Class 7: Machine Learning 1

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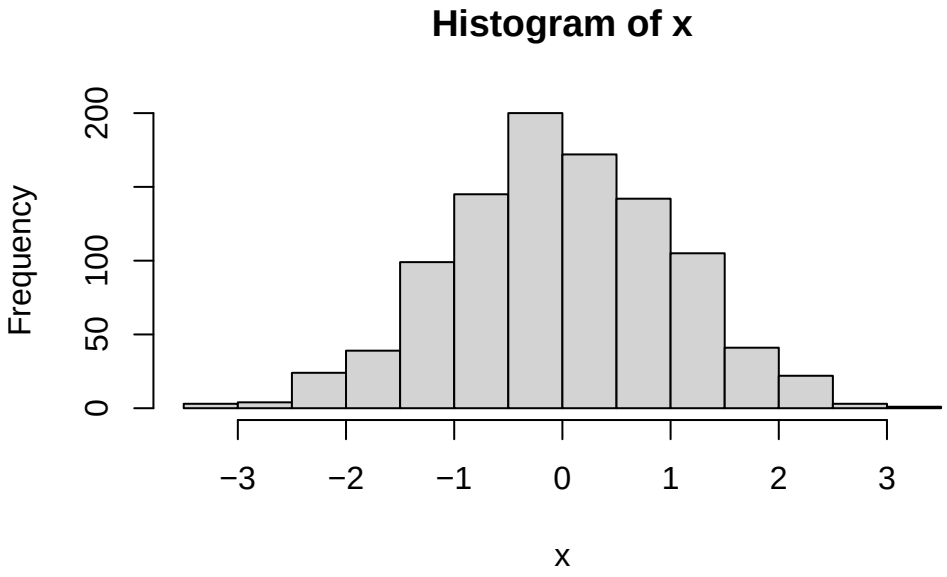
Clustering Methods

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

Kmeans

First, let's make up some data to cluster.

```
x <- rnorm(1000)
hist(x)
```

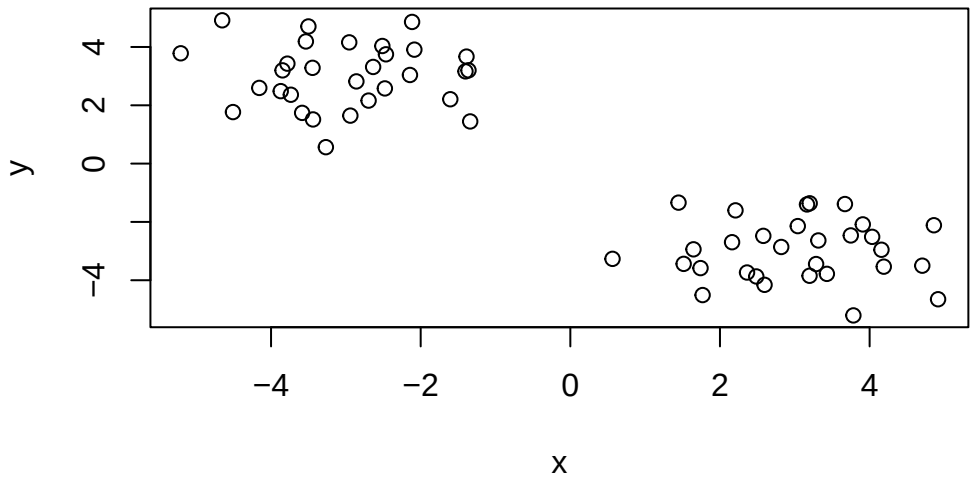


Make a vector of length 60 with 30 points centered at -3 and 30 points centered at +3.

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

I will now make a wee x and y dataset with 2 groups of points

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




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

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

Cluster means:
          x         y
1 -2.983616  3.016247
2  3.016247 -2.983616

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 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] 65.7638 65.7638
 (between_SS / total_SS =  89.1 %)

Available components:

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

Q. From your result object 'k', how many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q. What "component" of your result object details the cluster membership?

```
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 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
```

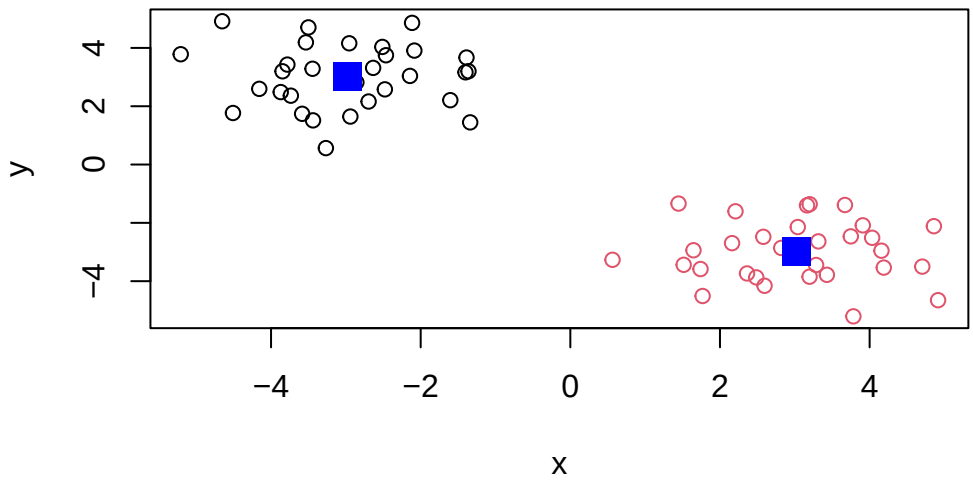
Q. Cluster centers?

```
k$centers
```

```
          x         y
1 -2.983616  3.016247
2  3.016247 -2.983616
```

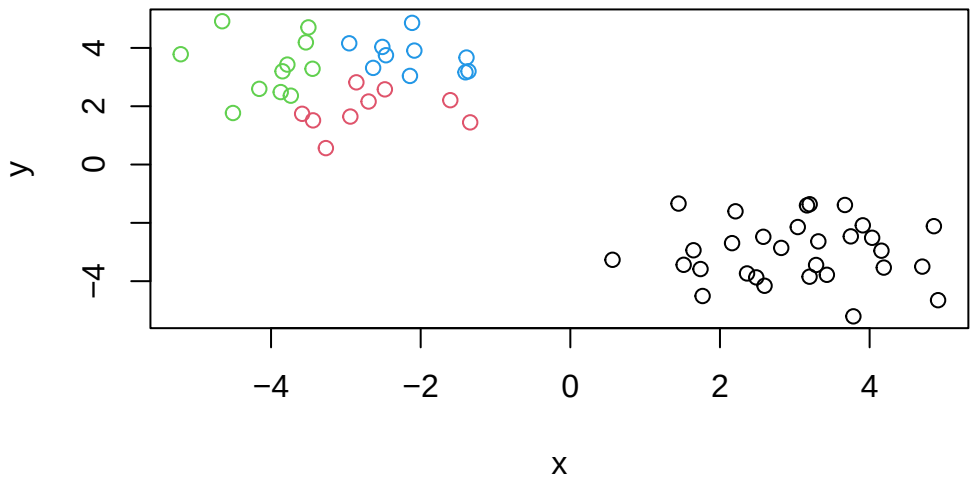
Q. Plot of our clustering results

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



We can cluster data into 4 groups.

```
# kmeans
k4 <- kmeans(x, centers=4)
# plot results
plot(x, col=k4$cluster)
```



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

Hierarchical Clustering

The main base R function for Hierarchical Clustering is `hclust()`. Unlike `kmeans()`, you cannot just pass it your data as input. You first need to calculate a distance matrix.

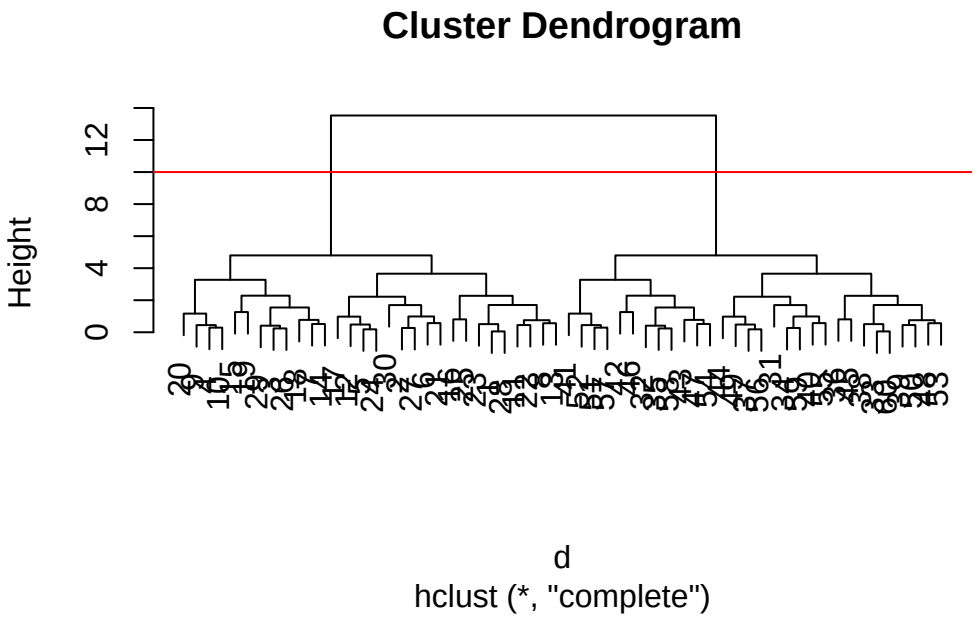
```
d <- dist(x)
hc <- hclust(d)
hc
```

```
Call:
hclust(d = d)

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

Use `plot()` to view results

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



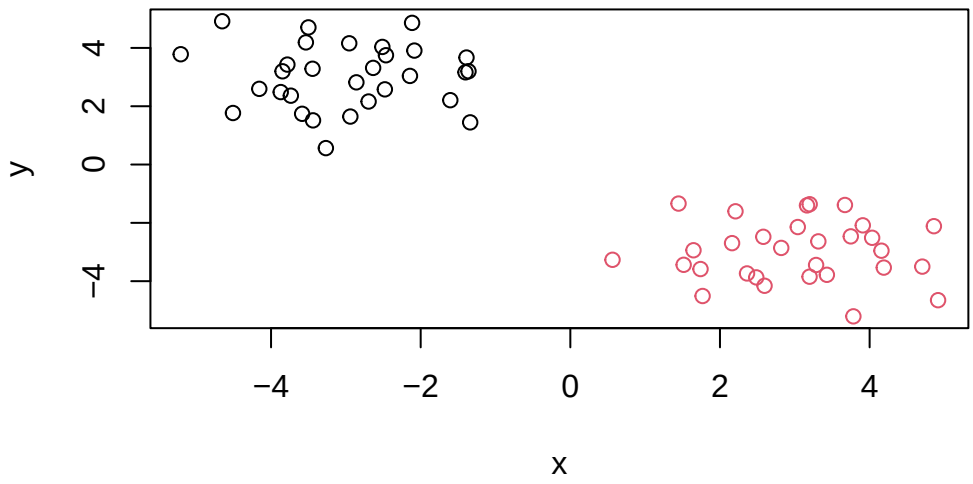
To make the "cut" and get our cluster membership vector we can use the `cutree()` function

```
grps <- cutree(hc, h=10)
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 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
```

Make a plot of our data colored by hclust results.

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



Principal Component Analysis (PCA)

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)
```

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

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

```
dim(x)
```

```
[1] 17  4
```

```
##Preview the first 6 rows
head(x)
```

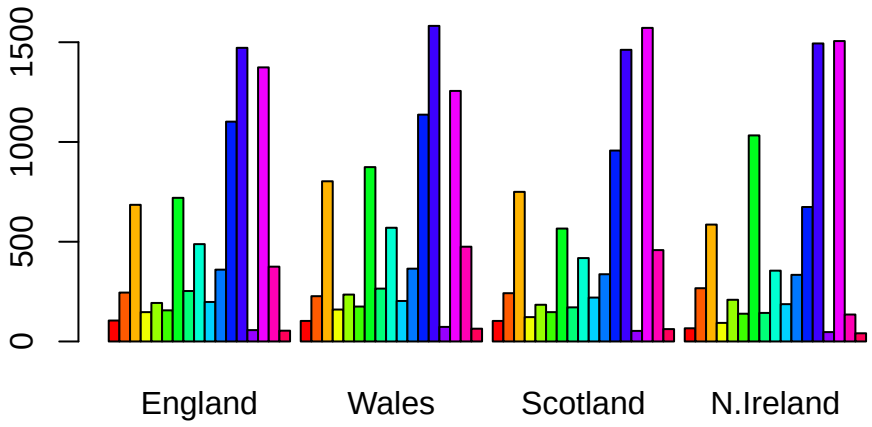
	England	Wales	Scotland	N.Ireland
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139

> 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?

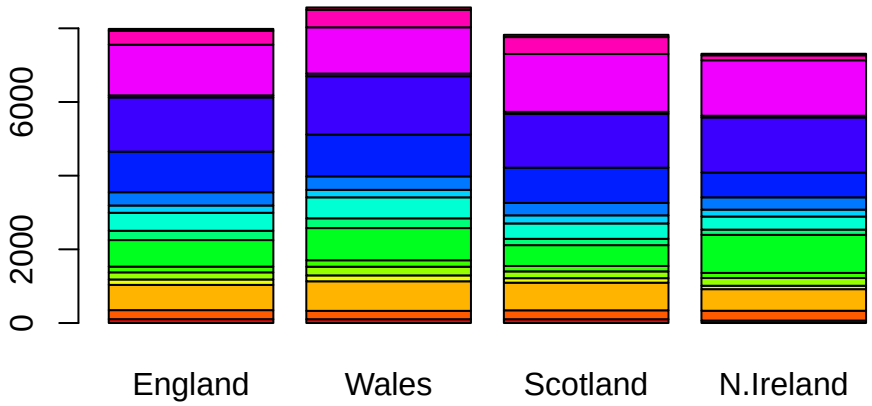
Setting the row.names argument is preferred, because the `rownames()` function will consistently delete the first row each time you run it.

> 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)))
```

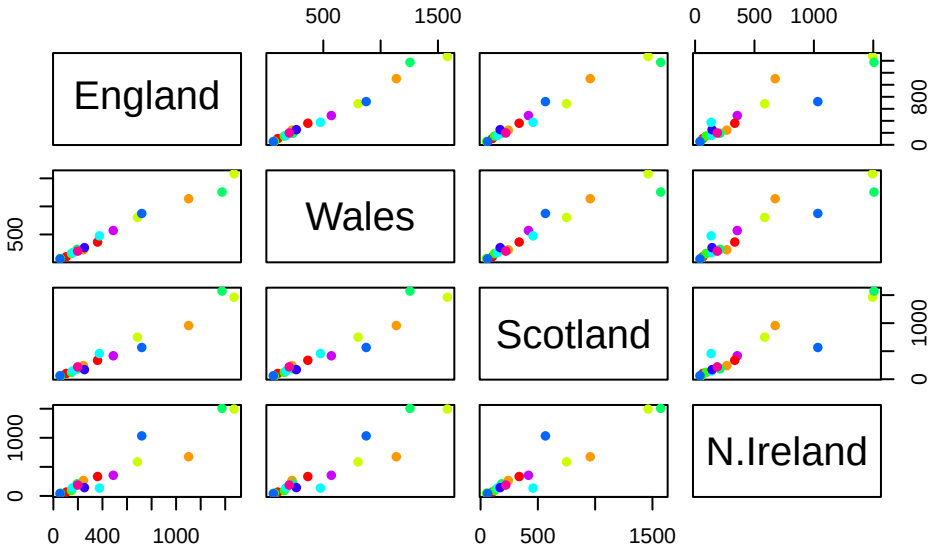


Changing `beside=T` to `beside=F`results in the correct barplot.

> Q5: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

If a point is on the diagonal, that means the values are all very similar (i.e. match the average). If a point is far from that diagonal, this means it deviates from the norm.

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



If a point lies on the diagonal,

> Q6: What is the main difference between N.Ireland and the other countries of the UK in terms of this data-set?

N. Ireland tends to consume less alcoholic beverages and fresh fruit and consumes more fresh potatoes and soft drinks.

PCA to the rescue

The main "base" R function for PCA is called `prcomp()`. Here we need to take the transpose of the data to switch the rows and columns.

```
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
```

Q: How much variance is captured in 2 PCs

96.5%

To make our main "PC score plot" (aka or "PC1 vs PC2 plot" or "PC plot" or "Coordination plot").

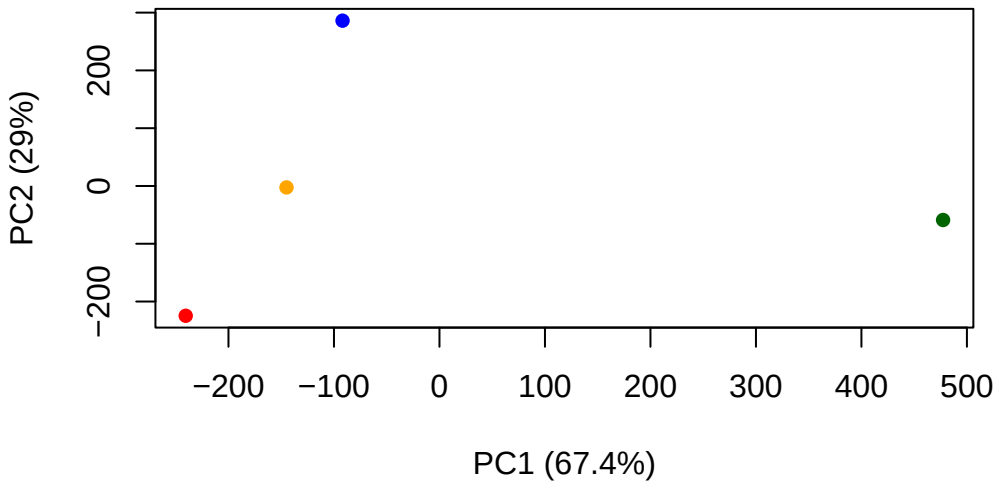
```
attributes(pca)
```

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

$class
[1] "prcomp"
```

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

```
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: the foods) contribute to the PCs.

This is contained in the `pca$rotation` object - folks often call this the "loadings" or "contributions" to the PCs.

```
pca$rotation
```

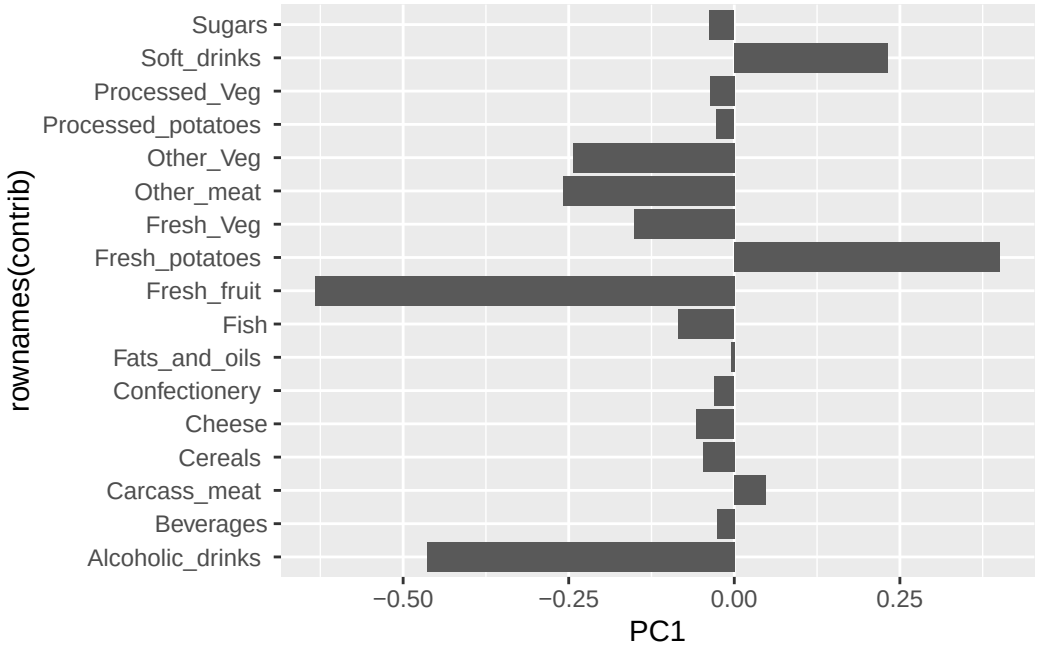
```
                           PC1          PC2         PC3          PC4
Cheese              -0.056955380  0.016012850  0.02394295 -0.694538519
Carcass_meat         0.047927628  0.013915823  0.06367111  0.489884628
Other_meat          -0.258916658 -0.015331138 -0.55384854  0.279023718
Fish                -0.084414983 -0.050754947  0.03906481 -0.008483145
Fats_and_oils       -0.005193623 -0.095388656 -0.12522257  0.076097502
Sugars              -0.037620983 -0.043021699 -0.03605745  0.034101334
Fresh_potatoes       0.401402060 -0.715017078 -0.20668248 -0.090972715
Fresh_Veg           -0.151849942 -0.144900268  0.21382237 -0.039901917
Other_Veg           -0.243593729 -0.225450923 -0.05332841  0.016719075
Processed_potatoes  -0.026886233  0.042850761 -0.07364902  0.030125166
Processed_Veg       -0.036488269 -0.045451802  0.05289191 -0.013969507
Fresh_fruit         -0.632640898 -0.177740743  0.40012865  0.184072217
Cereals             -0.047702858 -0.212599678 -0.35884921  0.191926714
Beverages           -0.026187756 -0.030560542 -0.04135860  0.004831876
Soft_drinks          0.232244140  0.555124311 -0.16942648  0.103508492
Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.316290619
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001847469
```

We can make a plot along PC1.

```
library(ggplot2)

contrib <- as.data.frame(pca$rotation)

ggplot(contrib) +
  aes(PC1, rownames(contrib)) +
  geom_col()
```


rownames(contrib)
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