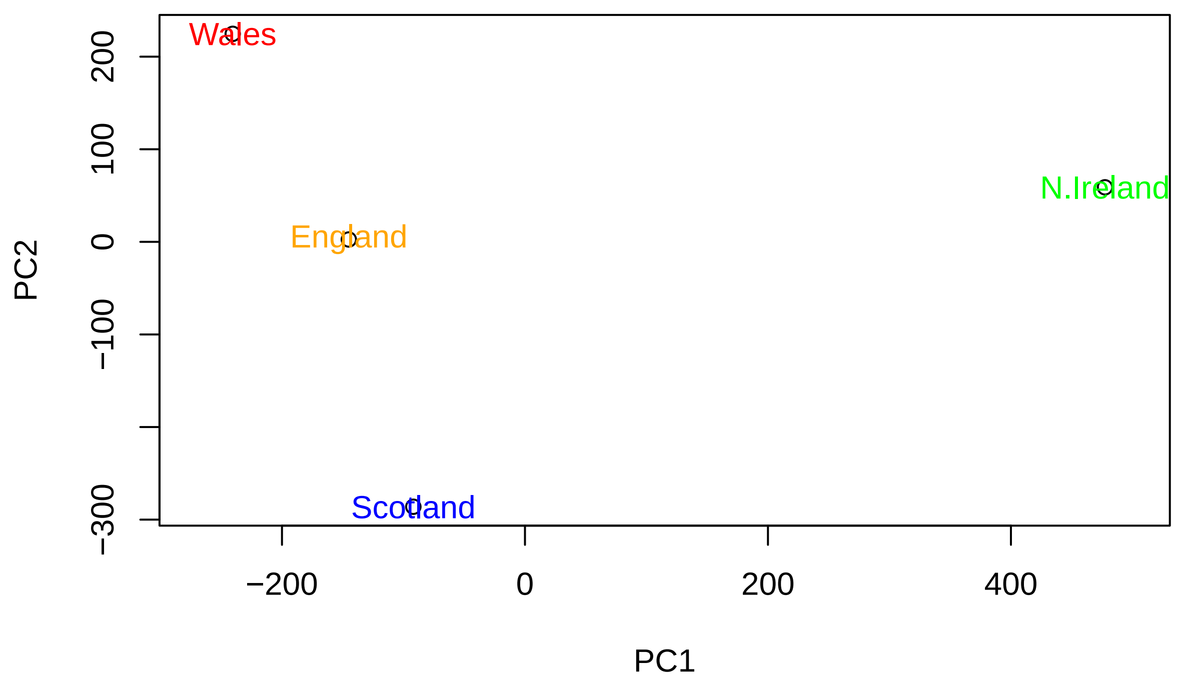
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
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.

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



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

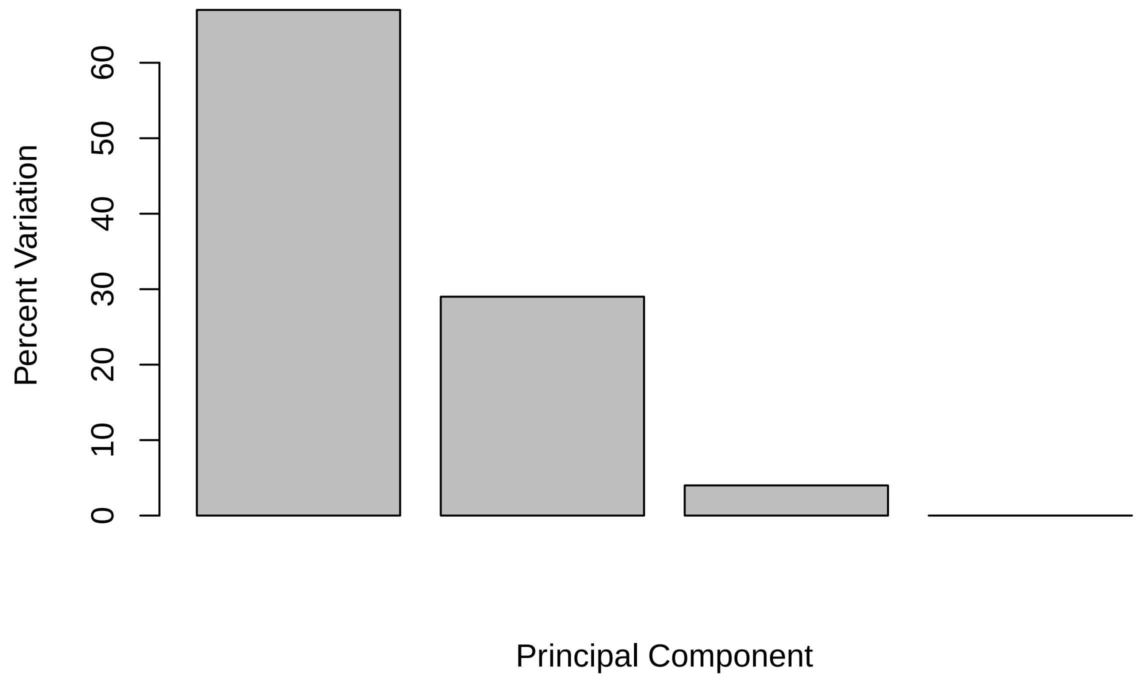
```
## [1] 67 29  4  0
```

```
# 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
```

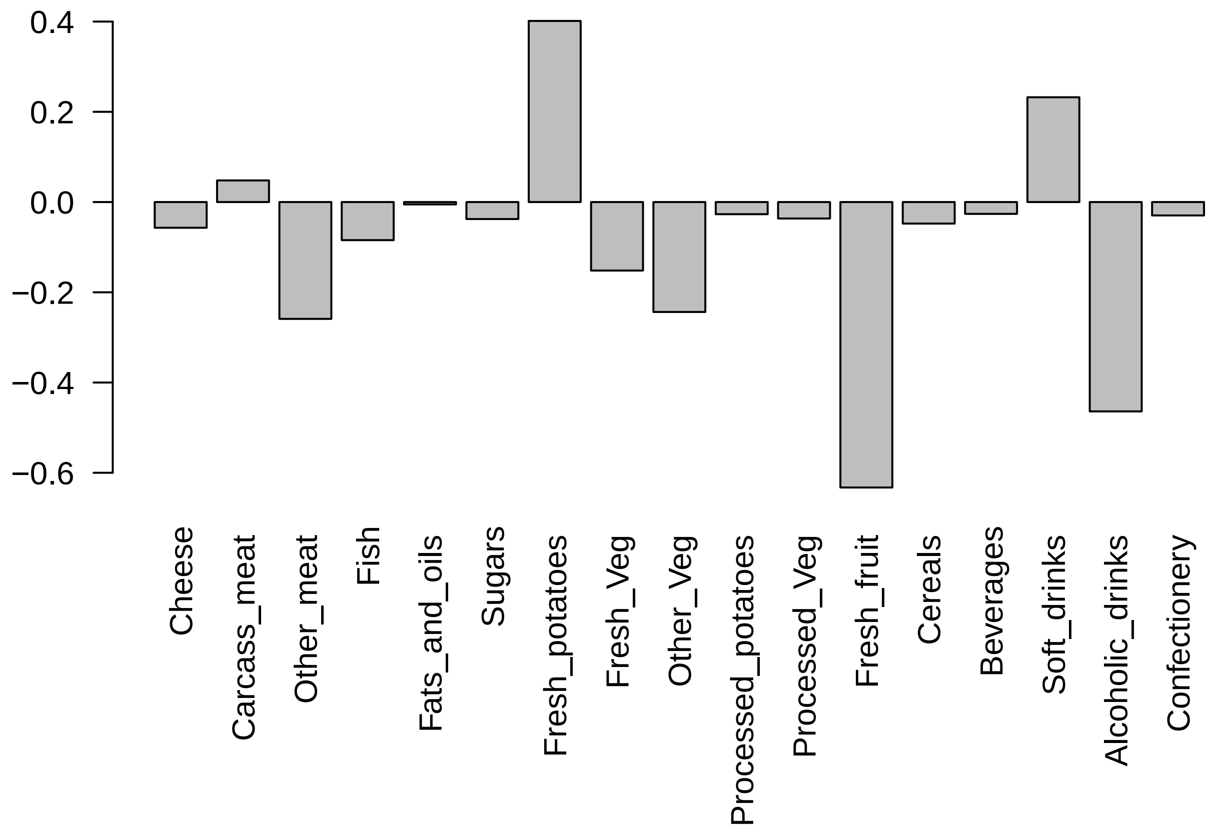
Make a plot.

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



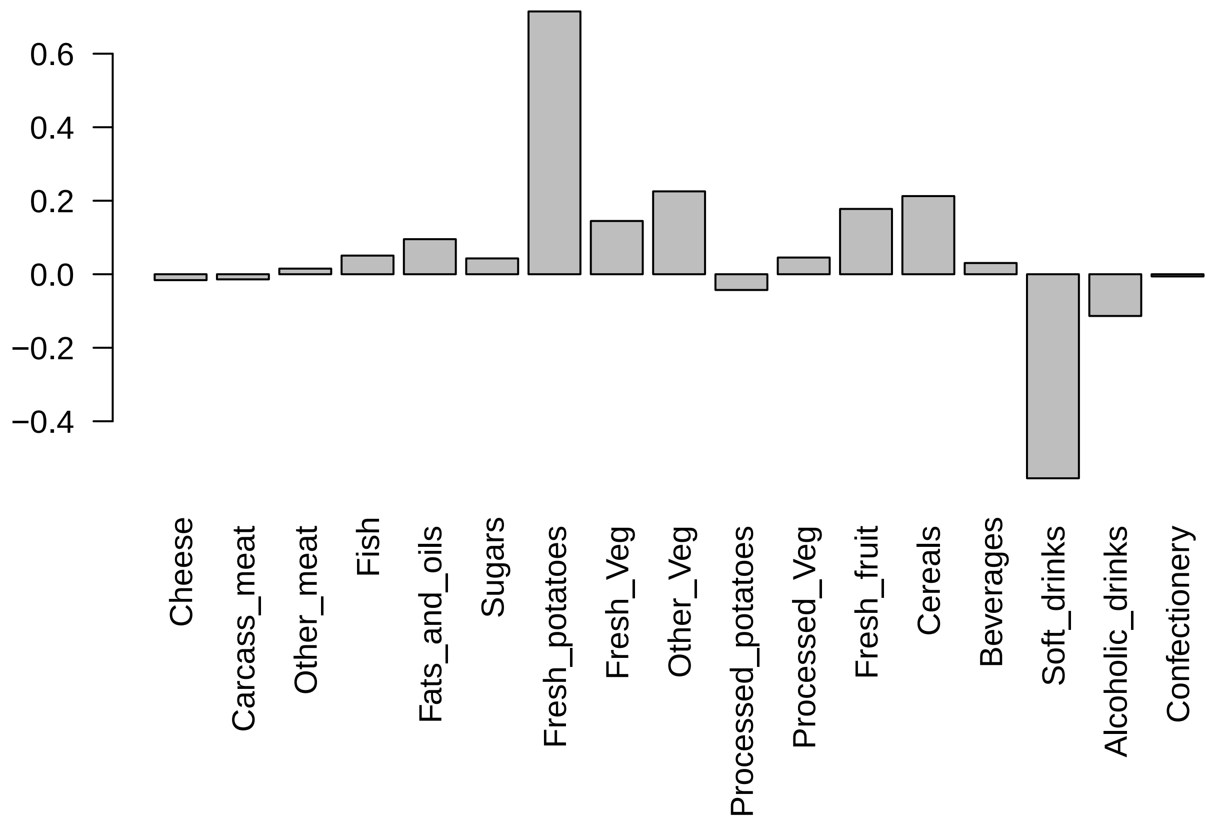
Digging deeper (variable loadings)

```
# Let's focus on PC1
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 prominently, and what does PC2 mainly tell us about?

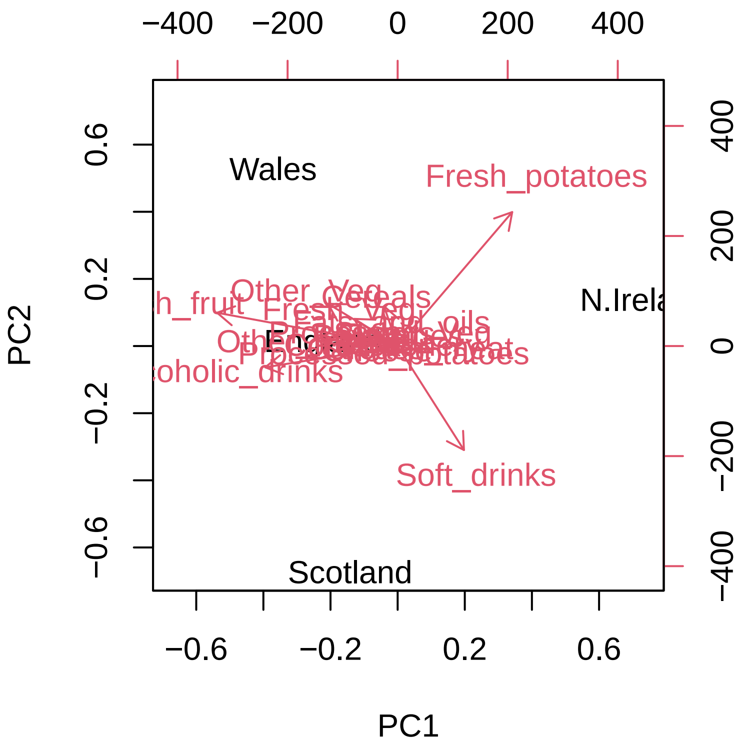
```
par(mar=c(10,3,0.35,0))
barplot(pca$rotation[,2], las=2)
```



Answer. The two groups that feature prominently are fresh potatoes and soft drinks. PC2 tells us that fresh potatoes (large positive loading score) pushes N. Ireland to the positive side of the plot and soft drinks (notable negative score) pushes the other countries to the left side of the plot. Overall, PC2 accounts for less variance (29%), which is displayed by the majority of loading scores being close to zero.

Biplots

```
# The inbuilt biplot() can be useful for small datasets
biplot(pca)
```



2. PCA of RNA-seq data

Q10. How many genes and samples are in this data set?

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

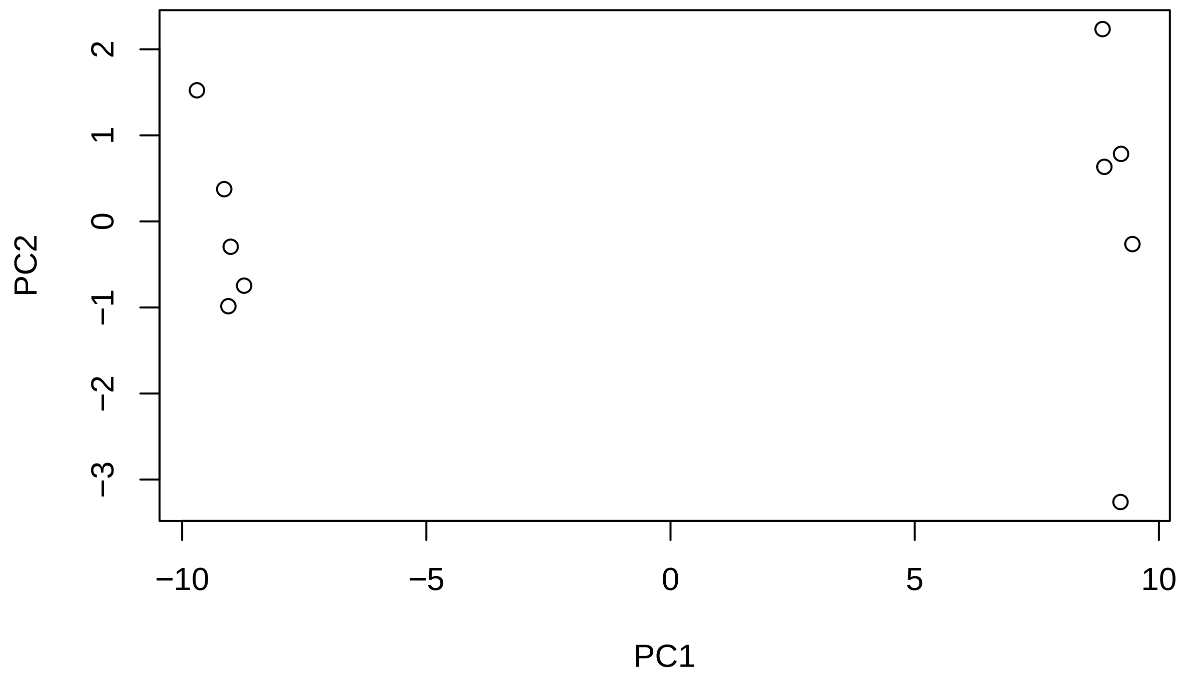
```
##          wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
## gene1  439 458  408  429 420  90  88  86  90  93
## gene2  219 200  204  210 187 427 423 434 433 426
## gene3 1006 989 1030 1017 973 252 237 238 226 210
## gene4  783 792  829  856 760 849 856 835 885 894
## gene5  181 249  204  244 225 277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

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

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

Answer: There are 100 genes and 10 samples in this data set.

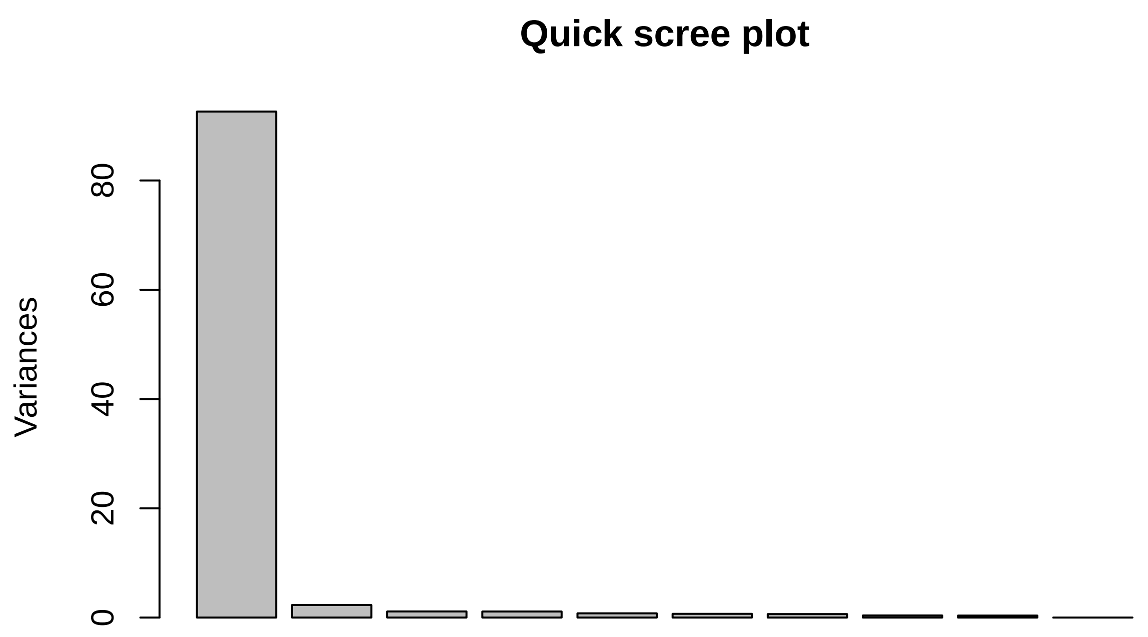
```r
# Again we have to take the transpose of our data
pca <- prcomp(t(rna.data), scale=TRUE)

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



```r
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
```

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

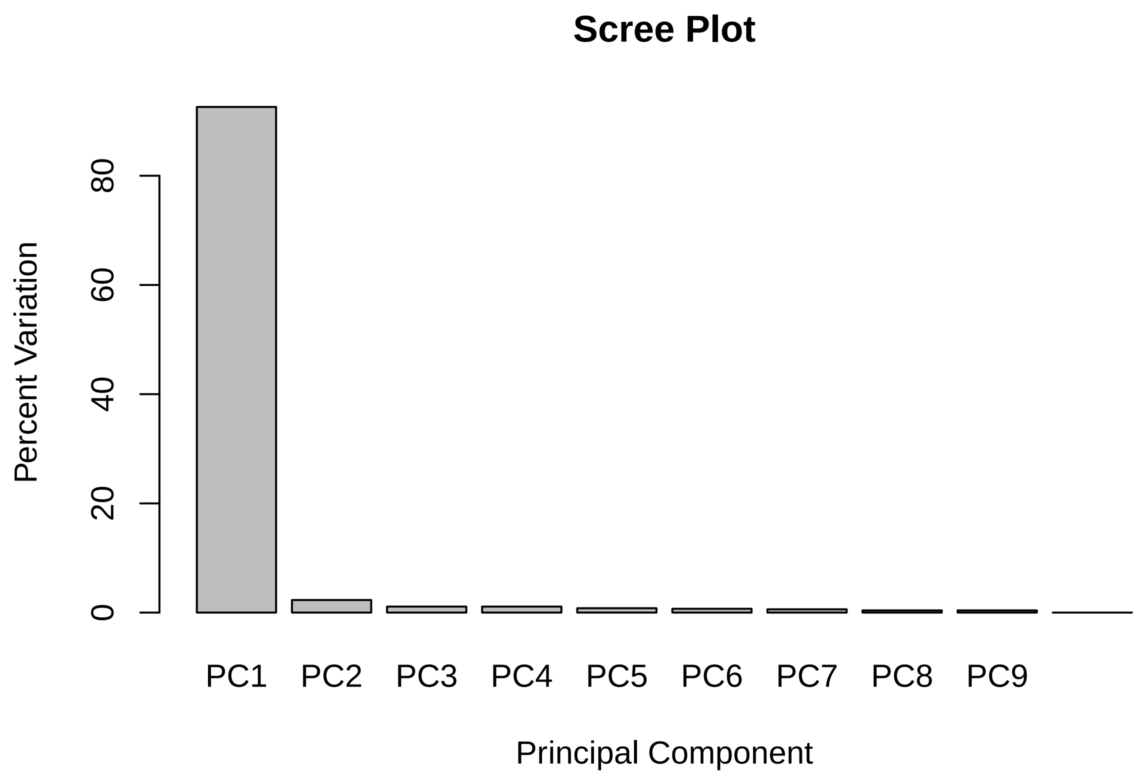


```
# Variance captured per PC
pca.var <- pca$sdev^2

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

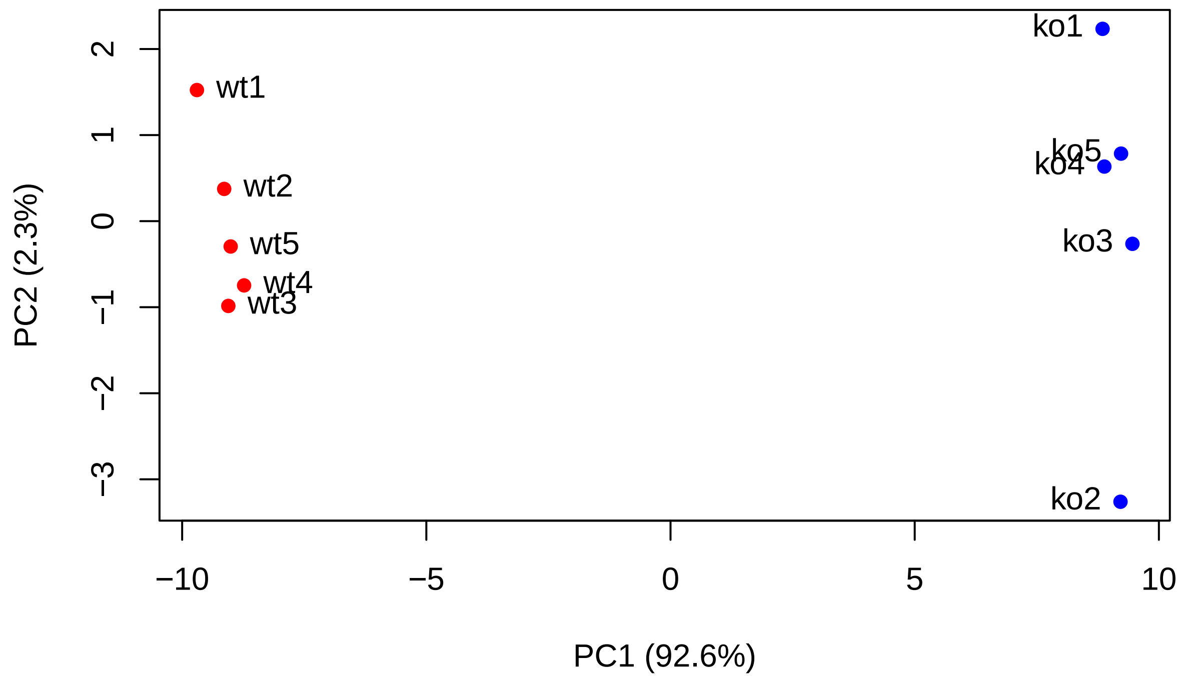
```
##  [1] 92.6  2.3  1.1  1.1  0.8  0.7  0.6  0.4  0.4  0.0
```

Make own scree-plot.

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

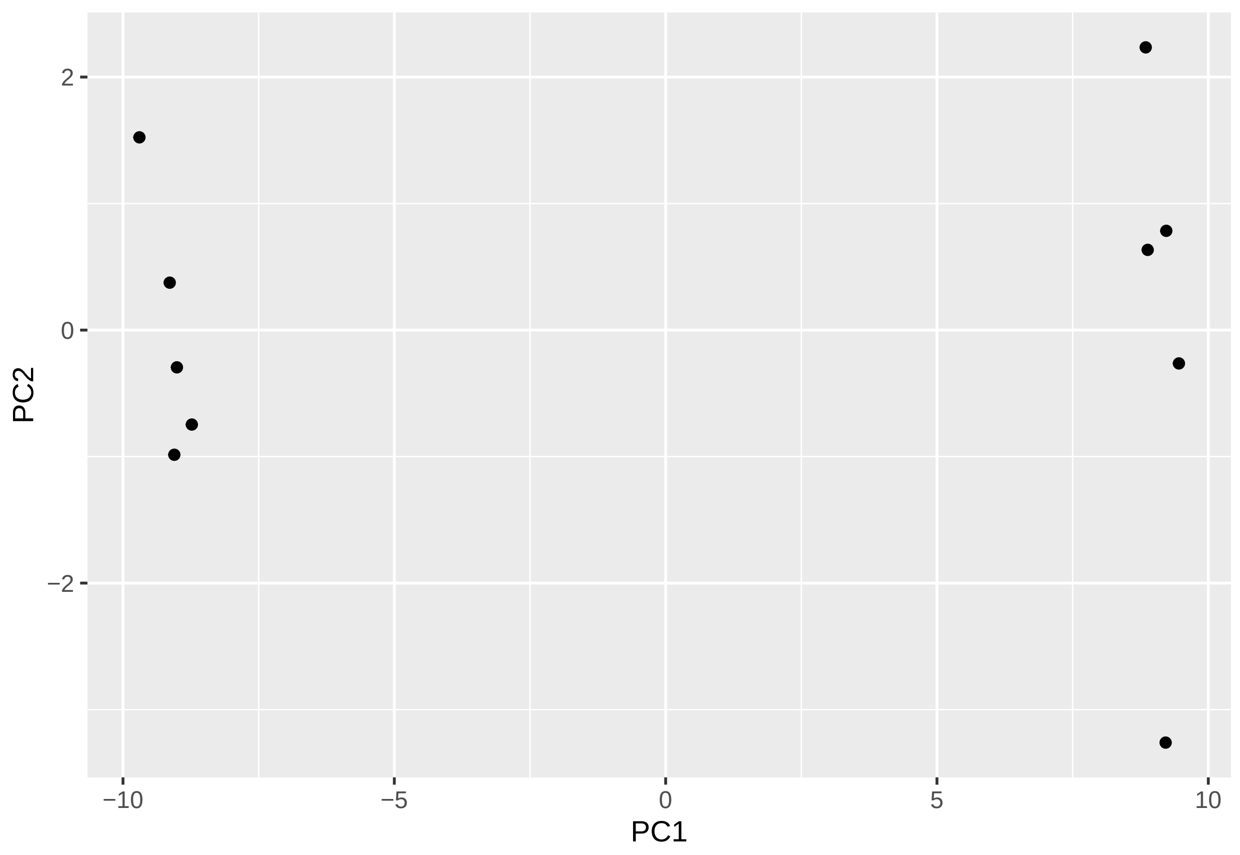


```r
# A vector of colors for wt and ko samples
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
colvec[grep("ko", colvec)] <- "blue"

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)))
```

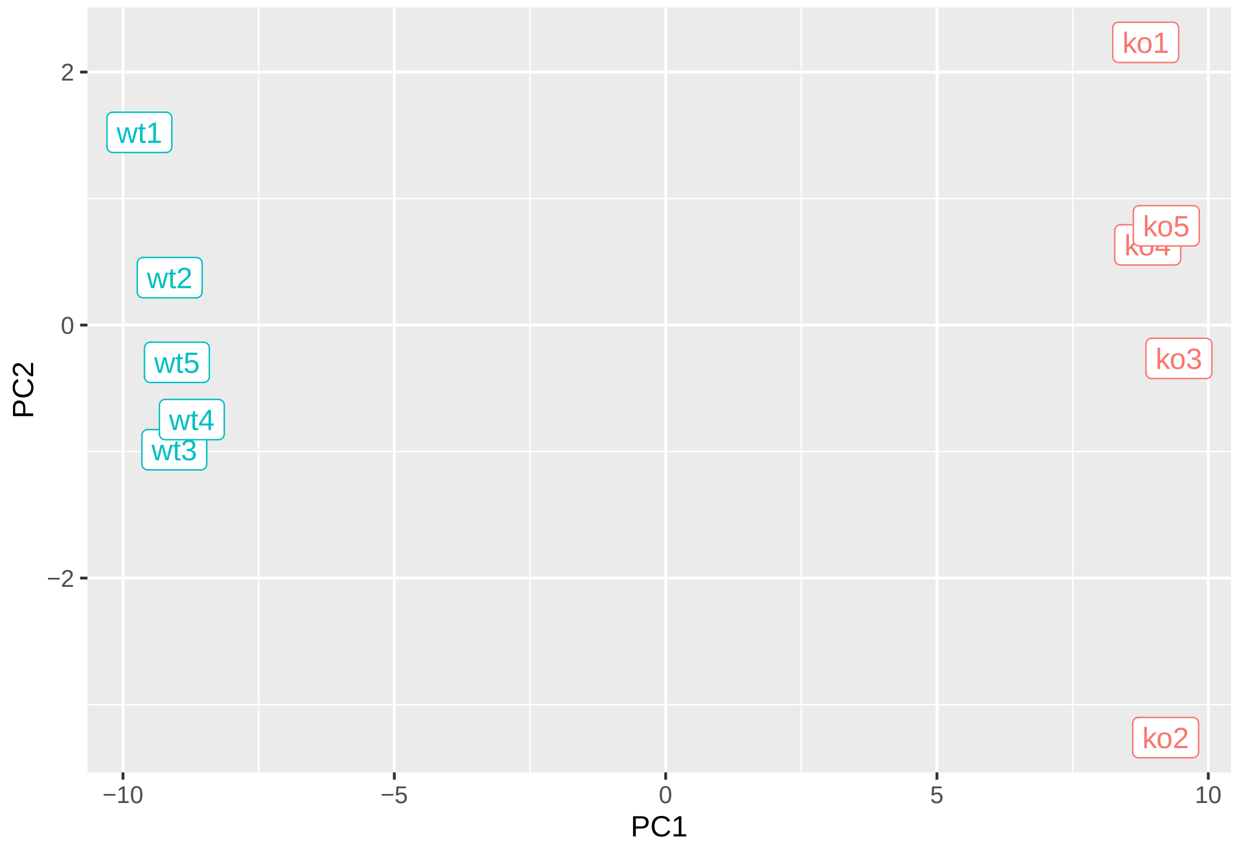


Using ggplot

```
library(ggplot2)
df <- as.data.frame(pca$x)

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

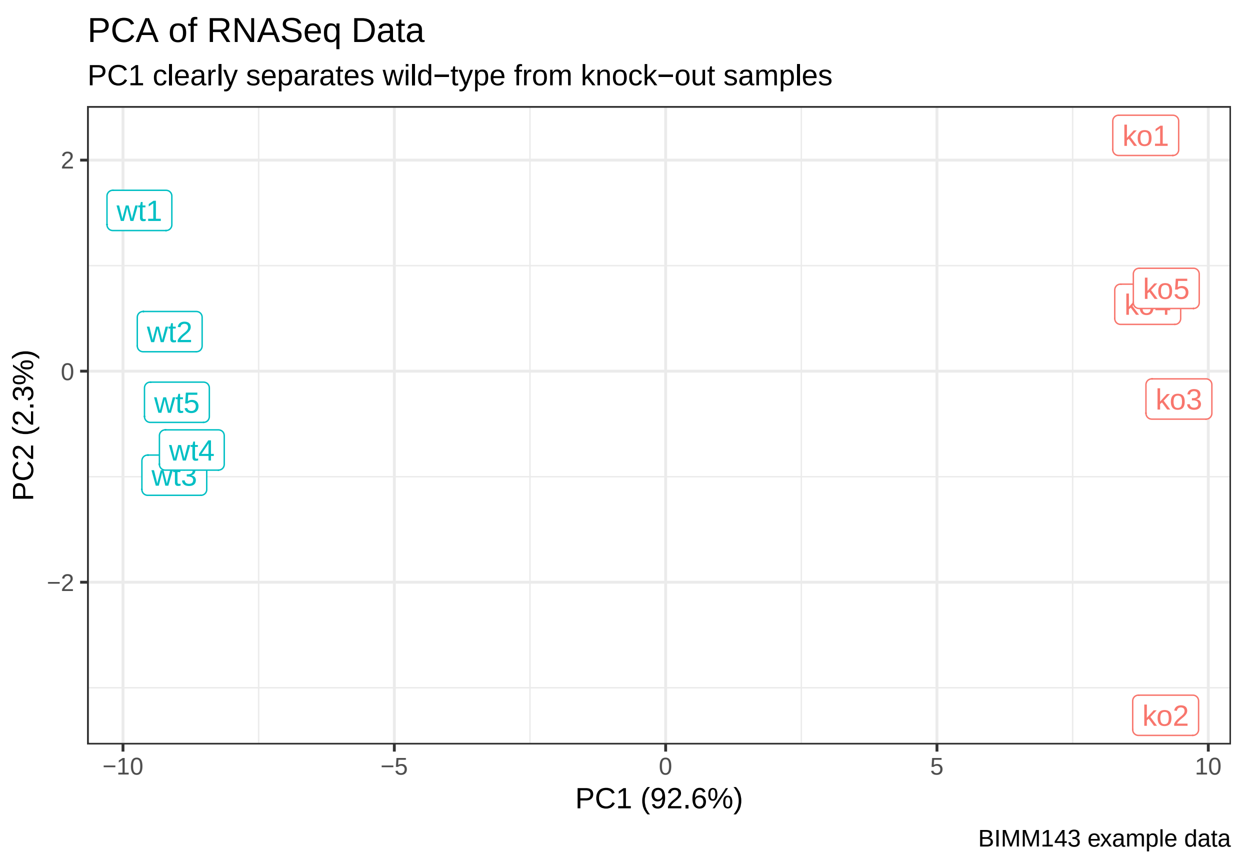


```
# Add a 'wt' and 'ko' "condition" column
df$samples <- colnames(rna.data)
df$condition <- substr(colnames(rna.data),1,2)

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



Now polish the plot.

```
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()
```


PCA of RNASeq Data
PC1 clearly separates wild−type from knock−out samples
ko1
wt1
ko5
ko4
wt2
ko3
wt5
wt4
wt3
ko2
2
0
−2
−10
−5
0
5
10
PC1 (92.6%)
PC2 (2.3%)
BIMM143 example data