Class07: Machine Learning

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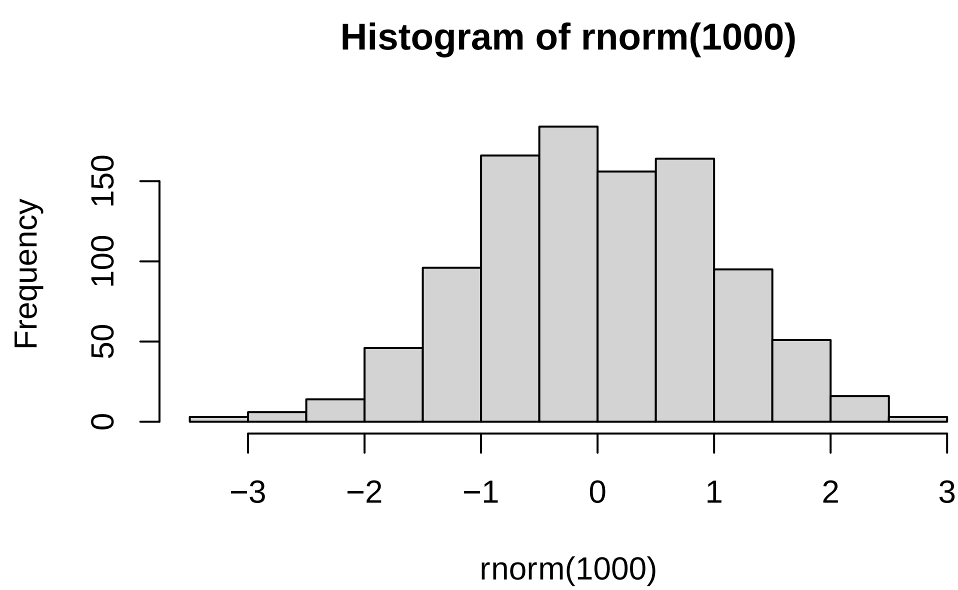
Today we will begin our exploration of some "classical" machine learning approaches. We will start with clustering:

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

There is only 1 required function with rnorm, "n"

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



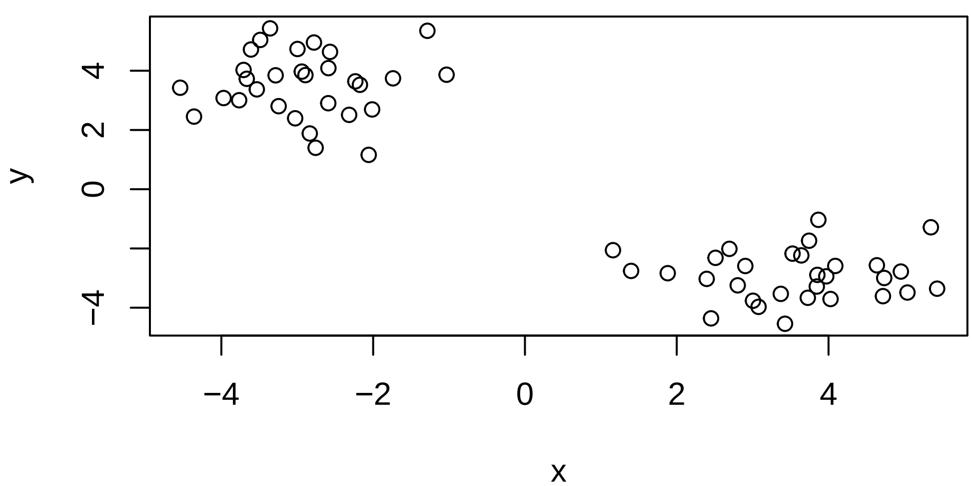
can merge these two norms together by turning them into a vector with c

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

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

```
             x        y
[1,] -2.997025 4.733777
[2,] -3.665120 3.726878
[3,] -2.316501 2.511003
[4,] -2.780075 4.952861
[5,] -2.013186 2.693706
[6,] -2.892175 3.852565
```

A peak at x with `plot()`

```r
plot(x)
```



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

```
k <- kmeans(x, centers = 4)
```

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

```
k$size
```

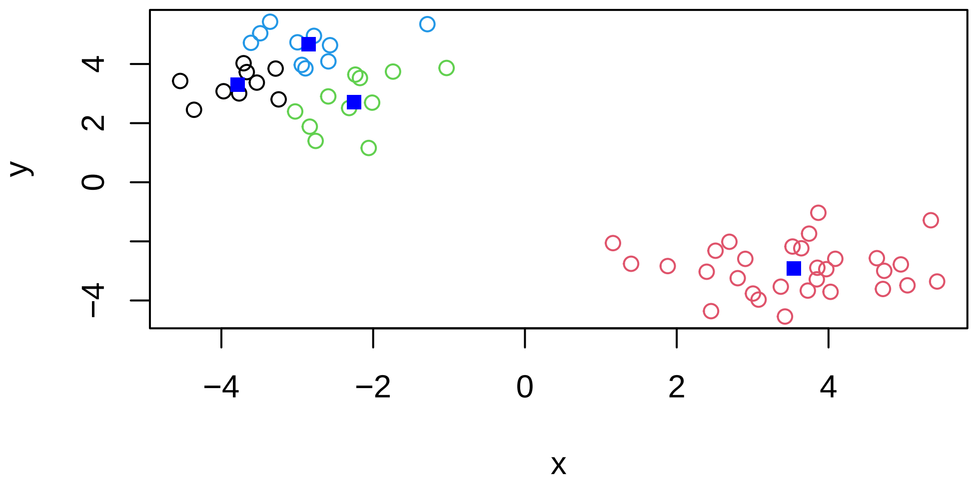
```
[1]  9 30 11 10
```

Q. What clusters do my data points reside in?

```
g <- k$cluster
```

Q. Can you make a plot of our data colored by cluster assignment - i.e. Make a result figure

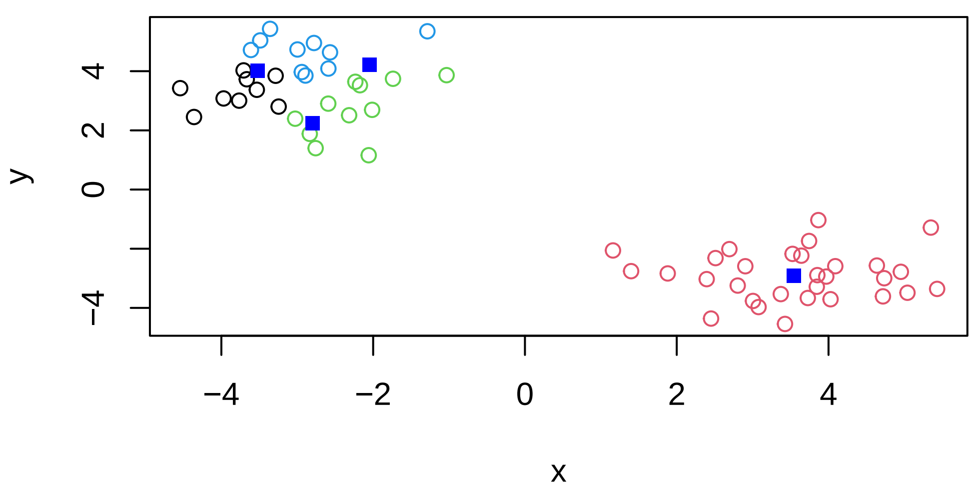
```
plot(x, col = c(g))
points(k$centers, col = "blue", pch = 15)
```



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

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

```
Warning in plot.xy(xy.coords(x, y), type = type, ...): "centers" is not a
graphical parameter
```



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

```r
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
k7 <- kmeans(x, centers = 7)$tot.withinss

c(k1, k2, k3, k4, k5, k6, k7)
```

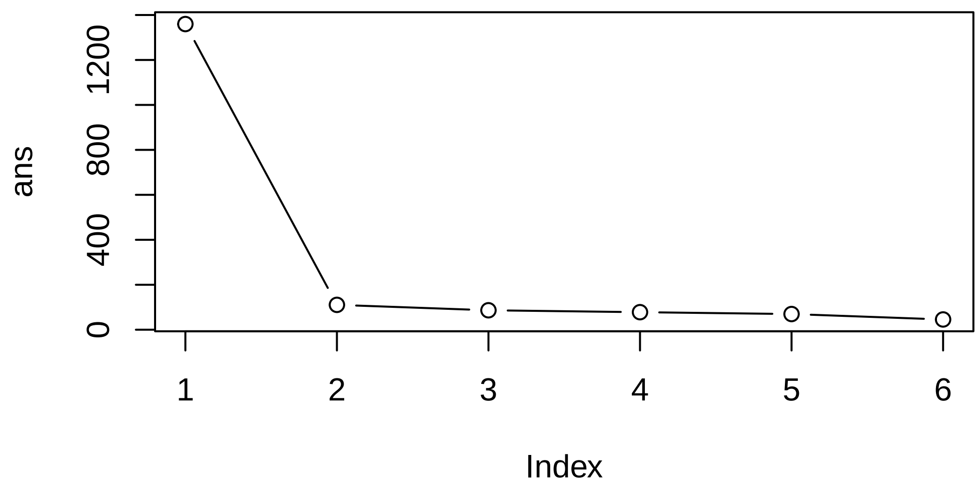
```
[1] 1359.75478  110.55026   86.41849   77.69505   70.23907   41.71409   42.39638
```

Or use a for loop

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

```
[1] 1359.75478  110.55026   86.41849   77.96975   69.68321   45.55144
```

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



##Hierarchical Clustering

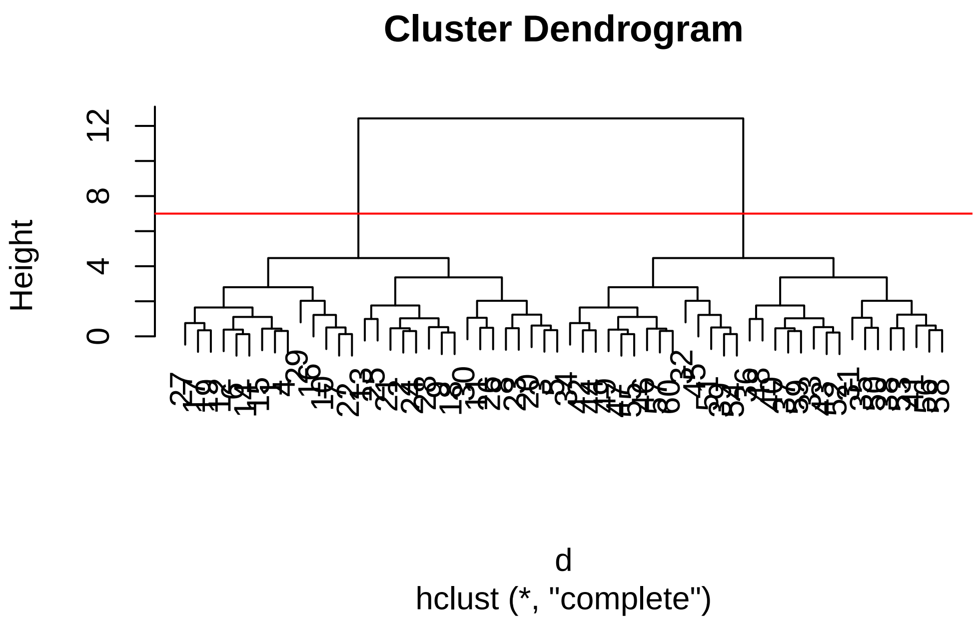
The main function in "base" R for this is called `hclust()`

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

```
Call:
```

```
hclust(d = d)

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

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



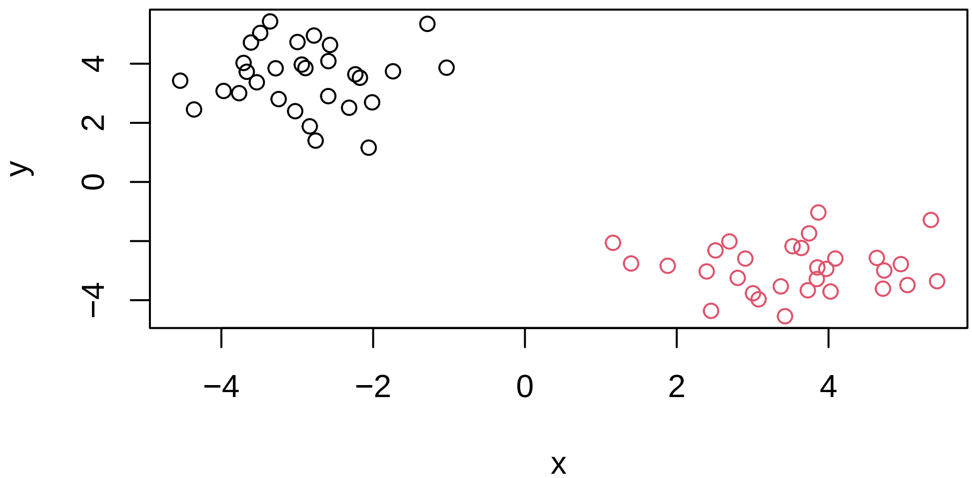
To obtain clusters from our `hclust` result object **hc** we "cut" the tree to yield different sub branches. For this use the `cutree()` function

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

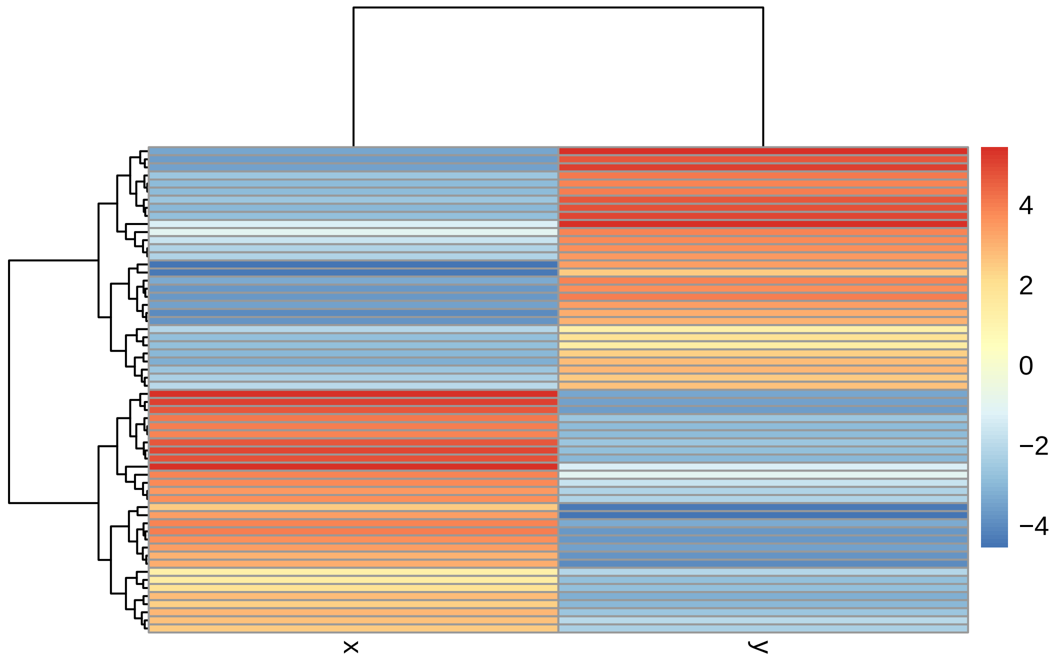
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

Results figure

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




```r
library(pheatmap)
pheatmap(x)
```



##Principal Component Analysis (PCA)

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

```
[1] 17
```

```
ncol(x)
```

```
[1] 5
```

> 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 5 columns in this data frame. I used nrow() and ncol()

```
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
```

```
# 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
```

```
dim(x)
```

```
[1] 17  4
```

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

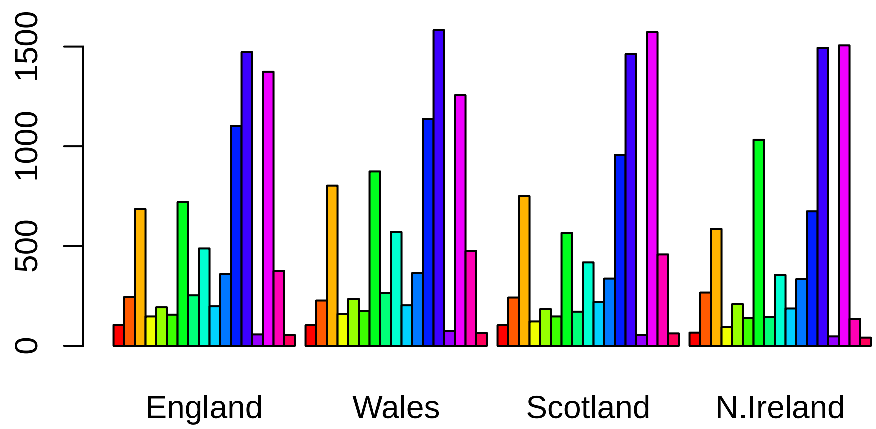
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
Fats_and_oils      193   235      184       209
Sugars  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

The second method shown above is more robust. Each time you run the code for the first method, a column gets subtracted, which is not ideal.

###Spotting major differences and trends

```r
# Using base R
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?

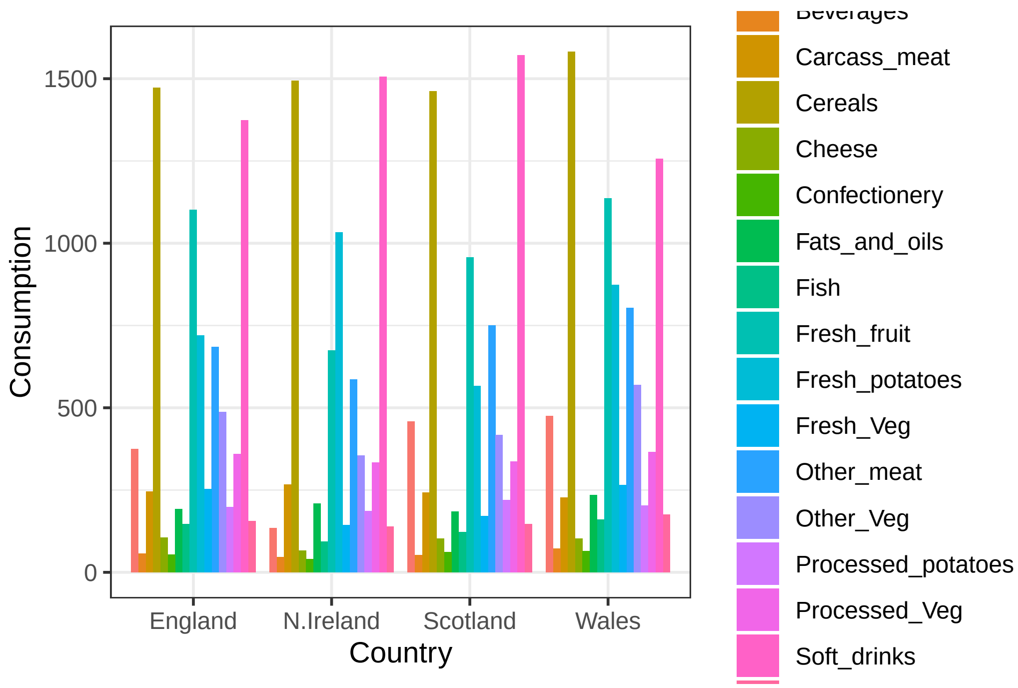
Changing the beside argument to false or taking it away will result in the different plot.

```r
library(tidyr)
x_long <- x |>
          tibble::rownames_to_column("Food") |>
          pivot_longer(cols = -Food,
                       names_to = "Country",
                       values_to = "Consumption")

dim(x_long)
```

```
[1] 68  3
```

```r
library(ggplot2)
ggplot(x_long) +
  aes(x = Country, y = Consumption, fill = Food) +
```

```r
  geom_col(position = "dodge") +
  theme_bw()
```



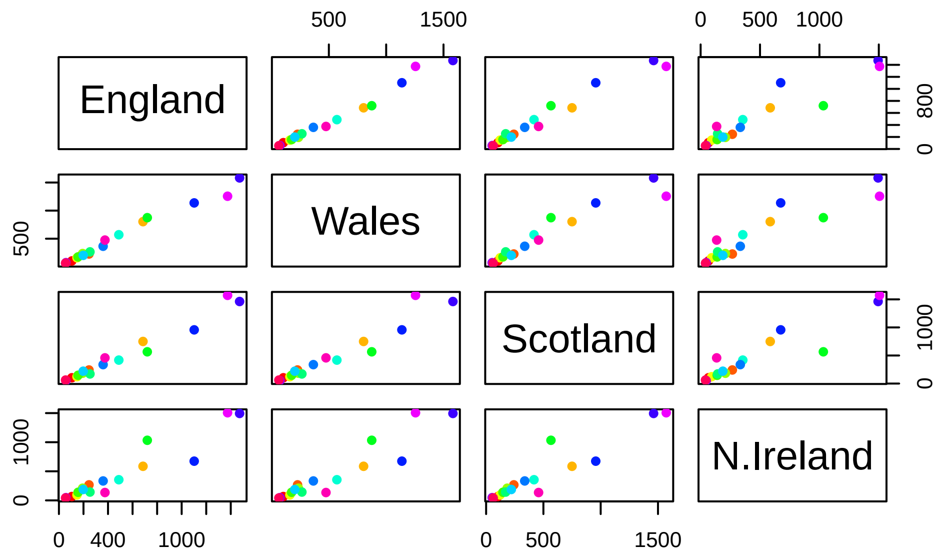
> Q4: Changing what optional argument in the above ggplot() code results in a stacked barplot figure?

Deleting the position = "dodge" argument results in a stacked barplot.

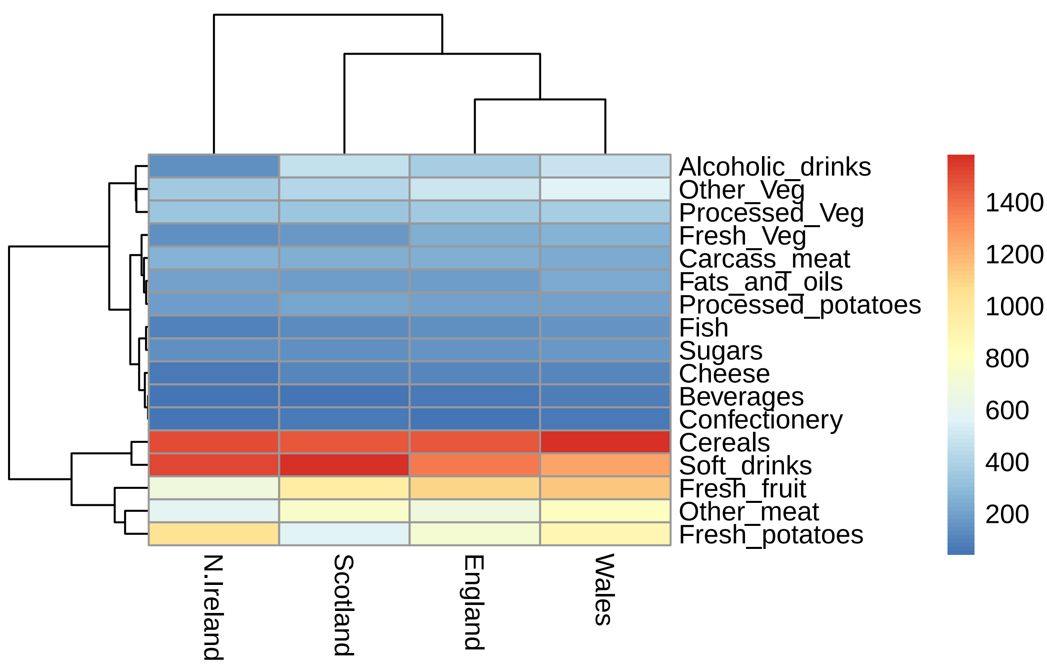
> Q5: We can use the pairs() function to generate all pairwise plots for our countries. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

Yes, when a country is listed, when looking at it from the row orientation, the country is listed on the y axis, but when looking at them through the column orientation, that is their x axis. When a point is on the diagonal for a given plot, it means that there is a positive correlation between the countries being compared and their consumption patterns for that food.

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




```r
library(pheatmap)

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



> Q6. Based on the pairs and heatmap figures, which countries cluster together and what does this suggest about their food consumption patterns? Can you easily tell what the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

It looks like Wales and England are quite similar in their consumption of these foods. It is still quite difficult to tell what is going on in the dataset.

##PCA to the rescue

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

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

```
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
```

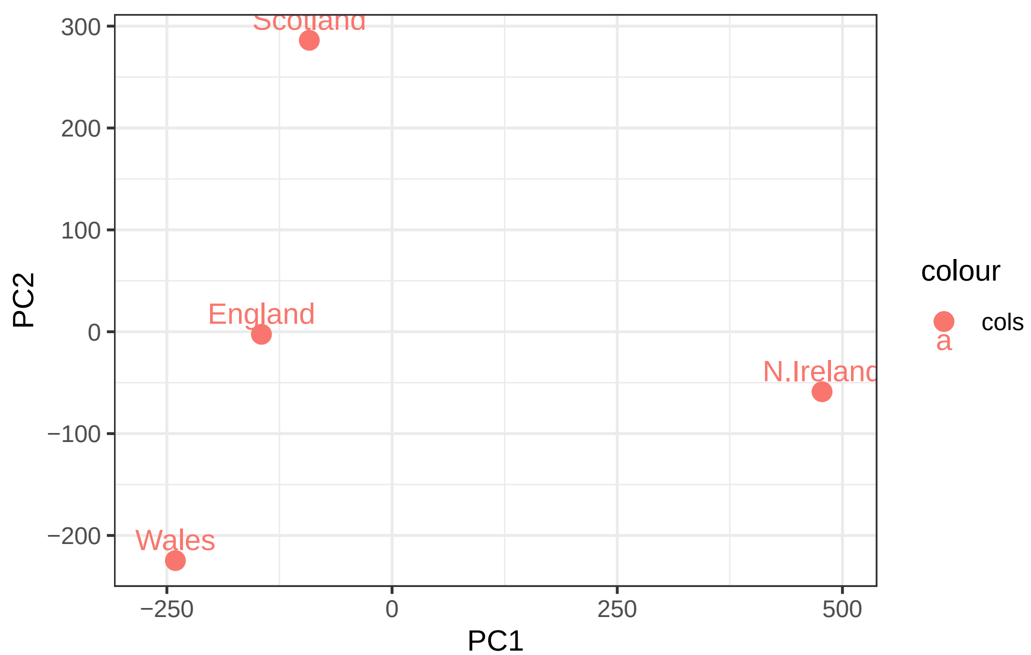
Our result object is called `pca` and it has a `$x` component that we will look at first

```
pca$x
```

```
                 PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -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
```

```
library(ggplot2)
cols <- c("orange", "red", "blue", "darkgreen")
# 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) +
```

```r
aes(x = PC1, y = PC2, label = rownames(pca$x), color = "cols") +
geom_point(size = 3) +
geom_text(vjust = -0.5) +
xlim(-270, 500) +
xlab("PC1") +
ylab("PC2") +
theme_bw()
```



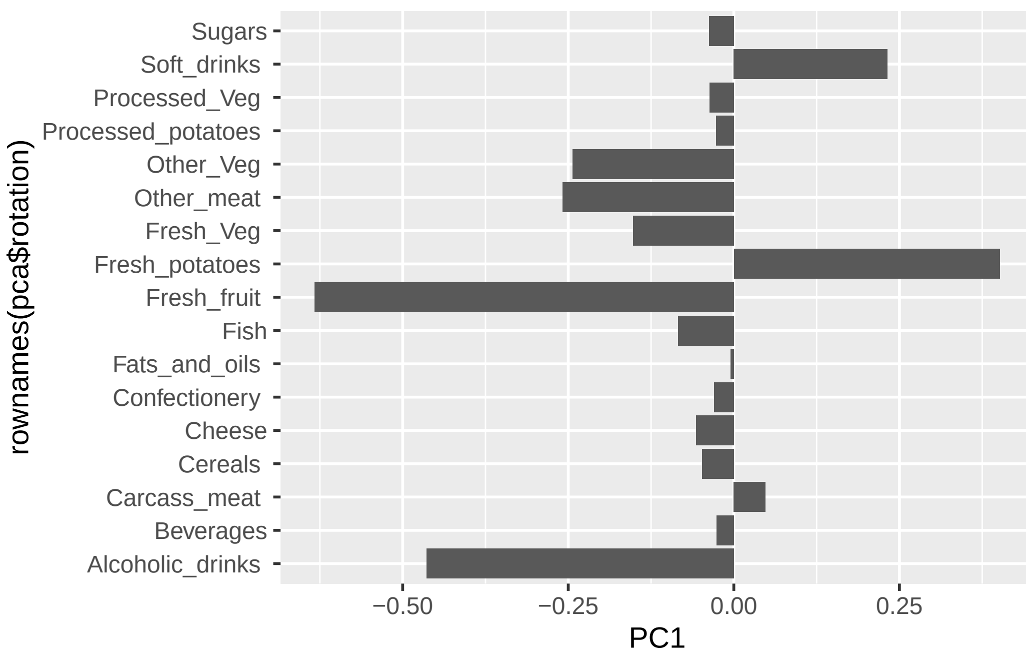
Another major result out of PCA is the so-called "variable loadings" pr `$rotation` that tells us how the original variables (foods) contribute to PCs (i.e. our new axis).

```r
pca$rotation
```

```
                            PC1          PC2         PC3          PC4
Cheese              -0.056955380  0.016012850  0.02394295 -0.694538519
Carcass_meat         0.047927628  0.013915823  0.06367111  0.489884628
Other_meat          -0.258916658 -0.015331138 -0.55384854  0.279023718
Fish                -0.084414983 -0.050754947  0.03906481 -0.008483145
Fats_and_oils       -0.005193623 -0.095388656 -0.12522257  0.076097502
Sugars              -0.037620983 -0.043021699 -0.03605745  0.034101334
Fresh_potatoes       0.401402060 -0.715017078 -0.20668248 -0.090972715
Fresh_Veg           -0.151849942 -0.144900268  0.21382237 -0.039901917
```

```
Other_Veg           -0.243593729 -0.225450923 -0.05332841  0.016719075
Processed_potatoes  -0.026886233  0.042850761 -0.07364902  0.030125166
Processed_Veg       -0.036488269 -0.045451802  0.05289191 -0.013969507
Fresh_fruit         -0.632640898 -0.177740743  0.40012865  0.184072217
Cereals             -0.047702858 -0.212599678 -0.35884921  0.191926714
Beverages           -0.026187756 -0.030560542 -0.04135860  0.004831876
Soft_drinks          0.232244140  0.555124311 -0.16942648  0.103508492
Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.316290619
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001847469
```

```r
ggplot(pca$rotation) + aes(PC1, rownames(pca$rotation)) + geom_col()
```

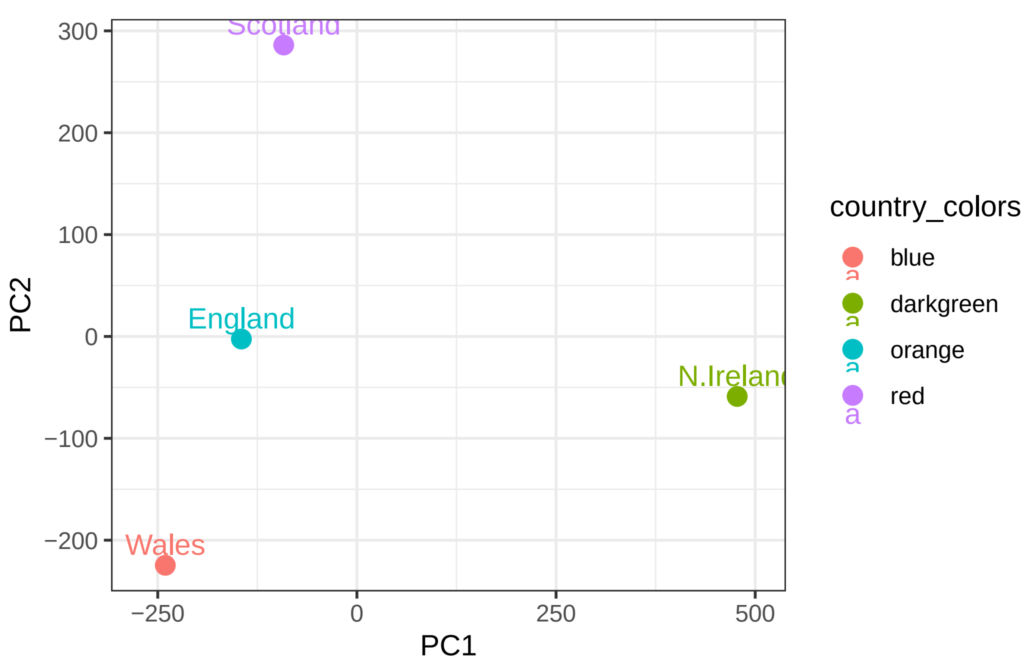



```r
pca <- prcomp( t(x) )
summary(pca)
```

```
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
```

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

```r
# Create a data frame for plotting
df <- as.data.frame(pca$x)
df$Country <- rownames(df)
country_colors <- c(
  "England" = "orange",
  "Scotland" = "blue",
  "Wales" = "red",
  "Ireland" = "darkgreen")
# Plot PC1 vs PC2 with ggplot
ggplot(pca$x) +
  aes(x = PC1, y = PC2, color = country_colors, label = rownames(pca$x)) +
  geom_point(size = 3) +
  geom_text(vjust = -0.5) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



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.

I could not get the right colors to appear for the right country for some reason!

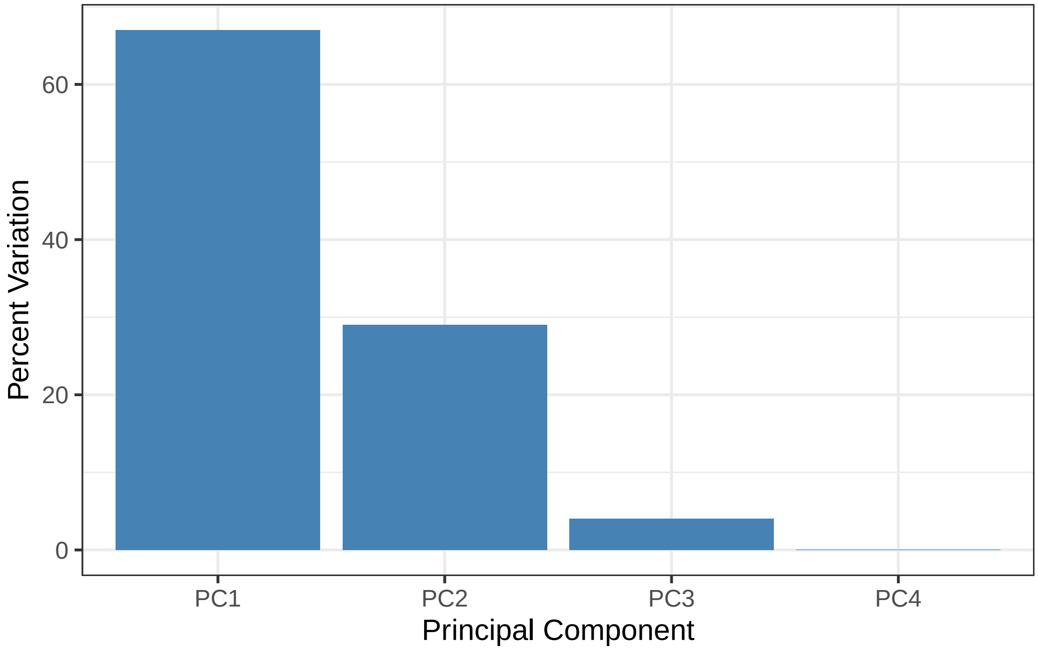
```r
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

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

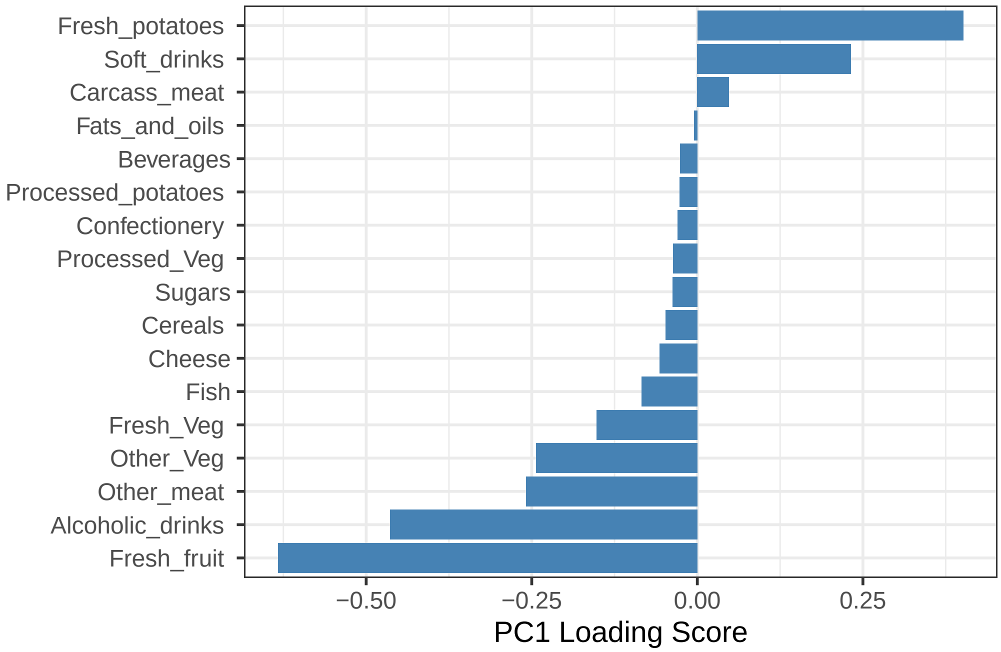
```r
z <- summary(pca)
z$importance
```

```
                             PC1       PC2      PC3          PC4
Standard deviation     324.15019 212.74780 73.87622 3.175833e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

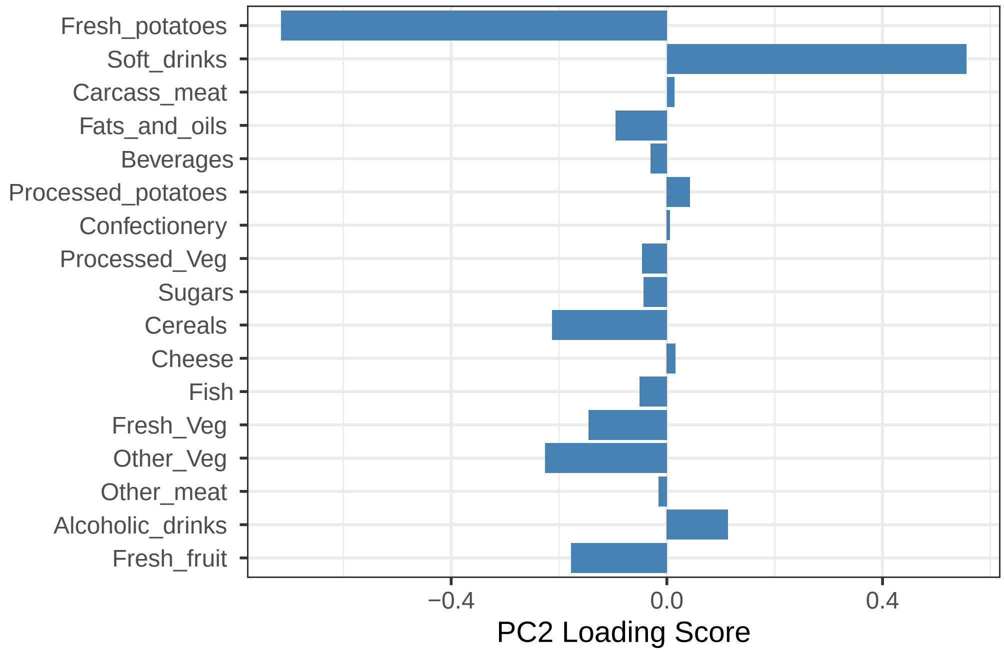
```r
variance_df <- data.frame(
  PC = factor(paste0("PC", 1:length(v)), levels = paste0("PC", 1:length(v))),
  Variance = v
)

ggplot(variance_df) +
  aes(x = PC, y = Variance) +
  geom_col(fill = "steelblue") +
  xlab("Principal Component") +
  ylab("Percent Variation") +
  theme_bw() +
  theme(axis.text.x = element_text(angle = 0))
```




```
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))
```




```
ggplot(pca$rotation) +
  aes(x = PC2,
      y = reorder(rownames(pca$rotation), PC1)) +
  geom_col(fill = "steelblue") +
  xlab("PC2 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```



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

Fresh potatoes and soft drinks are predominantly featured in PC2. This means that PC2 will tell us mainly about diets low in fresh potatoes and high in soft drinks.

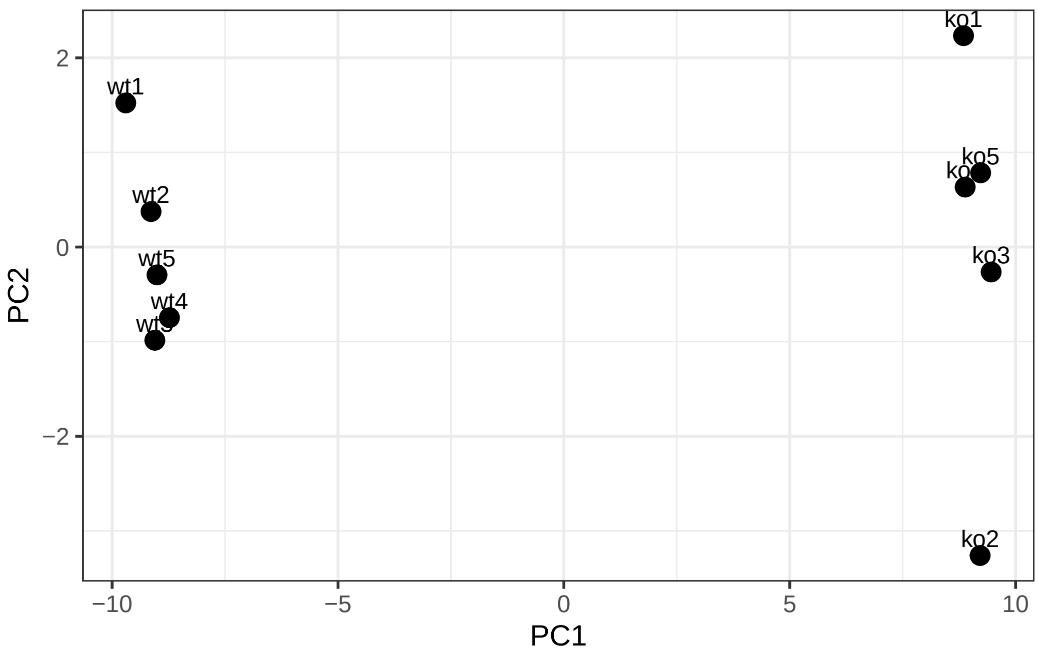
```
url2 <- "https://tinyurl.com/expression-CSV"
rna.data <- read.csv(url2, row.names=1)
head(rna.data)
```

```
       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
```

> Q9: How many genes and samples are in this data set?

There are 100 genes and 10 samples.

```r
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()
```

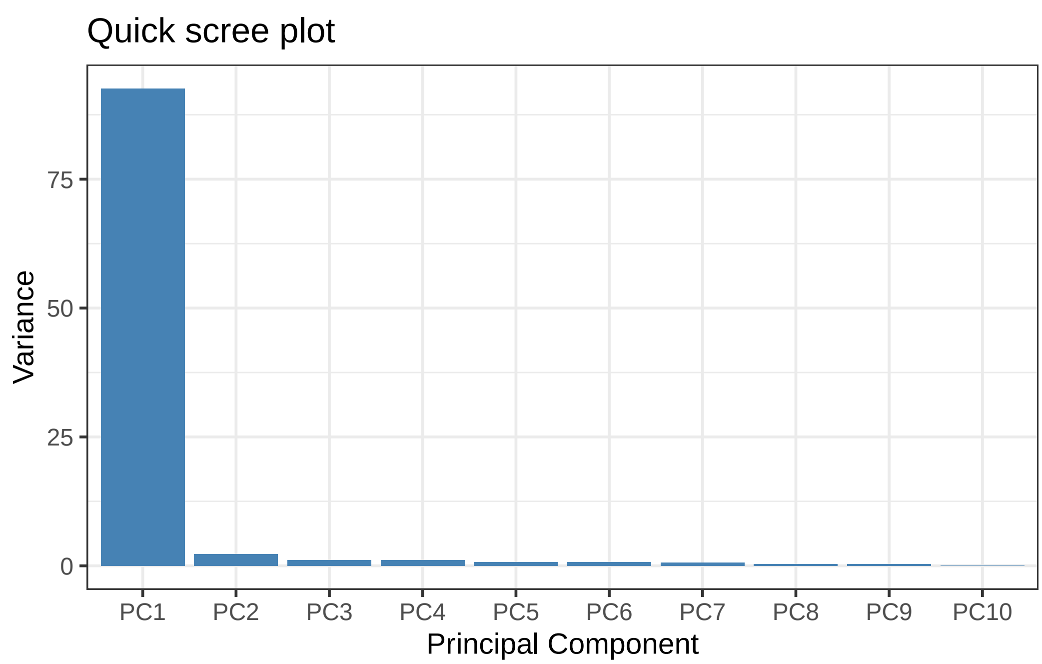



```r
summary(pca)
```

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

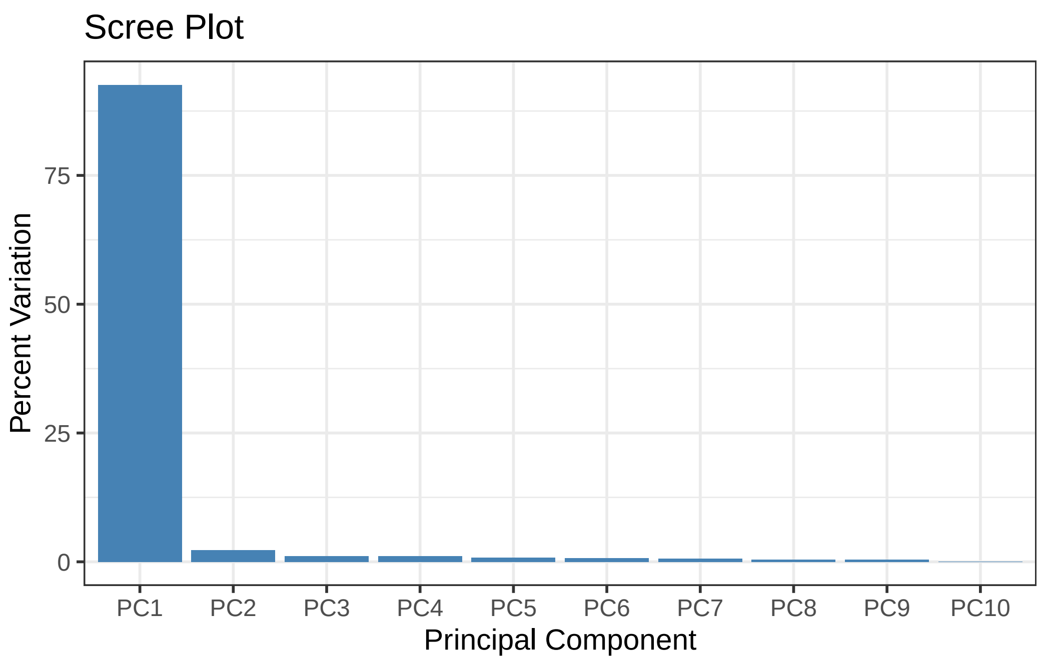
```
pca.var <- pca$sdev^2
pca.var.per <- round(pca.var/sum(pca.var)*100, 1)

# 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()
```



```r
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
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()
```




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

```r
# 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()
```