# Class 07: Clustering and PCA

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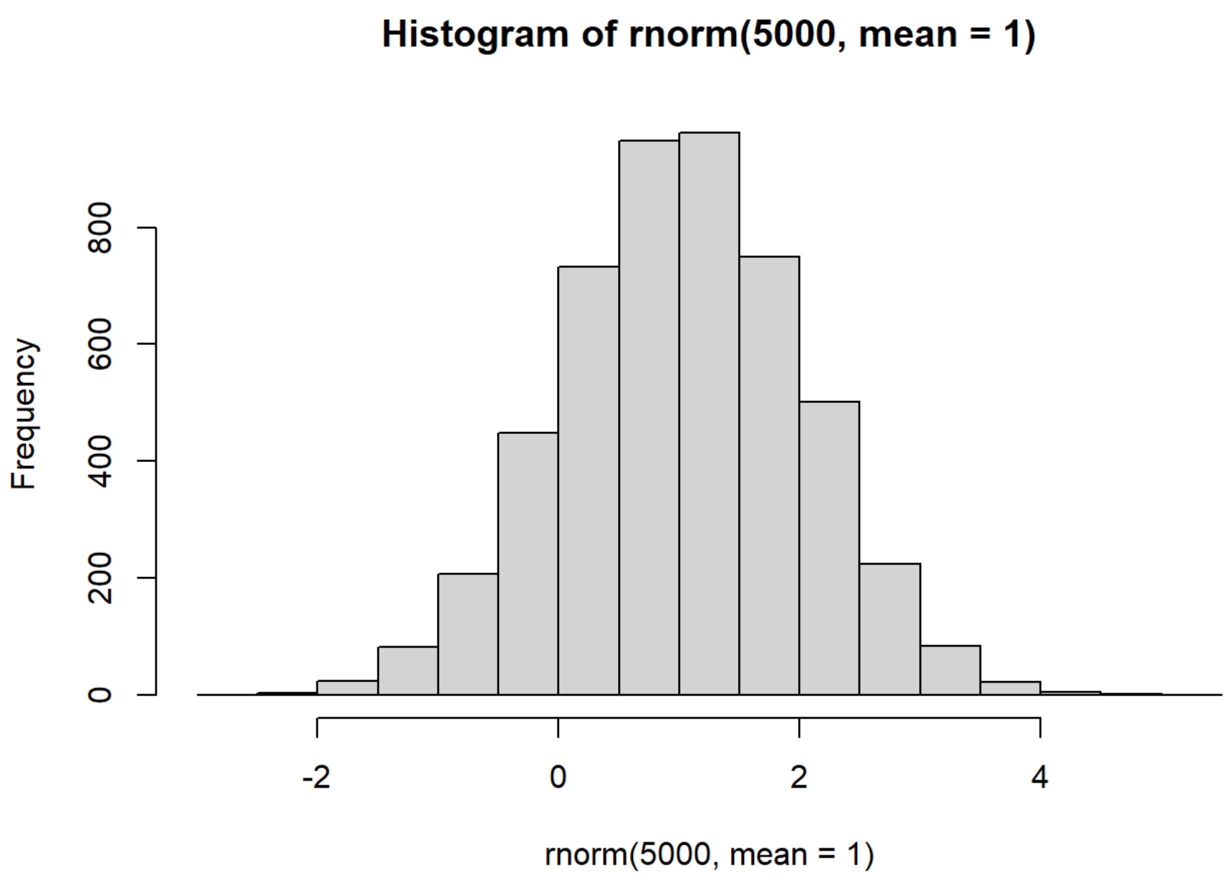
## Clustering

We can use the `rnorm()` function to get random numbers from a normal distribution around a given `mean`.

```
hist(rnorm(5000, mean=1))
```



Let's get 30 points with a mean of 3.

```
rnorm1 <- rnorm(30, mean=3)
rnorm1
```

```
 [1] 3.0748214 2.9140131 2.8095811 3.3477082 1.8936892 3.0385310 4.3540114
 [8] 3.4616944 3.1647144 2.9270168 2.2866782 3.1740964 4.3138157 2.6067250
[15] 2.3732292 0.9974841 2.5173488 2.3384774 4.4640759 1.9950615 2.5190661
[22] 4.6419446 2.2406096 2.1878564 2.9729941 2.1365422 3.6265074 2.5698465
[29] 3.1006287 3.1288489
```

```r
# rnorm2 <- rnorm(30, mean=-30)
# rnorm2

# x <- c(rnorm1, rnorm2)
# x

# cbind(rnorm1, rnorm2)

# rev( c(1:5) )

# y <- cbind( rev(rnorm1), rev(rnorm2) )
# y
```

```r
tmp <- c(rnorm(30, mean=3), rnorm(30, mean=-3))
tmp
```

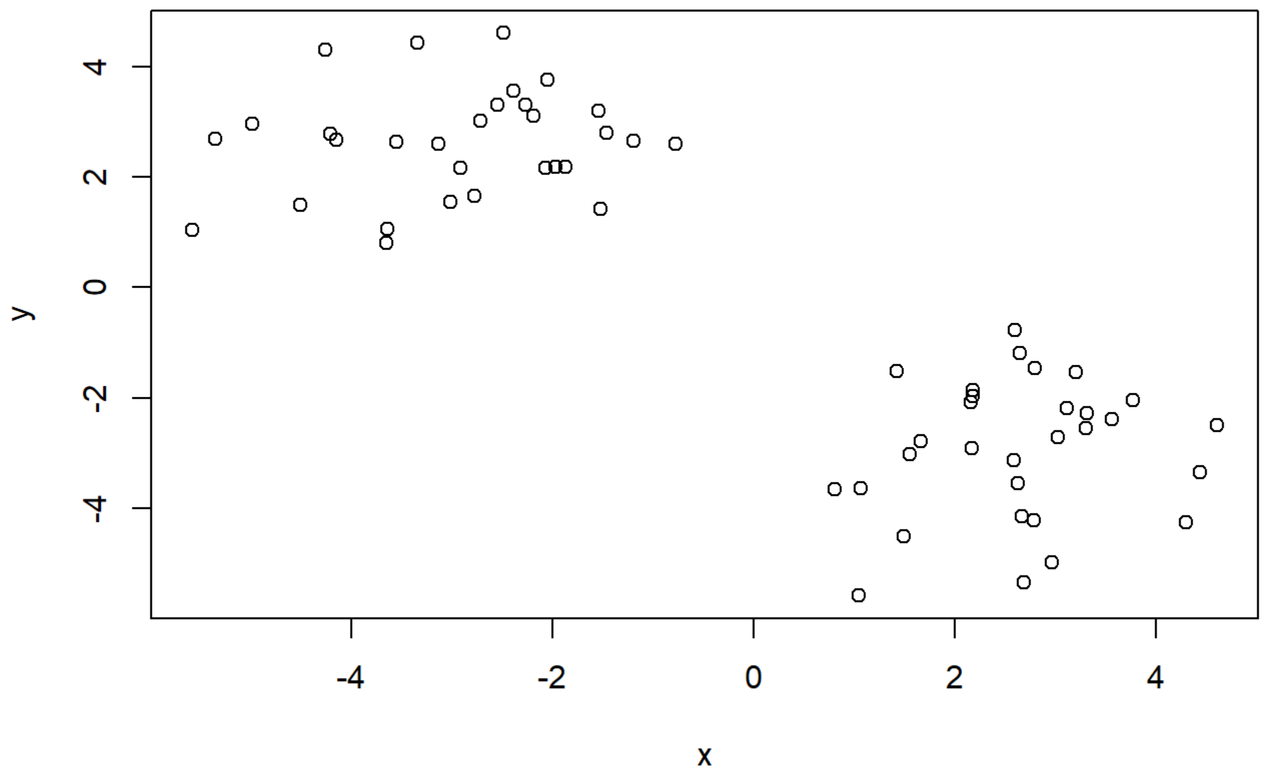
```
 [1]  3.3155838  3.0281034  3.1132274  1.6674582  2.6723357  2.6017949
 [7]  0.8060844  3.7709718  2.6909386  3.2099610  4.6087783  3.5689460
[13]  3.3064260  2.1808433  1.4968538  2.6327997  2.6495313  2.7852100
[19]  4.3061908  2.5943930  1.4287378  2.1639152  2.1851036  2.7958914
[25]  1.5567396  4.4431922  2.9681929  2.1740461  1.0456627  1.0657350
[31] -3.6415161 -5.5819856 -2.9105276 -4.9808150 -3.3396277 -3.0166921
[37] -1.4655752 -1.9640613 -2.0707050 -1.5187397 -3.1296481 -4.2587013
[43] -4.2100121 -1.1916937 -3.5529372 -4.5031799 -1.8651920 -2.5499362
[49] -2.3902640 -2.4904537 -1.5401178 -5.3479933 -2.0447769 -3.6523569
[55] -0.7781971 -4.1475101 -2.7760463 -2.1888957 -2.7191408 -2.2681572
```

```r
# Put these two together
x <- cbind(x=tmp, y=rev(tmp))
x
```

```
              x          y
 [1,]  3.3155838 -2.2681572
 [2,]  3.0281034 -2.7191408
 [3,]  3.1132274 -2.1888957
 [4,]  1.6674582 -2.7760463
 [5,]  2.6723357 -4.1475101
 [6,]  2.6017949 -0.7781971
 [7,]  0.8060844 -3.6523569
 [8,]  3.7709718 -2.0447769
 [9,]  2.6909386 -5.3479933
[10,]  3.2099610 -1.5401178
[11,]  4.6087783 -2.4904537
[12,]  3.5689460 -2.3902640
[13,]  3.3064260 -2.5499362
[14,]  2.1808433 -1.8651920
[15,]  1.4968538 -4.5031799
[16,]  2.6327997 -3.5529372
[17,]  2.6495313 -1.1916937
```

```
[18,]  2.7852100 -4.2100121
[19,]  4.3061908 -4.2587013
[20,]  2.5943930 -3.1296481
[21,]  1.4287378 -1.5187397
[22,]  2.1639152 -2.0707050
[23,]  2.1851036 -1.9640613
[24,]  2.7958914 -1.4655752
[25,]  1.5567396 -3.0166921
[26,]  4.4431922 -3.3396277
[27,]  2.9681929 -4.9808150
[28,]  2.1740461 -2.9105276
[29,]  1.0456627 -5.5819856
[30,]  1.0657350 -3.6415161
[31,] -3.6415161  1.0657350
[32,] -5.5819856  1.0456627
[33,] -2.9105276  2.1740461
[34,] -4.9808150  2.9681929
[35,] -3.3396277  4.4431922
[36,] -3.0166921  1.5567396
[37,] -1.4655752  2.7958914
[38,] -1.9640613  2.1851036
[39,] -2.0707050  2.1639152
[40,] -1.5187397  1.4287378
[41,] -3.1296481  2.5943930
[42,] -4.2587013  4.3061908
[43,] -4.2100121  2.7852100
[44,] -1.1916937  2.6495313
[45,] -3.5529372  2.6327997
[46,] -4.5031799  1.4968538
[47,] -1.8651920  2.1808433
[48,] -2.5499362  3.3064260
[49,] -2.3902640  3.5689460
[50,] -2.4904537  4.6087783
[51,] -1.5401178  3.2099610
[52,] -5.3479933  2.6909386
[53,] -2.0447769  3.7709718
[54,] -3.6523569  0.8060844
[55,] -0.7781971  2.6017949
[56,] -4.1475101  2.6723357
[57,] -2.7760463  1.6674582
[58,] -2.1888957  3.1132274
[59,] -2.7191408  3.0281034
[60,] -2.2681572  3.3155838
```

```r
plot(x)
```



## K-means clustering

Very popular clustering method for big data sets.

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

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

Cluster means:
          x         y
1  2.627788 -2.936515
2 -2.936515  2.627788

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] 73.01019 73.01019
 (between_SS / total_SS =  86.4 %)
```

```
Available components:

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

```
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
```

```
km$size
```

```
[1] 30 30
```

```
km$centers
```

```
          x         y
1  2.627788 -2.936515
2 -2.936515  2.627788
```

> Q: How many points are in each cluster?

```
# We can use km$size to see how many points are in each cluster
# In this case, there are 30 points in each cluster
km$size
```

```
[1] 30 30
```

> Q: What 'component' of your result object details:
>
> - cluster size?
> - cluster assignment/membership?
> - cluster center?

```
# Cluster size
km$size
```

```
[1] 30 30
```

```
# Membership
km$cluster
```

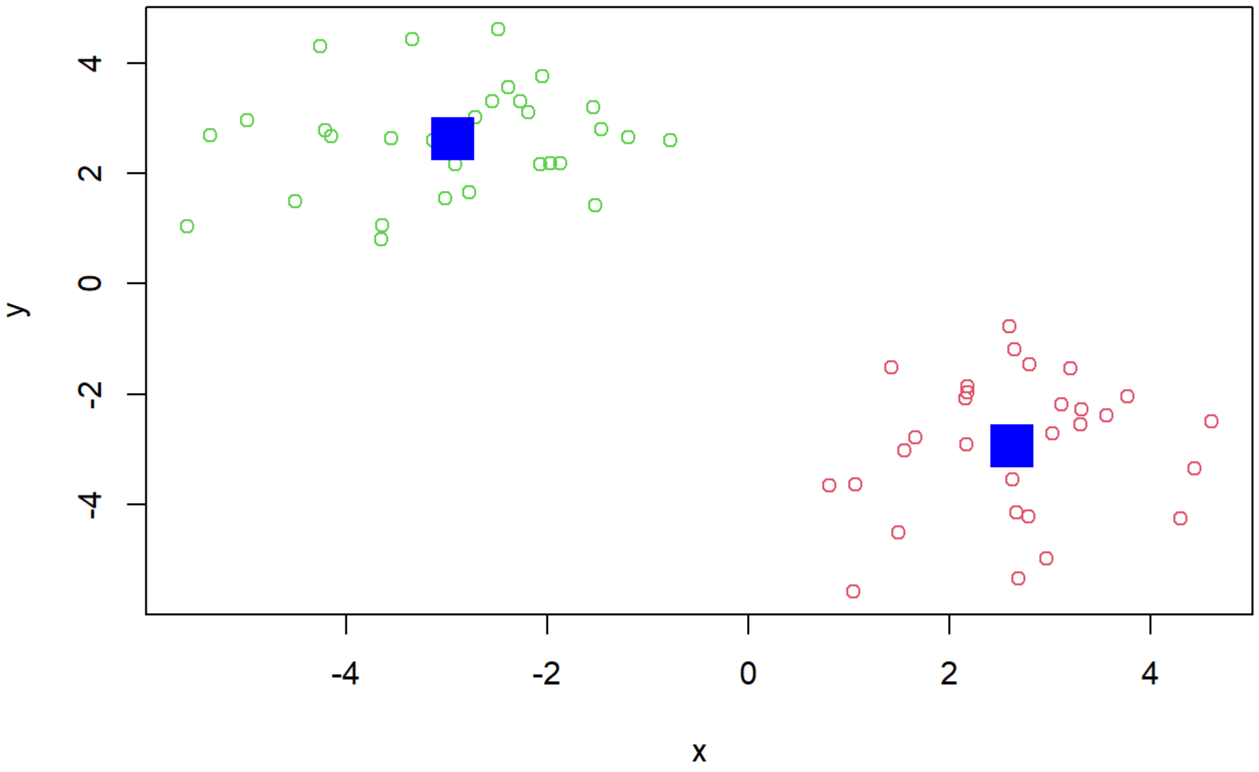
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

```
# Cluster center
km$centers
```

```
          x         y
1  2.627788 -2.936515
2 -2.936515  2.627788
```

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

```
mycols <- km$cluster
mycols <- mycols + 1
plot(x, col = mycols)
points(km$centers, col = 'blue', pch = 15, cex = 3)
```



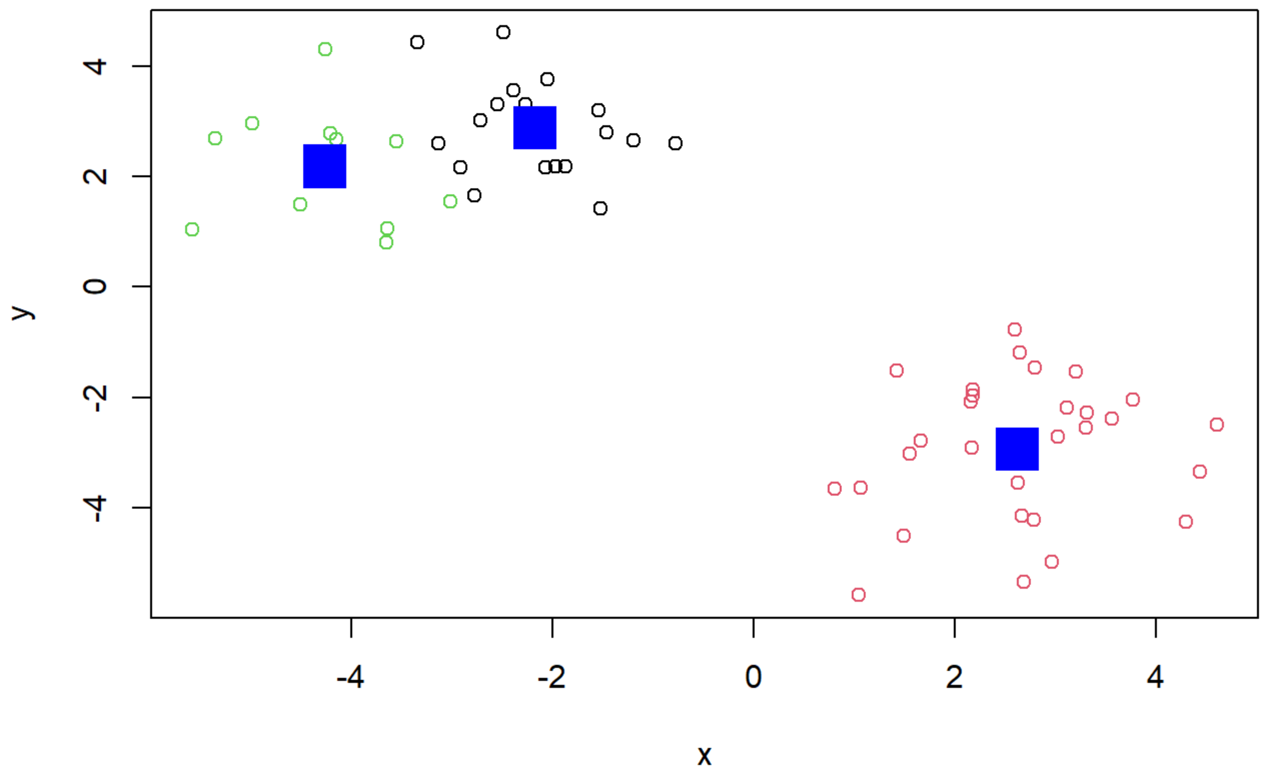
> Q: Let's cluster into 3 groups or same 'x' data and make a plot.

```
km2 <- kmeans(x, 3)
km2
```

```
K-means clustering with 3 clusters of sizes 19, 30, 11

Cluster means:
```

```
          x         y
1 -2.168513  2.884574
2  2.627788 -2.936515
3 -4.263064  2.184249

Clustering vector:
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 1 3 1 3 1 1
[39] 1 1 1 3 3 1 3 3 1 1 1 1 1 3 1 3 1 3 1 1 1 1

Within cluster sum of squares by cluster:
[1] 21.21938 73.01019 17.81023
 (between_SS / total_SS =  89.6 %)

Available components:

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

```r
plot(x, col = km2$cluster)
points(km2$centers, col = 'blue', pch = 15, cex = 3)
```



## Hierarchical Clustering

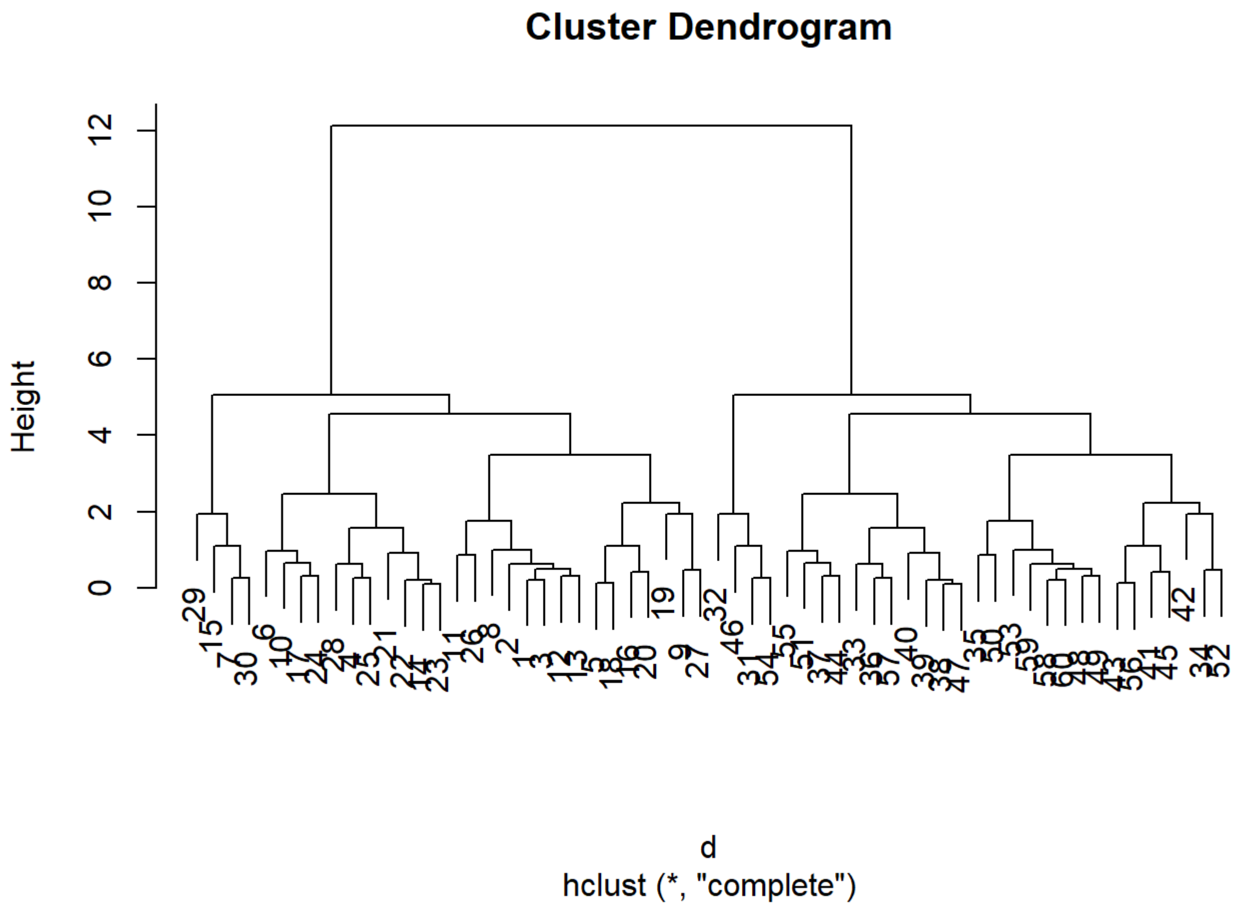
We can use the `hclust()` function for hierarchical clustering. Unlike `kmeans()` where we could just pass in our own data as input, we need to give `hclust()` a "distance matrix" (how far apart the points are, e.g. Euclidean distance `dist()` or other types of distance).

We will use the `dist()` function to start with.

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

```

Call:
hclust(d = d)

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

```
plot(hc)
```

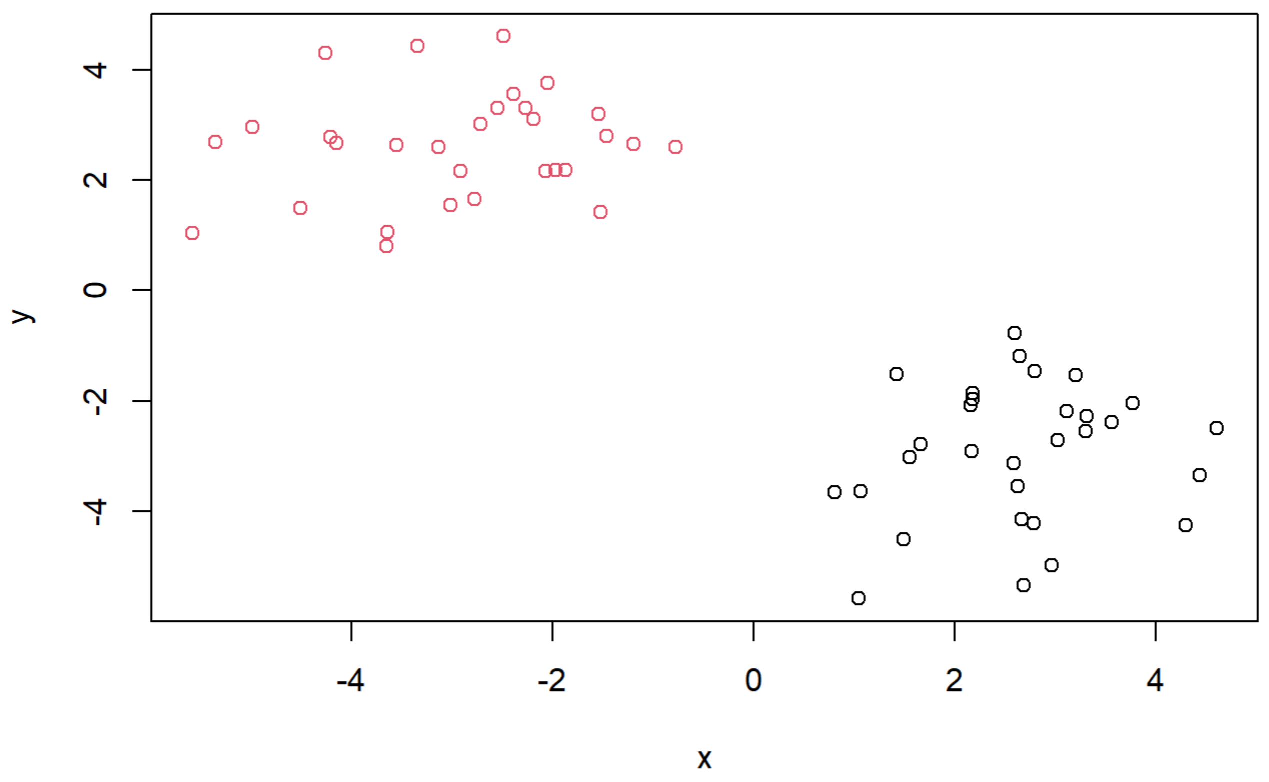


I can now "cut" my tree with the `cutree()` function to yield a cluster membership vector.

```r
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 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
```

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



You can also tell `cutree()` to cut where it yields "k" groups.

```r
cutree(hc, k=2)
```

```
 [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
```

# Lab 7: Principal Component Analysis (PCA)

## PCA of UK Foods

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)

# Q2: This solves the 'row-names problem'. In my opinion, this way is better since it automatical
```

```
# Finding number of rows and columns
dim(x)
```

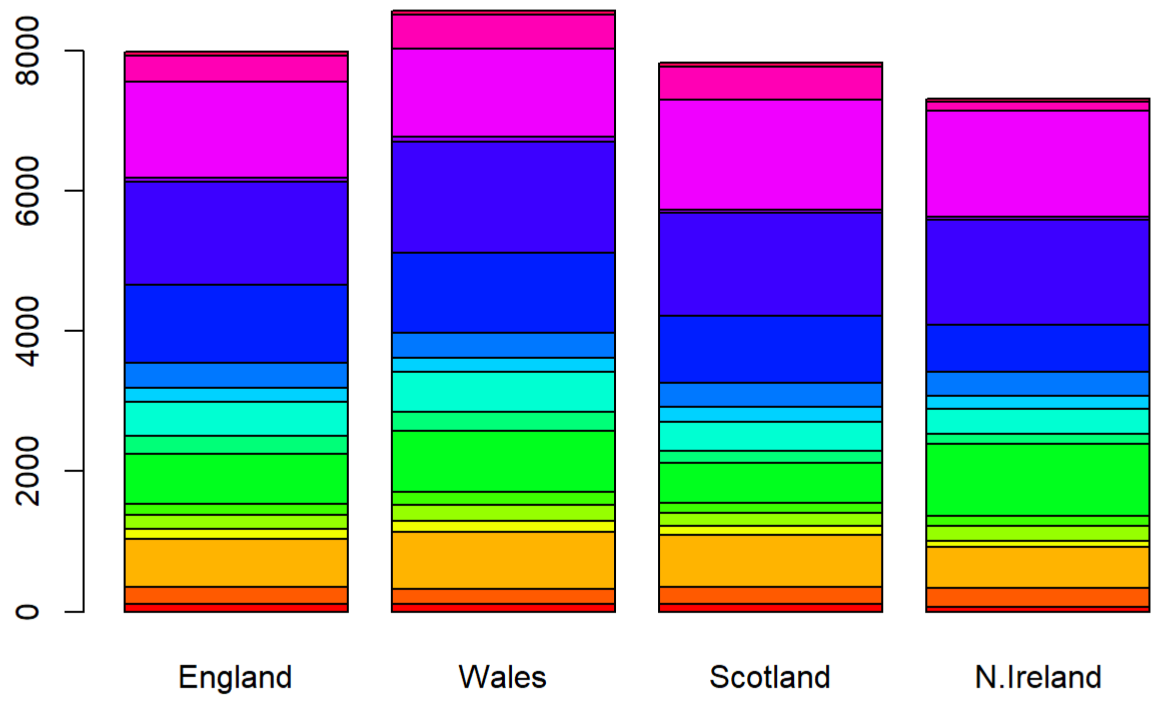
```
[1] 17  4
```

```
# Q1: We have 17 rows and 4 columns, where each column is a country.
```

```
# Using head to preview first 6 rows
head(x)
```

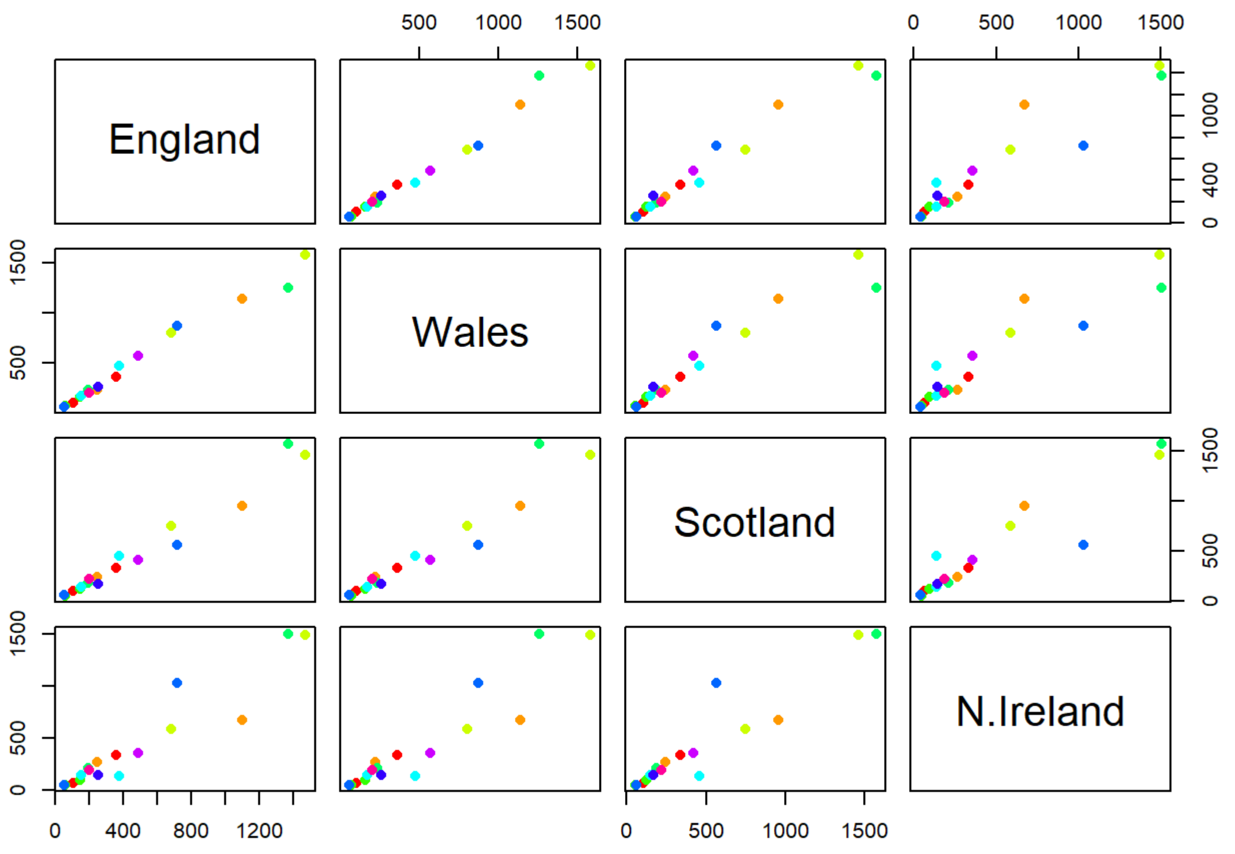
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
Fats_and_oils      193   235      184       209
Sugars  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

```
# Generating barplot
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



```
# Q3: We set beside=FALSE to change the barplot into a stacked format instead of the bars being s
```

```
# Generating pairwise plots.
pairs(x, col=rainbow(10), pch=16)
```



```
# Q5: If a point lines on the diagonal, then that means that the country on the y-axis and the co
```

> Q5: If a datapoint is on the diagonal, then the countries have the same amount of that product. If a datapoint is above the diagonal then the country on the y-axis has a higher amount of that product. If a datapoint is below the diagonal line (i.e. further to the right) then the country on the x-axis has more of that product.

> Q6: N. Ireland has more of the blue datapoint than other countries, since that datapoint is further to the right on the graph (below diagonal) when N. Ireland is plotted on the x-axis, and higher up on the graph (above diagonal) when N. Ireland is plotted on the y-axis.

The main PCA function in base R is called `prcomp()` it expects the transpose of our data.

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

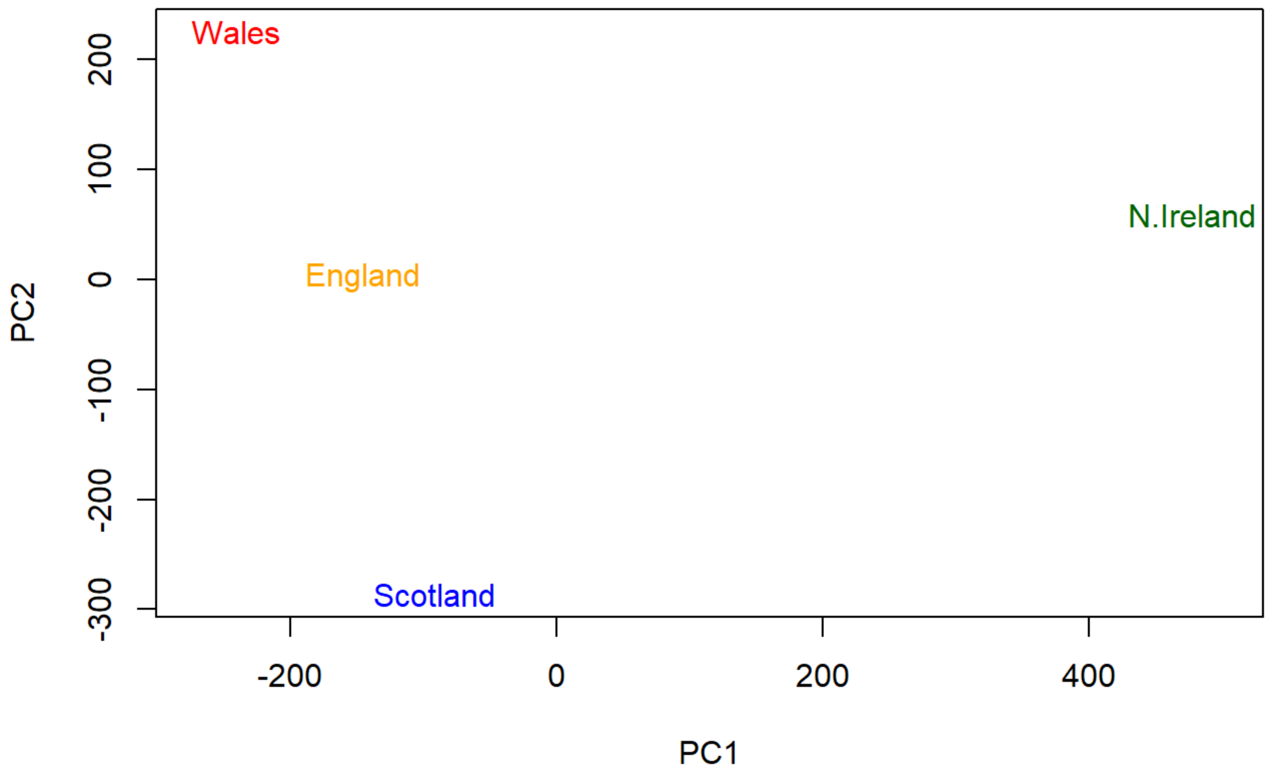
```
Importance of components:
                             PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 4.189e-14
```

```
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: Competing the pca plot code.
plot(pca$x[,1], pca$x[,2],
     xlab="PC1", ylab="PC2",
     col = 'transparent',
     pch = 16,
     xlim=c(-270,500))

# Q8: Customizing the plot by adding color.
text(pca$x[,1], pca$x[,2],
     colnames(x),
     col = c("orange", "red", "blue", "darkgreen"))
```


Wales
N.Ireland
England
Scotland
PC2
PC1