Class 7: Machine Learning 1

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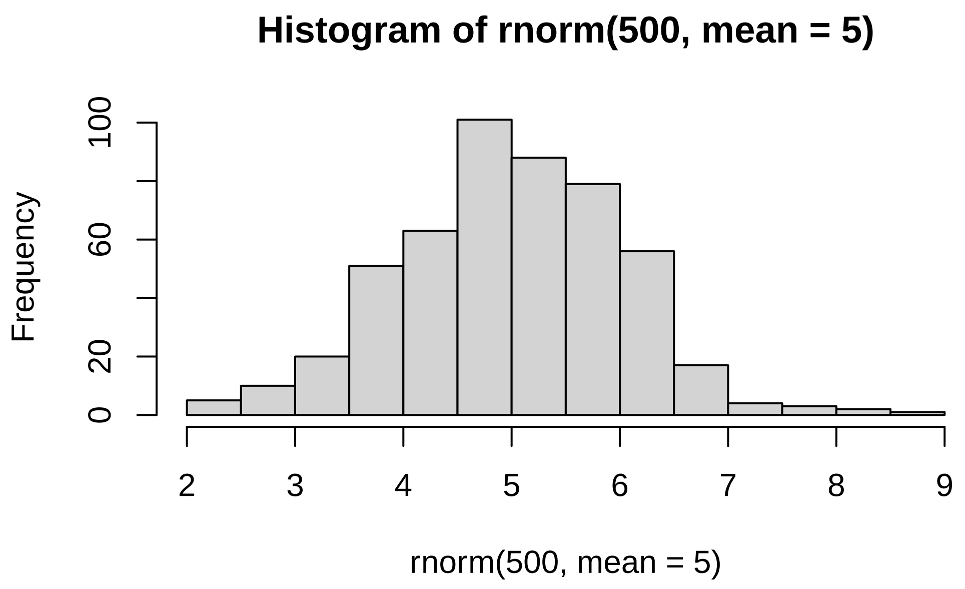
Today we will explore some fundamental machine learning methods including clustering and dimensionality reduction.

K-means clustering

To see how this works let's first makeup some data to cluster where we know what the answer should be. We can use the `rnorm()` function to help here:

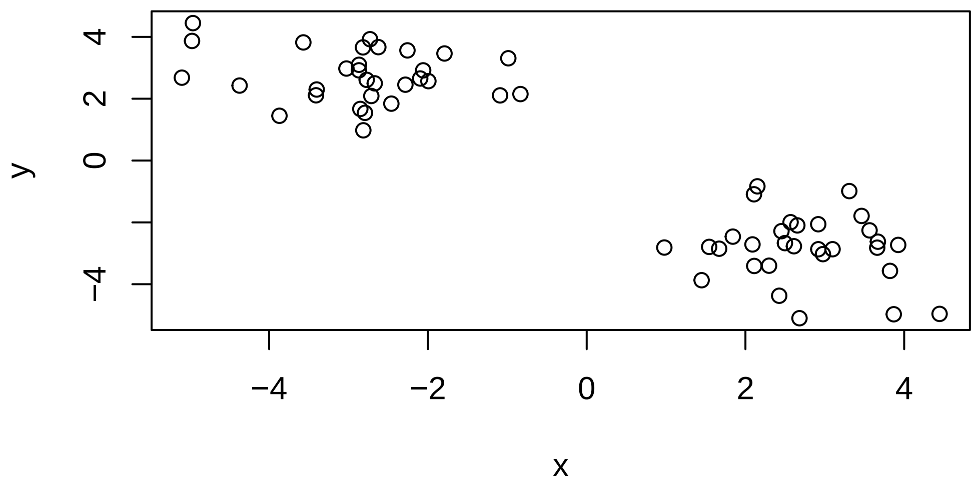
```r
hist(rnorm(500, mean = 5))
```



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

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

```r
plot(x)
```



The function for K-means clustering in “base” R is `kmeans()`

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

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

Cluster means:
          x         y
1  2.725280 -2.835451
2 -2.835451  2.725280

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 1 1 1 1 1 1 1 1
```

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

Within cluster sum of squares by cluster:
[1] 53.60948 53.60948
 (between_SS / total_SS =  89.6 %)

Available components:

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

To get at the results of the returned list object we can use the dollar $ syntax.

> Q. How many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

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

```
k$cluster
```

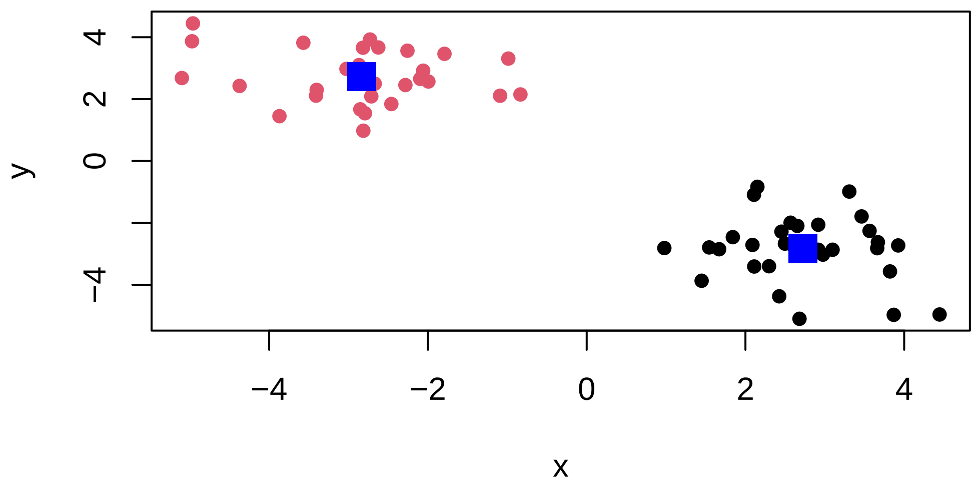
```
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

```
k$center
```

```
          x         y
1  2.725280 -2.835451
2 -2.835451  2.725280
```

> Q. Make a clustering results figure of the data colored by cluster membership and show cluster centers.

```r
plot(x, col = k$cluster, pch = 16)
points(k$centers, col = "blue", pch = 15, cex = 2)
```

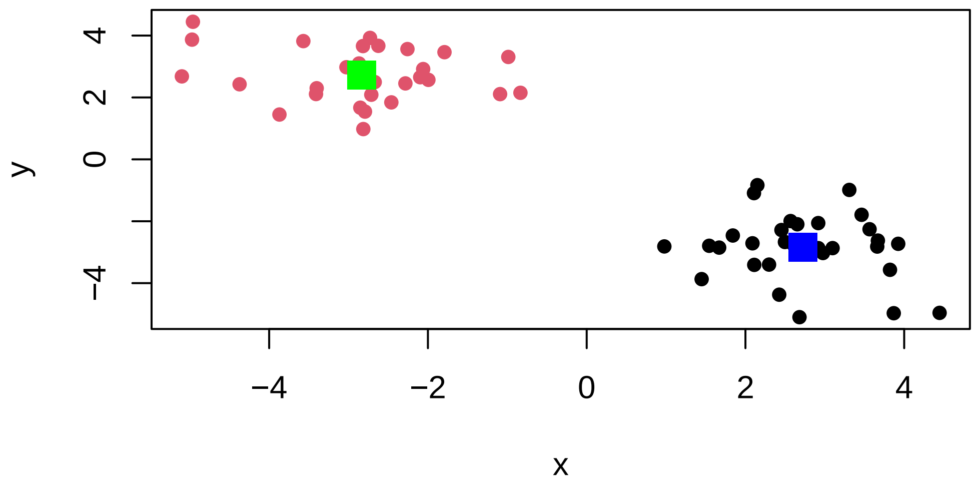


K-means clustering is very popular as it is very fast and relatively straight forward: it takes numeric data as input and returns the cluster membership vector etc.

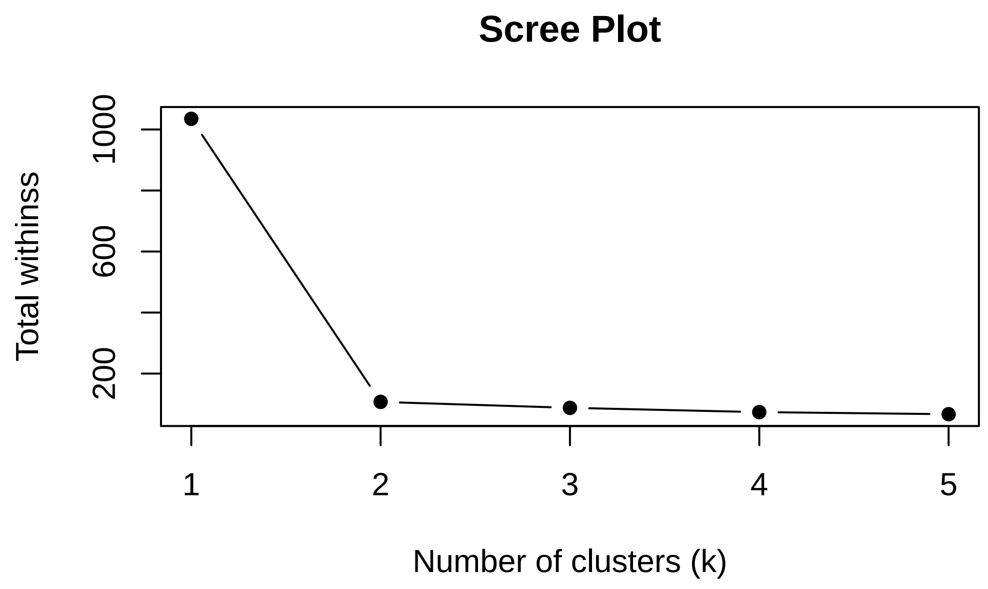
The “issue” is we tell `kmeans()` how many clusters we want!

> Q. Run k-means again and cluster 4 groups/clusters and plot the results as we did above?

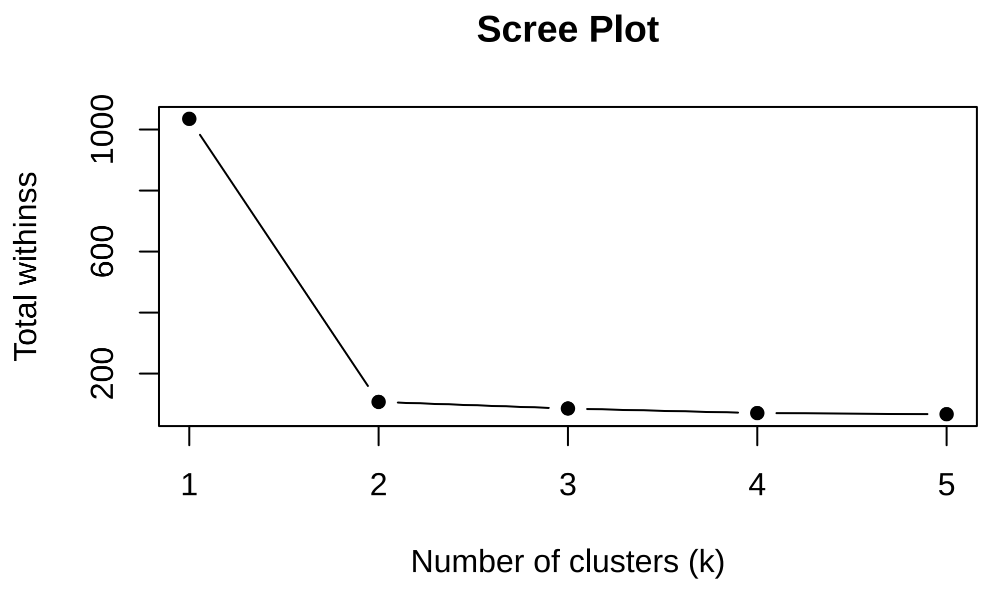
```r
k4 <- kmeans(x, centers = 4)
plot(x, col = k$cluster, pch = 16)
points(k$centers, col = c("blue", "green", "purple", "red"), pch = 15, cex = 2)
```



```
wss <- numeric()
for (k in 1:5) {
  wss[k] <- kmeans(x, centers = k)$tot.withinss
}
plot(1:5, wss, type = "b", xlab = "Number of clusters (k)", ylab = "Total withinss", main =
```



```
n <- NULL
for(i in 1:5) {
  n <- c(n, kmeans(x, centers = i)$tot.withinss)
}
plot(n, typ="b", xlab = "Number of clusters (k)", ylab = "Total withinss", main = "Scree Plo
```



The elbow point is the location on a scree plot where the total within-cluster sum of squares drops sharply as the number of clusters increases, but then levels off. This point represents the optimal number of clusters.

Next Hierarchical Clustering

The main "base" R function for Hierarchical Clustering is called `hclust()`. Here we can't just input our data we need to first calculate a distance matrix (e.g `dist()`) for our data and use this as input to `hclust()`

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

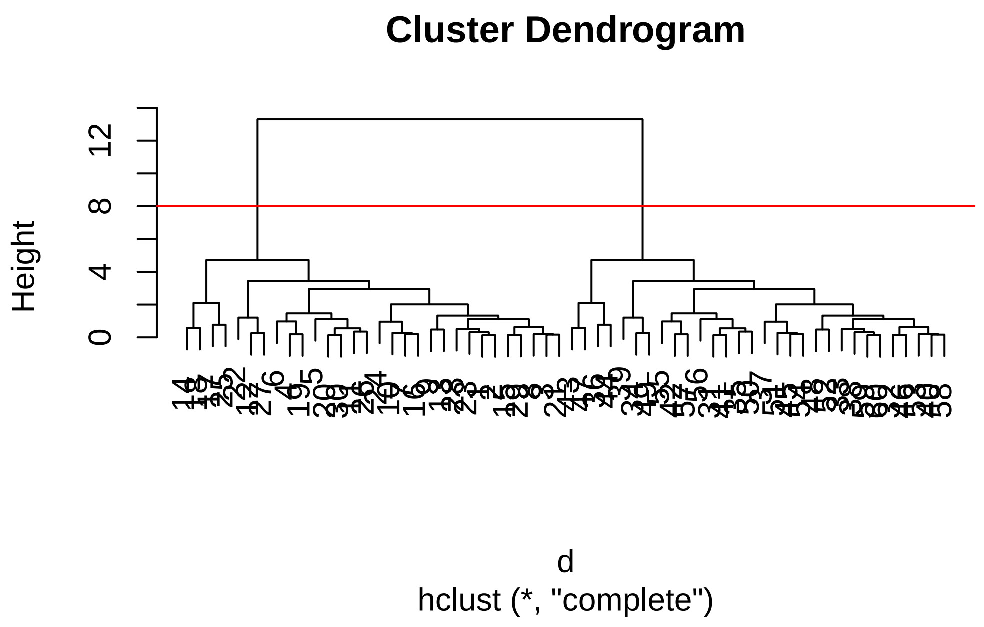
```

Call:
hclust(d = d)

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

There is a plot method for hclust results. Let's try it!

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



```r
cutree(hc, h=8)
```

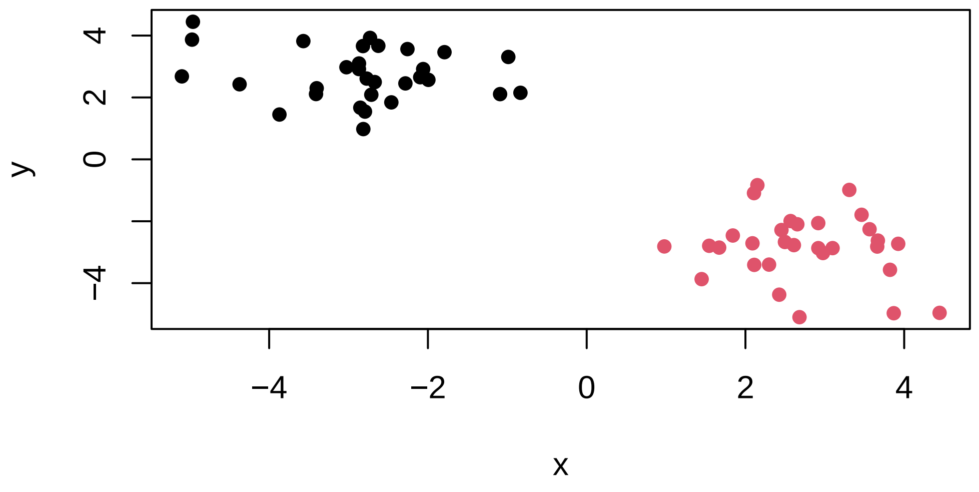
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

To get our cluster "membership" vector (i.e. our main clustering result) we an "cut" the tree at a given height that yields a given "k" groups.

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

> Q. Plot the data with our hclust result coloring

```r
plot(x, col = grps, pch = 16)
```



Principal Component Analysis (PCA)

PCA of UK food data

Import food data from an online CSV file:

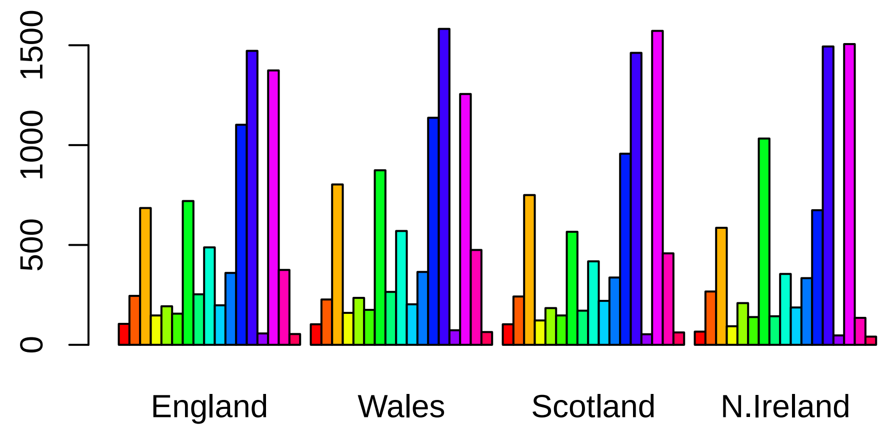
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
x
```

```
                    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
Fresh_potatoes          720   874      566      1033
Fresh_Veg               253   265      171       143
Other_Veg               488   570      418       355
Processed_potatoes      198   203      220       187
```

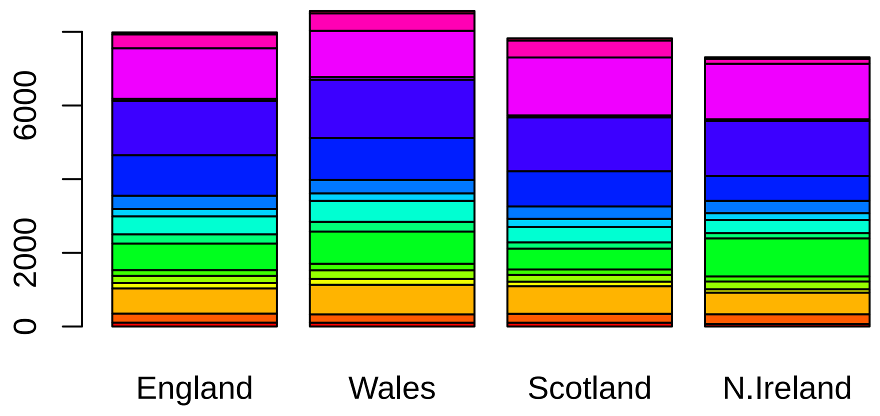
```
Processed_Veg           360   365       337        334
Fresh_fruit            1102  1137       957        674
Cereals                1472  1582      1462       1494
Beverages                57    73        53         47
Soft_drinks            1374  1256      1572       1506
Alcoholic_drinks        375   475       458        135
Confectionery            54    64        62         41
```

Some base figures:

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

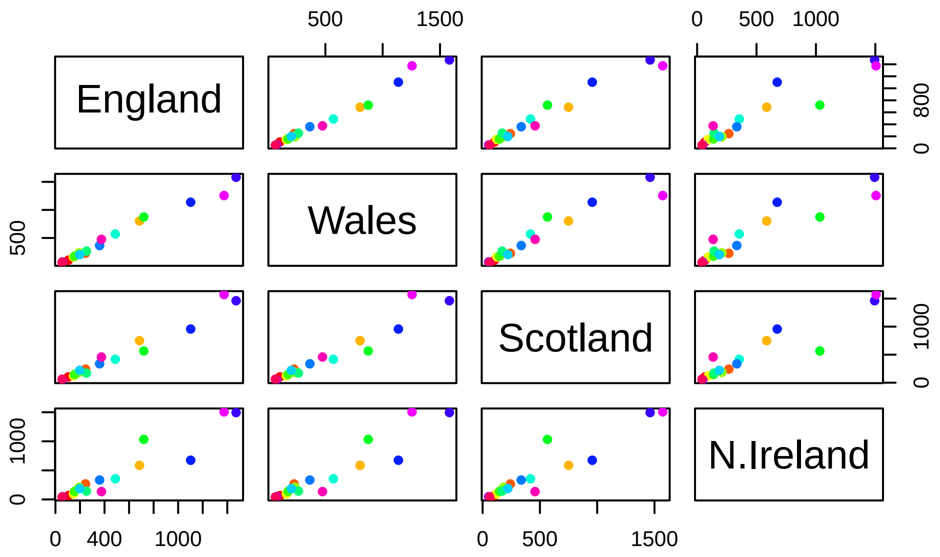


```r
barplot(as.matrix(x), col=rainbow(nrow(x)))
```



There is one plot that can be useful for small datasets:

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



Main point: it can be difficult to spot major trends and patterns even in relatively small multivariate datasets (here we only have 17 dimensions, typically we have 1000s).

PCA to the rescue

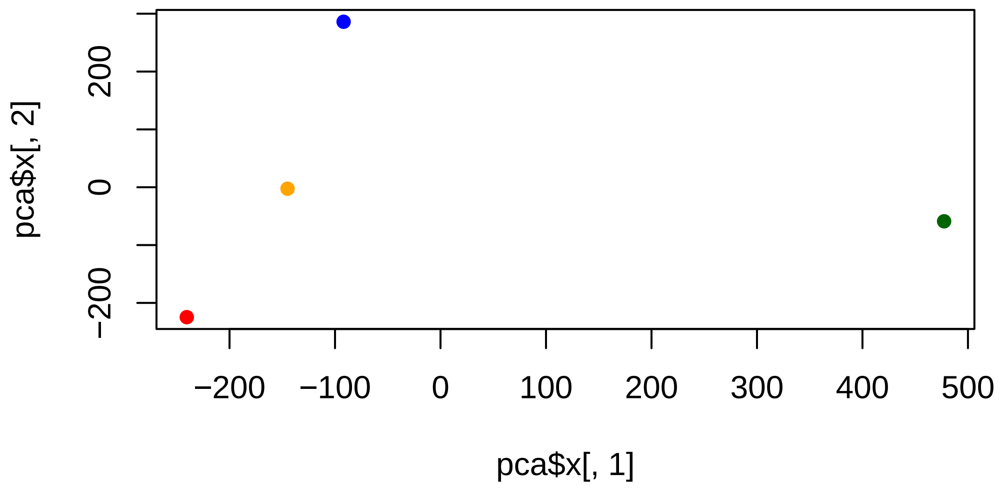
The main function in "base" R for PCA is called `prcomp()`

I will take the transpose of out data so the "foods" are in the columns:

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

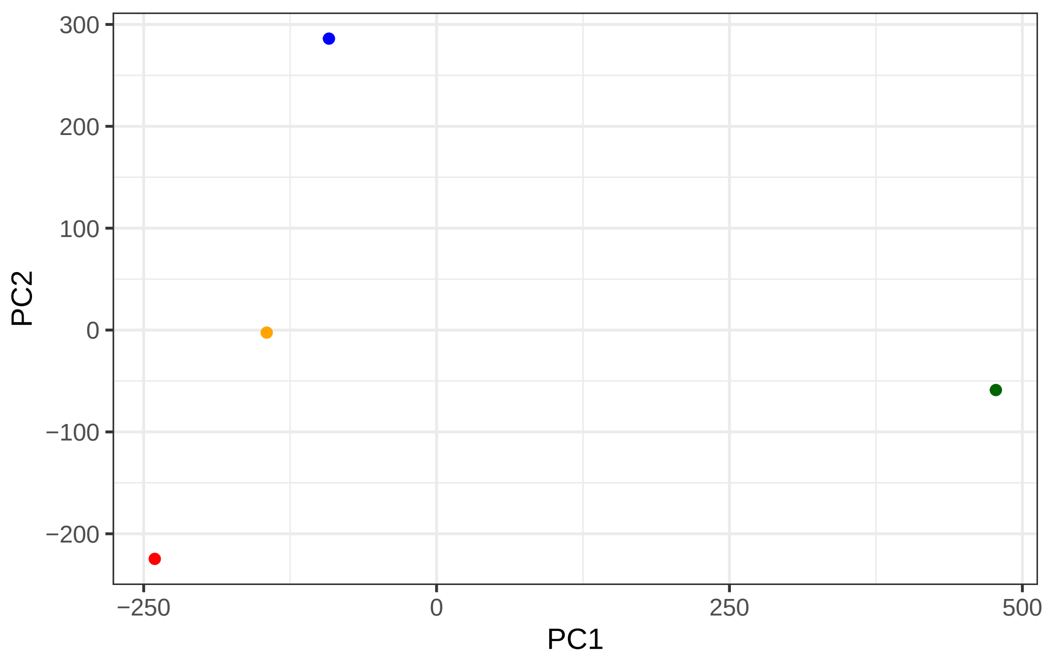
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 2.921e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
cols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=cols, pch=16)
```

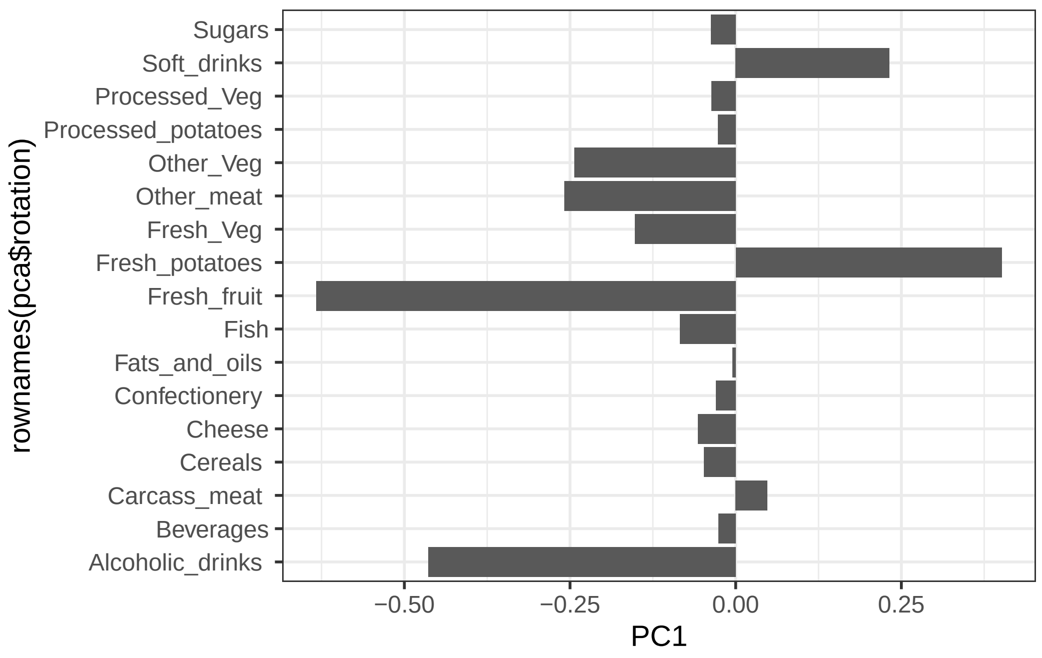


```r
library(ggplot2)
```

```r
ggplot(pca$x) +
  aes(PC1, PC2) +
  geom_point(col=cols) +
  theme_bw()
```



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



PCA looks super useful and we will come back to describe this further next time.