

Class 7: Machine learning 1

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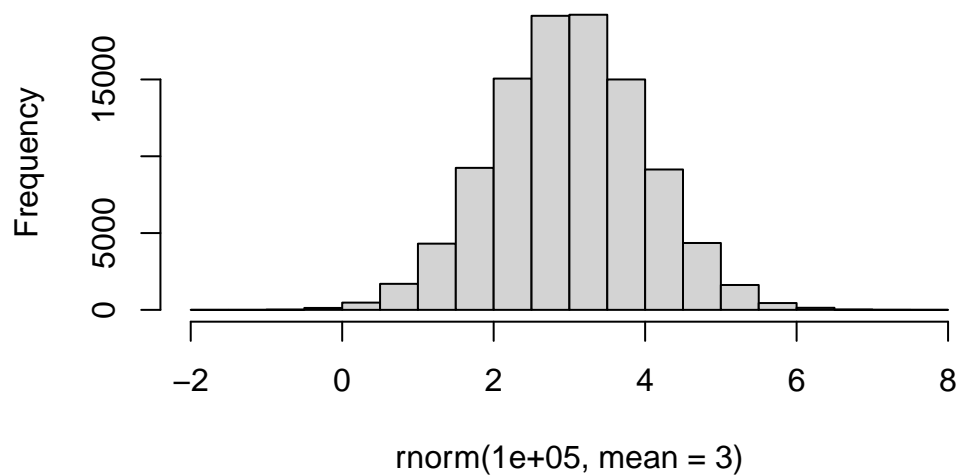
Today we will start our multi-part exploration of some key machine learning methods. We will begin with clustering- finding groupings in data, and then dimensionality reduction.

Clustering

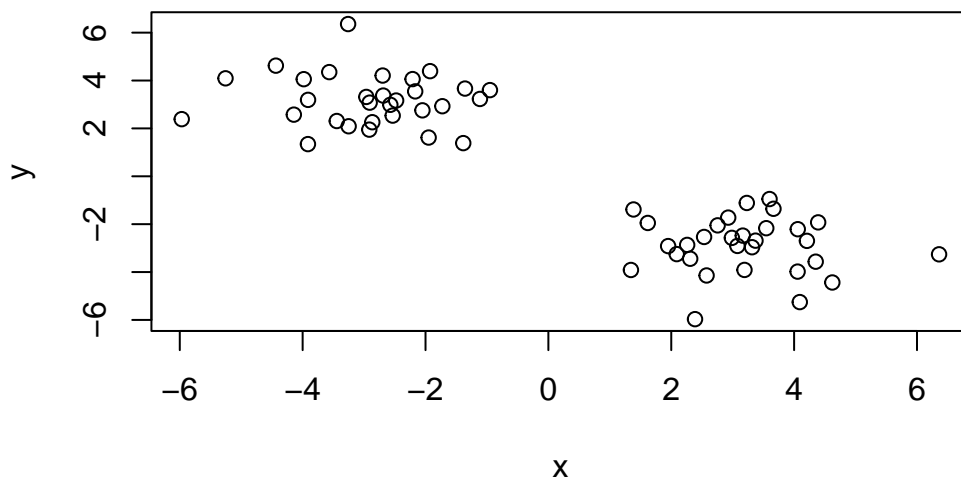
Let's start with "k-means" clustering. The main function in base R for this `kmeans()`

```
# Make up some data  
hist( rnorm(100000, mean=3) )
```

Histogram of `rnorm(1e+05, mean = 3)`



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



Now let's try out `kmeans()`

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

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

Cluster means:

	x	y
1	3.180747	-2.886454
2	-2.886454	3.180747

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 2 2 1 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 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

Within cluster sum of squares by cluster:

Available components:

```
attributes(km)
```

```
$class
[1] "kmeans"
```

km\$size

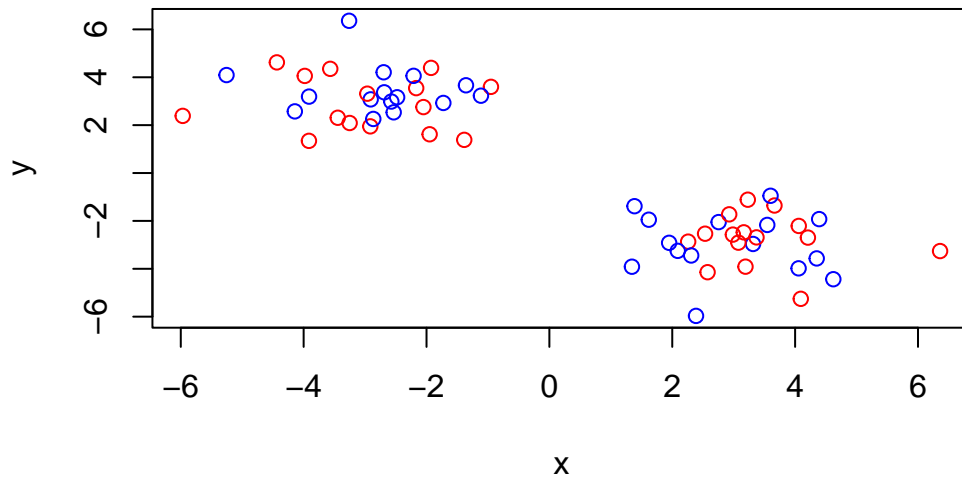
Q. What component of your result object details cluster assignment/membership?

[illegible]

km\$centers

Q. Make a plot of your data showing your clustering results (groupings/clusters and cluster centers).

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

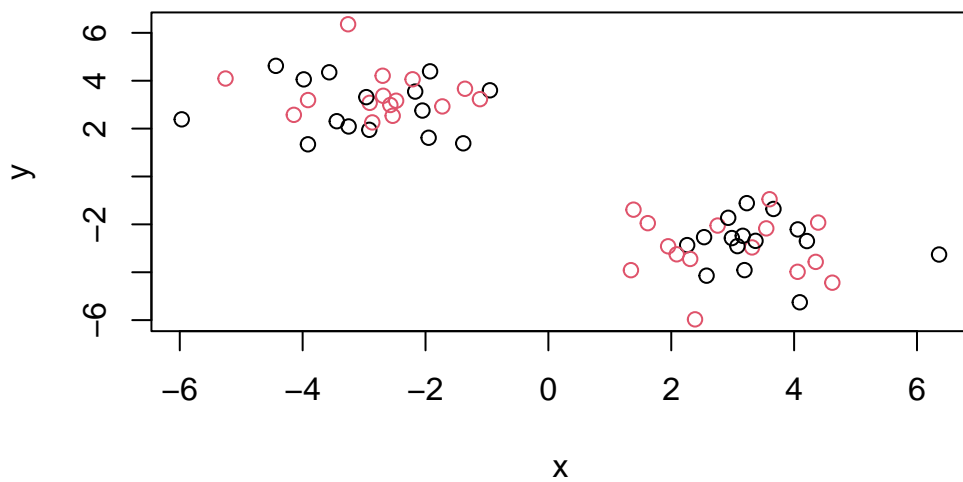


```
c(1:5) + c(100,1)
```

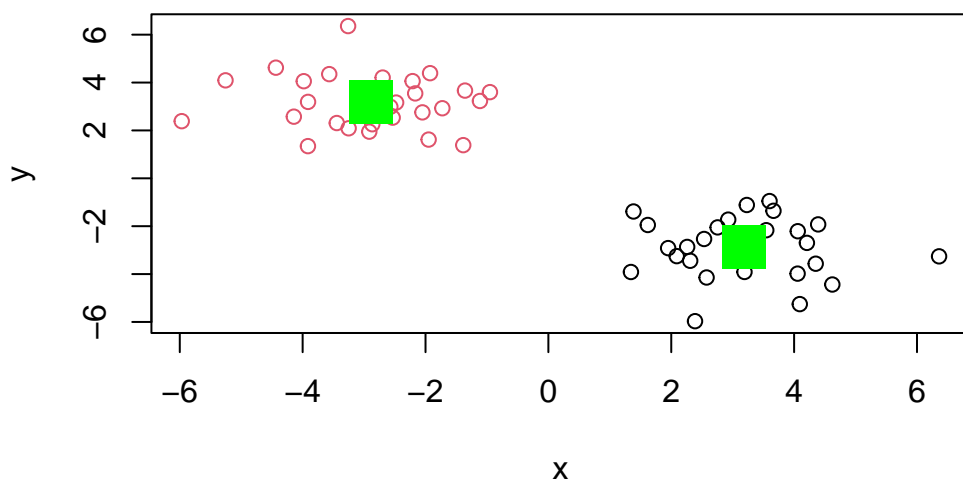
Warning in c(1:5) + c(100, 1): longer object length is not a multiple of shorter object length

```
[1] 101    3 103    5 105
```

```
plot(x, col=c(1,2))
```

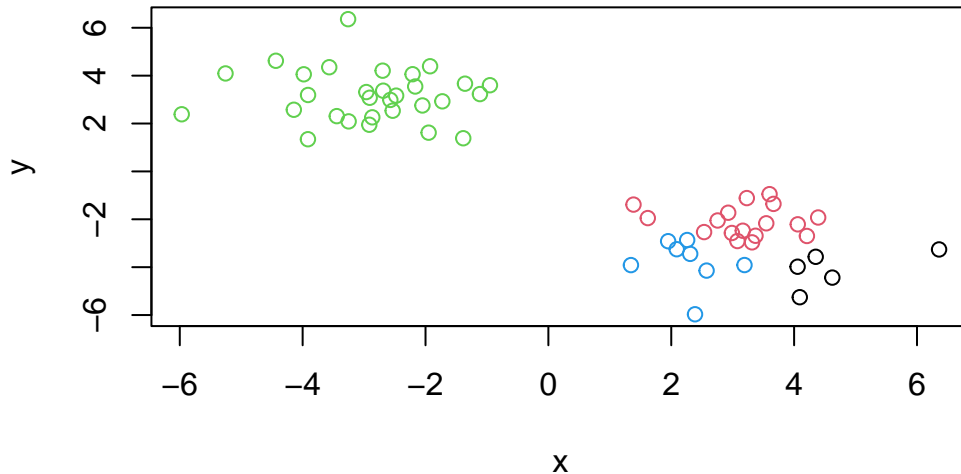


```
plot(x, col=km$cluster)
points(km$centers, col="green", pch=15, cex=3)
```



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 an even smaller number of clusters.

The main function in base R for this 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
```

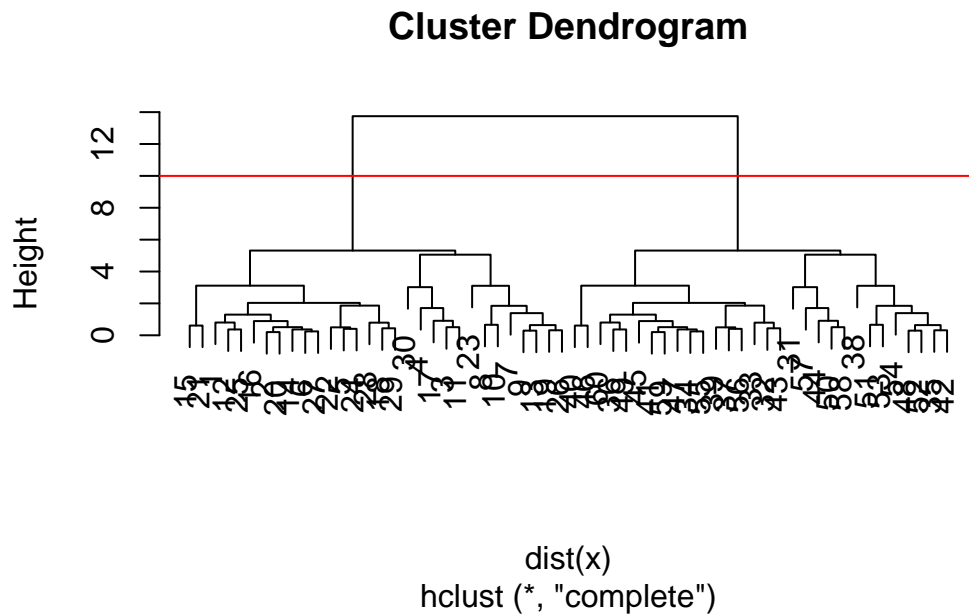
Call:

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

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

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

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

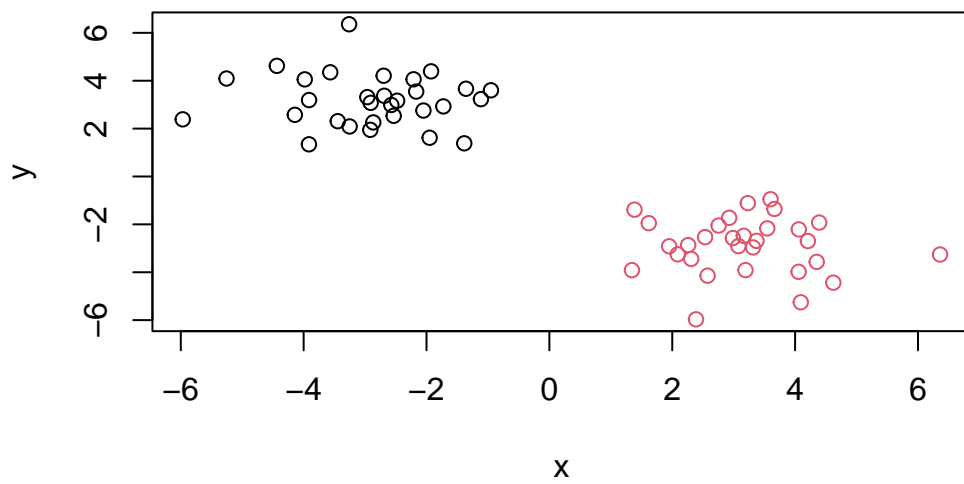


To get my main result (my cluster membership vector) I need to “cut” my tree using the function `cutree()`

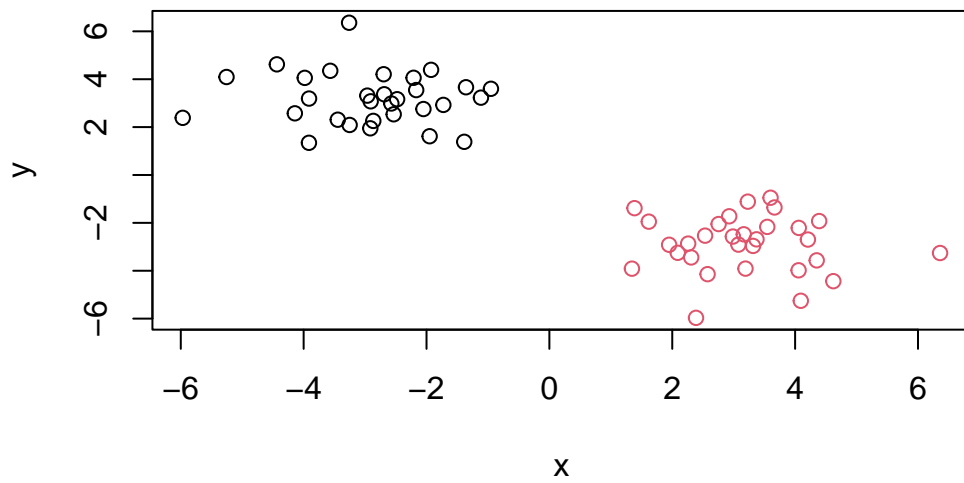
```
grps <- cutree(hc, h=10)
grps
```

[illegible]

```
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 smaller subset of new variables (called PCs) that are a useful bases for further analysis, like visualization, clustering, etc.

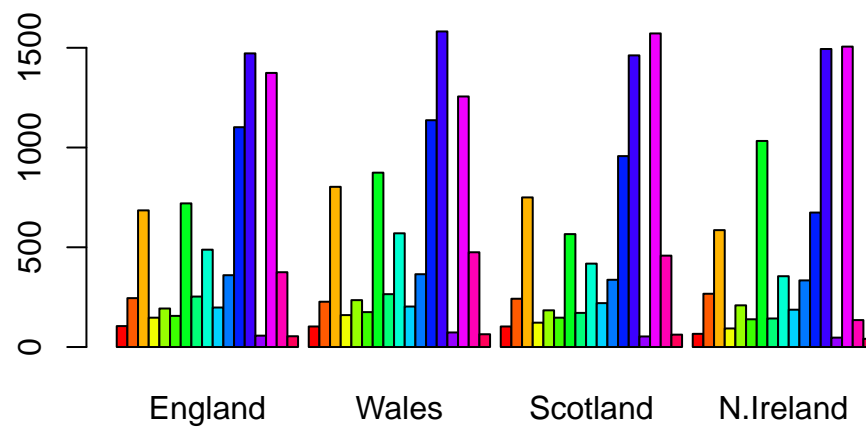
Data import

Read data about crazy eating trends in the UK and N. Ireland

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names=1)
x
```

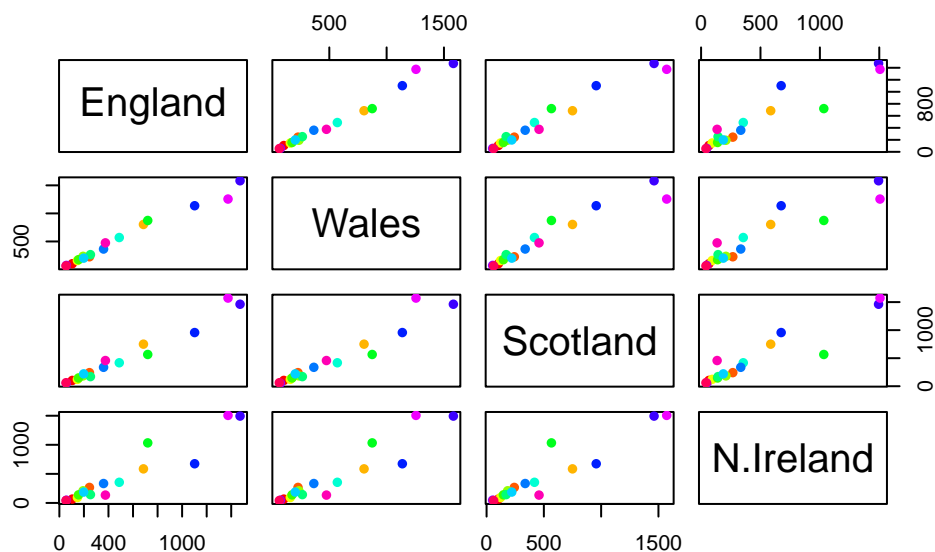
	England	Wales	Scotland	N.Ireland
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139
Fresh_potatoes	720	874	566	1033
Fresh_Veg	253	265	171	143
Other_Veg	488	570	418	355
Processed_potatoes	198	203	220	187
Processed_Veg	360	365	337	334
Fresh_fruit	1102	1137	957	674
Cereals	1472	1582	1462	1494
Beverages	57	73	53	47
Soft_drinks	1374	1256	1572	1506
Alcoholic_drinks	375	475	458	135
Confectionery	54	64	62	41

```
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 paris 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 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	2.921e-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"
```

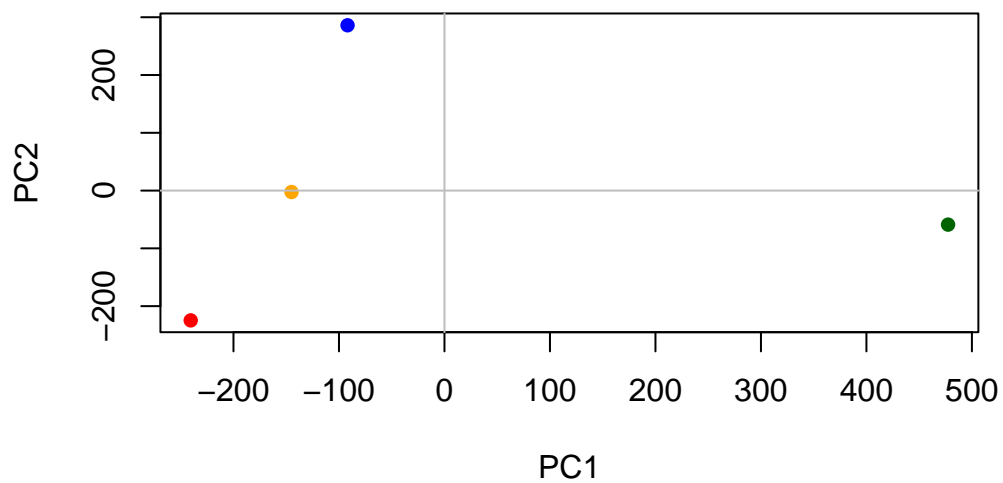
```
$class  
[1] "prcomp"
```

```
pca$x
```

	PC1	PC2	PC3	PC4
England	-144.99315	-2.532999	105.768945	-9.152022e-15
Wales	-240.52915	-224.646925	-56.475555	5.560040e-13
Scotland	-91.86934	286.081786	-44.415495	-6.638419e-13
N.Ireland	477.39164	-58.901862	-4.877895	1.329771e-13

A major PCA result viz is called a “PCA plot” (a.k.a a score plot, a 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 tell sus 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	-0.409382587
Carcass_meat	0.047927628	0.013915823	0.06367111	0.729481922
Other_meat	-0.258916658	-0.015331138	-0.55384854	0.331001134
Fish	-0.084414983	-0.050754947	0.03906481	0.022375878
Fats_and_oils	-0.005193623	-0.095388656	-0.12522257	0.034512161
Sugars	-0.037620983	-0.043021699	-0.03605745	0.024943337
Fresh_potatoes	0.401402060	-0.715017078	-0.20668248	0.021396007
Fresh_Veg	-0.151849942	-0.144900268	0.21382237	0.001606882
Other_Veg	-0.243593729	-0.225450923	-0.05332841	0.031153231
Processed_potatoes	-0.026886233	0.042850761	-0.07364902	-0.017379680
Processed_Veg	-0.036488269	-0.045451802	0.05289191	0.021250980
Fresh_fruit	-0.632640898	-0.177740743	0.40012865	0.227657348
Cereals	-0.047702858	-0.212599678	-0.35884921	0.100043319
Beverages	-0.026187756	-0.030560542	-0.04135860	-0.018382072
Soft_drinks	0.232244140	0.555124311	-0.16942648	0.222319484
Alcoholic_drinks	-0.463968168	0.113536523	-0.49858320	-0.273126013
Confectionery	-0.029650201	0.005949921	-0.05232164	0.001890737

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