Class 7: Machine Learning I

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Today we are going to learn how to apply different machine learning methods, beginning with clustering:

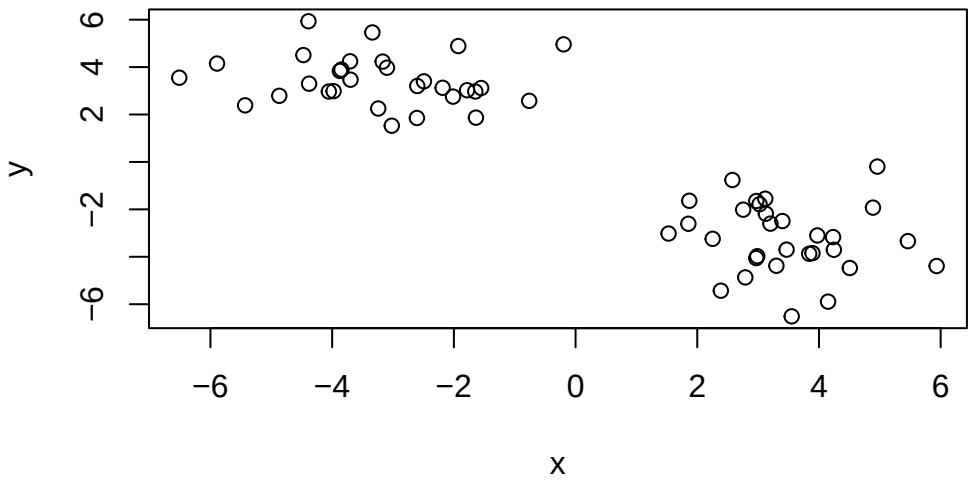
The goal here is to find groups/clusters in your input data.

First I will make up some data with clear groups. For this I will use the `rnorm()` function.

```
rnorm(10)
```

```
 [1]  2.26070856  0.20089428  0.12024632  1.07663978 -0.01075139 -0.15497909
 [7]  1.78958333  1.77835457 -0.76674235  0.94105325
```

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




```
km <- kmeans(z, 2)
km
```

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

Cluster means:
          x         y
1  3.440302 -3.212620
2 -3.212620  3.440302

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 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

Within cluster sum of squares by cluster:
[1] 95.16456 95.16456
 (between_SS / total_SS =  87.5 %)

Available components:

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

```r
attributes(km)
```

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

$class
[1] "kmeans"
```

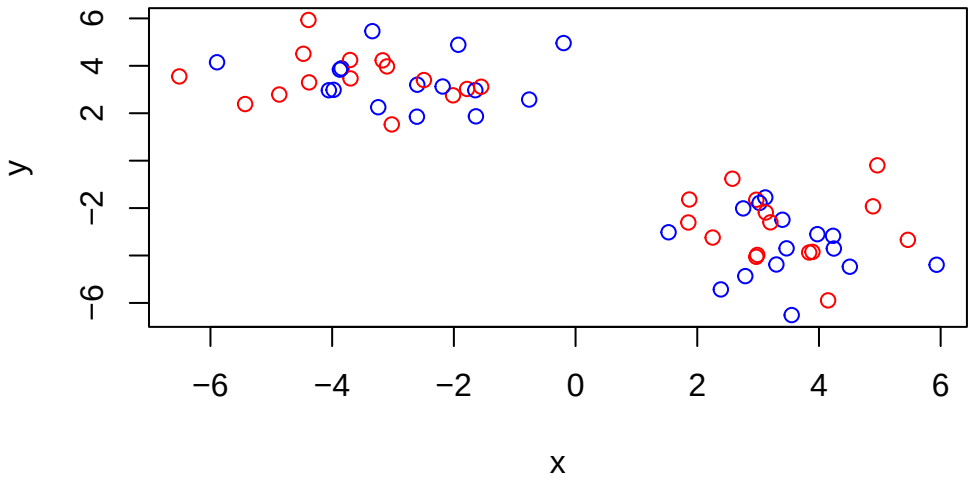
```r
km$center
```

```
          x         y
1  3.440302 -3.212620
2 -3.212620  3.440302
```

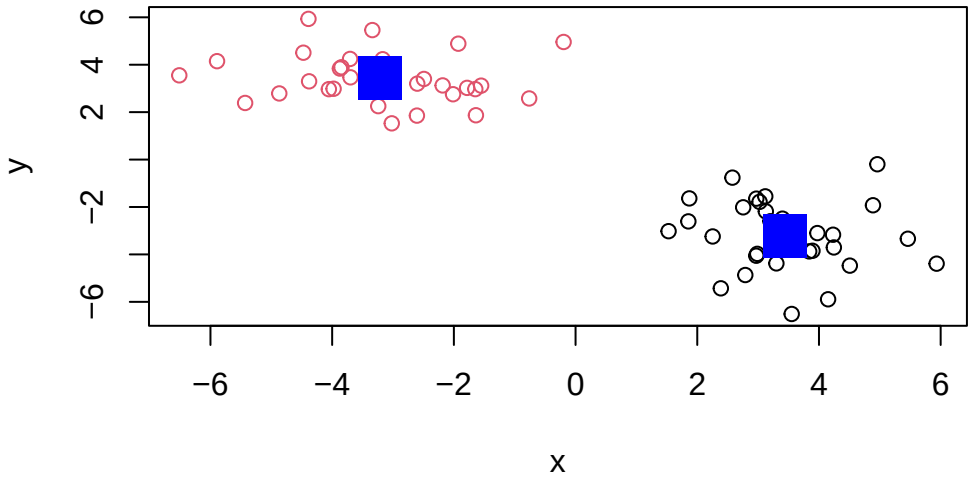
```r
km$cluster
```

```
 [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 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
```

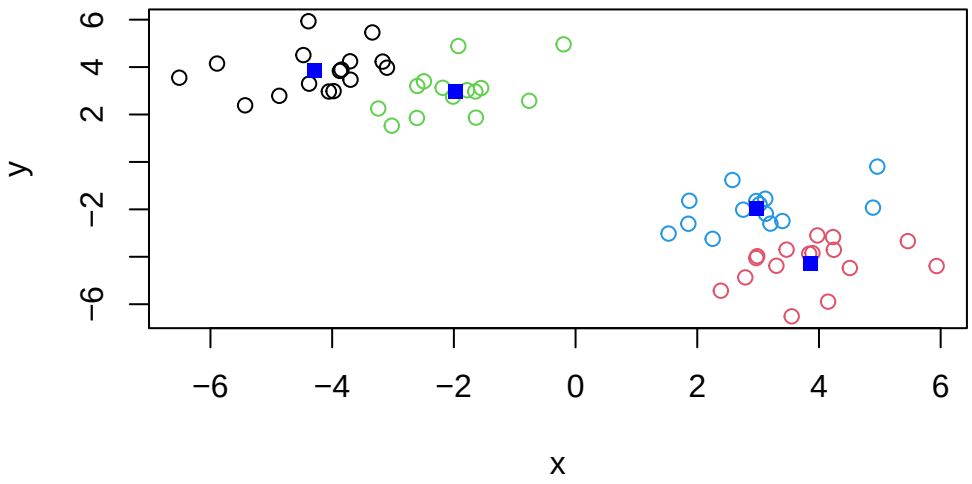
```r
plot(z, col = c("red", "blue"))
```



```r
plot(z, col = km$cluster)
points(km$center, col = "blue", pch = 15, cex = 3)
```




```r
km_2 <- kmeans(z, 4)
plot(z, col = km_2$cluster)
points(km_2$center, col = "blue", pch = 15, cex = 1)
```



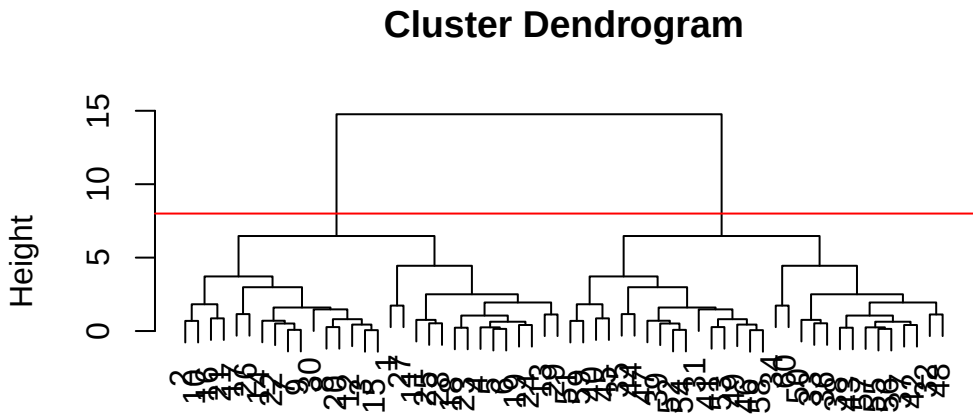
Hierarchical Clustering

Let's take our same made-up data **z** and see how hclust works.

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

```
Call:
hclust(d = d)

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

```
plot(hc)
abline(h=8, col = "red")
```

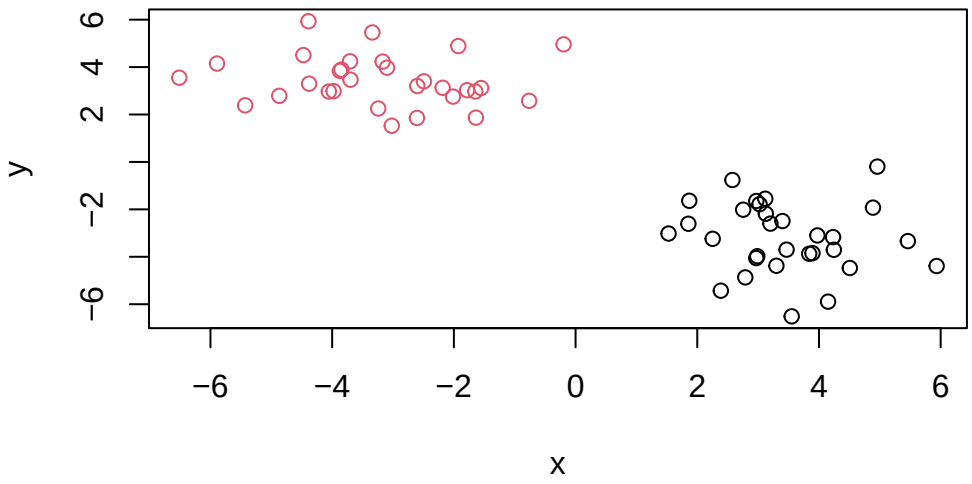


d
hclust (*, "complete")

```
grps <- cutree(hc, h=8)
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 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
```

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



1. PCA of UK food data

Read data from UK UK on food consumption in different parts of the UK

```
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

Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions? There are 17 rows and 4 columns

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? Generally, I would prefer the method used in this code, as it is a much simpler way of solving this issue. However, since the method involving reading the data file again is much more thorough, it would be more failsafe.

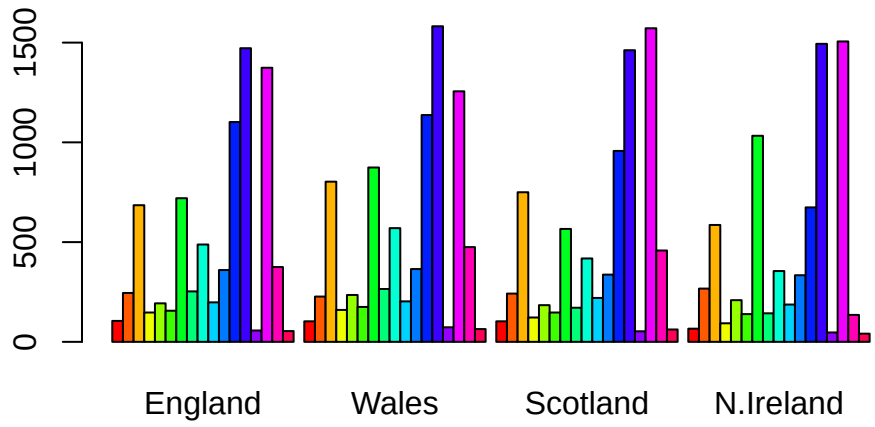
```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

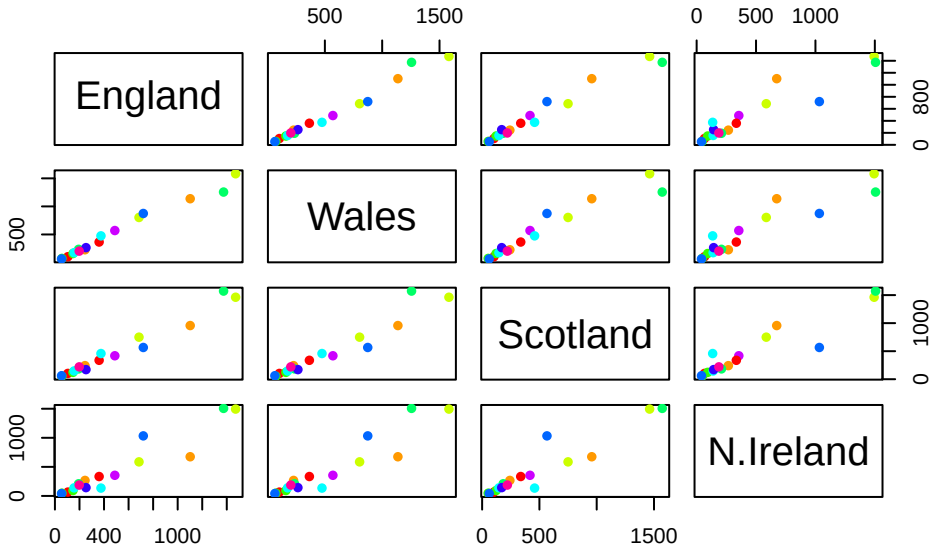
```
[1] 4
```

```
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 beside to false causes that change. Leaving it out would have the same effect because the default setting for beside is false.

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



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? This plot compares the consumption of different foods in the countries, two countries at a time. Therefore, a point lying on the diagonal means that it is consumed in a similar amount in both countries on the graph.

Q6. What is the main differences between N. Ireland and the other countries of the UK in terms of this data-set? Northern Ireland has a lot less in `other meats` and much more in `fresh potatoes`.

Its hard to see structure and trends in even this small data-set. How will we ever do this when we have big datasets with 1000s or 10s of thousands of things we are measuring …

##PCA to the rescue

Let's see how PCA deals with this dataset. Main function in base R to do PCA is called `prcomp()`

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

```
Importance of components:
                            PC1      PC2      PC3        PC4
Standard deviation     324.1502 212.7478 73.87622 3.176e-14
```

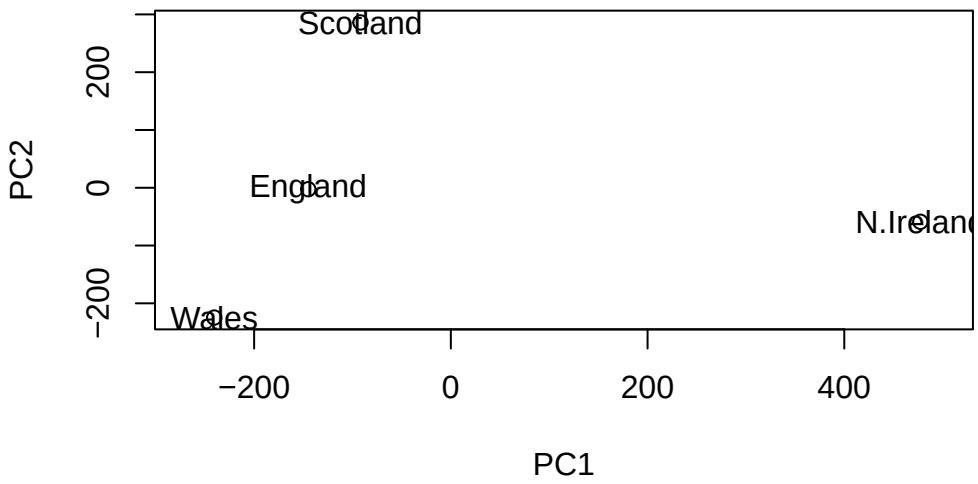
```
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

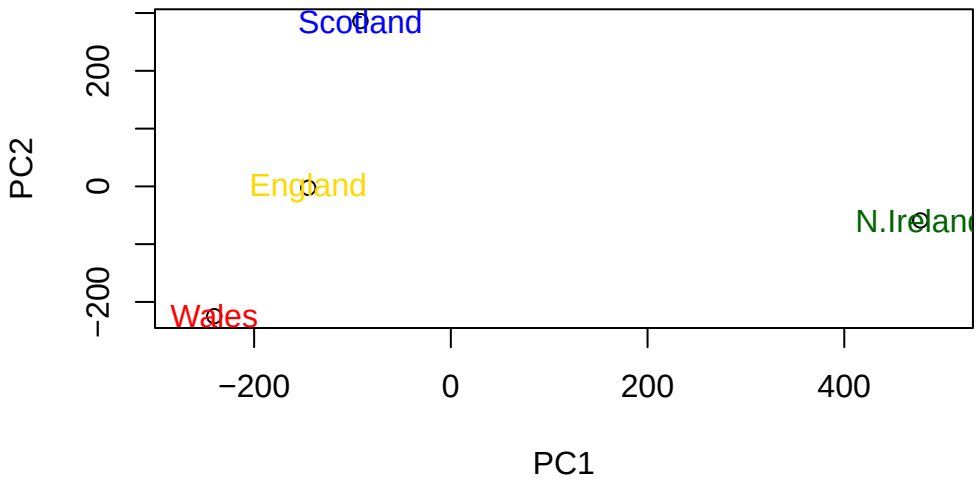
Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
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.

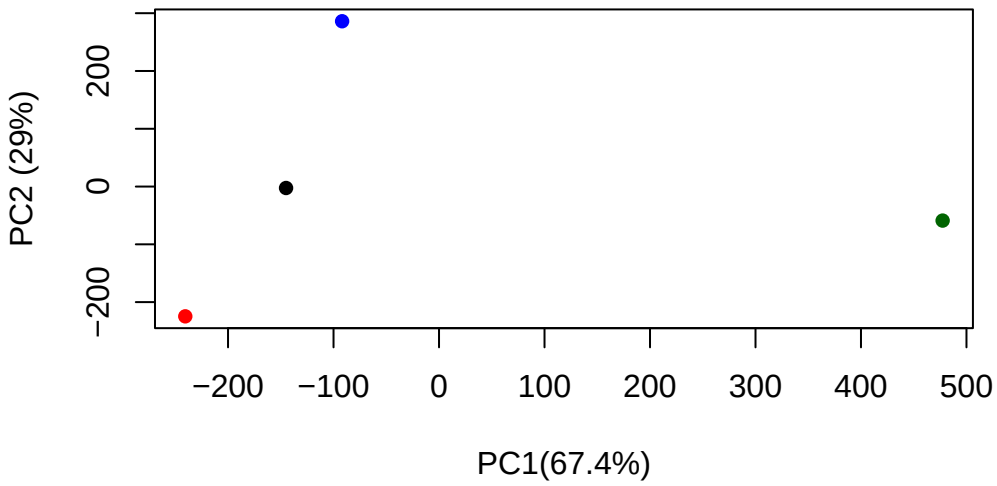
```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x), col = c("gold", "red", "blue", "darkgreen"))
```



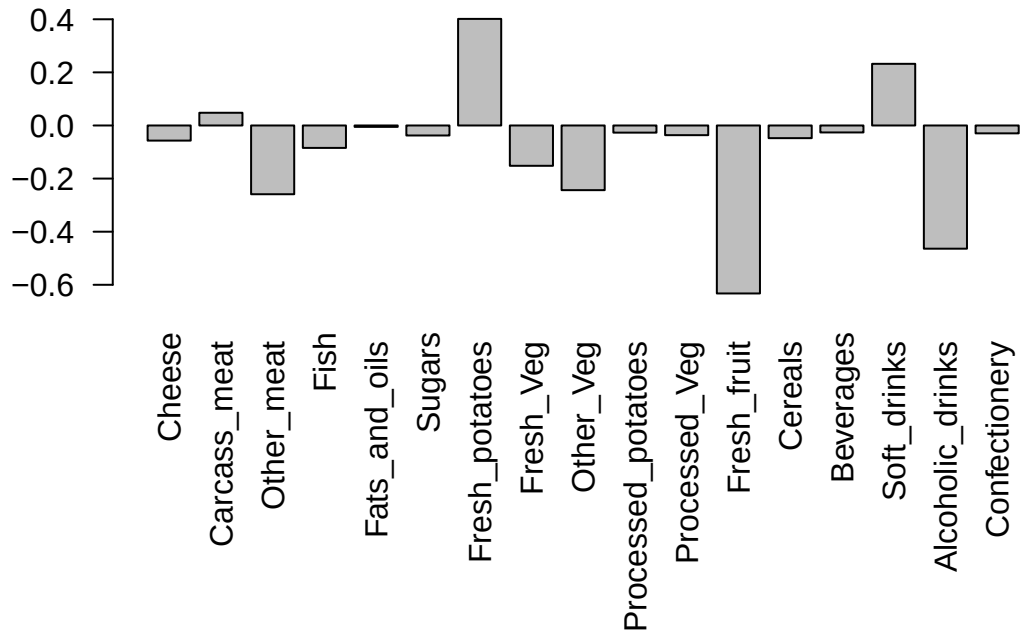

```
pca$x
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -4.894696e-14
Wales     -240.52915 -224.646925 -56.475555  5.700024e-13
Scotland   -91.86934  286.081786 -44.415495 -7.460785e-13
N.Ireland  477.39164  -58.901862  -4.877895  2.321303e-13
```

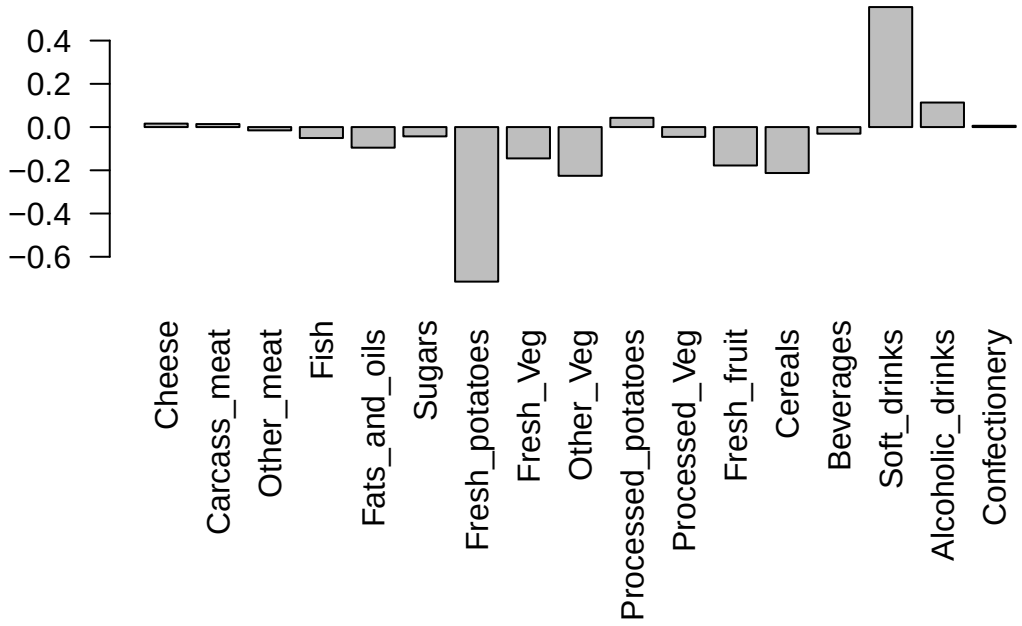
```
plot(pca$x[,1], pca$x[,2],
     col=c('black', "red", "blue", "darkgreen"), pch = 16,
     xlab= "PC1(67.4%)", ylab = "PC2 (29%)")
```




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

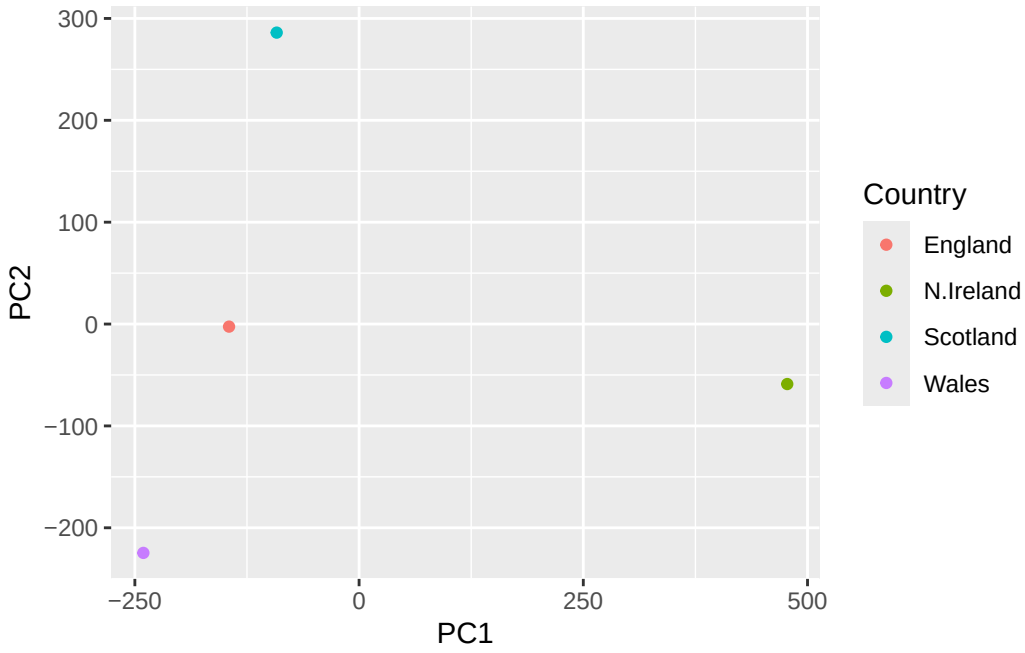


```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```

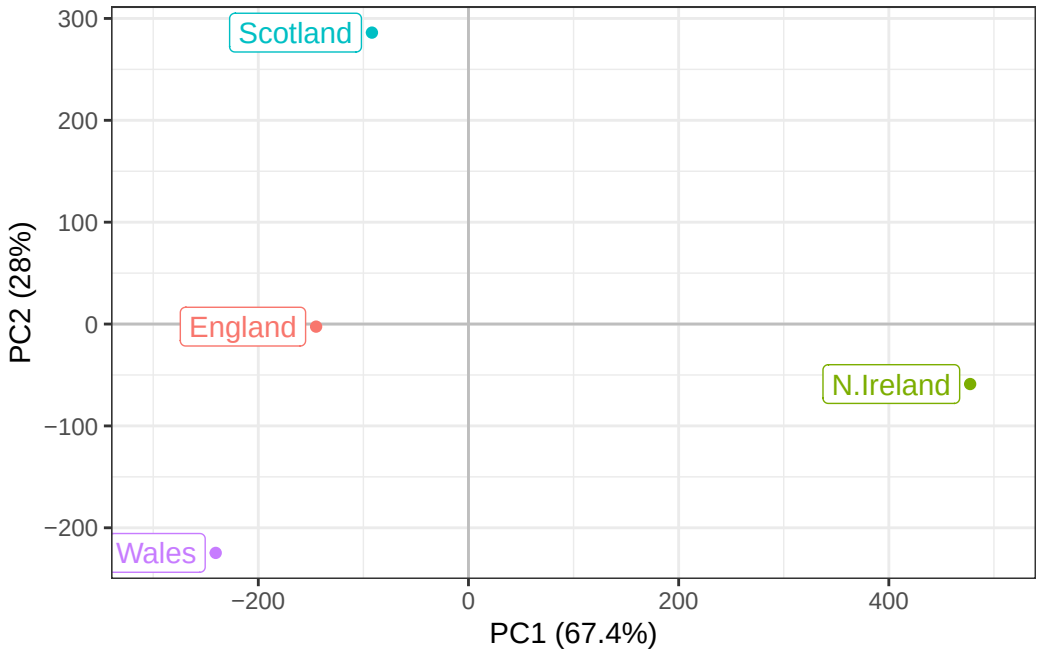


Q9: Generate a similar 'loadings plot' for PC2. What two food groups feature prominantely and what does PC2 maninly tell us about? The two groups that feature prominently in this plot are fresh potatoes and soft drinks. This tells us what food groups account for most of the variance in PC2.

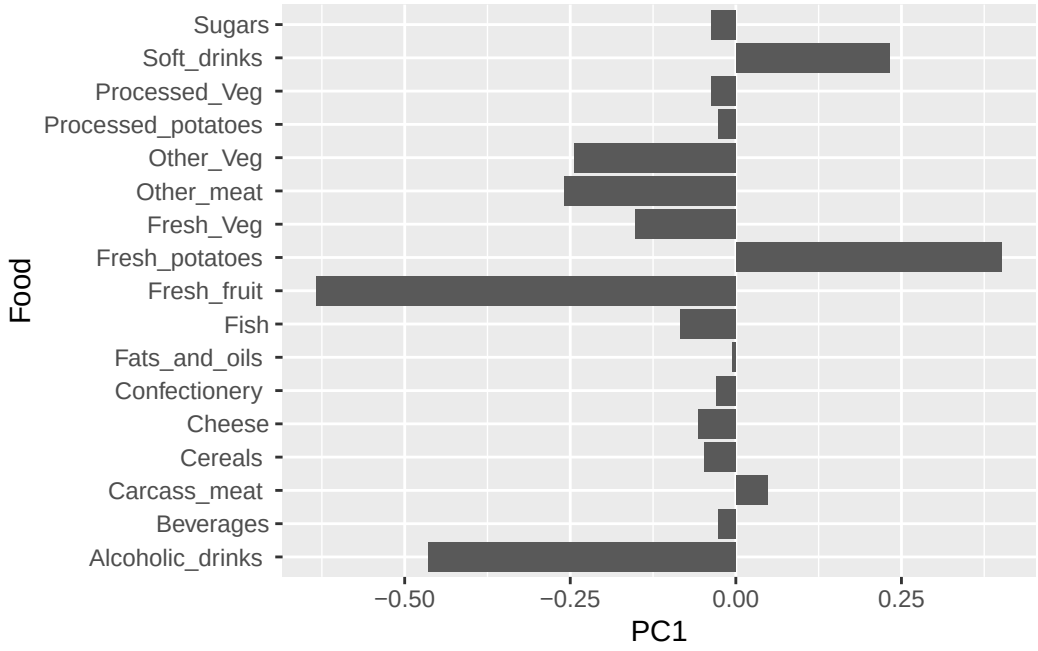
```
library(ggplot2)

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

# Our first basic plot
ggplot(df_lab) +
  aes(PC1, PC2, col=Country) +
  geom_point()
```



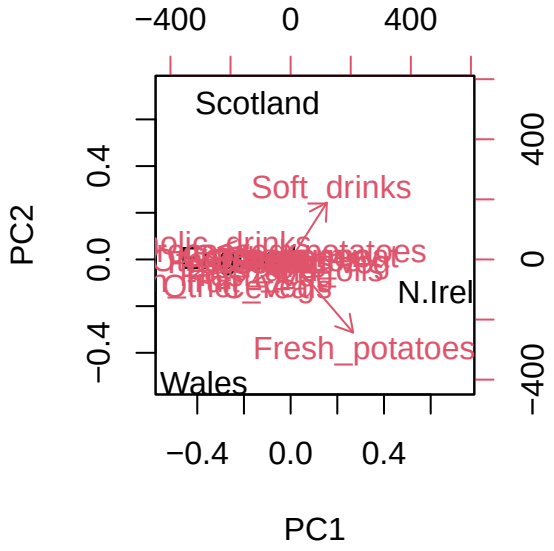

```
ggplot(df_lab) +
  aes(PC1, PC2, col=Country, label=Country) +
  geom_hline(yintercept = 0, col="gray") +
  geom_vline(xintercept = 0, col="gray") +
  geom_point(show.legend = FALSE) +
  geom_label(hjust=1, nudge_x = -10, show.legend = FALSE) +
  expand_limits(x = c(-300,500)) +
  xlab("PC1 (67.4%)")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




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

ggplot(ld_lab) +
  aes(PC1, Food) +
  geom_col()
```


Sugars
Soft_drinks
Processed_Veg
Processed_potatoes
Other_Veg
Other_meat
Fresh_Veg
Fresh_potatoes
Fresh_fruit
Fish
Fats_and_oils
Confectionery
Cheese
Cereals
Carcass_meat
Beverages
Alcoholic_drinks
Food
−0.50
−0.25
0.00
0.25
PC1

```
biplot(pca)
```


−400
0
400
Scotland
Soft_drinks
N.Irel
Fresh_potatoes
Wales
0.4
0.0
−0.4
400
0
−400
−0.4
0.0
0.4
PC2
PC1

```
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
```

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

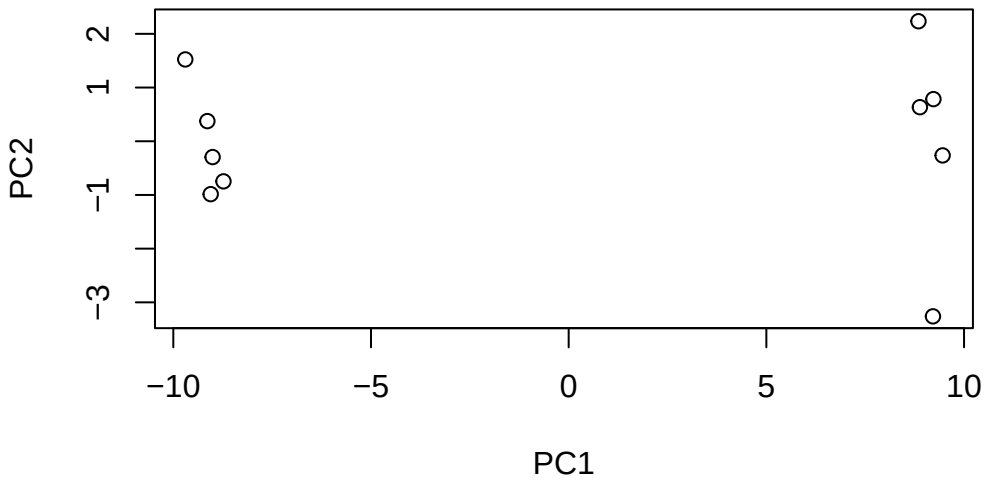
```
[1] 100
```

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

```
[1] 10
```

Q10: How many genes and samples are in this data set? 10 samples and 100 genes

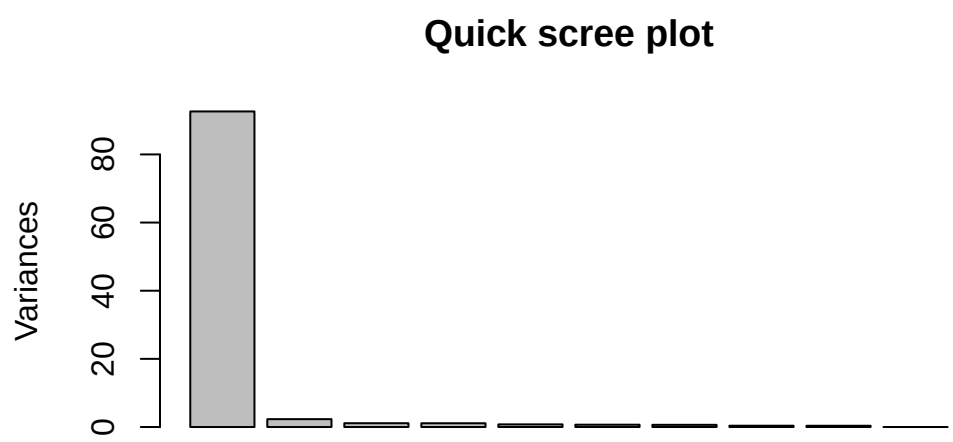
```
pca <- prcomp(t(rna.data), scale=TRUE)
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
```




```
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 3.457e-15
Proportion of Variance 0.00385 0.00364 0.000e+00
Cumulative Proportion  0.99636 1.00000 1.000e+00
```

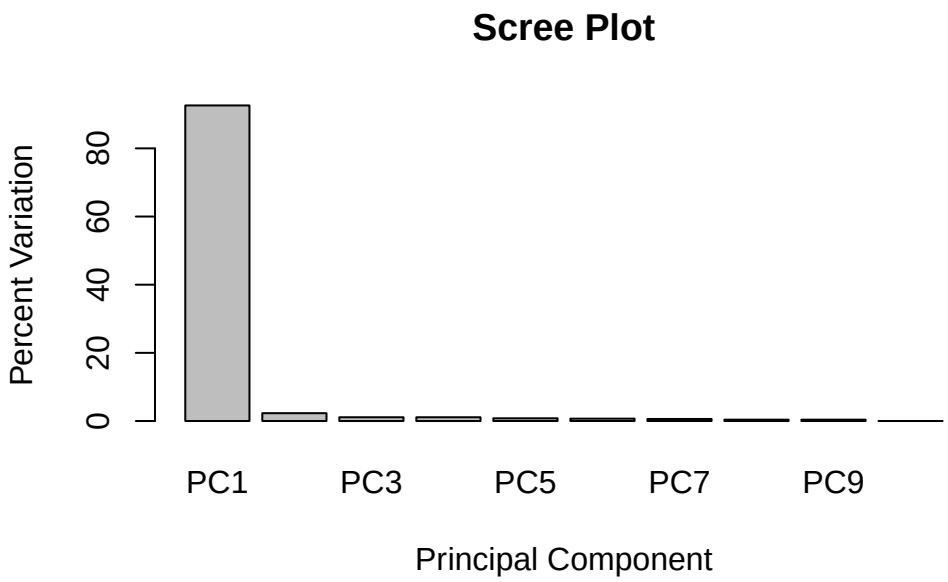
```
plot(pca, main="Quick scree plot")
```



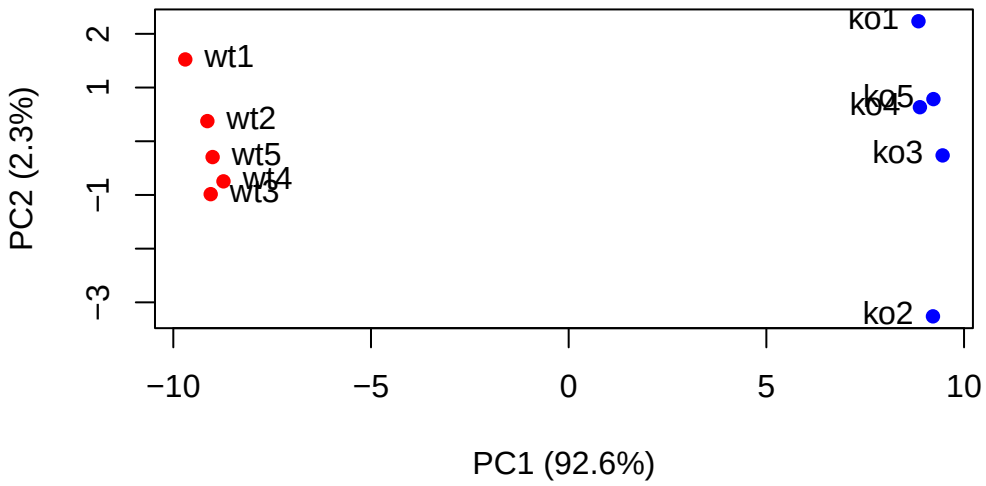

```
## Variance captured per PC
pca.var <- pca$sdev^2

## 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
```

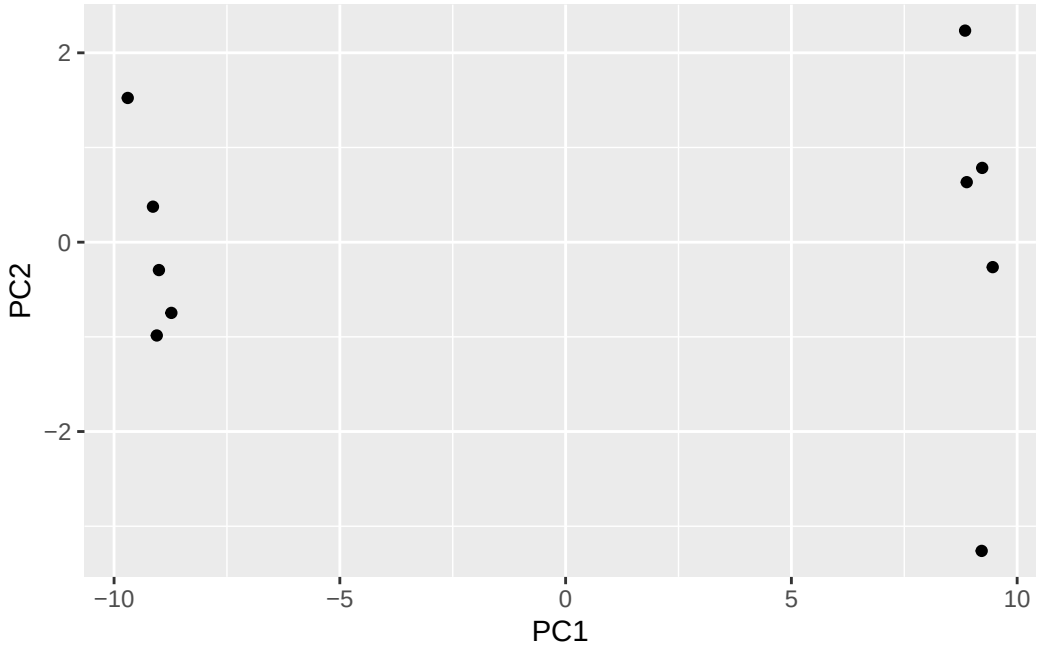
```
barplot(pca.var.per, main="Scree Plot",
        names.arg = paste0("PC", 1:10),
        xlab="Principal Component", ylab="Percent Variation")
```



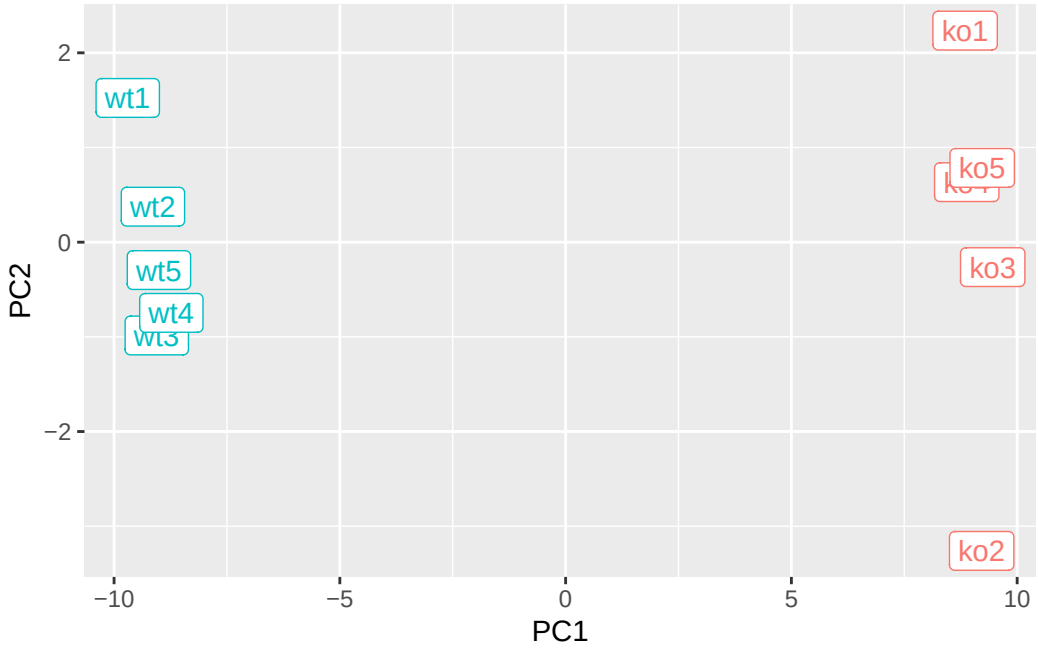

```
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
colvec[grep("ko", colvec)] <- "blue"

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)))
```



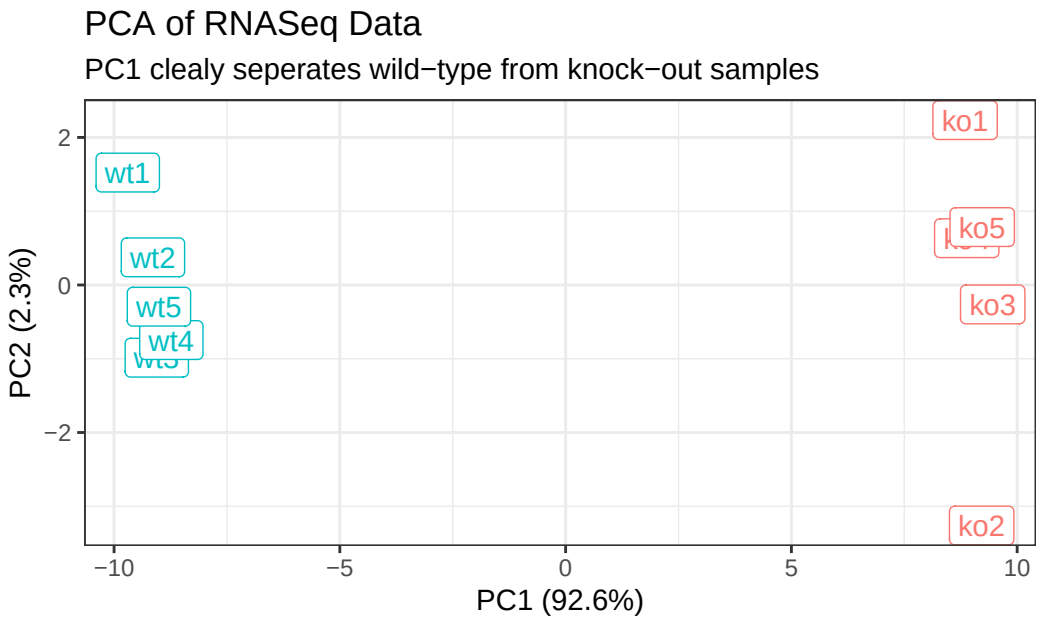

```
library(ggplot2)

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

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




```
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 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()
```




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


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

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

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