Class 7: Machine Learning 1

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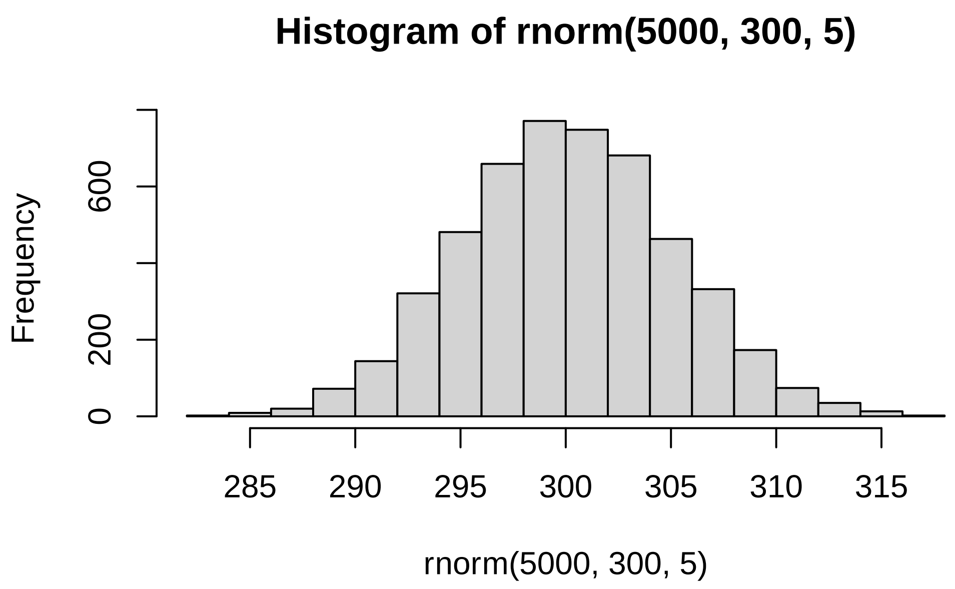
Background

Today we will begin our exploration of some important machine learning methods, namely **clusterring** and **dimensionality reduction**.

Let's make up some input data for clustering where we know what the natural "clusters" are.

The function `rnorm()` can be useful here.

```r
hist(rnorm(5000, 300, 5))
```

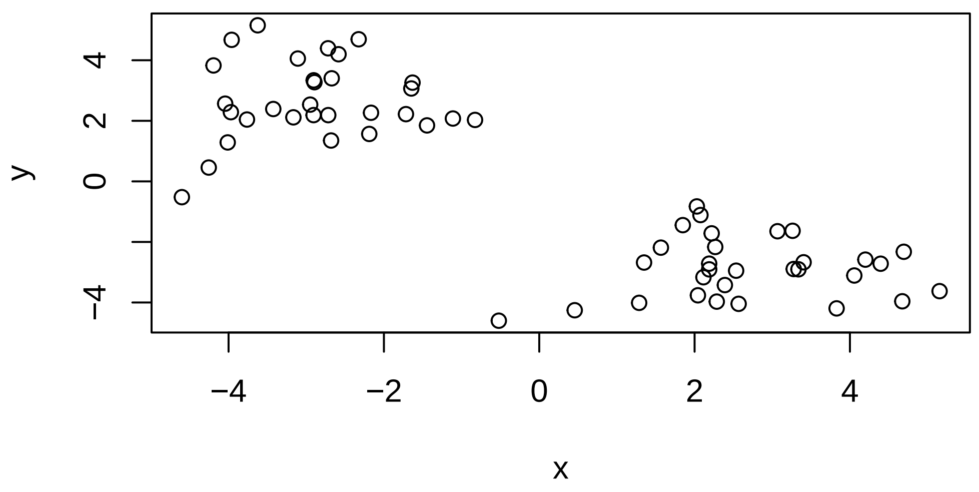


Q. Generate 30 random numbers centered at + 3 and -3

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

x <- cbind(x= tmp, y=rev(tmp))

plot(x)
```



K-means clustering

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

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

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

Cluster means:
          x         y
1 -2.873557  2.674594
2  2.674594 -2.873557

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] 76.60792 76.60792
 (between_SS / total_SS =  85.8 %)

Available components:

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

Q. What component of the results object details the cluster sizes?

```r
km$size
```

```
[1] 30 30
```

Q. What component of the results object details the cluster centers?

```r
km$centers
```

```
          x         y
1 -2.873557  2.674594
2  2.674594 -2.873557
```

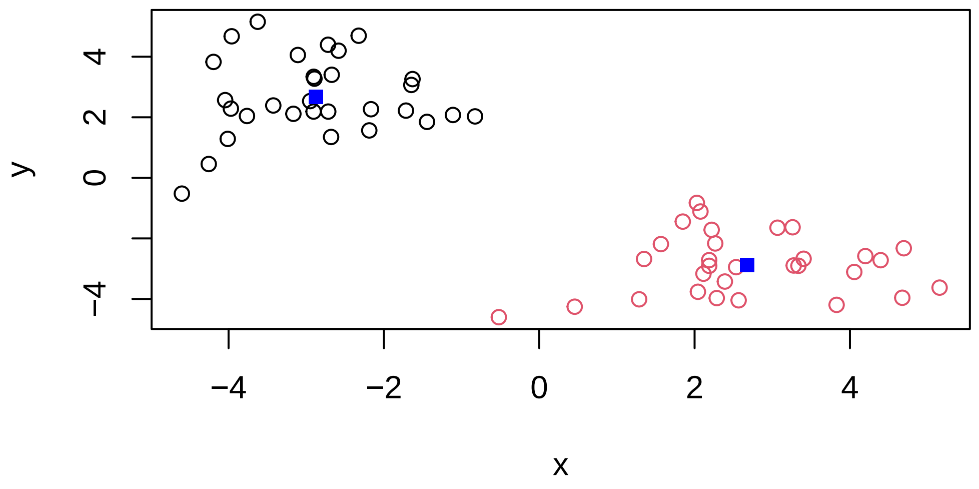
Q. What component of the results object details the cluster membership vector (i.e. our main result of which points lie in which cluster)

```r
km$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
```

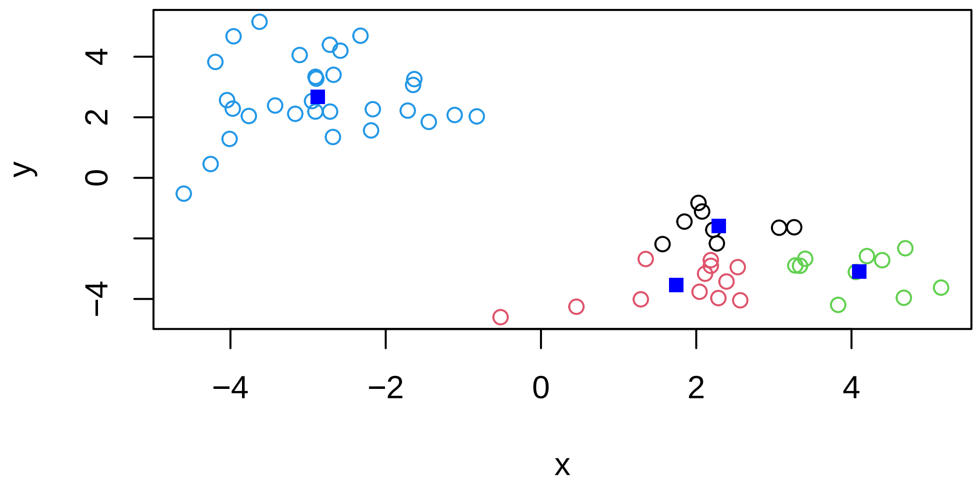
Q. Plot our clustering results with points colored by cluster and also add the cluster centers as new points colored blue?

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



Q. Run `kmeans()` again and this time produce 4 clusters and call your result object `k4`

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



The metric

```
k4$tot.withinss
```

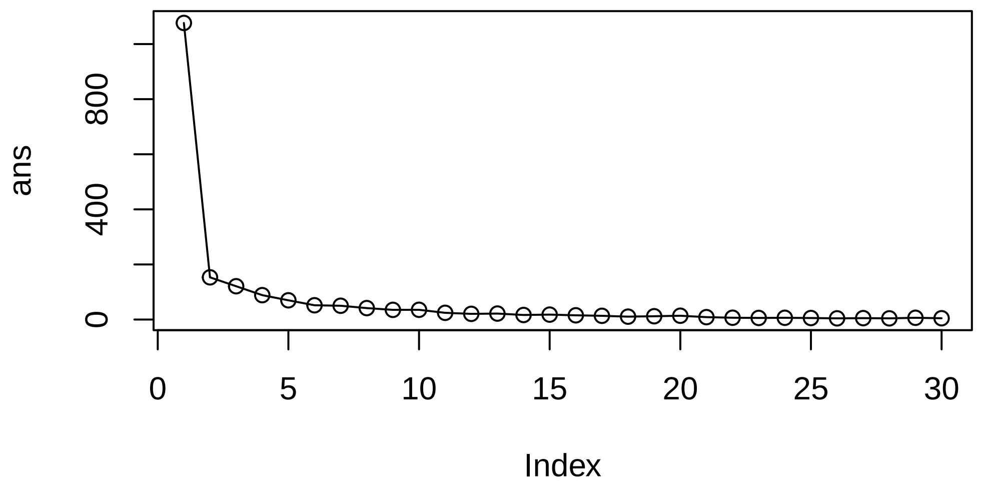
```
[1] 102.1992
```

> Q. Let's try different number of K(centers) from 1 to 30 and see what the best result is?

```
ans <- NULL
for (i in 1:30){
ans <- c(ans, kmeans(x,centers = i)$tot.withinss)
}
ans
```

```
 [1] 1076.675070  153.215848  120.890409   88.564969   69.873721   51.790720
 [7]   50.056354   41.547306   35.097239   35.334373   24.402346   20.612429
[13]   21.670084   16.574259   17.906721   15.364529   13.516267   10.500297
[19]   11.941704   13.868758    8.708025    6.595800    5.822908    6.368789
[25]    5.502479    4.368836    5.140008    4.295194    6.359370    4.731376
```

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



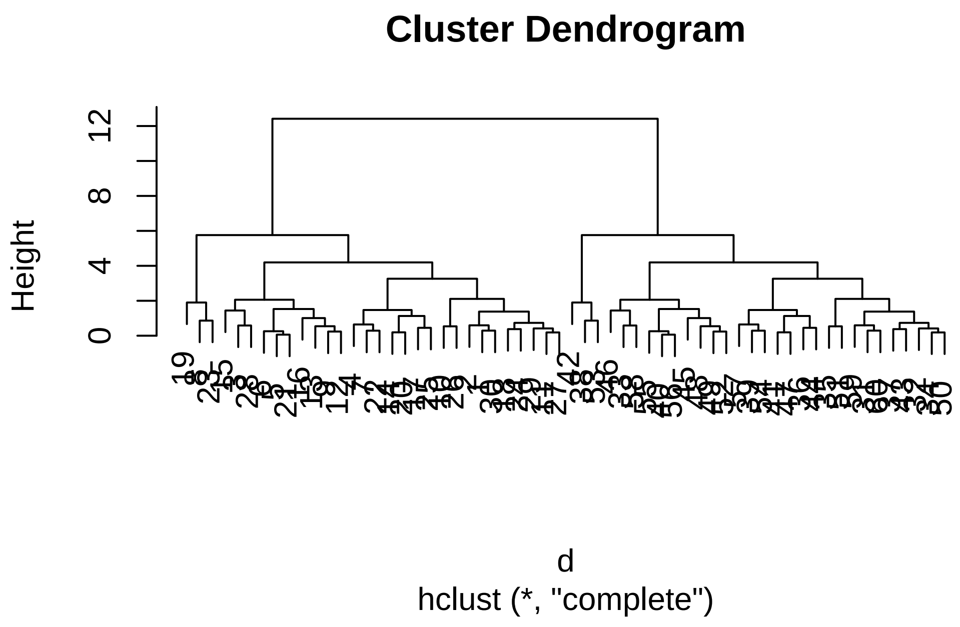
`tot.withnss` shows how tight the cluster it is. The lower the value the tighter the clusters group.

Key-Point: K-means will impose a clustering structure on your data even if it is not there - it will always give you the answer you asked for even if that answer is silly!

Hierarchical Clustering

The main function for Hierarchical Clustering is called `hclust()`. Unlike `kmeans()` (which does all the work for you) you can't just pass `hclust()` our raw input data. It needs a "distance matrix" like the one returned from the `dist()` function.

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



To extract our cluster membership vector from a `hclust()` result object we have to "cut" our tree at a given height to yield separate "groups"/"branches".

To do this we use the `cutree()` function on our `hclust()` objection:

```
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
```

```
table(grps, km$cluster)
```

```
grps  1  2
   1  0 30
   2 30  0
```

PCA of UK food data

Import the data set of food consumption in the UK

```r
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
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
7      Fresh_potatoes      720   874      566      1033
8           Fresh_Veg      253   265      171       143
9           Other_Veg      488   570      418       355
10 Processed_potatoes      198   203      220       187
11      Processed_Veg      360   365      337       334
12        Fresh_fruit     1102  1137      957       674
13            Cereals     1472  1582     1462      1494
14           Beverages      57    73       53        47
15        Soft_drinks     1374  1256     1572      1506
16   Alcoholic_drinks      375   475      458       135
17      Confectionery       54    64       62        41
```

> Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?

```r
dim(x)
```

```
[1] 17  5
```

One soltion to set the row names is by hand…

```r
#rownames(x)
rownames(x) <- x[,1]
```

To remove the first column I can use the minus index trick

```r
x <- x[,-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
```

A better way to do this is to set the row names to the first collumn with `read.csv()`

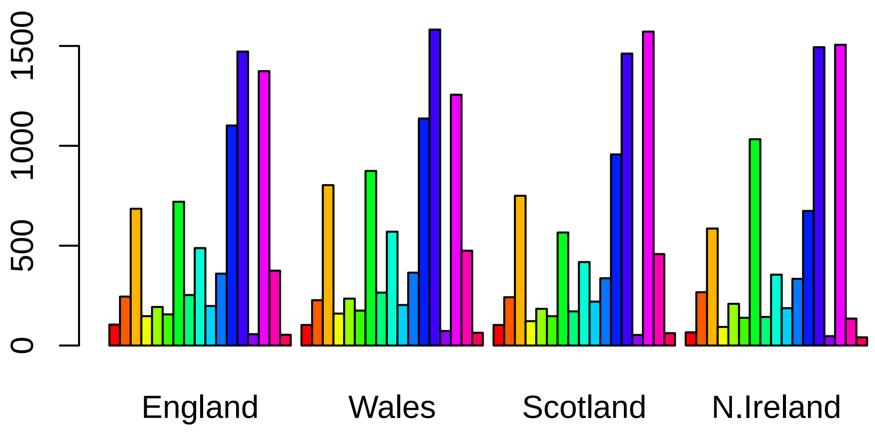
```r
x <- read.csv(url, row.names = 1)
x
```

```
                    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
```

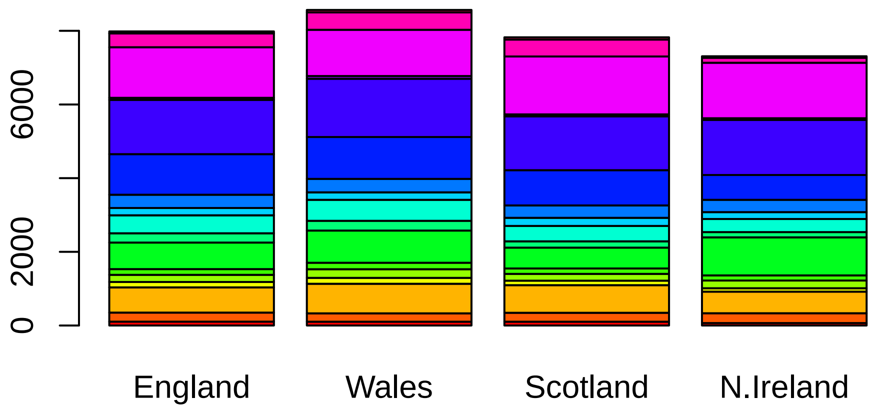
Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

Spotting major differences and trends

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

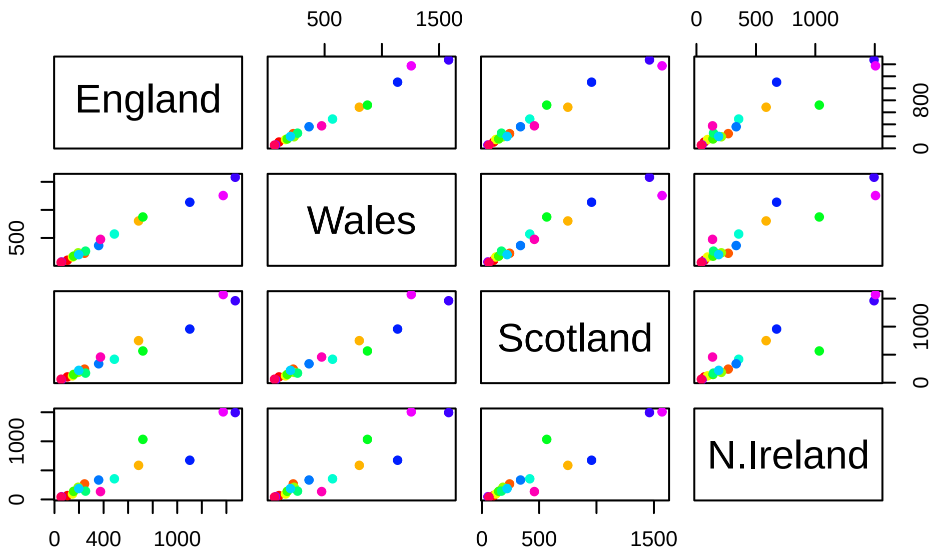


```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```

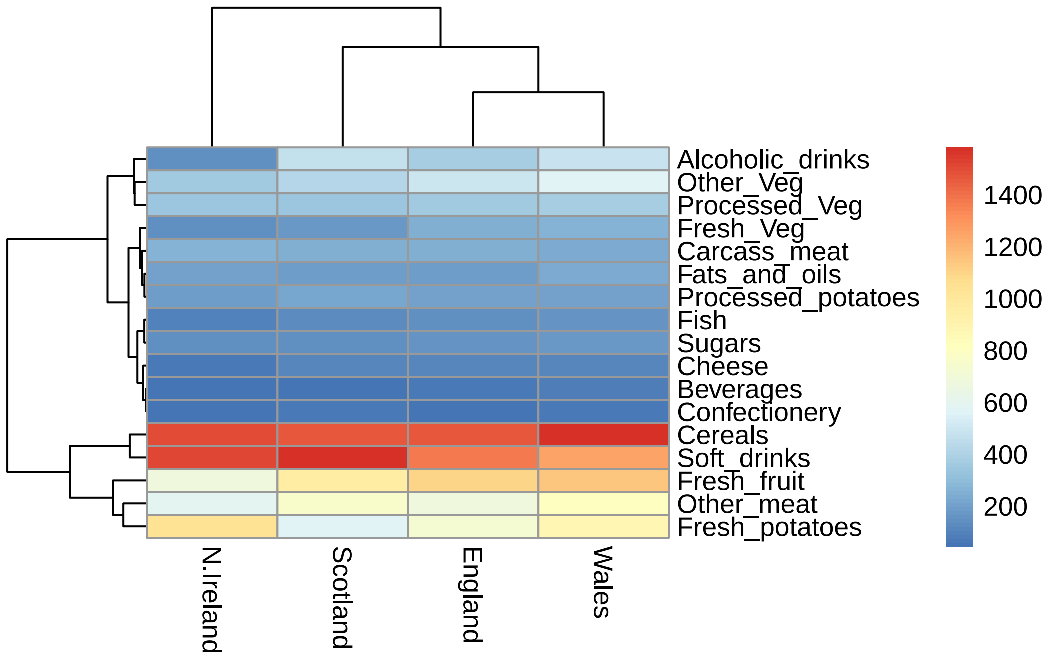


Pairs plots and heatmaps

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



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



PCA to the rescue

The main PCA function in "base R" is called `prcomp()`. This function wants the transpose of our food data as input (i.e. the foods as columns and the countries as rows).

```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
```

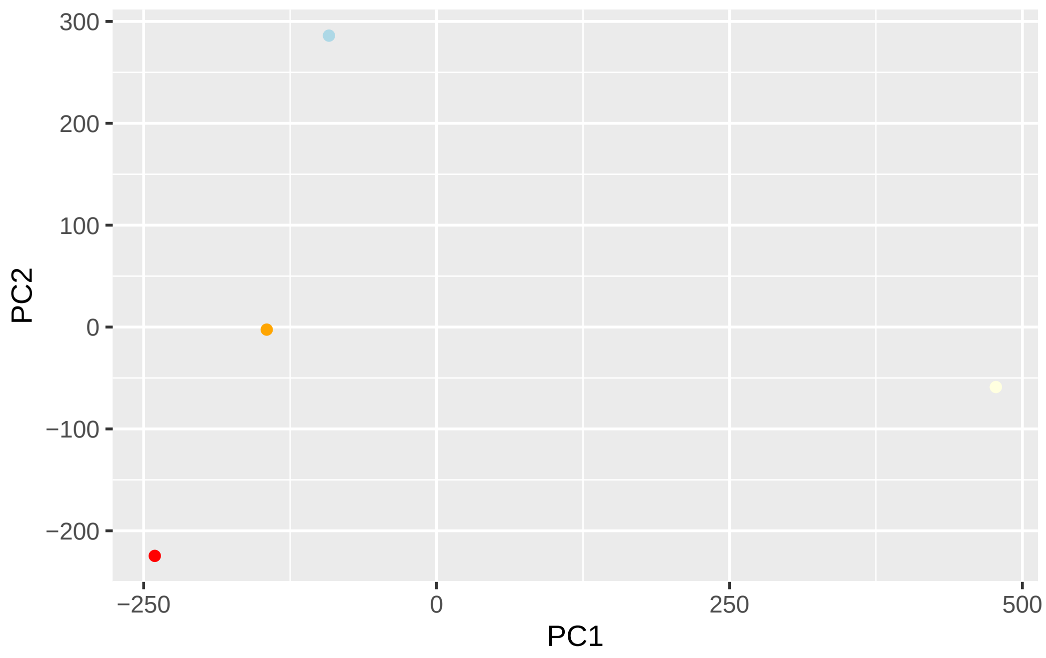
```r
attributes(pca)
```

```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"       

$class
[1] "prcomp"
```

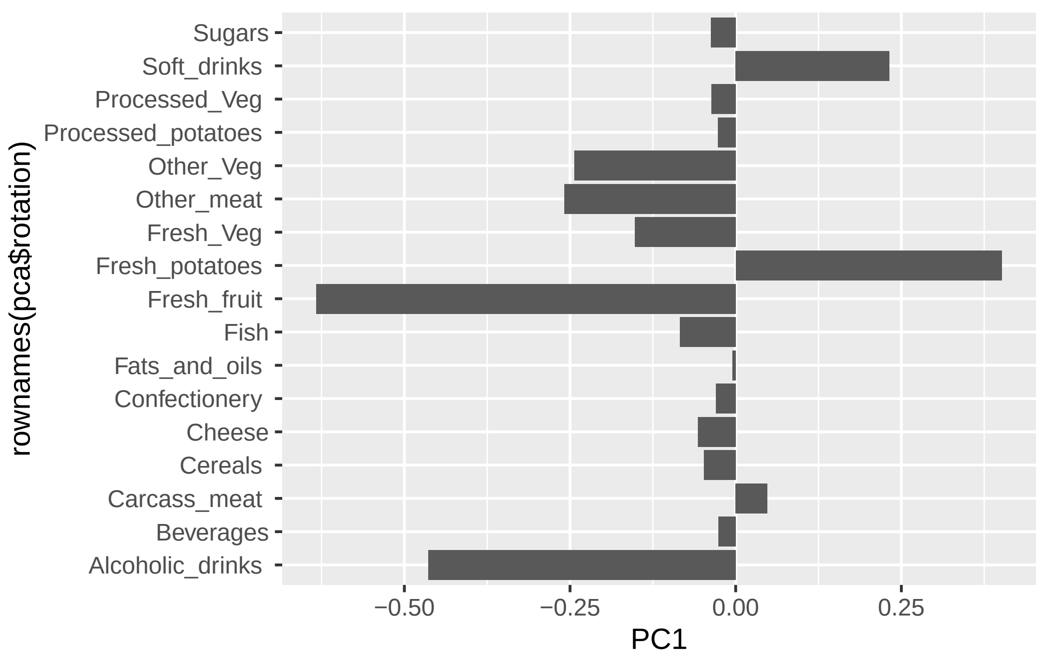
To make one of main PCA result figures we turn to `pca$x` the scores along our new PCs. This is called "PC plot" or "score plot" or "Ordination plot" …

```r
library(ggplot2)
my_cols <- c("orange", "red", "lightblue", "lightyellow")
ggplot(pca$x)+ aes(PC1,PC2, label= rownames(pca$x)) +
  geom_point(col= my_cols)
```



the second major result figure is called a "loadings plot" of "variable contributions plot" or "weight plot"

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


rownames(pca$rotation)
Sugars
Soft_drinks
Processed_Veg
Processed_potatoes
Other_Veg
Other_meat
Fresh_Veg
Fresh_potatoes
Fresh_fruit
Fish
Fats_and_oils
Confectionery
Cheese
Cereals
Carcass_meat
Beverages
Alcoholic_drinks
−0.50
−0.25
0.00
0.25
PC1