Class07 Machine Learning 1

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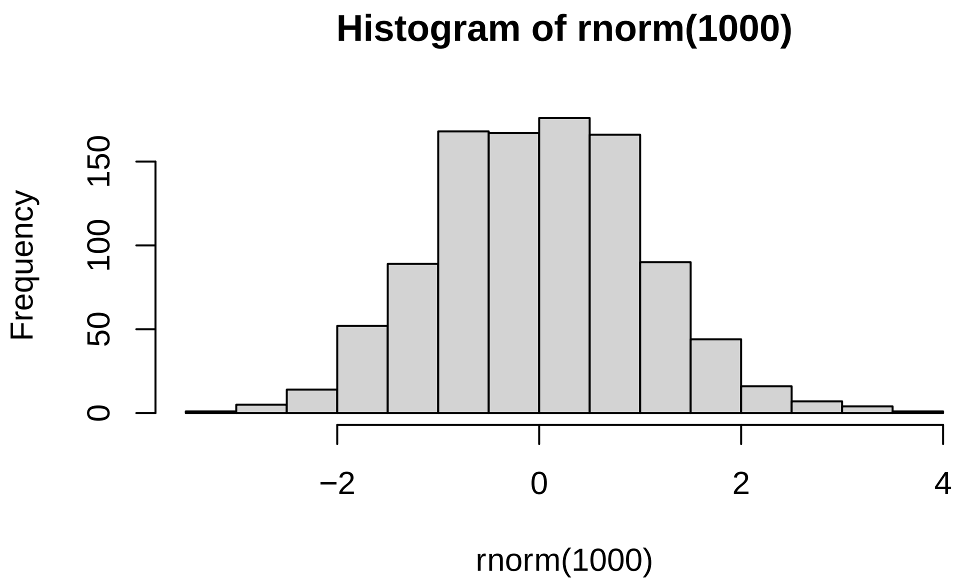
Today we will begin our exploration of some "classical" machine learning approaches. We will start will clustering:

Let's first make up some data to cluster where we know what the answer should be.

```r
hist( rnorm(1000) )
```



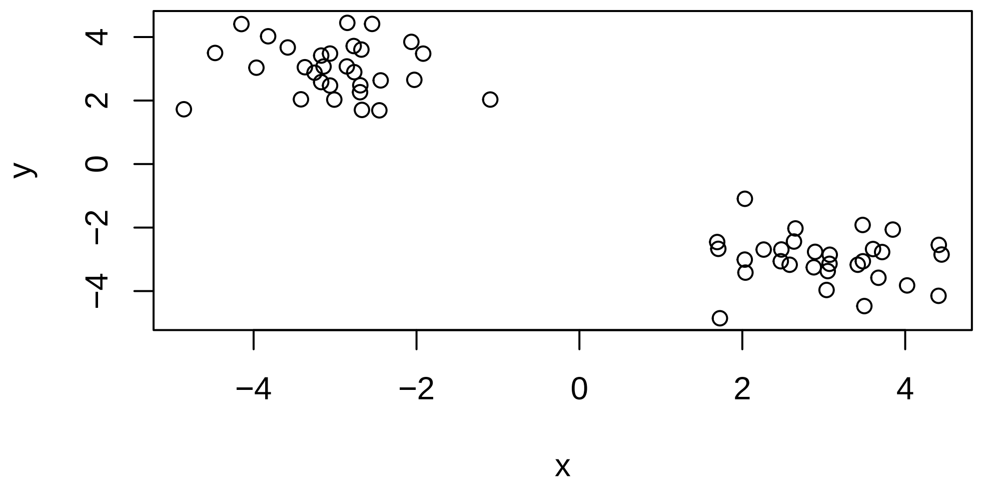
```r
x <- c(rnorm(30,mean=-3), rnorm(30,mean=3))
y <- rev(x)

x <- cbind(x,y)
head(x)
```

```
             x        y
[1,] -2.545408 4.412533
[2,] -3.581017 3.671296
[3,] -2.855466 3.073373
[4,] -3.821666 4.023172
[5,] -3.418836 2.038392
[6,] -2.764325 2.893790
```

plot x

```r
plot(x)
```



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

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

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

Cluster means:
          x         y
1 -3.000652  3.010232
2  3.010232 -3.000652

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] 36.76886 36.76886
 (between_SS / total_SS =  93.6 %)

Available components:

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

> Q. How big are the clusters (i.e. their size)?

```r
k$size
```

```
[1] 30 30
```

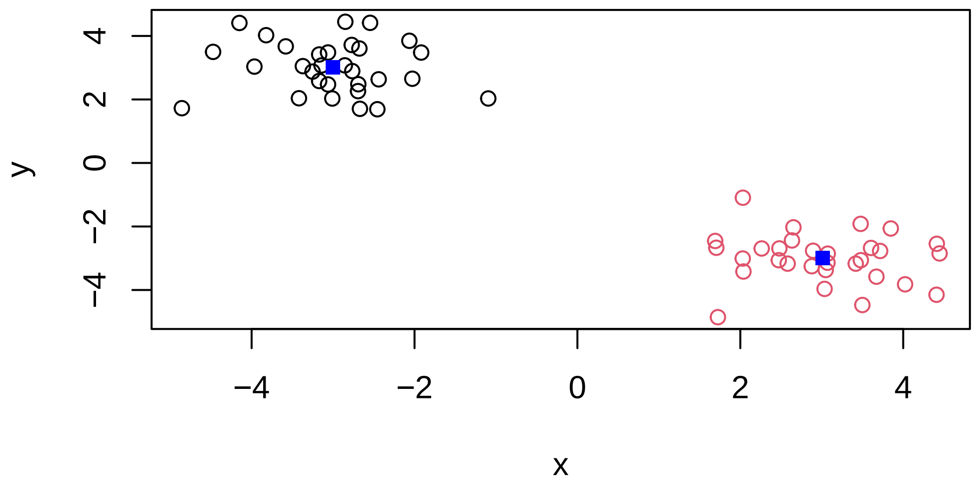
> Q. What clusters do my data points reside in?

```r
k$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
```

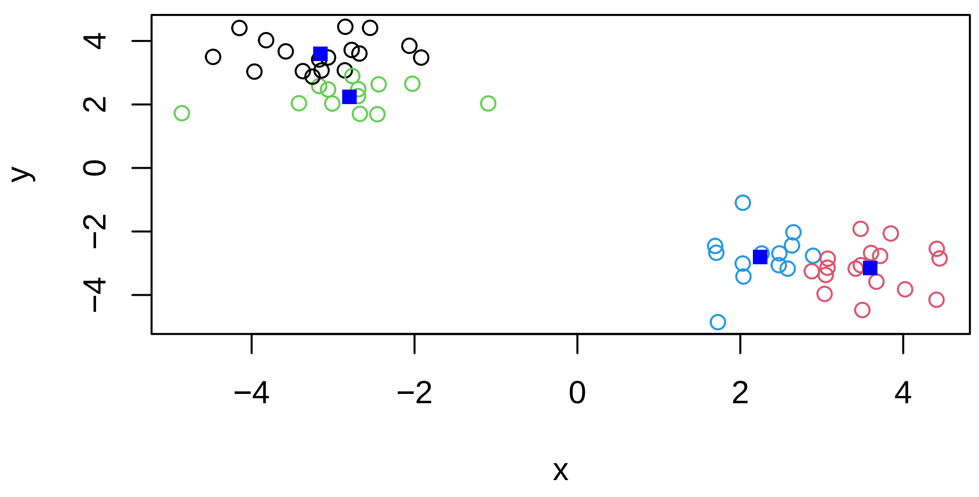
> Q. Make a plot of our data colored by cluster assignment(i.e. make a result figure)

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



Q. Cluster with k-means into 4 clustrs and plot your results as above.

```
k4 <- kmeans(x, centers=4)
plot(x,col=k4$cluster)
points(k4$centers,col="blue",pch=15)
```



Q. Run kmeans with center (i.e. values of k) equal 1 to 6

```
k1 <- kmeans(x, centers=1)$tot.withinss
k2 <- kmeans(x, centers=2)$tot.withinss
k3 <- kmeans(x, centers=3)$tot.withinss
k4 <- kmeans(x, centers=4)$tot.withinss
k5 <- kmeans(x, centers=5)$tot.withinss
k6 <- kmeans(x, centers=6)$tot.withinss

ans <- c(k1,k2,k3,k4,k5,k6)
```

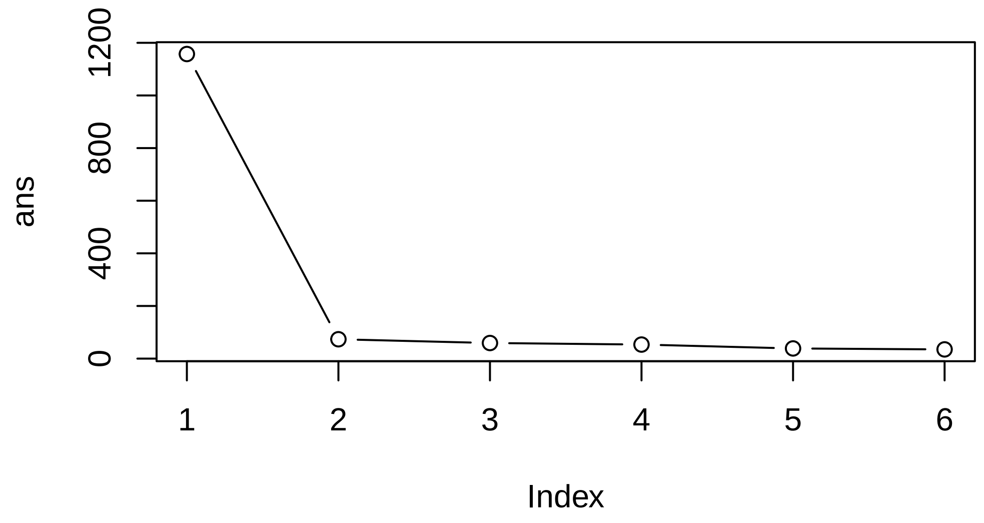
Or use a `for` loop

```
ans <- NULL
for(i in 1:6){
  km <- kmeans(x, centers=i)
  ans[i] <- km$tot.withinss
}
ans
```

```
[1] 1157.45952   73.53773   59.17998   53.34115   38.60985   34.91535
```

Make a "screen-plot"

```r
plot(ans,typ="b")
```



Hierarchical Clustering

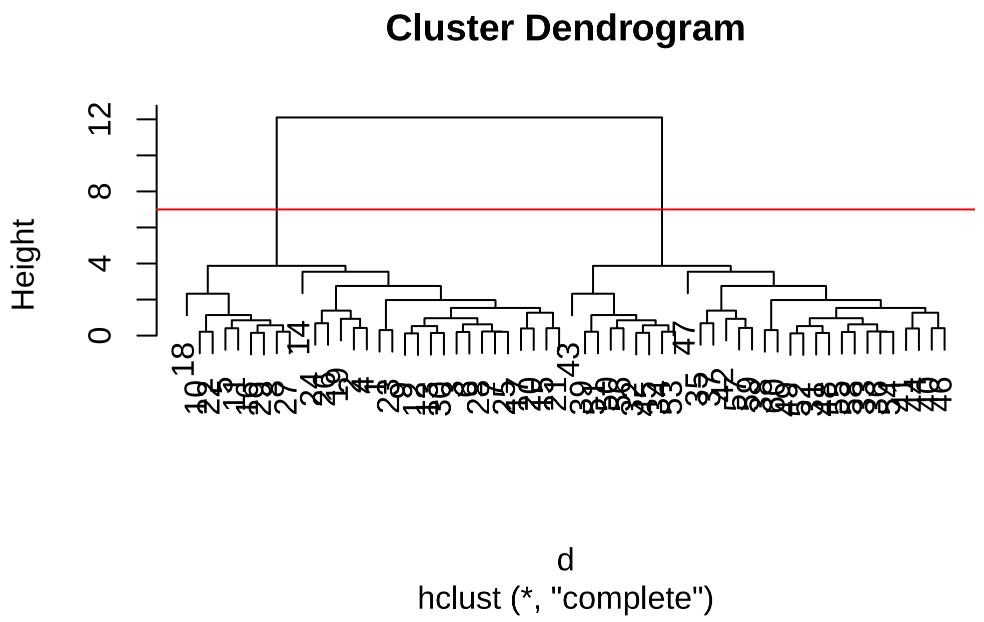
The main function in "base" R for this is called `hclust()`.

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

```
Call:
hclust(d = d)

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

```
plot(hc)
abline(h=7,col="red")
```

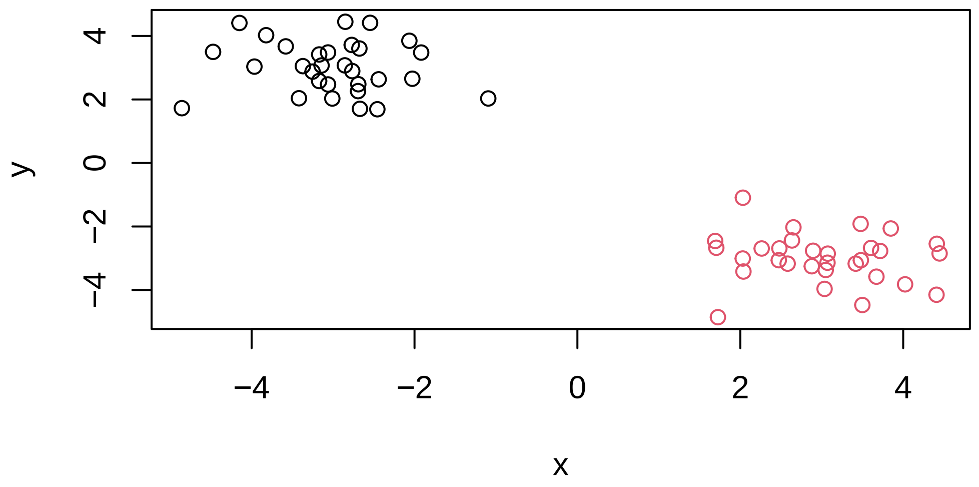


To obtain clusters from our `hclust` result object **hc**, we cut the tree to yield different sub branches For this we use the `cutree()` function.

```
grps <- cutree(hc,h=7)
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 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
```

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



PCA

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

Q1. 17 rows and 5 column dim(x)

Q2. I like the first approach as the code feels more straight-forward to me. Running it more than one time could remove the informatin we want.

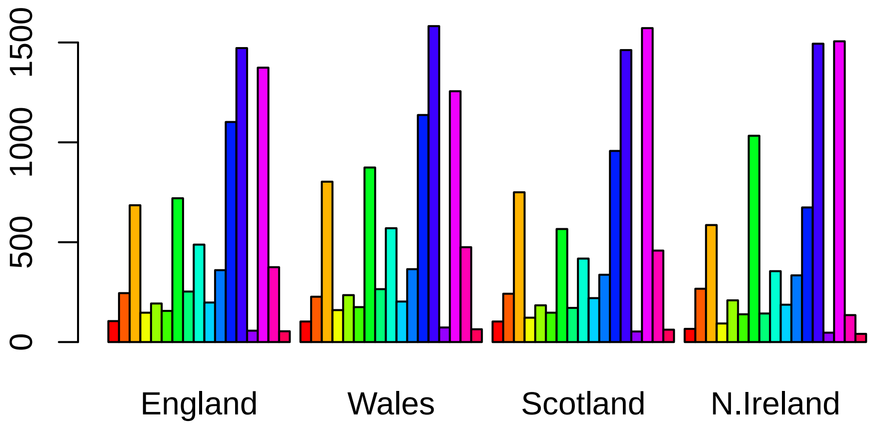
Q3. beside = FALSE

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

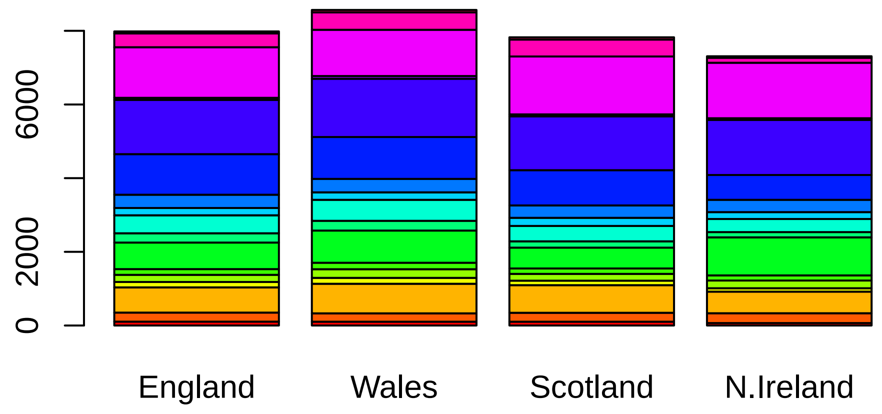
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
```

```
Fats_and_oils       193   235       184        209
Sugars              156   175       147        139
```

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

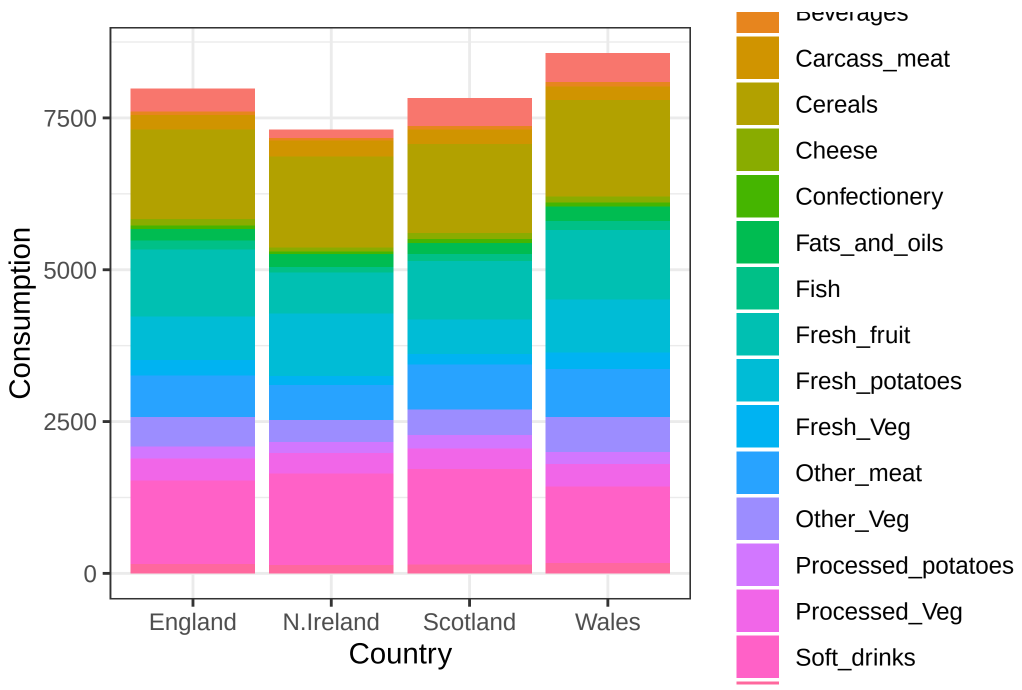


```
barplot(as.matrix(x), beside=FALSE, col=rainbow(nrow(x)))
```



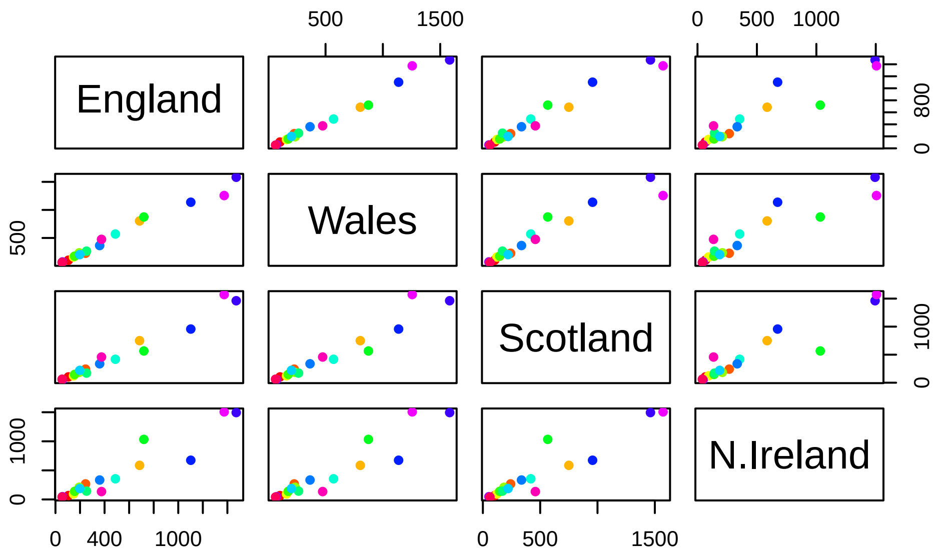
Q4. Delete the position = “dodge” argument

```
library(tidyr)
library(ggplot2)
x_long <- x |>
          tibble::rownames_to_column("Food") |>
          pivot_longer(cols = -Food,
                       names_to = "Country",
                       values_to = "Consumption")
ggplot(x_long) +
  aes(x = Country, y = Consumption, fill = Food) +
  geom_col() +
  theme_bw()
```

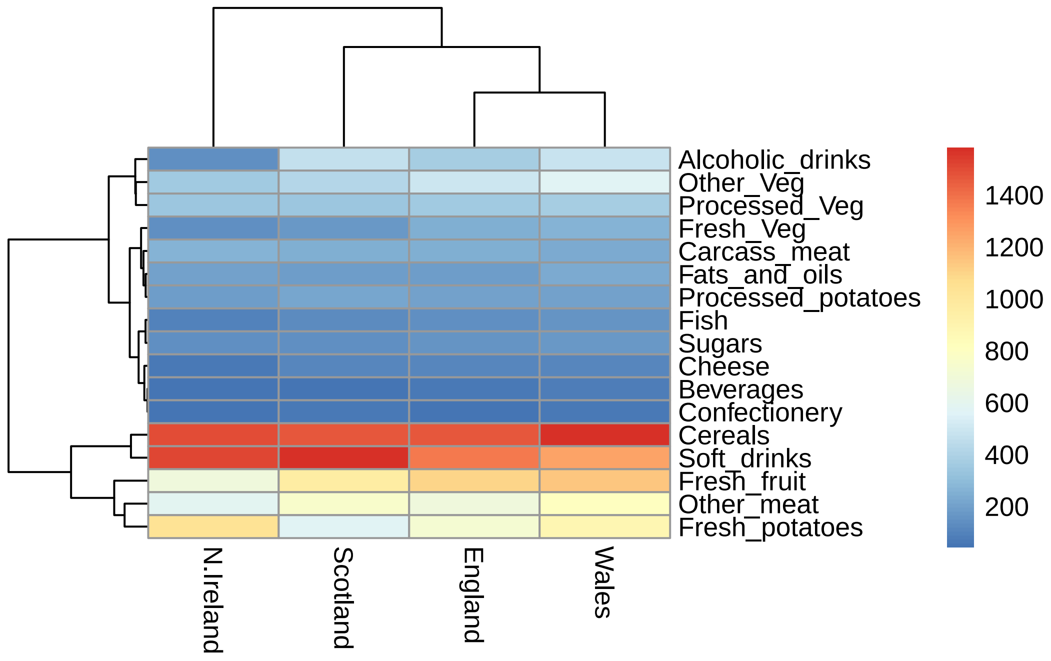


Q5. Plots above and below each diagonal countries are replicates. Each plot represents compairson between the two countries vertical to the plot. Each dot represents a food item. The position of the dot represents the consumption amount in each country. The dot would be on the diagonal of the plot if two countries consum about the same amount of that particular food.

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



```r
library(pheatmap)
pheatmap( as.matrix(x) )
```



Q6. Scotland, England, and Wales are clustered together in contrast to N.Ireland. This result indicates that N.Ireland has a different food consumption pattern than the other three countries. Main differences are a little hard to spot since the color is not that different.

PCA to the rescue

The main function in "base" R for PCA is called `prcomp()`.

As we want to do a PCA on the food data for the different countries, we will want the foods in the columns.

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

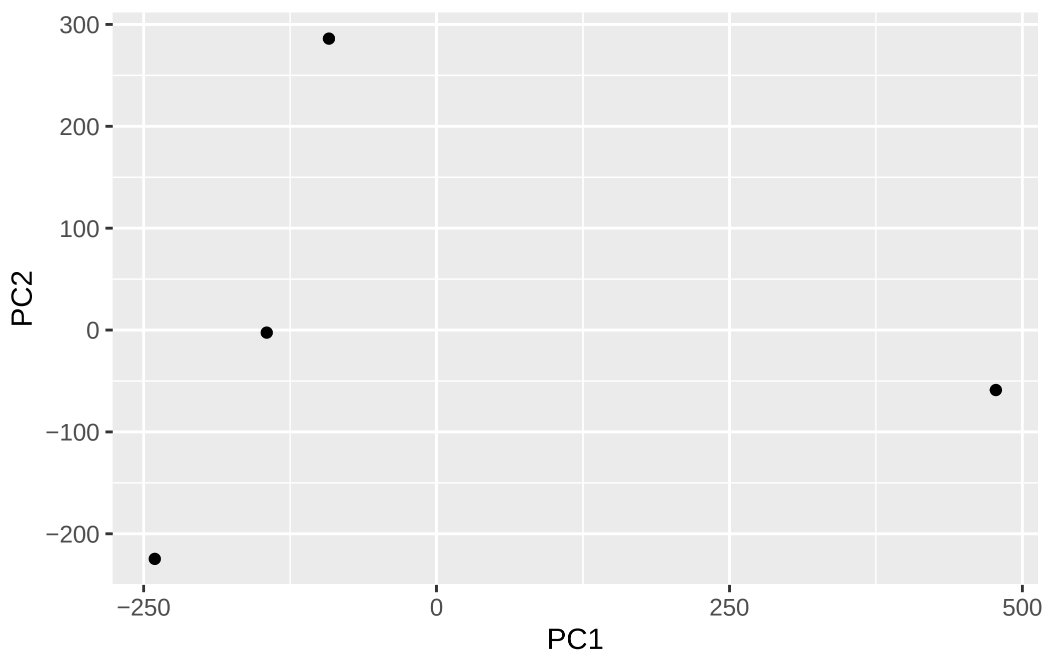
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 2.921e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

Our result object is called `PCA` and it has a `$x` component that we will look at first.

```
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
```

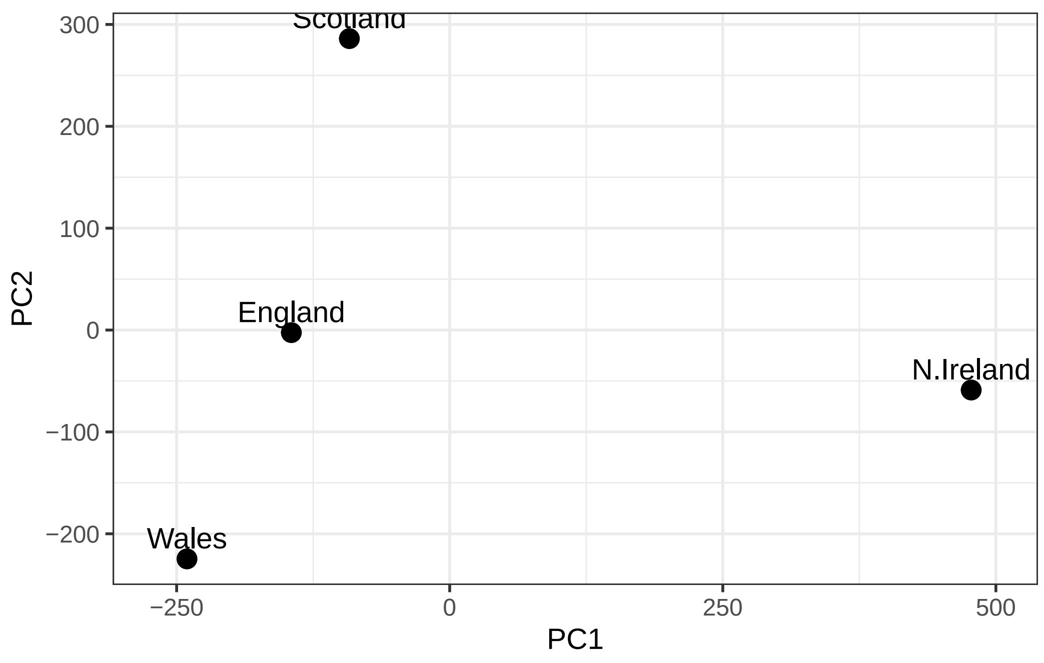
```
ggplot(PCA$x) + aes(PC1,PC2) + geom_point()
```



Q7. The finished code is below.

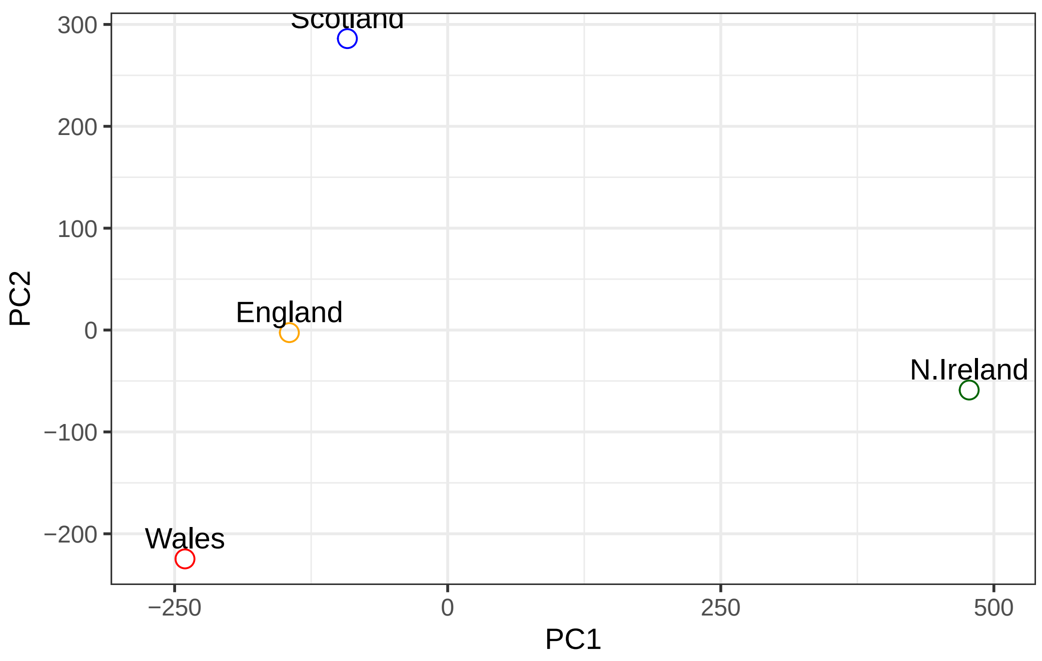
```
# Create a data frame for plotting
df <- as.data.frame(PCA$x)
df$Country <- rownames(df)

# Plot PC1 vs PC2 with ggplot
ggplot(PCA$x) +
  aes(x = PC1, y = PC2, label = rownames(PCA$x)) +
  geom_point(size = 3) +
  geom_text(vjust = -0.5) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



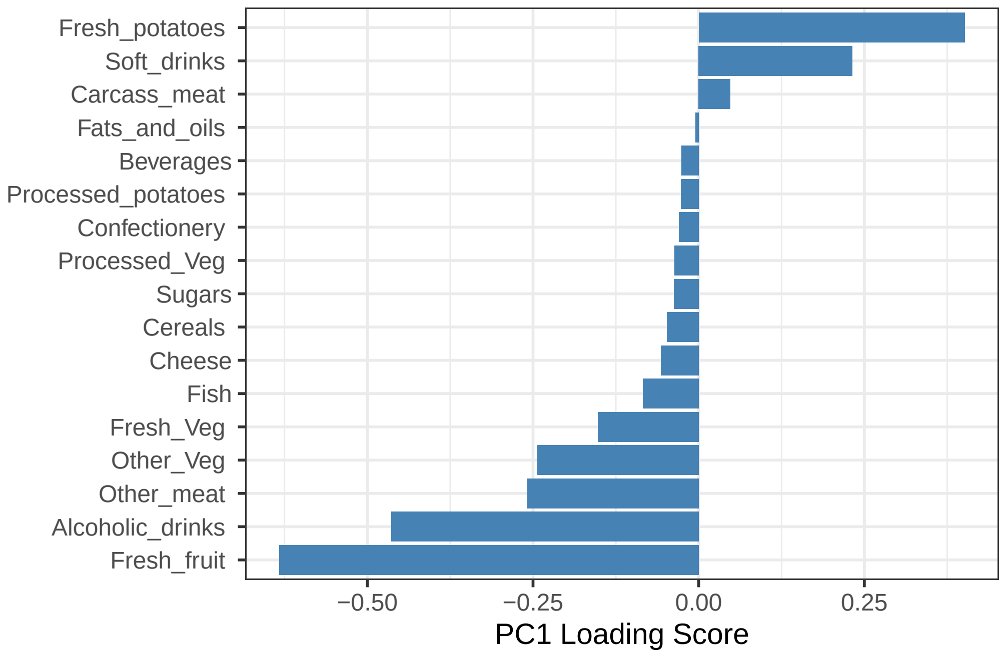
Q8.

```
ggplot(PCA$x) +
  aes(x = PC1, y = PC2, label = rownames(PCA$x)) +
  geom_point(size = 3,color=c('orange', 'red', 'blue', 'darkgreen'), pch = 1) +
  geom_text(vjust = -0.5) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



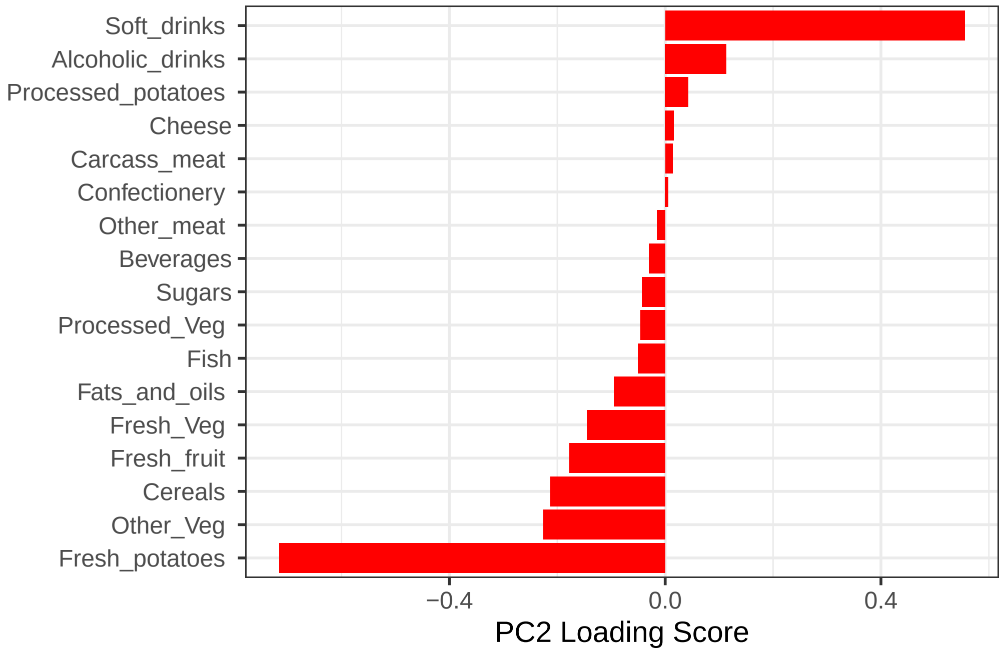
Another major result out of PCA is the so-called "variable loadings" or `$rotation` that tells us how the original variables (foods) contribute to PCs.

```
ggplot(PCA$rotation) +
  aes(x = PC1,
      y = reorder(rownames(PCA$rotation), PC1)) +
  geom_col(fill = "steelblue") +
  xlab("PC1 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```



Q9. Soft drinks and alcoholic drinks feature prominently in PC2. PC2 mainly tells us that consumption of soft and alcoholic drinks separates Scotland from the cluster that contains the rest of three countries.

```
ggplot(PCA$rotation) +
  aes(x = PC2,
      y = reorder(rownames(PCA$rotation), PC2)) +
  geom_col(fill = "red") +
  xlab("PC2 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```



RNA-seq data exploration

Q10. 100 genes and 10 samples

```
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
```

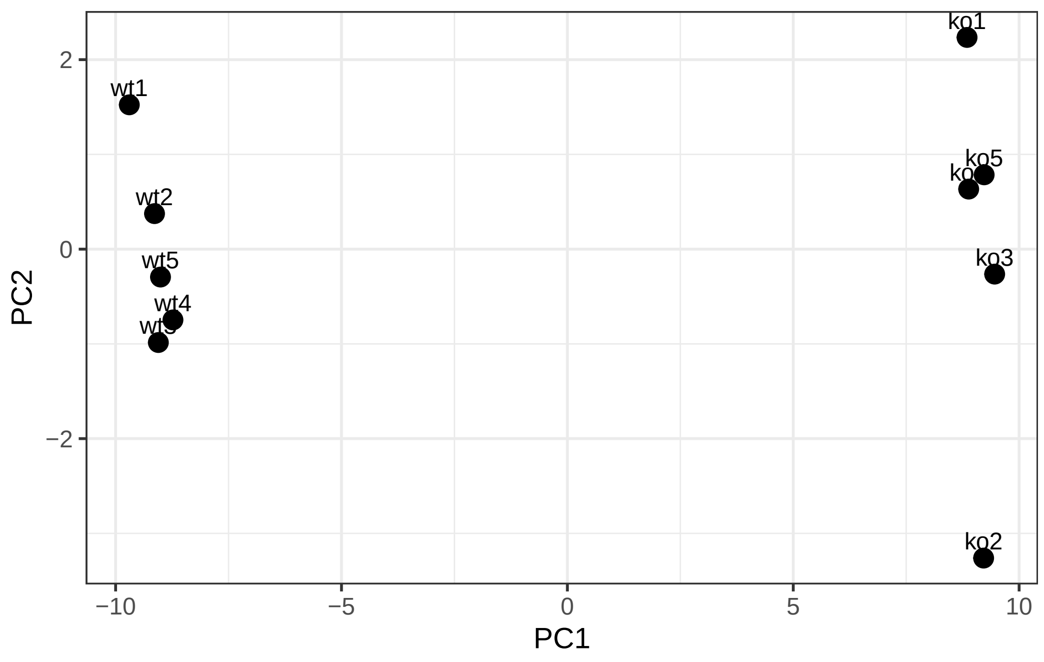
```
dim(rna.data)
```

```
[1] 100  10
```

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

# Create data frame for plotting
df <- as.data.frame(pca$x)
df$Sample <- rownames(df)

## Plot with ggplot
ggplot(df) +
  aes(x = PC1, y = PC2, label = Sample) +
  geom_point(size = 3) +
  geom_text(vjust = -0.5, size = 3) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



```r
summary(pca)
```

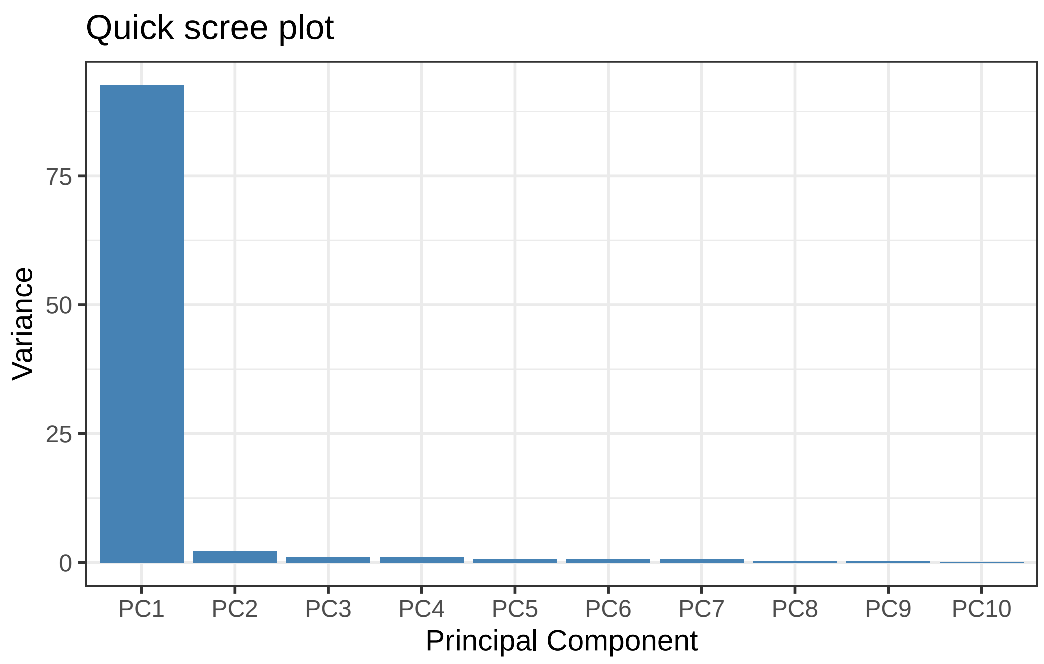
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     9.6237 1.5198 1.05787 1.05203 0.88062 0.82545 0.80111
Proportion of Variance 0.9262 0.0231 0.01119 0.01107 0.00775 0.00681 0.00642
```

```
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 3.3e-15
Proportion of Variance 0.00385 0.00364 0.0e+00
Cumulative Proportion  0.99636 1.00000 1.0e+00
```

```r
# Calculate variance explained
pca.var <- pca$sdev^2
pca.var.per <- round(pca.var/sum(pca.var)*100, 1)

# Create scree plot data
scree_df <- data.frame(
  PC = factor(paste0("PC", 1:10), levels = paste0("PC", 1:10)),
  Variance = pca.var[1:10]
)

ggplot(scree_df) +
  aes(x = PC, y = Variance) +
  geom_col(fill = "steelblue") +
  ggtitle("Quick scree plot") +
  xlab("Principal Component") +
  ylab("Variance") +
  theme_bw()
```

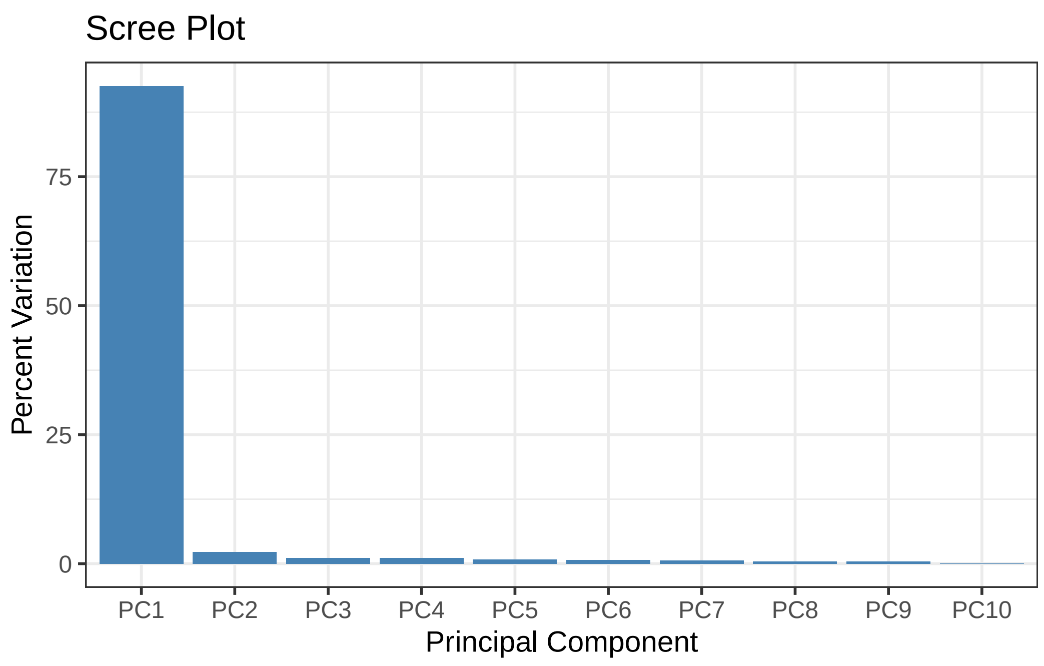


```
pca.var.per
```

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

```
# Create percent variance scree plot
scree_pct_df <- data.frame(
  PC = factor(paste0("PC", 1:10), levels = paste0("PC", 1:10)),
  PercentVariation = pca.var.per[1:10]
)

ggplot(scree_pct_df) +
  aes(x = PC, y = PercentVariation) +
  geom_col(fill = "steelblue") +
  ggtitle("Scree Plot") +
  xlab("Principal Component") +
  ylab("Percent Variation") +
  theme_bw()
```

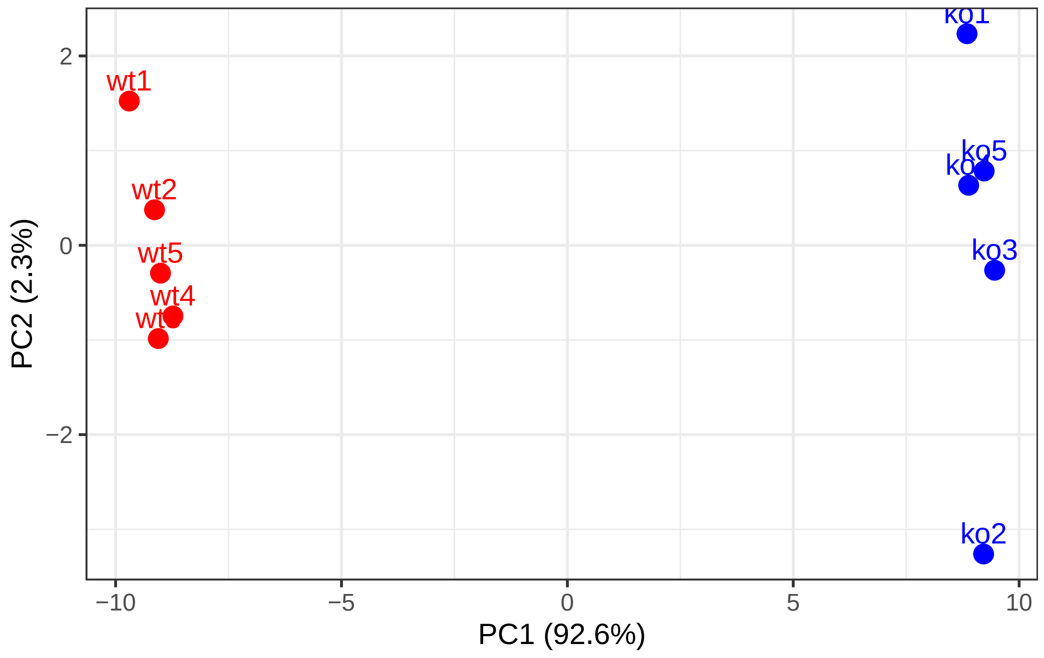


```
## A vector of colors for wt and ko samples
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
```

```
colvec[grep("ko", colvec)] <- "blue"

# Add condition to data frame
df$condition <- substr(df$Sample, 1, 2)
df$color <- colvec

ggplot(df) +
  aes(x = PC1, y = PC2, color = color, label = Sample) +
  geom_point(size = 3) +
  geom_text(vjust = -0.5, hjust = 0.5, show.legend = FALSE) +
  scale_color_identity() +
  xlab(paste0("PC1 (", pca.var.per[1], "%)")) +
  ylab(paste0("PC2 (", pca.var.per[2], "%)")) +
  theme_bw()
```



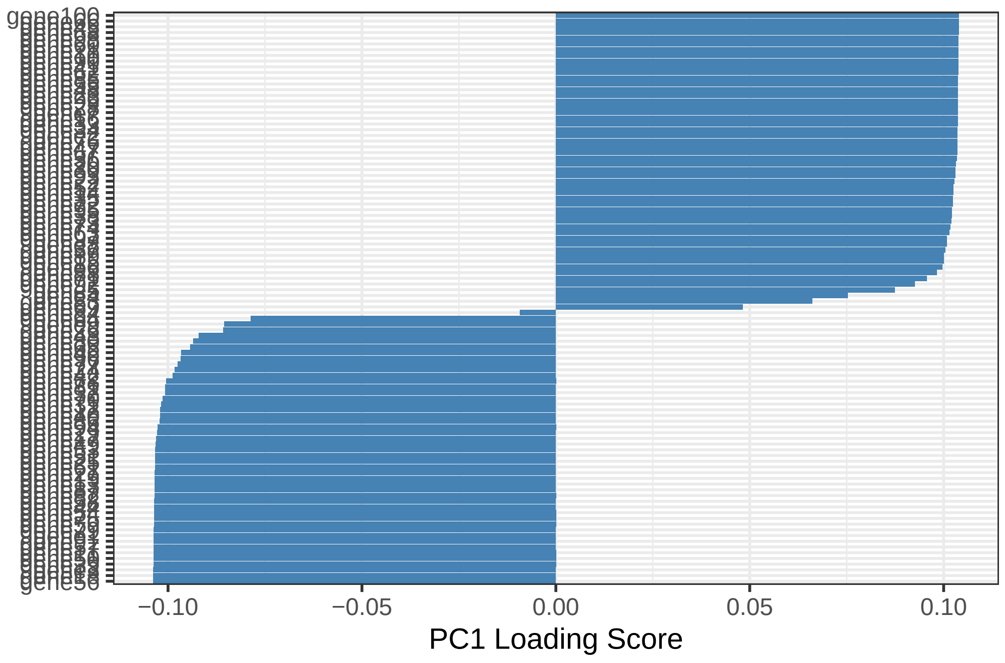
```
loading_scores <- pca$rotation[,1]

## 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"
```

```
ggplot(pca$rotation) +
  aes(x = PC1,
      y = reorder(rownames(pca$rotation), PC1)) +
  geom_col(fill = "steelblue") +
  xlab("PC1 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```


gene100
gene50
PC1 Loading Score