Class 7: Machine Learning 1

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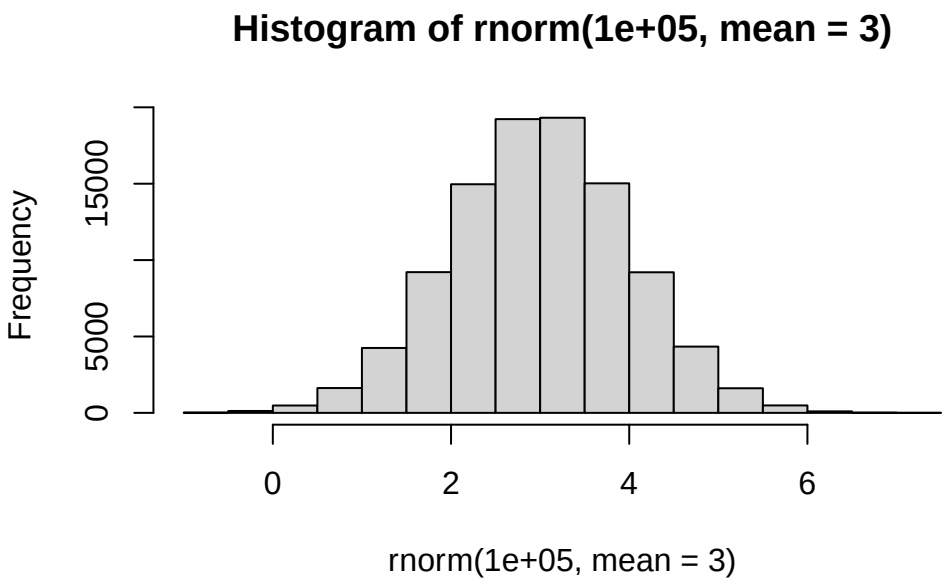
Today we will start our multi-part exploration of some key machine learning methods. We will begin clustering - finding groupingsn in data and then dimensionality reduction.

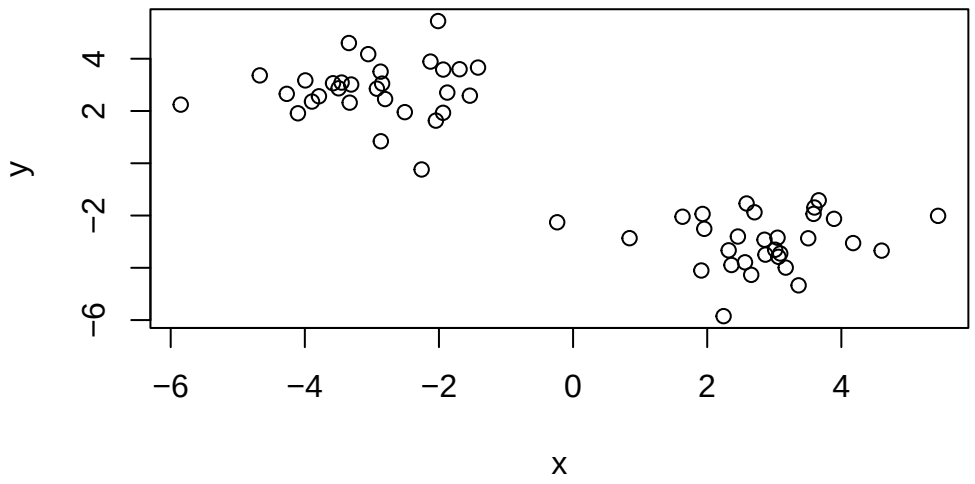
Clustering

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

```
# Make up some data
hist(rnorm(100000, mean =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  2.828713 -2.993415
2 -2.993415  2.828713

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] 64.83399 64.83399
 (between_SS / total_SS =  88.7 %)

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 components of your result object details cluster assignment/membership?

```
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
```

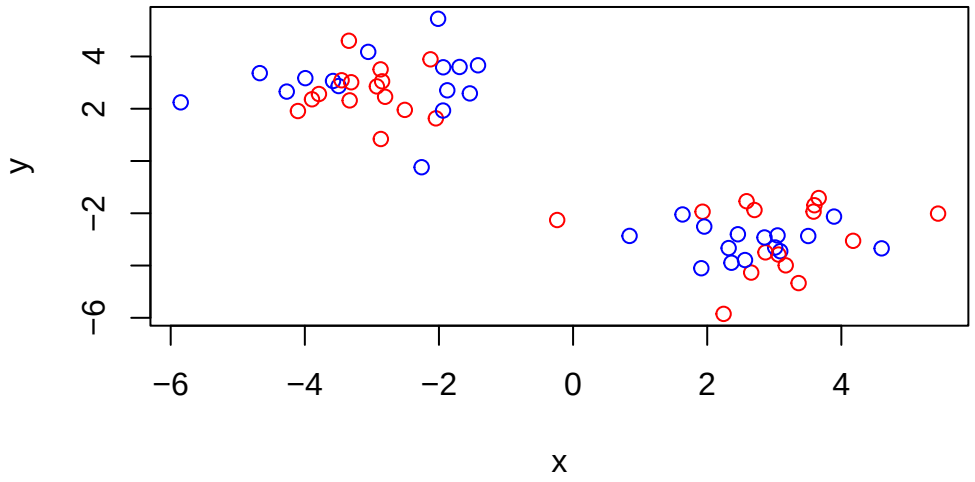
Q. What are centers/mean values of each cluster?

```
km$centers
```

```
          x         y
1  2.828713 -2.993415
2 -2.993415  2.828713
```

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

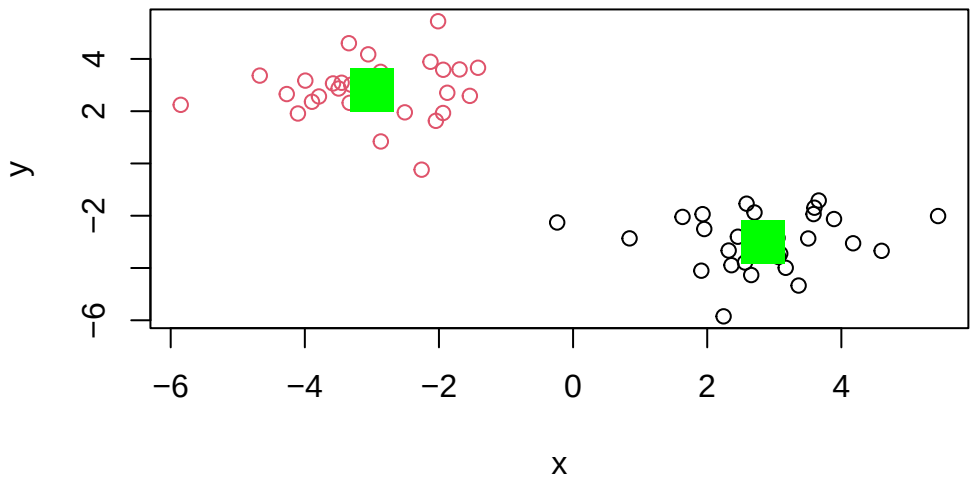
```
plot(x, col = c("red","blue"))
```




```
c(1:5) + c(100)
```

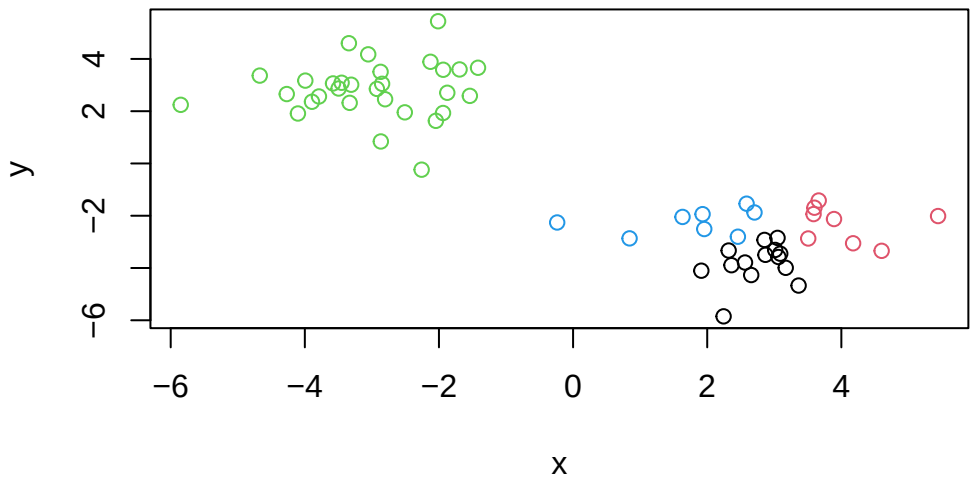
```
[1] 101 102 103 104 105
```

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



Q. Run ‘kmeans()’ again and cluster in 4 groups and plot the results.

```
km4 <- kmeans(x, centers = 4)

plot(x, col=km4$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.

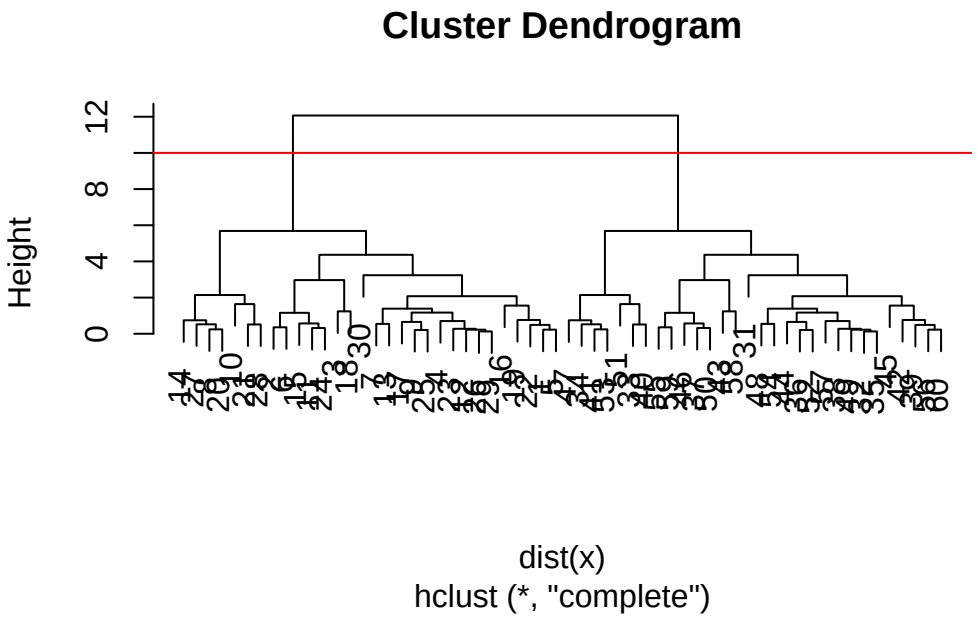
The main function in base R is for this is called 'hclust()'. This function does not take our input data directly but wants a "distance matrix" that details how (dis)similar all our input points are to each other.

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

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

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

The printout above is not very useful (unlick that from kmeans) but there is a useful 'plot()' method.

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

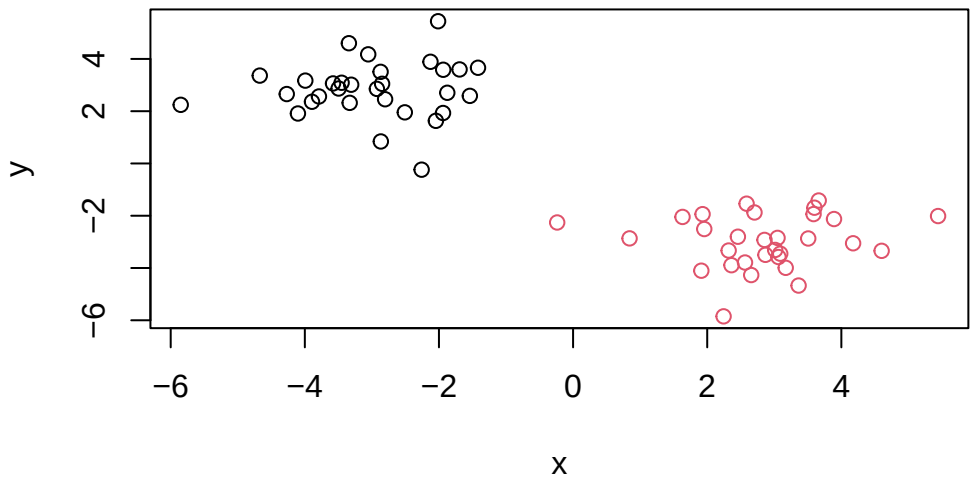


To get my main result (my cluster membership vector) I need to "cut" my tree using the function 'cutree()'

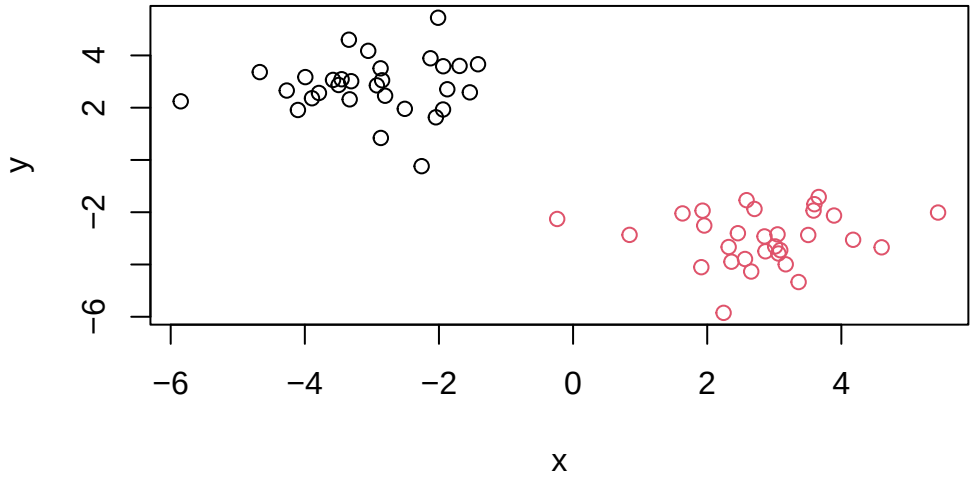
```
grps <- cutree(hc,h = 10)
grps
```

```
 [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)
```




```
plot(x, col = cutree(hc,h = 6))
```



Principal Component Analysis (PCA)

The goal of PCA is to reduce the dimensionality of a dataset down to some smalelr subsets oif new variables (called PCs) thata re a useful bases for further analysis, like visualization, clustering, etc.

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
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
7     Fresh_potatoes     720   874      566      1033
8          Fresh_Veg     253   265      171       143
9          Other_Veg     488   570      418       355
10 Processed_potatoes     198   203      220       187
11     Processed_Veg     360   365      337       334
12       Fresh_fruit    1102  1137      957       674
13           Cereals    1472  1582     1462      1494
14         Beverages      57    73       53        47
15       Soft_drinks    1374  1256     1572      1506
16   Alcoholic_drinks     375   475      458       135
17     Confectionery      54    64       62        41
```

```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

```
[1] 5
```

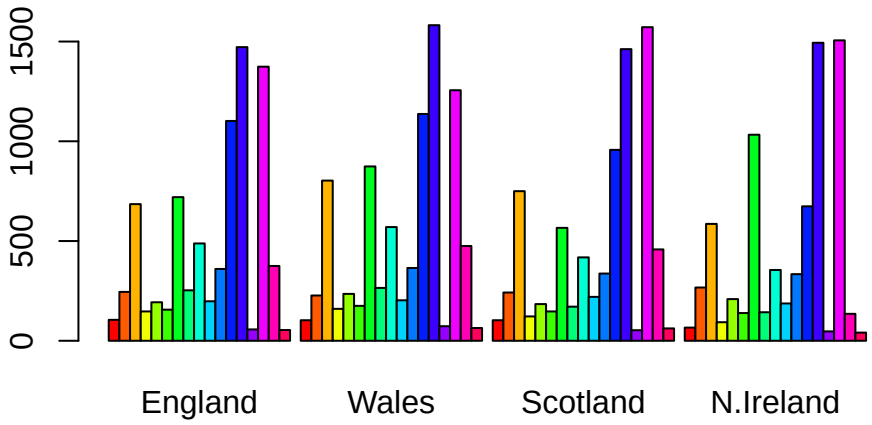
```
x <- read.csv(url, row.names=1)
head(x)
```

```
              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
```

```
dim(x)
```

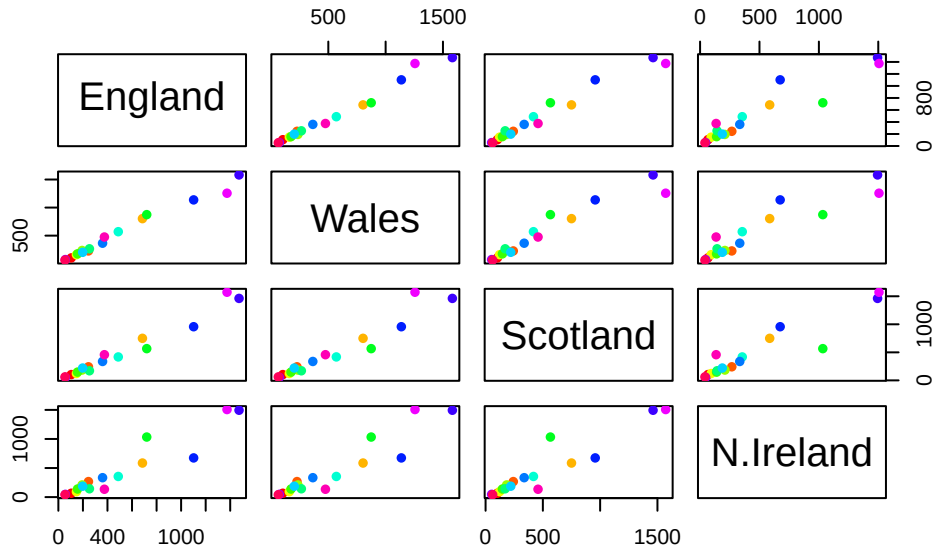
```
[1] 17  4
```

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



The so-called "pairs" plot can be useful for small datasets:

```
# rainbow(nrow(x))
pairs(x, col=rainbow(nrow(x)), pch=16)
```



So the pairs plot is useful for small datasets but it can be lots 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 the tranpose 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)
```

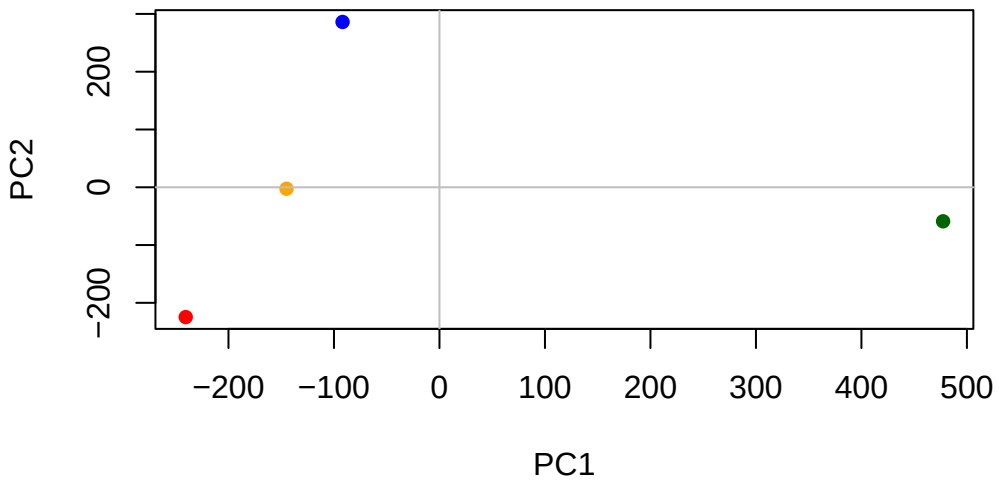
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$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 is called a "PCA plot" (aka: score plot, biplot, PC1 vs PC2 plot, ordientation 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.