Class 7: Machine Learning 1

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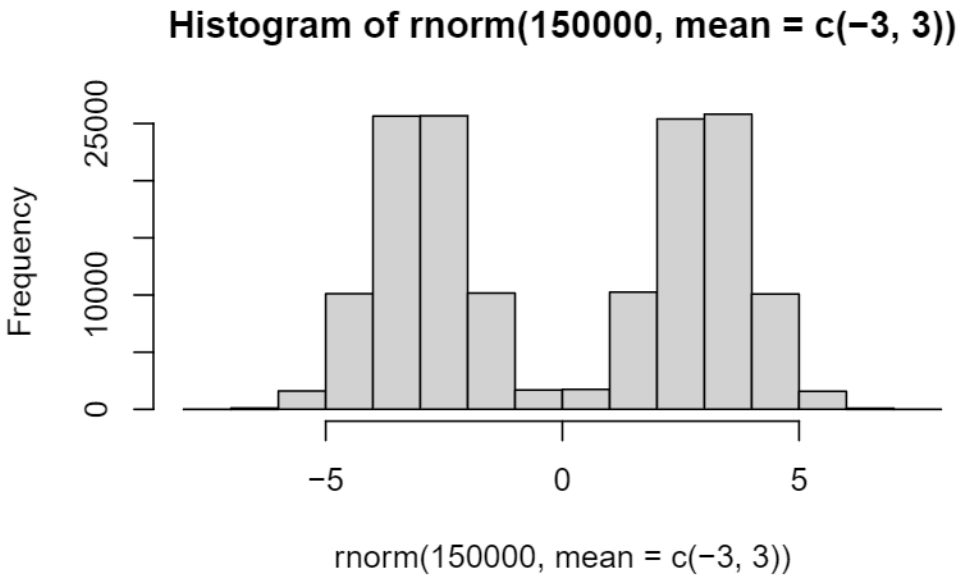
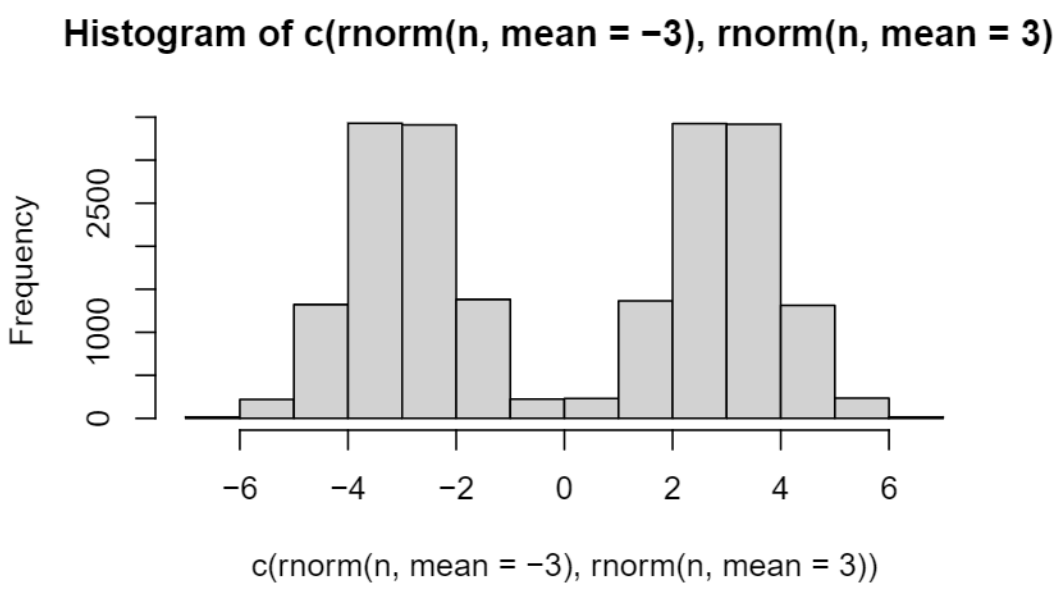
Before we get into clustering methods let's make some sample data to cluster where we know what the answer should be.

To help with this I will use the `rnorm()` function.

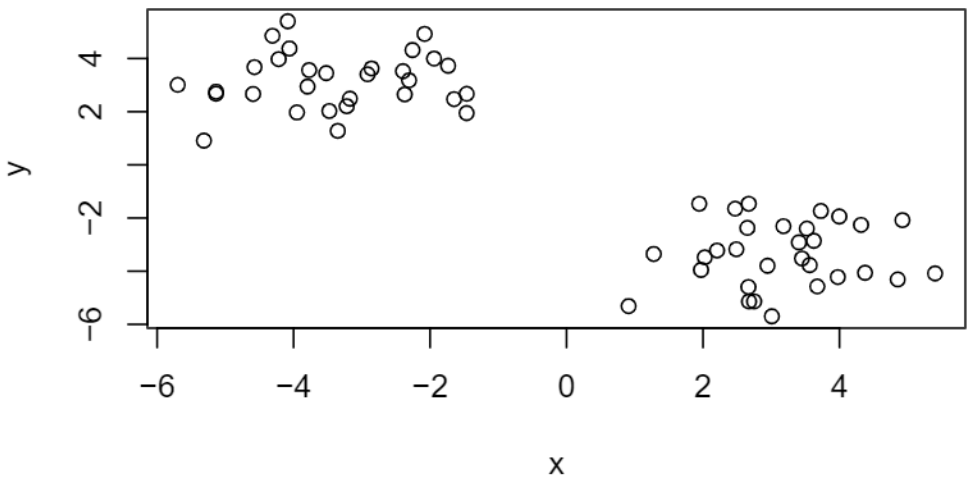
```
hist(rnorm(150000, mean = c(-3,3)))
```




```
n=10000
hist(c(rnorm(n, mean=-3), rnorm(n, mean=3)))
```




```r
n=30
x <- c(rnorm(n, mean=3), rnorm(n, mean=-3))
y <- rev(x)
z <- cbind(x,y)
plot(z)
```



K-means clustering

The function in base R for k-means clustering is called `kmeans()`.

```
km <- kmeans(z, centers = 2)
km
```

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

Cluster means:
          x         y
1 -3.361148  3.154906
2  3.154906 -3.361148

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 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] 75.39334 75.39334
 (between_SS / total_SS =  89.4 %)
```

```
Available components:

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

```
km$centers
```

```
          x         y
1 -3.361148  3.154906
2  3.154906 -3.361148
```

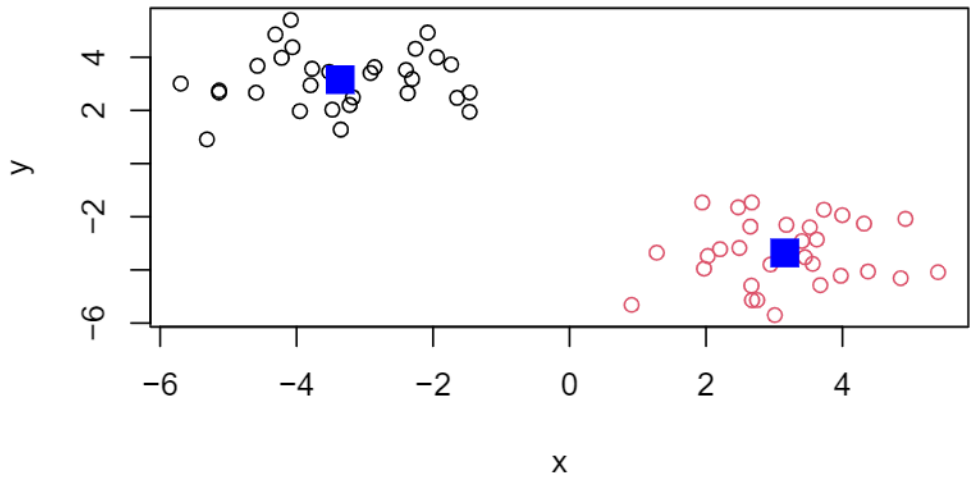
Q. Print out the cluster membership vector (i.e. our main answer)

```
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 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
```

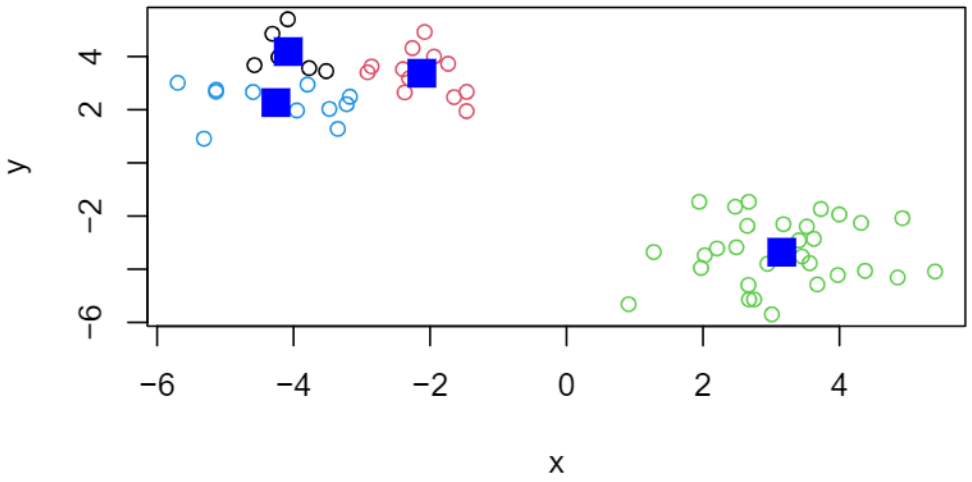
Plot with clustering result and add cluster centers:

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



Q. Can you cluster our data in z into four clusters please?

```
km_4 <- kmeans(z, centers = 4)
plot(z, col=km_4$cluster)
points(km_4$centers, col="blue", pch=15, cex=2)
```



Hierarchical Clustering

The main function for hierarchical clustering in base R is called `hclust()`

Unlike `kmeans()` I cannot just pass in my data as input I first need a distance matrix from my data.

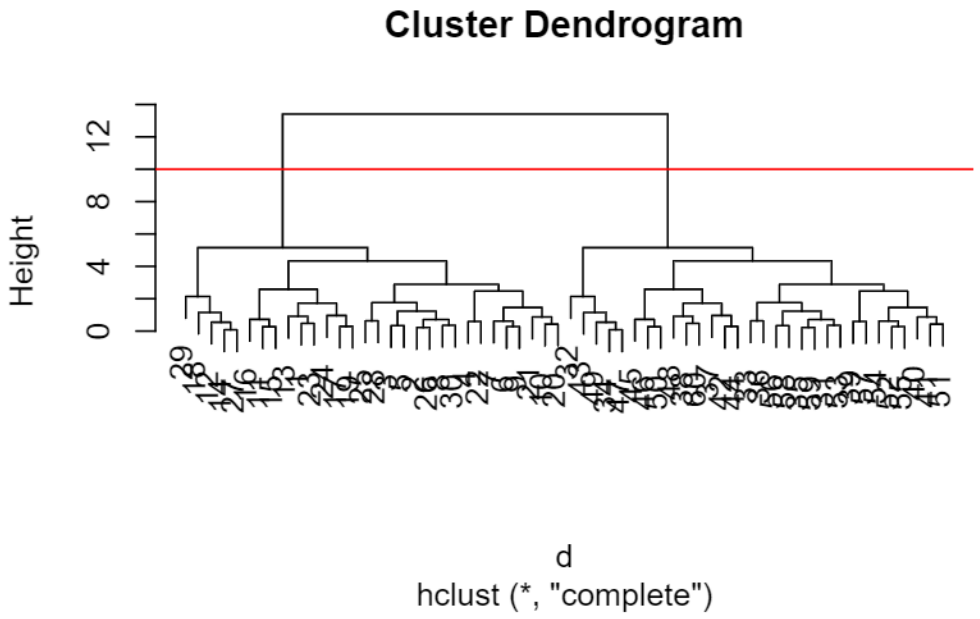
```
d <- dist(z)
hc <- hclust(d)
hc
```

```
Call:
hclust(d = d)
```

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

There is a specific hclust plot() method...

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

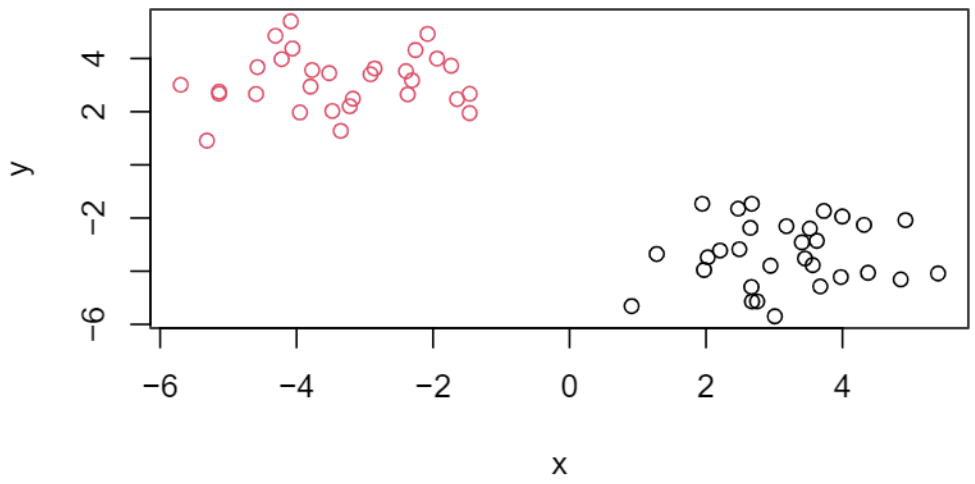


To get my main clustering result (i.e. the membership vector) I can "cut" my tree at a given height. To do this I will use the `cutree()` function

```
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 2 2
```

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



Principal Component Analysis

PCA is a multivariate statistical technique for reducing data set dimensionality.

PCA of UK food data

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
dim(x)
```

```
[1] 17  5
```

```
head(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
```

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

```
dim(x)
```

```
[1] 17  4
```

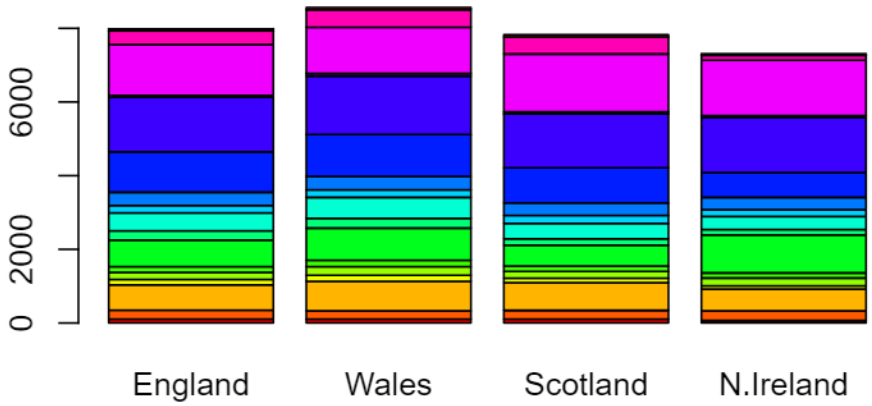
Q1. There are 17 rows and 5 columns. You can find this out by using nrow() and ncol() together or just dim().

```
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
```

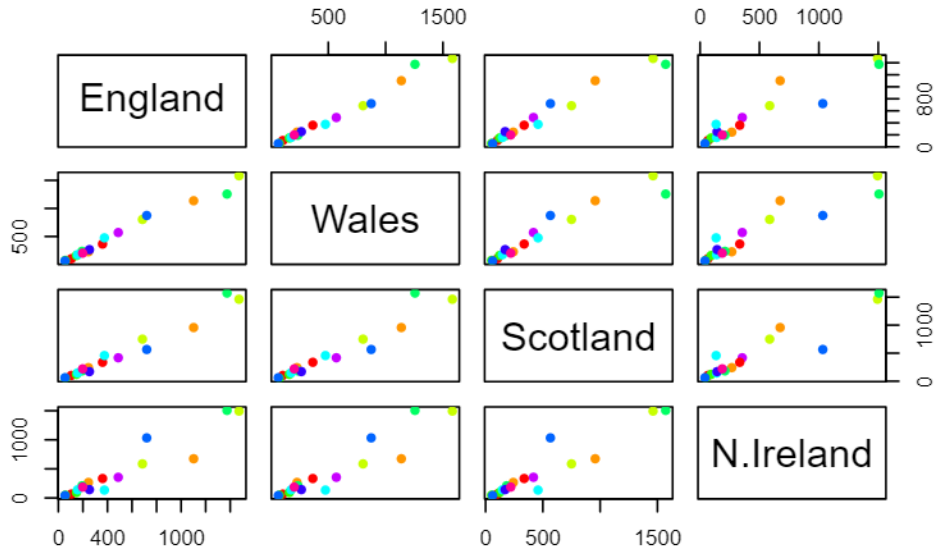
Q2. I like the second approach better because it's more concise and because if you run the first approach multiple times you'll just keep deleting columns.

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



Q3. I changed beside=T to beside=F.

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



Q5. The code above plots each pair of countries against each other and color codes the food types. You can determine which countries are being compared based on the row/column that each subplot is in. If a point lies on the diagonal, then both countries consume a roughly equal amount of food in that category.

PCA to the rescue

The main function to do PCA in base R is called `prcomp()`.

Note that I need to take the transpose of this particular data as that is what the `prcomp()` help page was asking for.

```
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
```

Let's see what is inside our result object pca that we just calculated:

```
attributes(pca)
```

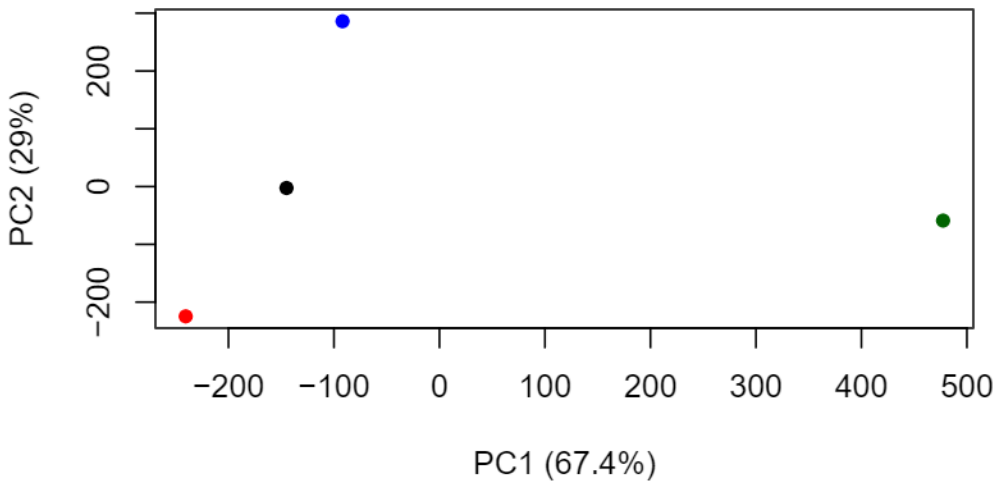
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

```
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
```

To make our main result figure, called a "PC plot" (or "score plot", "ordination plot" or PC1 vs PC2 plot)

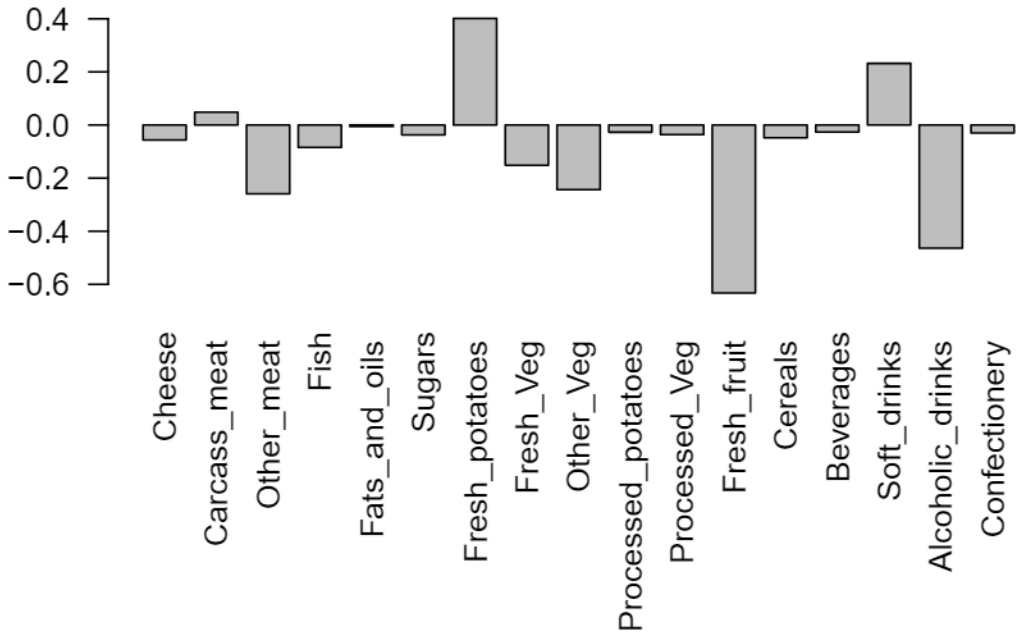
```
plot(pca$x[,1], pca$x[,2], col=c("black", "red", "blue", "darkgreen"),
     pch=16, xlab='PC1 (67.4%)', ylab=('PC2 (29%)'))
```



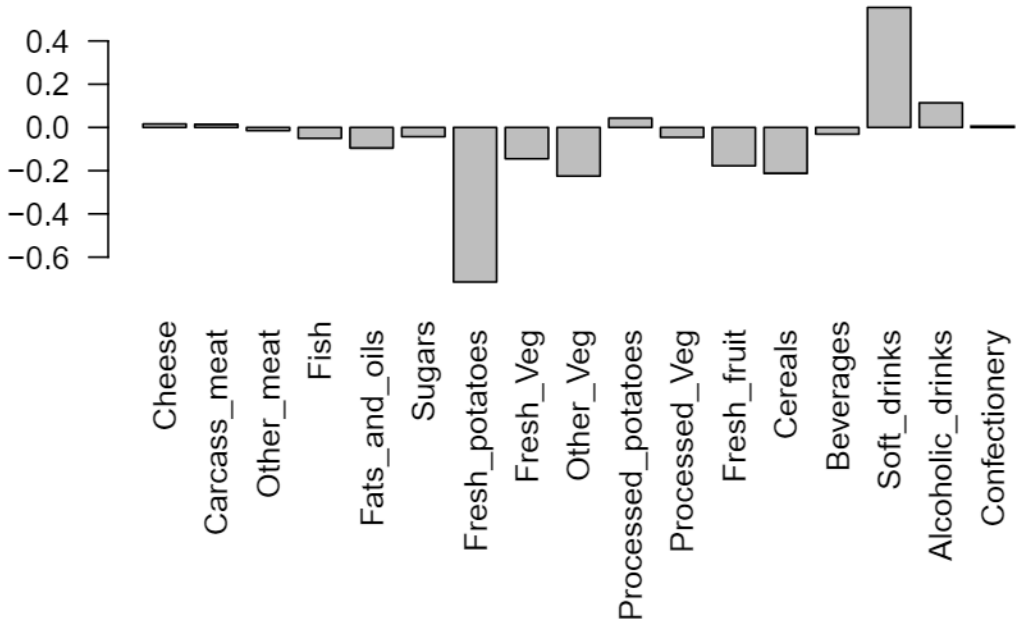
Variable loadings plot

Can give us insight on how the original variables (in this case the foods) contribute to our new PC axis

```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```




```
# Scotland
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```


0.4
0.2
0.0
−0.2
−0.4
−0.6
Cheese
Carcass_meat
Other_meat
Fish
Fats_and_oils
Sugars
Fresh_potatoes
Fresh_Veg
Other_Veg
Processed_potatoes
Processed_Veg
Fresh_fruit
Cereals
Beverages
Soft_drinks
Alcoholic_drinks
Confectionery