Class 7: Introduction to Machine Learning Lab

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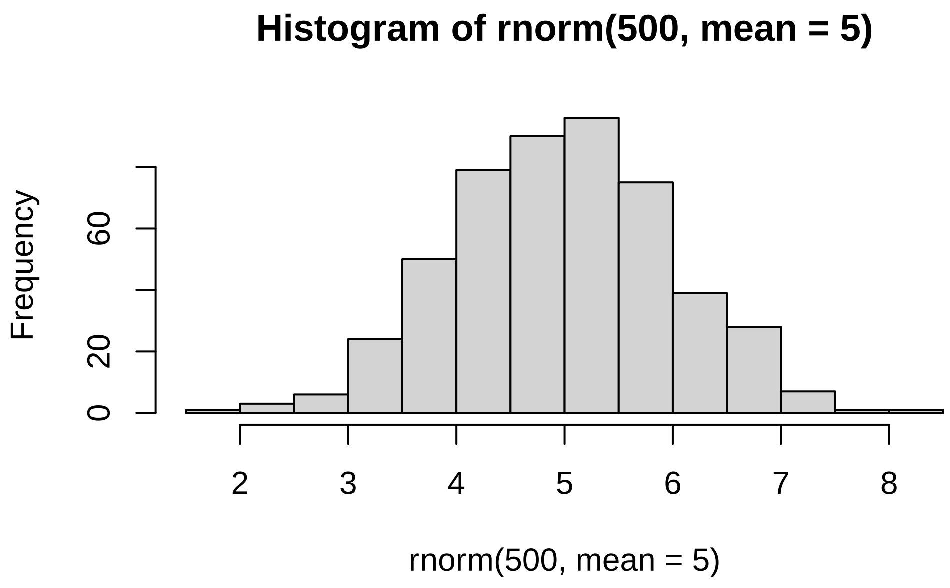
Today we will explore some fundamental machine learning methods including clustering and dimensionality reduction.

K-means clustering

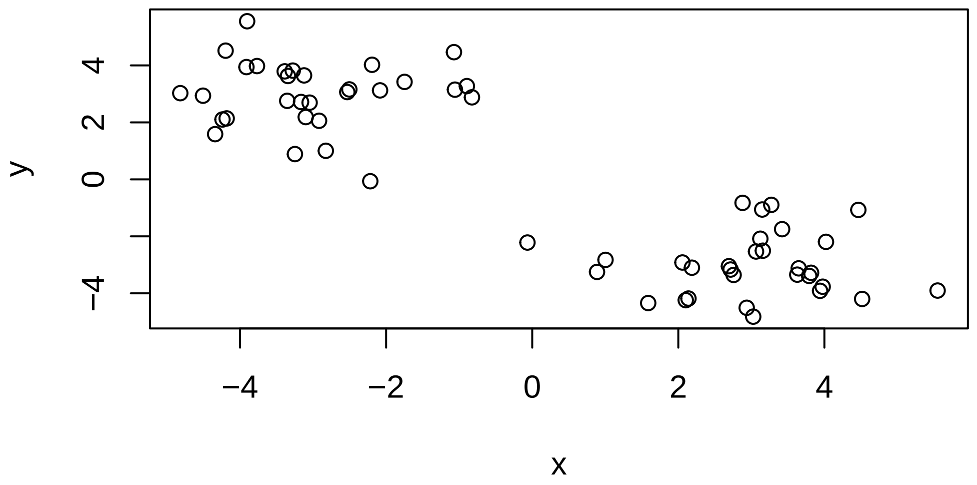
To see how this works, let's first makeup some data to cluster where we know what the answer should be. We can use the `rnorm()` fuction to help here:

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



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

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



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

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

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

Cluster means:
          x         y
1 -2.992952  2.981686
2  2.981686 -2.992952

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] 74.84455 74.84455
 (between_SS / total_SS =  87.7 %)

Available components:

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

To get the results of the returend list object, we can use the dollor $ syntax

Q1. How many points are in each cluster?

```
km$size
```

```
[1] 30 30
```

Q2. What 'component' of your result object details - cluster assignment/membership? - cluster center?

```
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
```

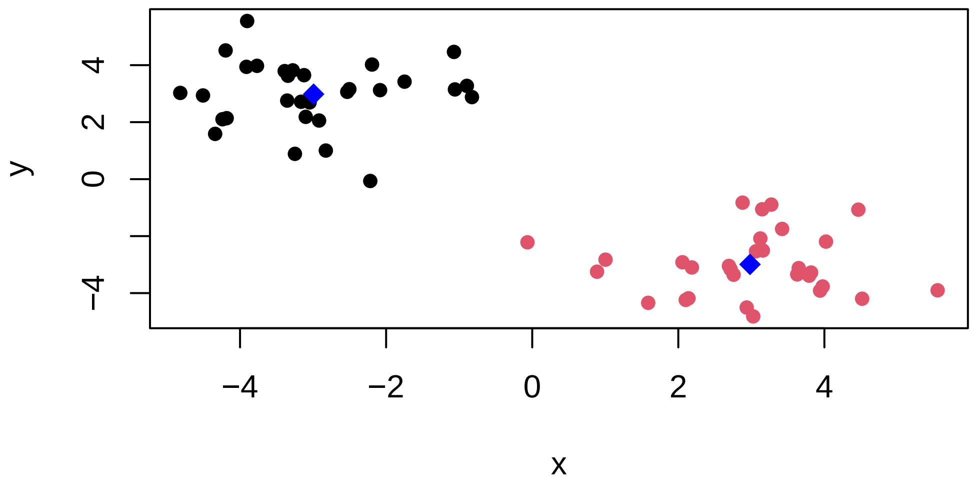
```
km$centers
```

```
          x         y
1 -2.992952  2.981686
2  2.981686 -2.992952
```

Q3. Make a clustering result figure of the data colored by cluster membership.

```
plot(x, col=km$cluster, pch=16)
# if col=c("red", "blue), the vector would recycle to length of 60 alternating colors

points(km$centers, col="blue", pch=18, cex=1.5)
```

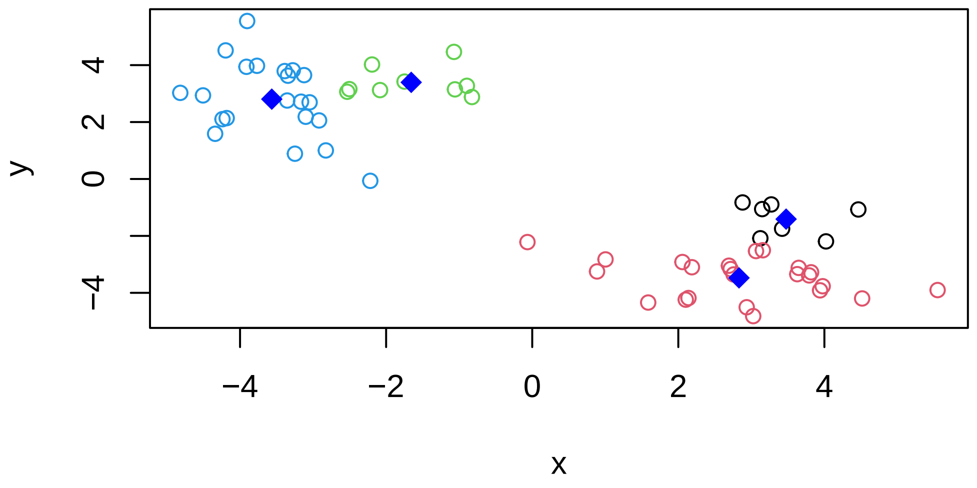


K-means clustering is very popular as it is very fast and relatively straightforward: it takes numeric data as input and returns the cluster membership vector etc.

The *"issue"* is that we tell `kmeans()` how many clusters we want.

> Q4. Run kmeans again and cluster into 4 groups and plot the results like we did above.

```r
km2 <- kmeans(x, centers=4)
plot(x, col=km2$cluster)
points(km2$centers, col="blue", pch=18, cex=1.5)
```



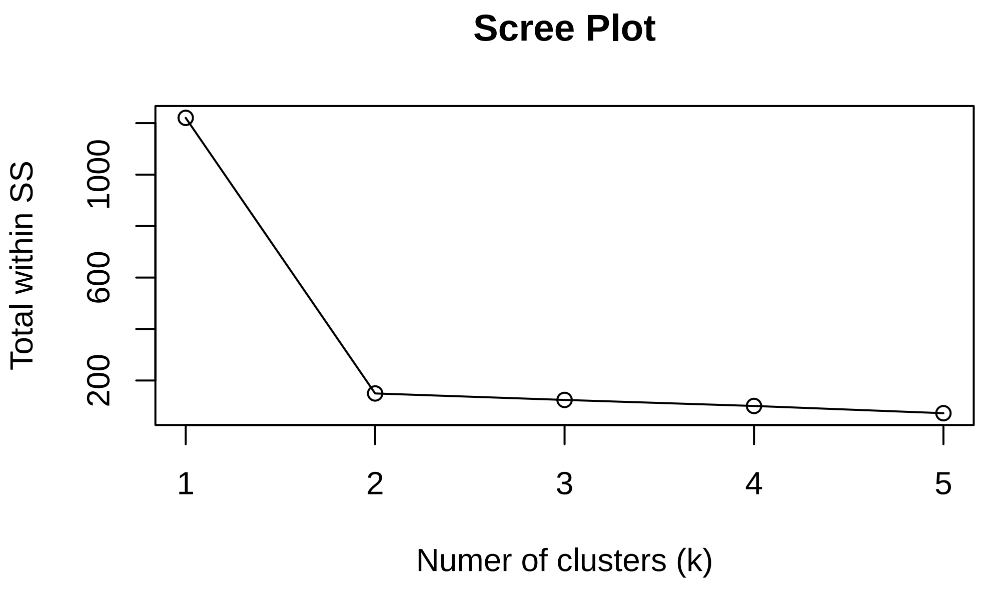
```r
# Within Sum of Square
mean(km$withinss)
```

```
[1] 74.84455
```

Scree plot

```r
ssvec <- c()

for(i in 1:5){
  km <- kmeans(x, centers = i)
  ssvec[i] <- km$tot.withinss
}
plot(c(1:5), ssvec, type="o", xlab="Numer of clusters (k)", ylab="Total within SS", main="Sc
```



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 out data and use this as input to `hclust()`.

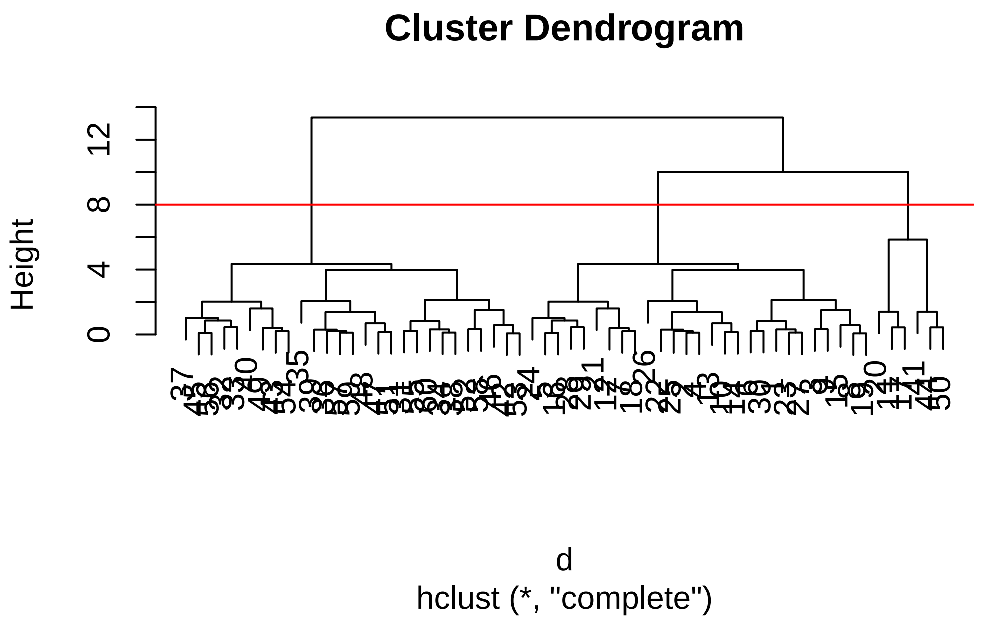
```r
d <- dist(x)
hc <- hclust(d)
hc
```

```
Call:
hclust(d = d)

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

There is a plot method for class `hclust` results. Lets try

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



To get our cluster membership vector (i.e. out main cluster result), we can *cut the tree* at a given height or at a height that yields a given “k”.

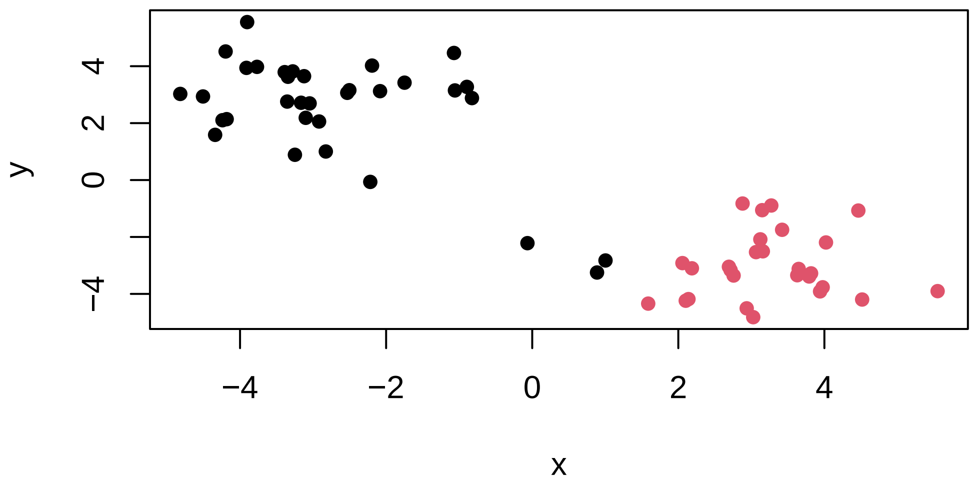
```r
cutree(hc, h=8)
```

```
 [1] 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 2 1 1 2 1 1 1 1 1 1 1 1 1 1 3 3 3 3 3 3 3 3
[39] 3 3 2 3 3 2 3 3 3 3 3 2 3 3 3 3 3 3 3 3 3 3
```

```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

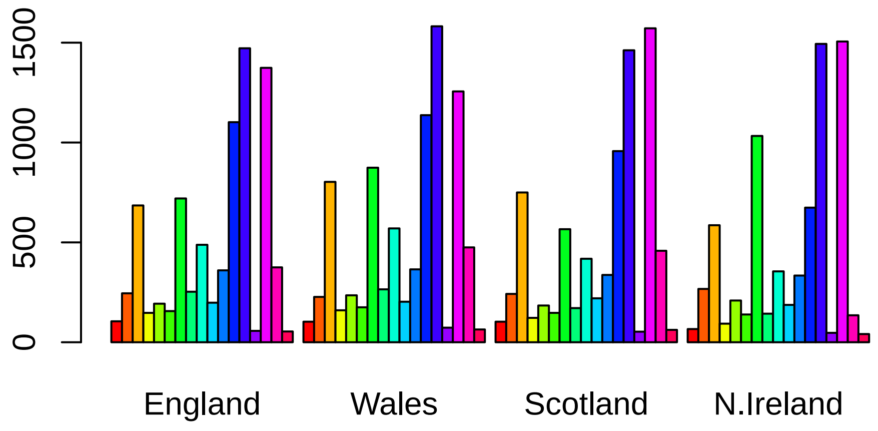
Import food data from an online CSV file:

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

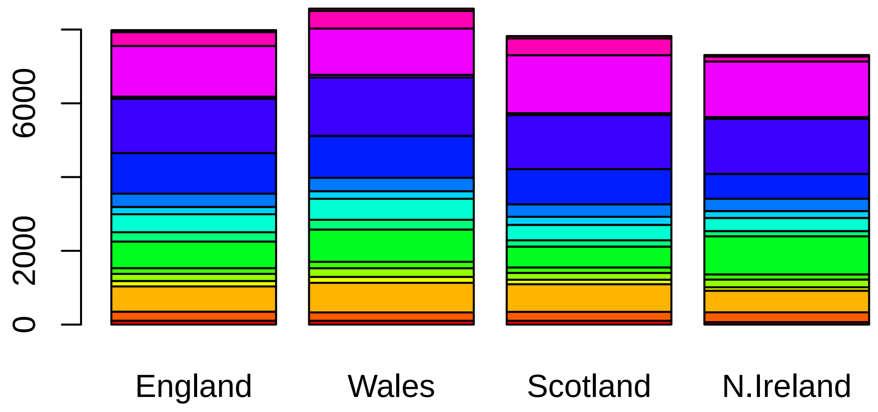
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
Fats_and_oils      193   235      184       209
Sugars  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

Some base figures

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

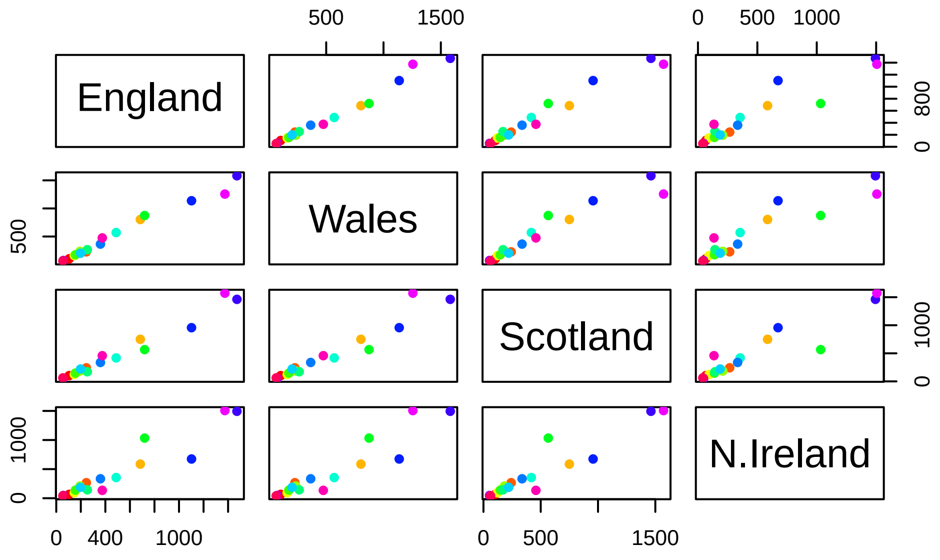


```
# Stacked bar chart - NOT useful
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



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

```
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()`.

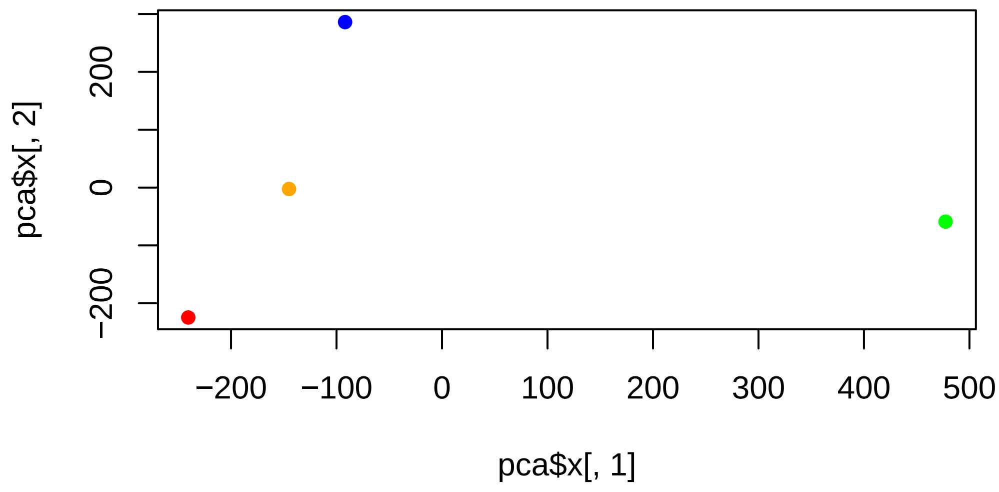
I will take the transpose of our data so the "foods" are in columns.

```
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
```

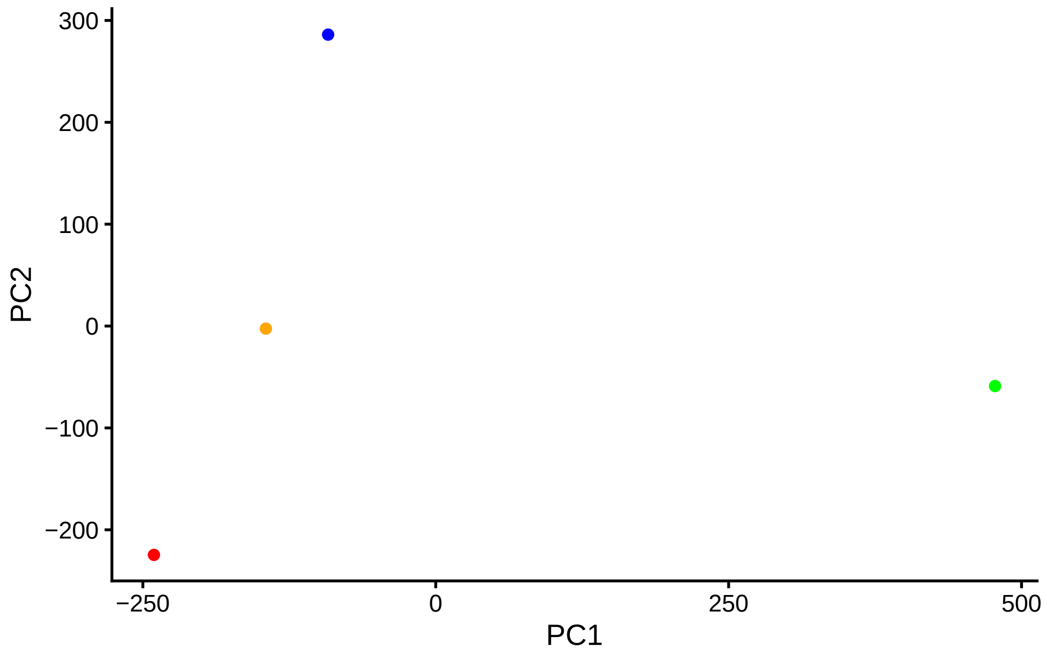
```
# See how PC1 and PC2 captured 96% of the variance -> good enough representative of the data
```

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

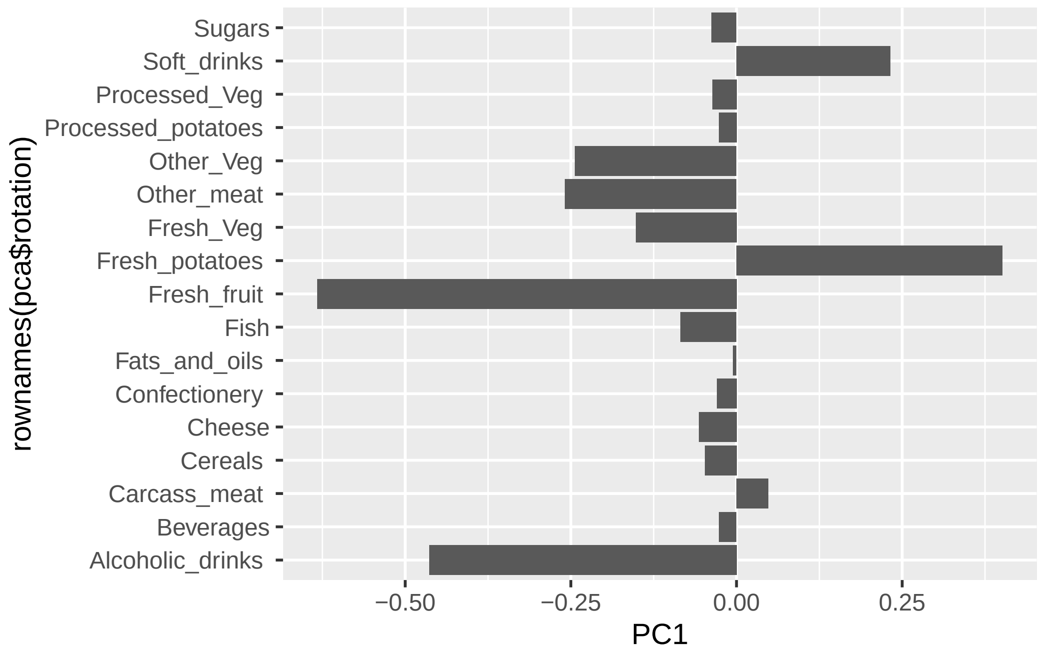


```r
library(ggplot2)
```

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



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



```r
# How much each variable weighs in the PCA
```

PCA looks really useful and we will come back to discuss this further next class (Class 8).