Class 7: Machine Learning 1

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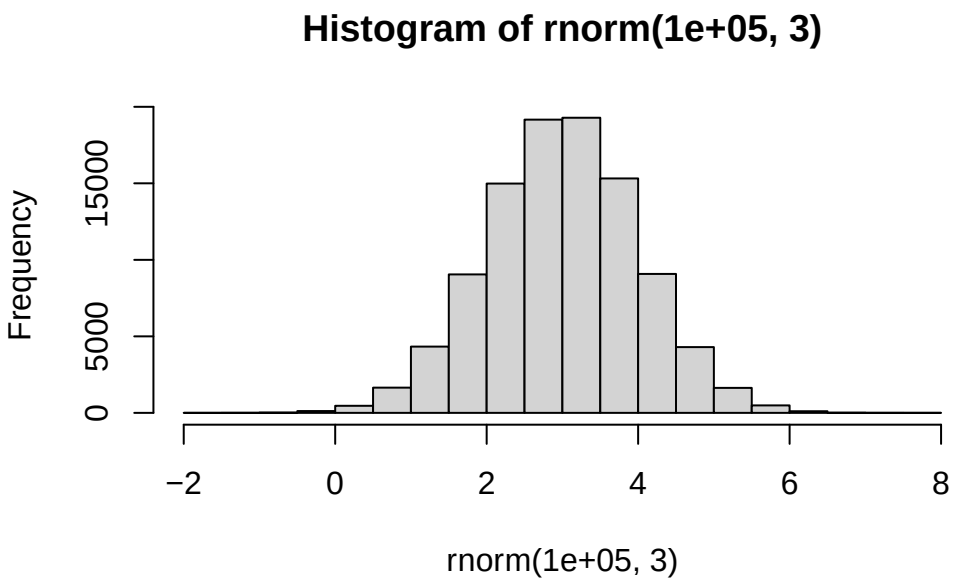
Today we will start out multi-part exploration of some key meachine learning methods. We will being with clustering - findings groupings of like data, and then dimensionallity reduction

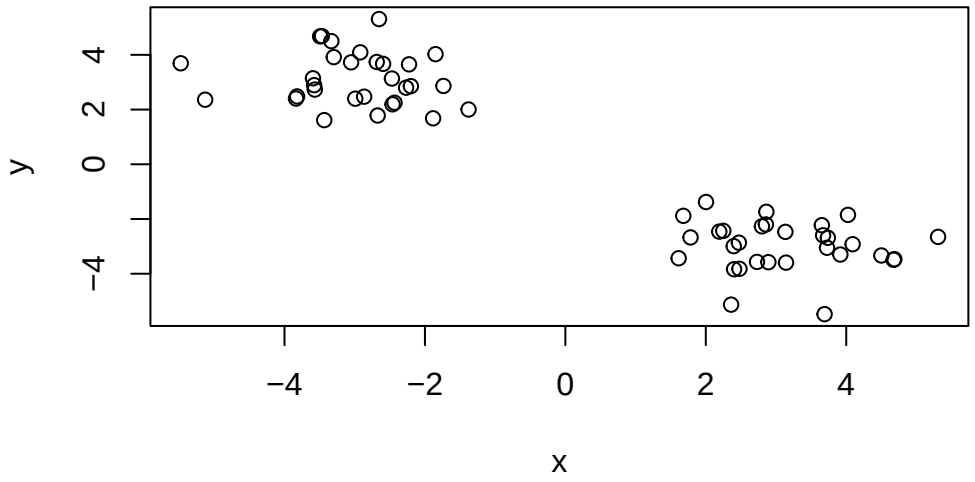
Clustering

Let's start with "k-means" clustering The main function in base R for this is `k-means()`

```
# make up some data
hist(rnorm(100000, 3))
```



```r
tmp <- c(rnorm(30, -3), rnorm(30, +3))
x <- cbind(x=tmp, y=rev(tmp))
plot(x)
```



Now let's try out `kmeans()`

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

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

Cluster means:
          x         y
1 -2.979572  3.124148
2  3.124148 -2.979572

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 2 2

Within cluster sum of squares by cluster:
```

```
[1] 51.38598 51.38598
 (between_SS / total_SS =  91.6 %)

Available components:

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

```
attributes(km)
```

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

$class
[1] "kmeans"
```

Q. How many points in each cluster

```
km$size
```

```
[1] 30 30
```

Q. What component of your results object details cluster assignment/membership?

```
km$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 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
```

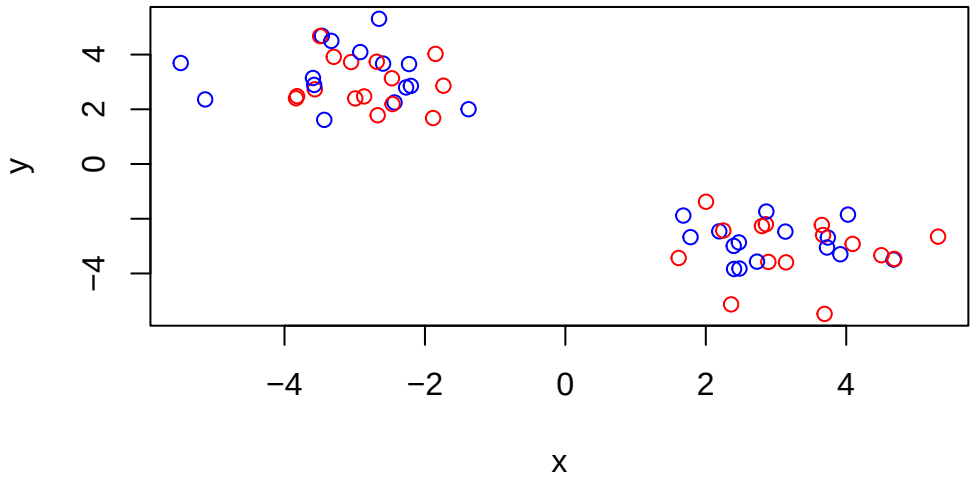
Q. What are centers/mean values of each cluster

```
km$centers
```

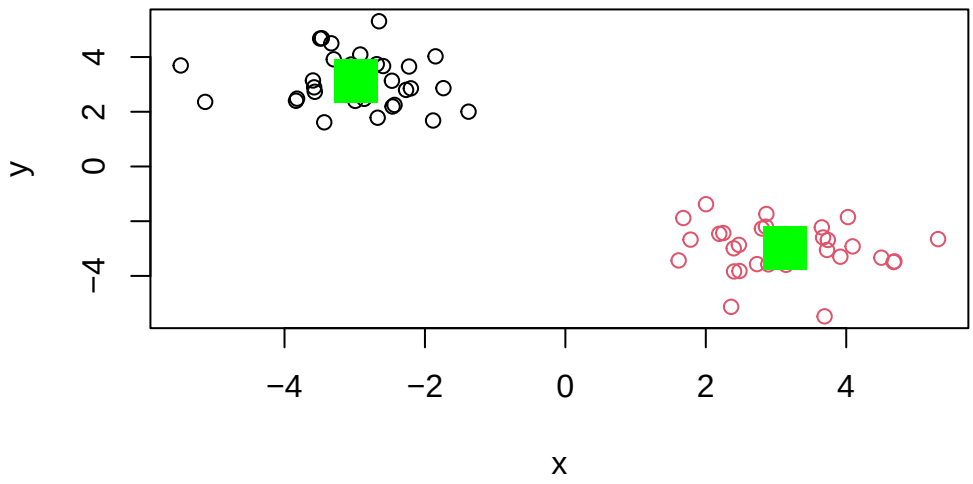
```
          x         y
1 -2.979572  3.124148
2  3.124148 -2.979572
```

Q. Make a plot of your data showing your clustering results

```r
plot(x, col=c("red","blue"))
```

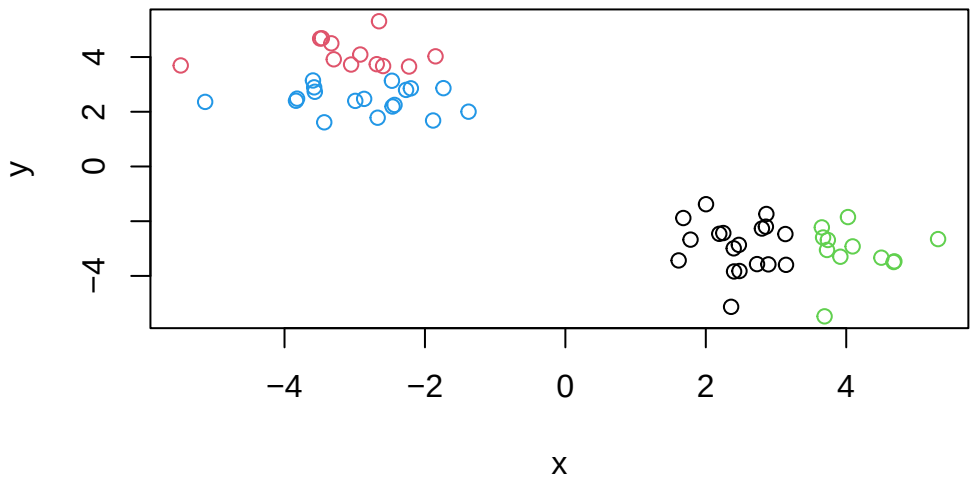



```r
plot(x, col=km$cluster)
points(km$centers, col="green", pch=15, cex=3)
```



Q. Run`kmeans()` again and cluster into 4 groups and plot the results.

```
km_new <- kmeans(x, 4)
plot(x, col=km_new$cluster)
```



Hierarchical Clustering

This form of clustering aims to reveal the structure in your data by progressively grouping points into a ever smaller number of clusters

The main function in base R for this is called `hclust()`. This function does not take our input data directly but wants a "distance matrix" that details how dis-similar all our input points are to each other.

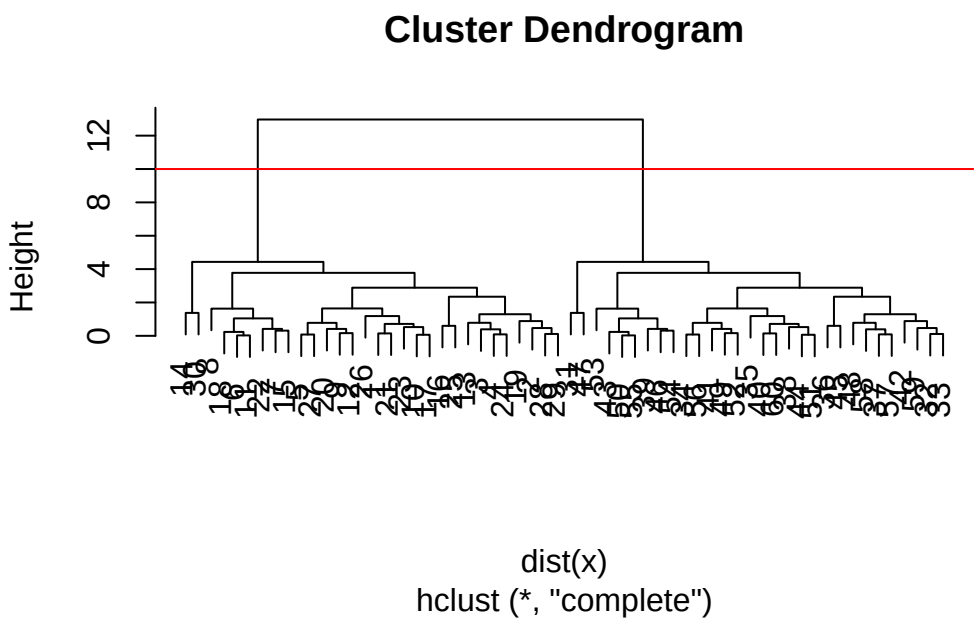
```
hc <- hclust(dist(x))
hc
```

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

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

The print out above is not very useful (unlick that from kmeans) but there is a useful `plot()` method.

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

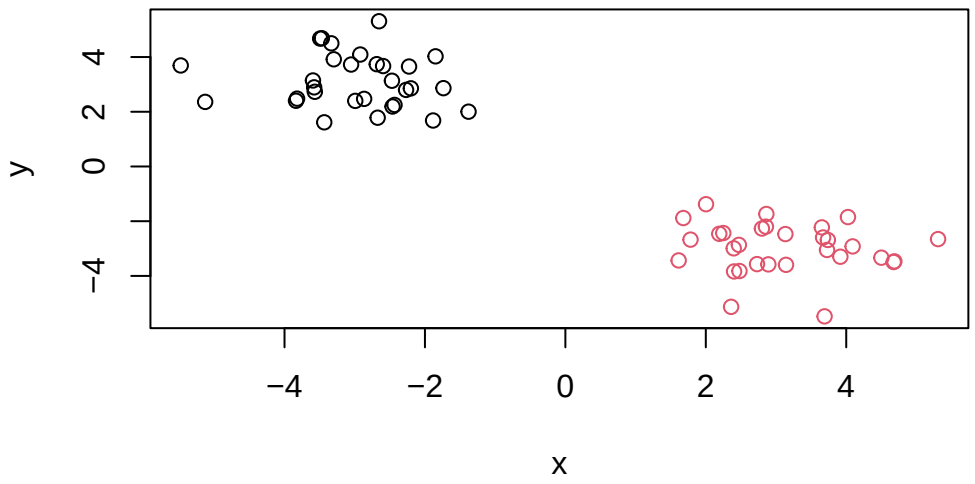


To get my main result (my cluster membership vector) I need to "cut" my tree using the function `cutree()`

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



Principal Component Analysis (PCA)

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

Q1. How many rows and columns are in the dataset?

```
dim(x)
```

```
[1] 17  5
```

```
head(x, 6)
```

```
              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
```

Faster method to change row names:

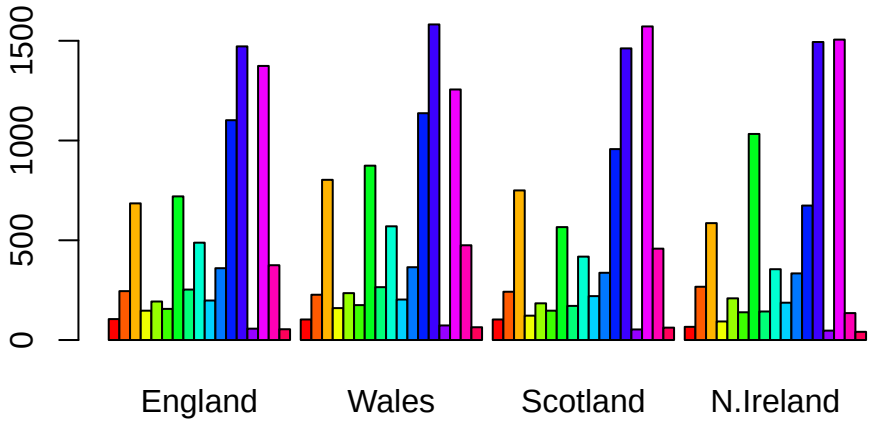
```
  x <- read.csv(url, row.names=1)
  head(x)
```

```
               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. Which approch to solving the row-names problem do you prefer

I prefer the second method, since it is much shorter, requiring only 1 line of code. It is also more well-defined, since running the first version multiple times will keep shifting the row header column

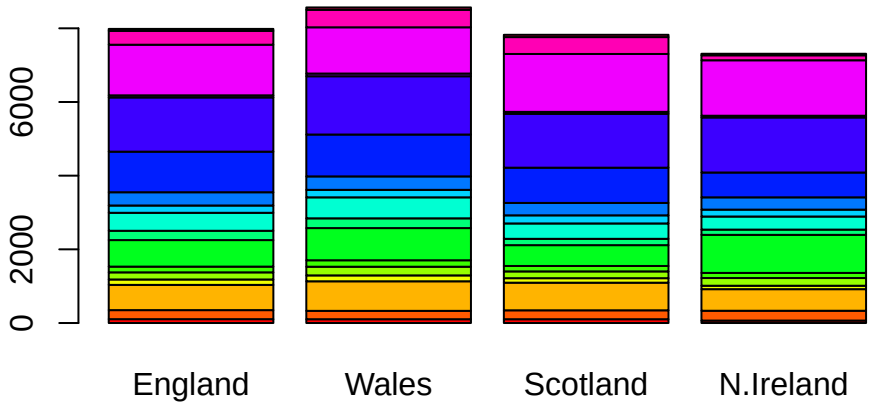
```
  barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



Q3. Changing what optional arguemtn results in a stacked barplot?

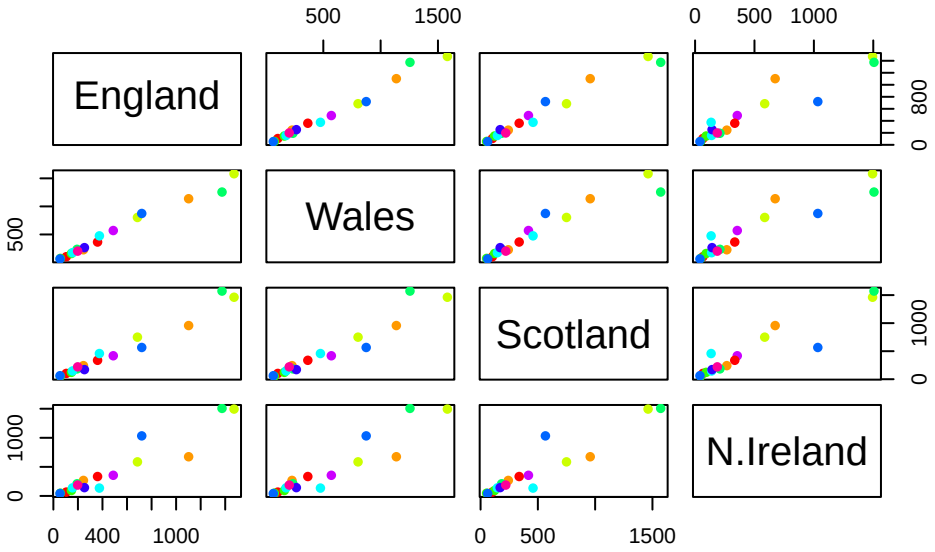
Changes besides to False or deleting this argument

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



The so-called “pairs” plto canbe useful for small datasets

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



So, the pairs plot is useful for small datasets but it can be lot of work to interpret and gets intractable for larger datasets.

so PCA to the rescue...

The main function to do PCA in base R is called `prcomp()`. This function wants thr transpose of our data in this case.

```
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
```

```
attributes(pca)
```

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

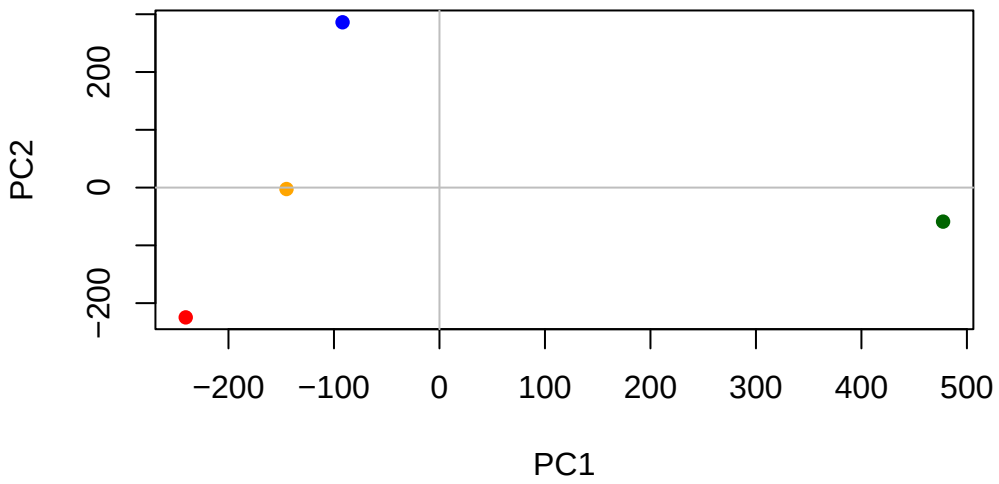
```
$class
[1] "prcomp"
```

```
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
```

A major PCA result visualization is called a "PCA Plot" (aka a score plot, biplot, PC1 vs PC2 plot, ordination plot)

```
mycols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=mycols, pch=16,
     xlab="PC1", ylab="PC2")
abline(h=0, col="gray")
abline(v=0, col="gray")
```



Another important output from PCA is called the "loadings" vector or the "rotation" component - this tells us how much the original variables (the foods in this case) contribute to the new 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
```

PCA looks to be a super useful method for gaining some insight into high-dimensional data that is difficult to examine in other ways.