Class 07: Machine Learning

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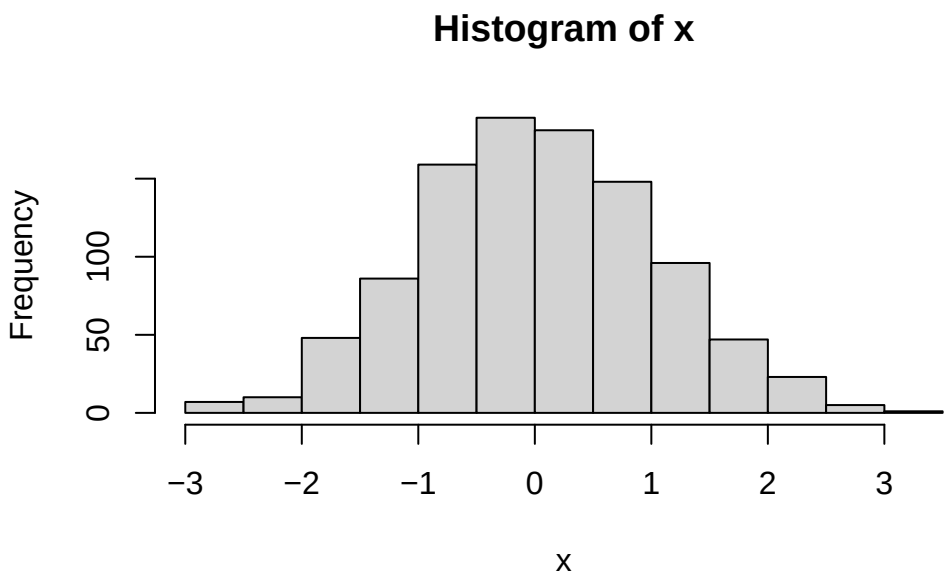
Clustering Methods

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

Kmeans

First, let's make up some data

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

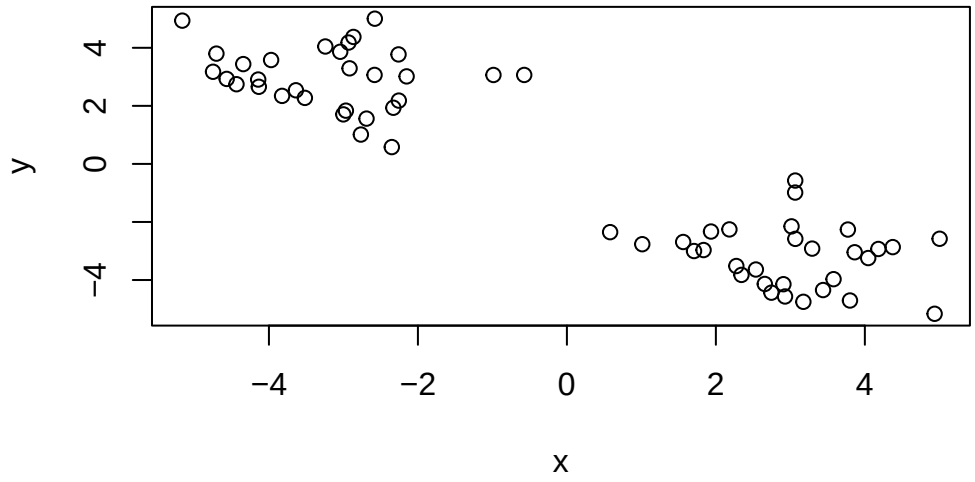


Make a vector of length 60 with 30 points centered at -3 and 30 points centered at +3

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

I will now make a 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 -3.189607  2.962623
2  2.962623 -3.189607

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] 66.84807 66.84807
 (between_SS / total_SS =  89.5 %)

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 2
```

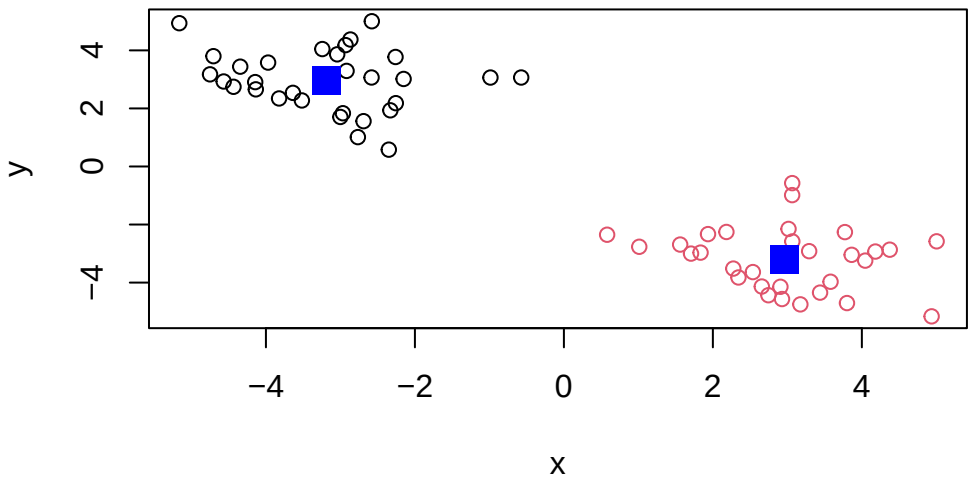
Q. Cluster centers?

```
k$centers
```

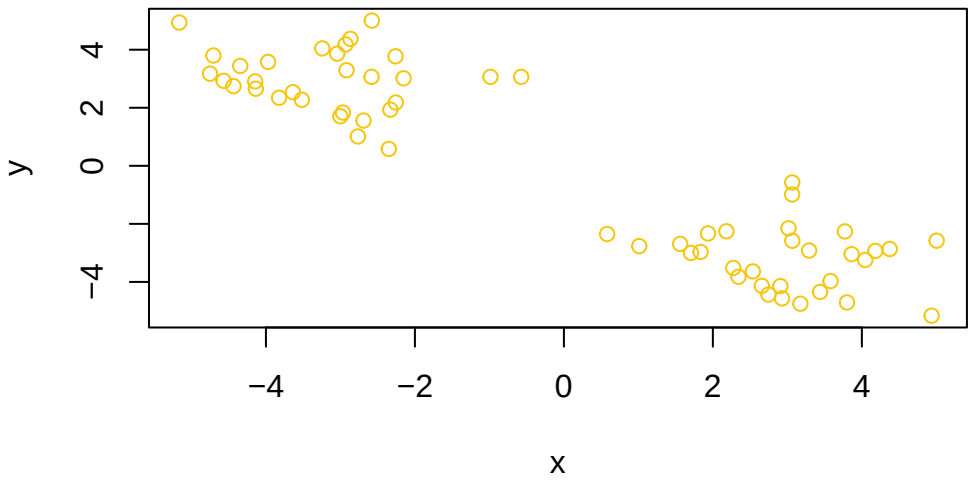
```
          x         y
1 -3.189607  2.962623
2  2.962623 -3.189607
```

Q. Plot of our clustering results

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




```
plot(x, col=7)
```

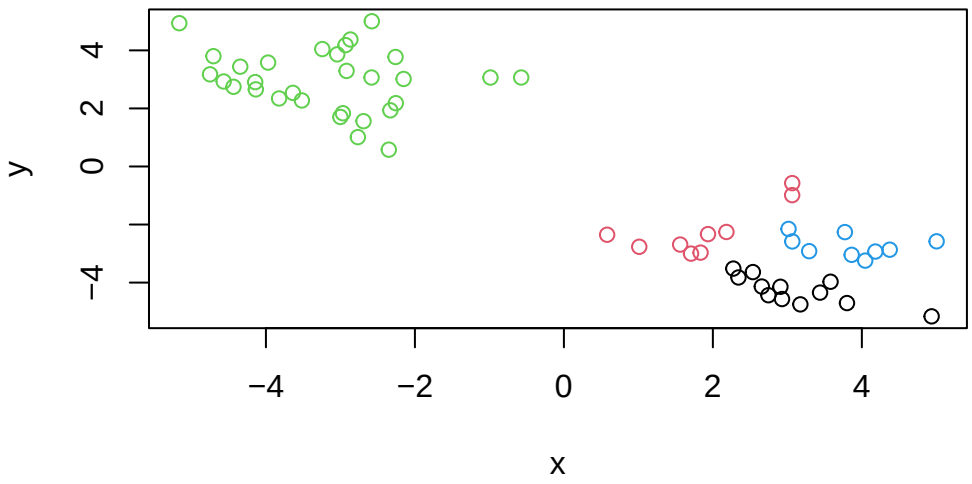


We can cluster into 4 groups

```r
# kmeans
k4 <- kmeans(x, centers = 4)
k4
```

```
K-means clustering with 4 clusters of sizes 12, 9, 30, 9

Cluster means:
          x         y
1  3.110277 -4.266340
2  1.882276 -2.213219
3 -3.189607  2.962623
4  3.846096 -2.730352

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 4 4 1 1 4 4 1 4
[39] 2 1 1 2 1 1 1 1 1 2 4 2 2 1 2 4 2 4 4 1 2 2

Within cluster sum of squares by cluster:
[1]  8.800224 11.429589 66.848069  4.437106
 (between_SS / total_SS =  92.8 %)

Available components:

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

```r
# 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

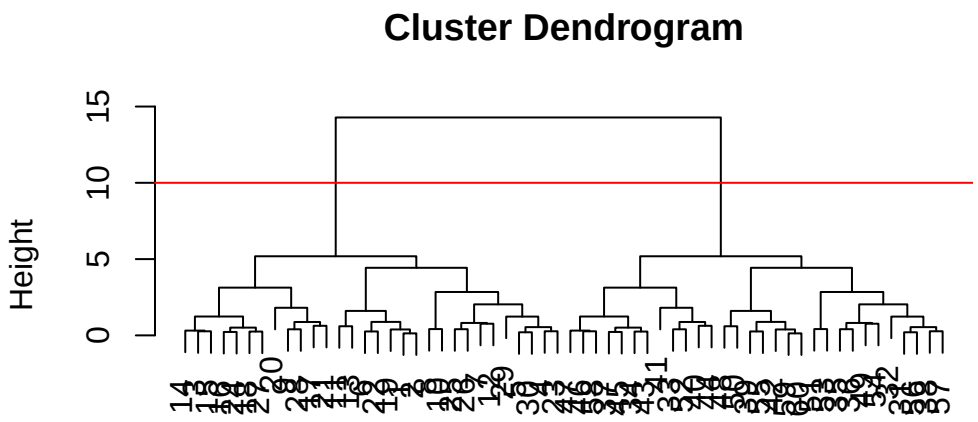
The main base R function for Hierarchical Clustering is `hclust()` Unlike `kmeans()` you can not just pass it your data as input. You first need to calculate a distance matrix.

```
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")
```



d
hclust (*, "complete")

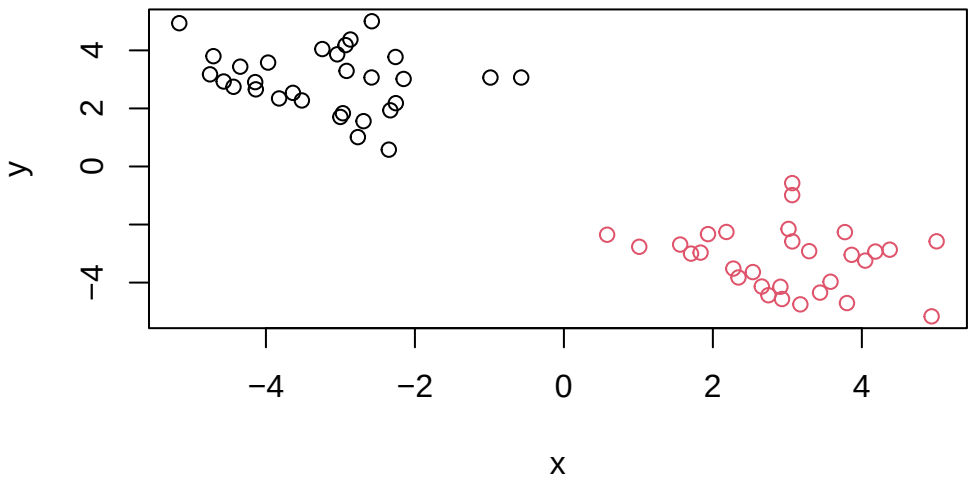
To make the "cut" and get our cluster membership vector we can use the `cutree()` function.

```
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
```

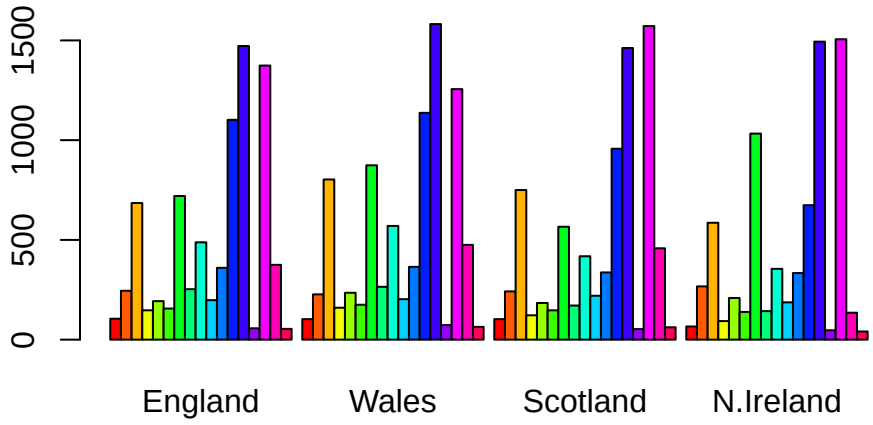
Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?

```
dim(x)
```

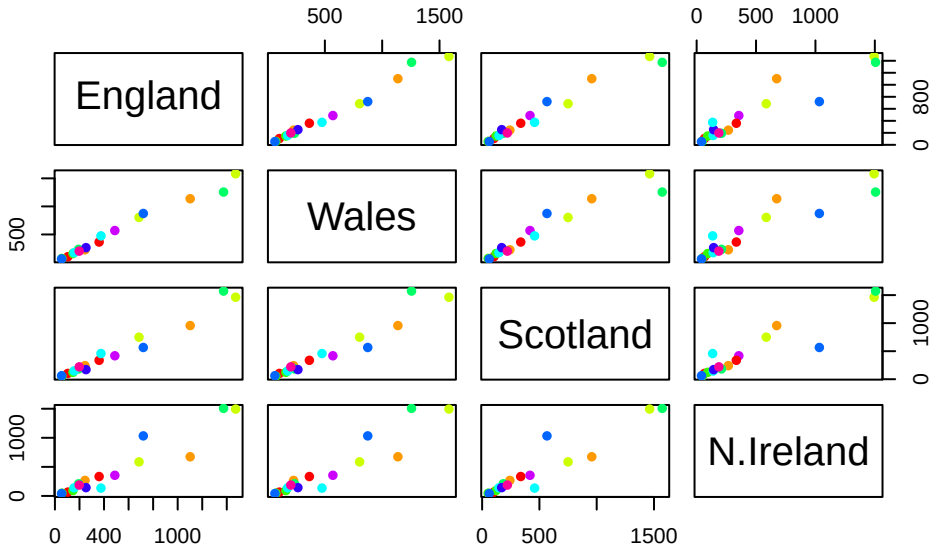
```
[1] 17  4
```

There are 17 rows and 4 columns in my x date frame

```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
barplot(as.matrix(x), beside=T, 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()`. Here we need to take the transpose of our input so countries are in the rows and food as the 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? A. 96.5%

To make our main "PC score plot" (a.k.a "PC1 vs PC2 plot" or "PC plot" or "ordination plot").

```
attributes(pca)
```

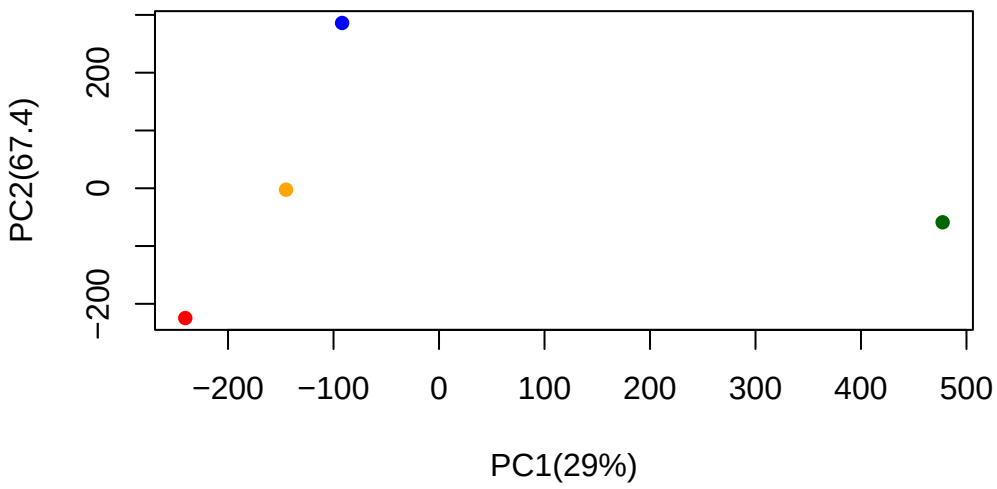
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$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 -4.894696e-14
Wales     -240.52915 -224.646925 -56.475555  5.700024e-13
Scotland   -91.86934  286.081786 -44.415495 -7.460785e-13
N.Ireland  477.39164  -58.901862  -4.877895  2.321303e-13
```

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



Another important result from PCA is how the original variables (in this case the food) contribute to the PCA.

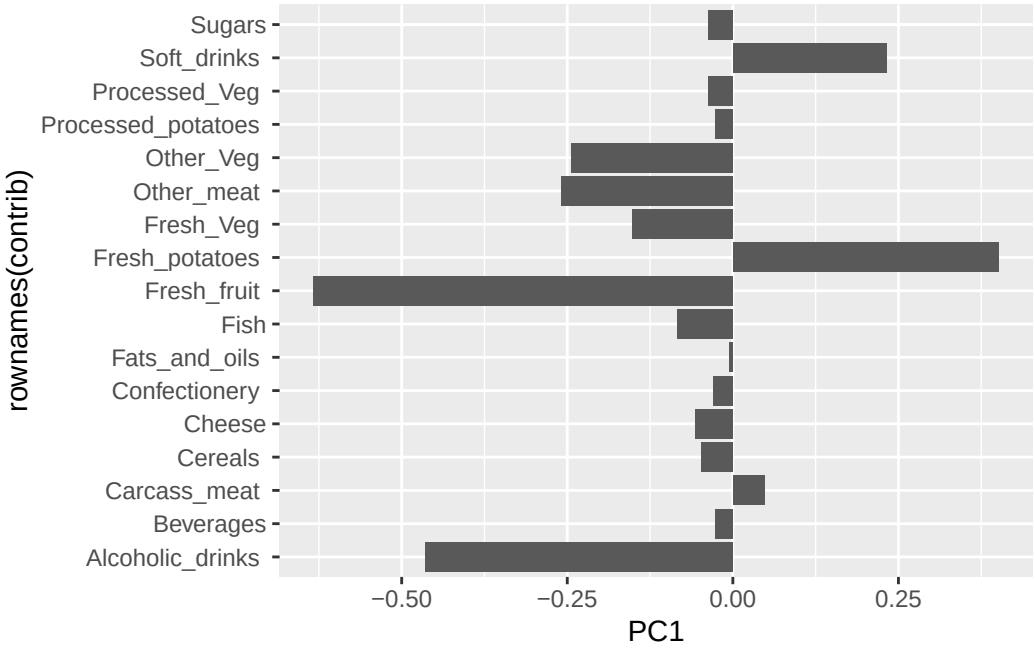
This is contained in the `pca$rotation` onject - folks often call this the "loadings" or "contributions" to the PCS

```
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