Class 7

Sabrina Koldinger (A16368238)

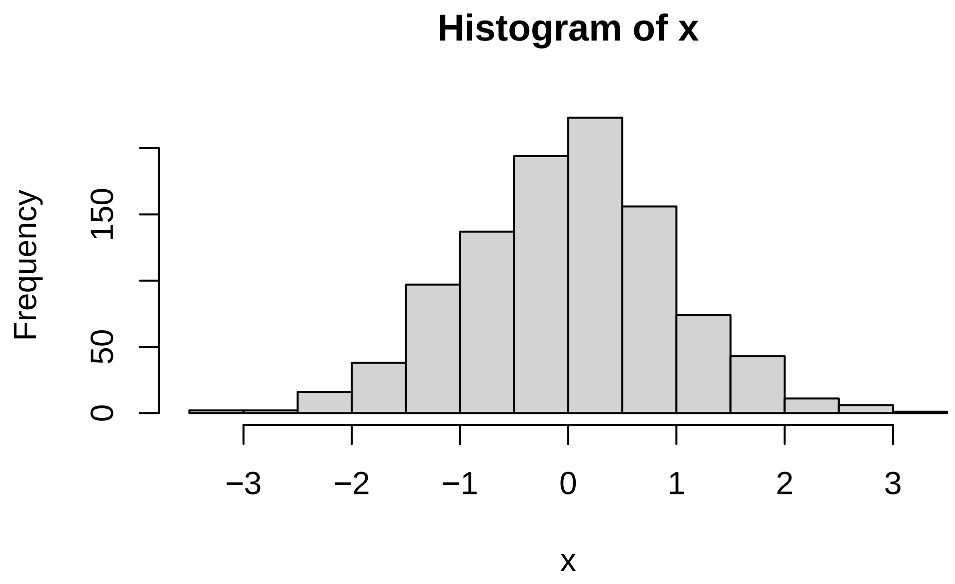
Class 7 Clustering methods

The broad goal here is to find groupings in your input data.

kmeans

First, make some data to cluster.

```
x=rnorm(1000)
hist(x)
```



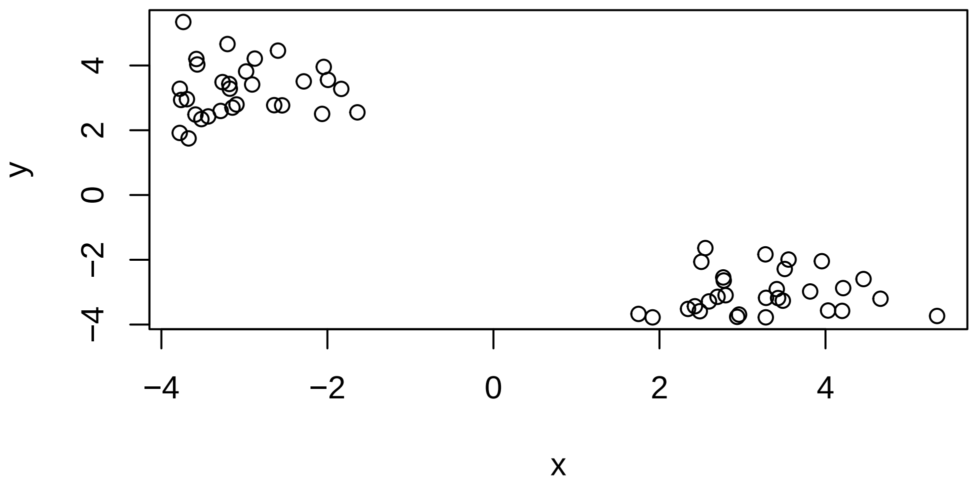
MAke a vector of length 60 with 30 points centered at -3 and 30 points centered at 3.

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

```
 [1] -1.993215 -2.545352 -3.672325 -2.906536 -3.095059 -3.517621 -3.777858
 [8] -1.832730 -2.063347 -3.761910 -3.567369 -2.284752 -3.692237 -2.978851
[15] -1.638371 -2.640830 -3.262984 -2.595547 -3.577998 -3.182104 -3.286236
[22] -3.143687 -3.435739 -3.203561 -3.735788 -2.044038 -3.778846 -3.589206
[29] -2.874677 -3.175576  3.283563  4.212834  2.485628  1.917040  3.955702
[36]  5.343970  4.662216  2.426890  2.699276  2.596221  3.428800  4.200494
[43]  4.457996  3.486060  2.774215  2.552768  3.815276  2.958822  3.508970
[50]  4.031265  2.935926  2.504427  3.276542  3.280792  2.344021  2.796407
[57]  3.413238  1.747618  2.768272  3.554944
```

I will now make a small x and y data set with 2 groups of points.

```
x= cbind(x=tmp, y=rev(tmp))
plot(x)
```



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

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

Cluster means:
          x         y
1 -3.028478  3.247340
2  3.247340 -3.028478

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] 32.15525 32.15525
 (between_SS / total_SS =  94.8 %)

Available components:

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

Question: from your result object `k` how many point are in each cluster?

```r
k$size
```

```
[1] 30 30
```

Question: What "component" of your result object details the cluster membership?

```r
k$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
```

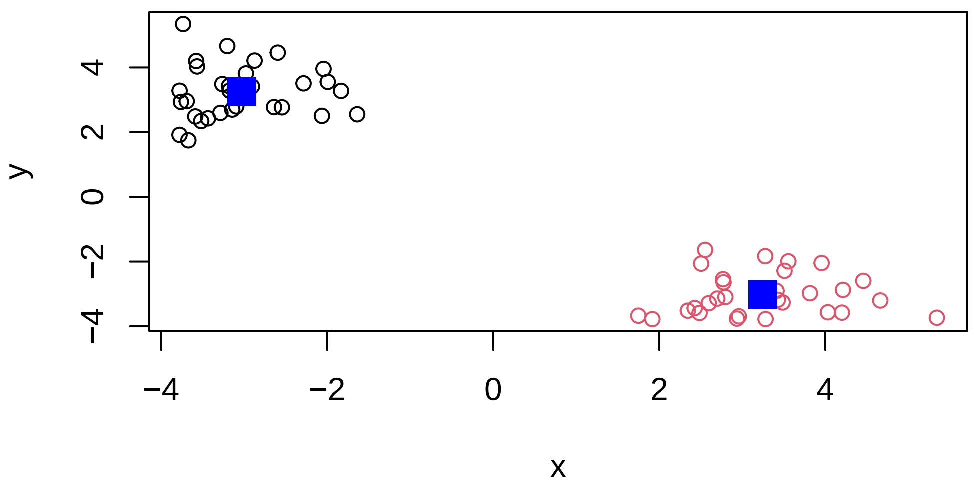
Question: what about cluster center?

```r
k$centers
```

```
          x         y
1 -3.028478  3.247340
2  3.247340 -3.028478
```

Plot clusters

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



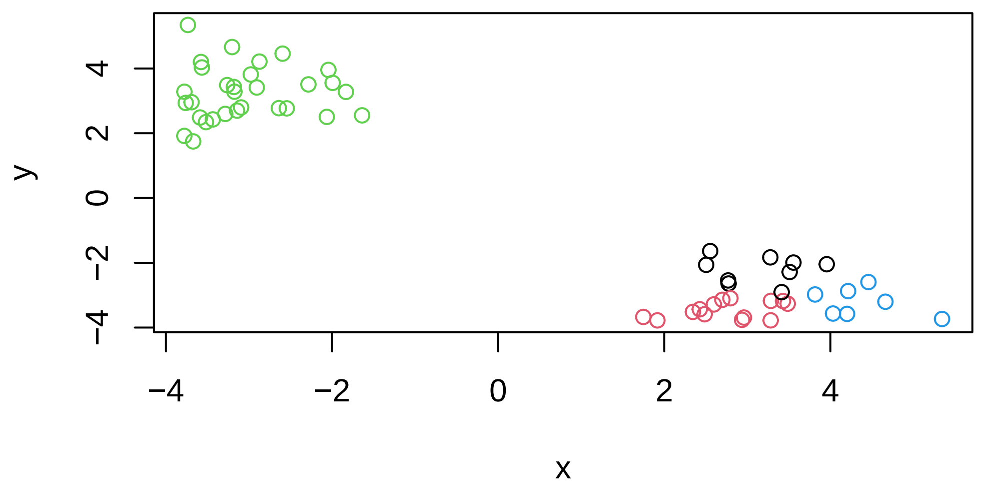
We can cluster into 4 groups

```
k4=kmeans(x,centers=4)
k4
```

```
K-means clustering with 4 clusters of sizes 9, 14, 30, 7

Cluster means:
          x         y
1  3.145453 -2.216575
2  2.741933 -3.455099
3 -3.028478  3.247340
4  4.389150 -3.219113
```

```
Clustering vector:
 [1] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 2 4 2 2 1 4 4 2
[39] 2 2 2 4 4 2 1 1 4 2 1 4 2 1 1 2 2 2 1 2 1 1

Within cluster sum of squares by cluster:
[1]  3.441073  4.585824 32.155249  2.597549
 (between_SS / total_SS =  96.6 %)

Available components:

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

```
plot(x, col=k4$cluster)
```



A big limitation of kmeans is that it does what you ask even if the clusters are silly.

hclust

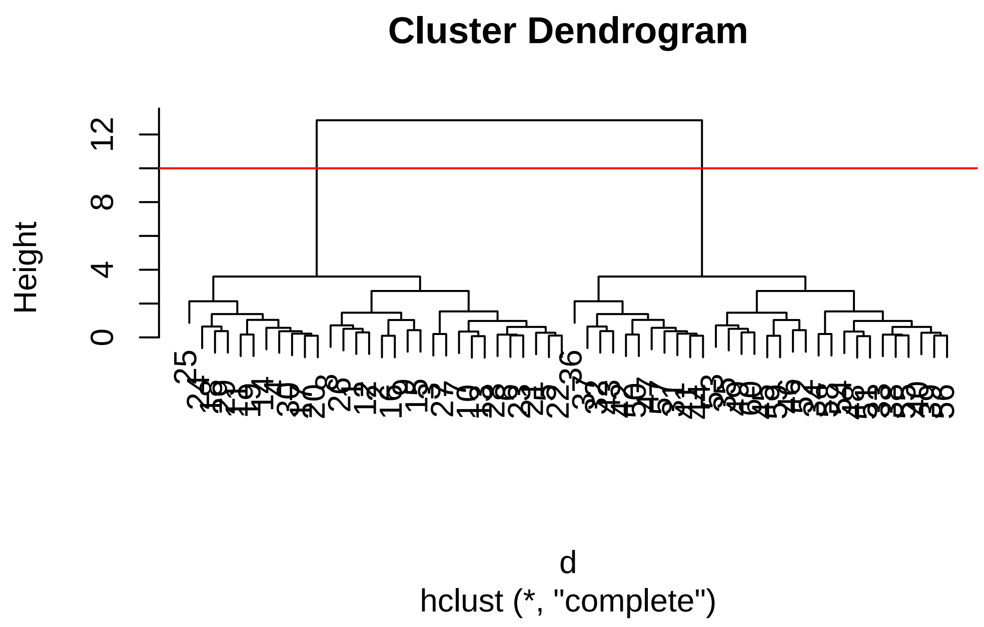
The main base R function for Hierarchical clustering is `hclust`. unlike `kmeans`, you can not just pass it your data as an input. You need to calculate a distance matrix.

```r
d=dist(x)
hc=hclust(d)
hc
```

```

Call:
hclust(d = d)

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

Use `plot()`

```r
plot(hc)
abline(h=10, col="red")
```

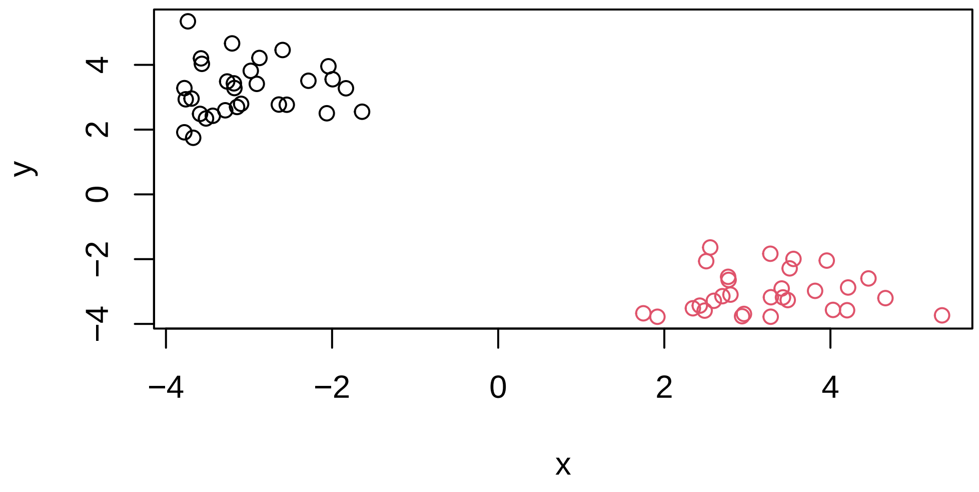


To make the "cut" and get our cluster membership vector we can use the `cutree()` function. Make a plot of our data colored by hclust results.

```
groups=cutree(hc, h=10)
groups
```

```
 [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
```

```
plot(x, col=groups)
```



PCA- Principal Component Analysis

Here we will do Principal Component Analysis (PCA) on some food data from the UK.

```
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
```

```
#dont do this
#rownames(x)=x[,1]
#x=x[,-1]
```

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

```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

```
[1] 4
```

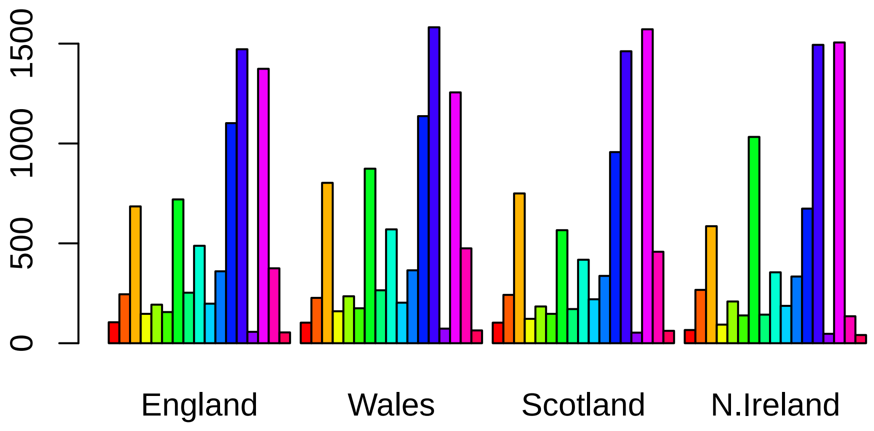
17 rows and 4 columns

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?

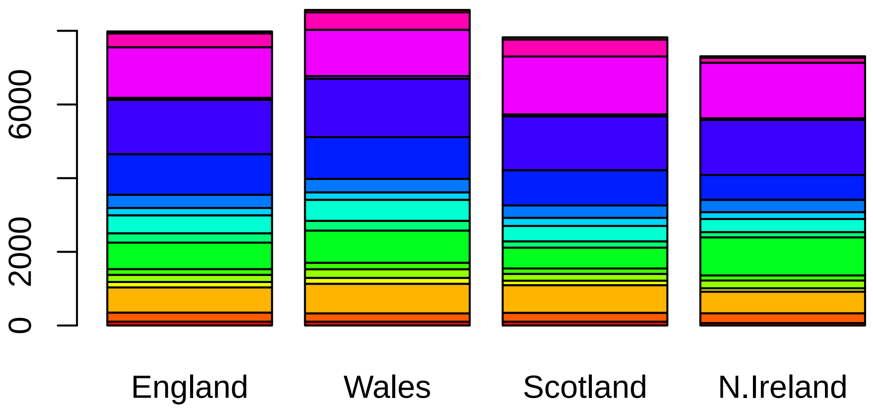
It is more effective to use the `row.names=1` since it will not end up removing columns of data if run multiple times.

Q3: Changing what optional argument in the above barplot() function results in the following plot?

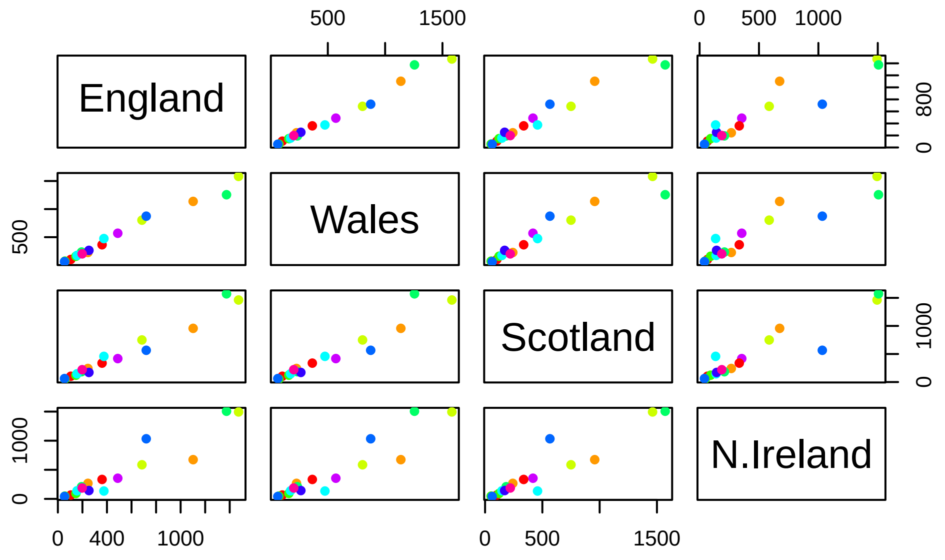
```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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



```
pairs(x, col=rainbow(10), pch=16)
```



PCA to the rescue

The main “base” R function for PCA is called `prcomp()`.

```
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
```

How much variance is captured in 2 PCs. 96.5%

To make our main “PC score plot” or PC1 vs PC2 plot”, “PC plot”, or ” ordination plot”.

```
attributes(pca)
```

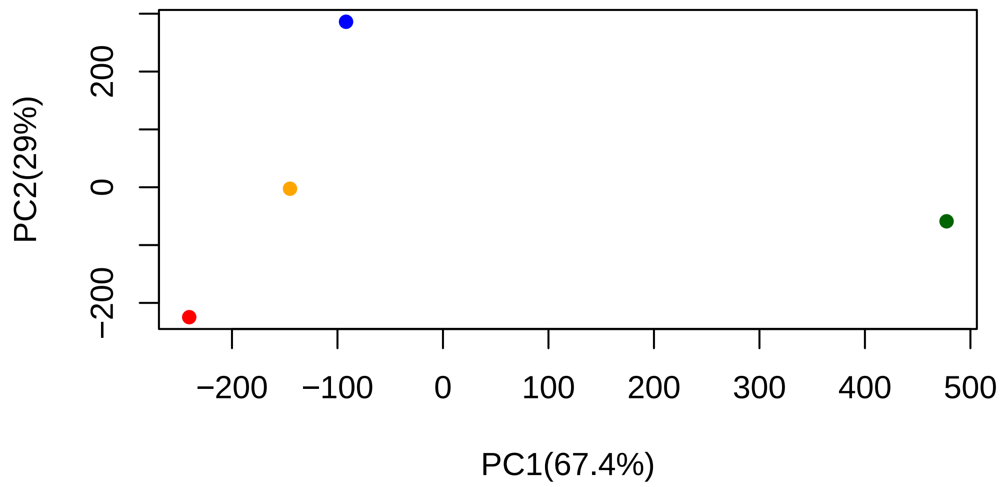
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"       

$class
[1] "prcomp"
```

We are after the `pca$x` result component to make our main PCA plot.

```
pca$x
```

```
                 PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -9.152022e-15
Wales     -240.52915 -224.646925 -56.475555  5.560040e-13
Scotland   -91.86934  286.081786 -44.415495 -6.638419e-13
N.Ireland  477.39164  -58.901862  -4.877895  1.329771e-13
```

```
mycols=c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=mycols, pch=16, xlab="PC1(67.4%)", ylab="PC2(29%)")
```



Another important result from PCA is how the original variables (in this case foods) contribute to the PCs. This is contained in the `pca$rotation` object- people often call this the "loadings" or "contributions" to the PCs.

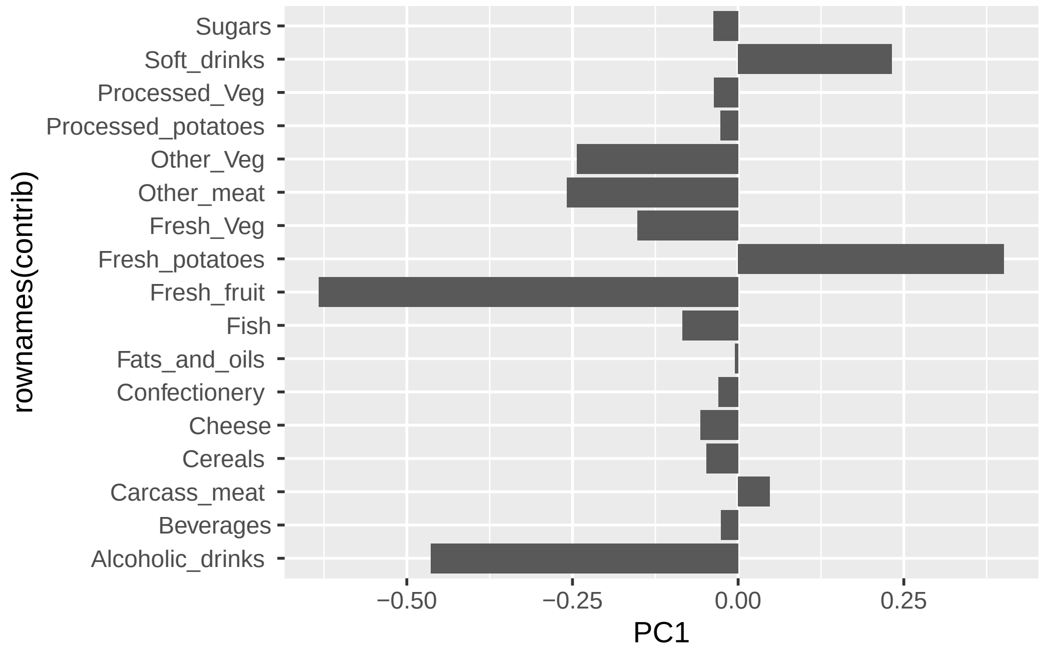
```
pca$rotation
```

```
                            PC1          PC2         PC3          PC4
Cheese             -0.056955380  0.016012850  0.02394295 -0.409382587
Carcass_meat        0.047927628  0.013915823  0.06367111  0.729481922
Other_meat         -0.258916658 -0.015331138 -0.55384854  0.331001134
Fish               -0.084414983 -0.050754947  0.03906481  0.022375878
Fats_and_oils      -0.005193623 -0.095388656 -0.12522257  0.034512161
Sugars             -0.037620983 -0.043021699 -0.03605745  0.024943337
Fresh_potatoes      0.401402060 -0.715017078 -0.20668248  0.021396007
Fresh_Veg          -0.151849942 -0.144900268  0.21382237  0.001606882
Other_Veg          -0.243593729 -0.225450923 -0.05332841  0.031153231
Processed_potatoes -0.026886233  0.042850761 -0.07364902 -0.017379680
Processed_Veg      -0.036488269 -0.045451802  0.05289191  0.021250980
Fresh_fruit        -0.632640898 -0.177740743  0.40012865  0.227657348
Cereals            -0.047702858 -0.212599678 -0.35884921  0.100043319
Beverages          -0.026187756 -0.030560542 -0.04135860 -0.018382072
Soft_drinks         0.232244140  0.555124311 -0.16942648  0.222319484
```

```
Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.273126013
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001890737
```

We can make a plot along PC1

```
library(ggplot2)
contrib= as.data.frame(pca$rotation)
ggplot(contrib)+ aes(PC1, rownames(contrib))+geom_col()
```


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
rownames(contrib)
PC1