Class07

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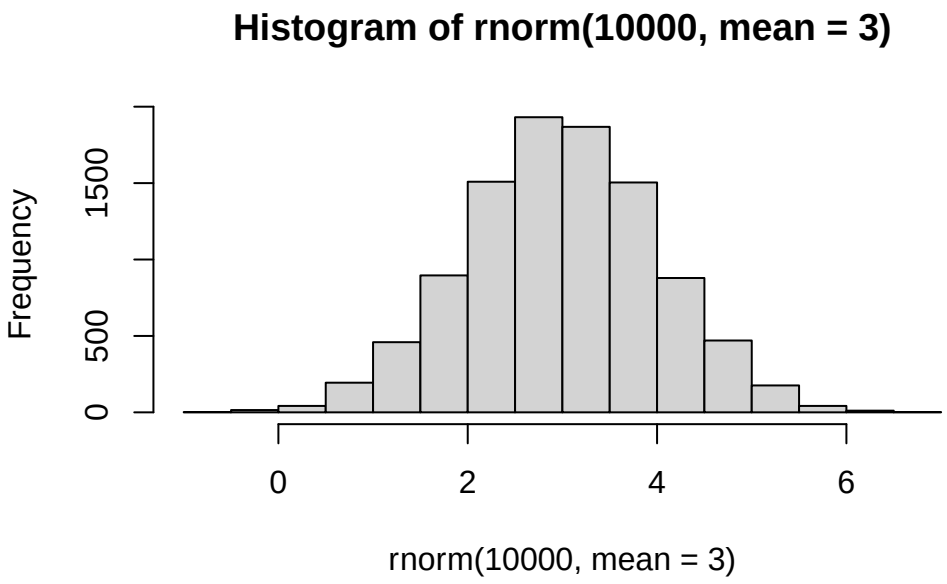
Today we will start our multi-part exploration of some key machine learning mehtods. We will begin with clustering - finding groupings in data, and then dimensionality reduction.

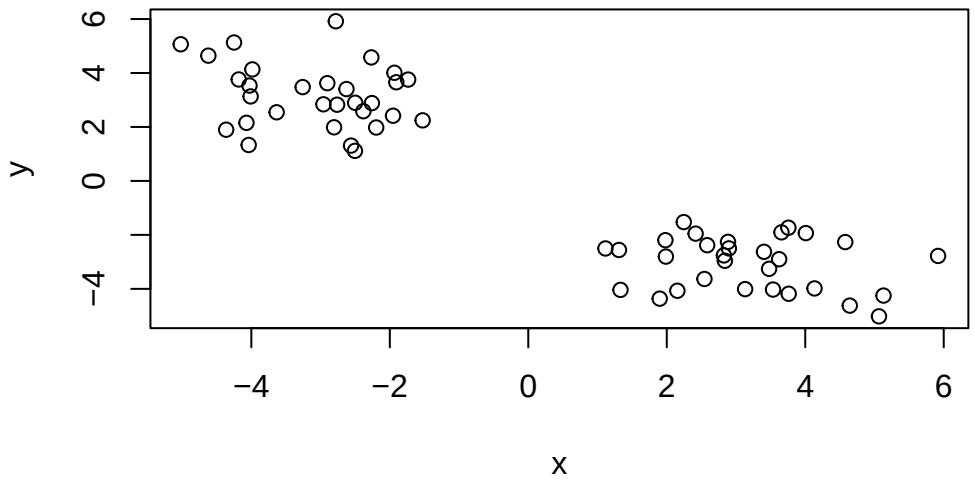
clustering

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

```
# make up some data
hist( rnorm(10000, mean=3))
```




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



now lets try out `kmeans()`

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

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

Cluster means:
          x         y
1  3.161081 -3.067238
2 -3.067238  3.161081

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] 68.68854 68.68854
 (between_SS / total_SS =  89.4 %)

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 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
```

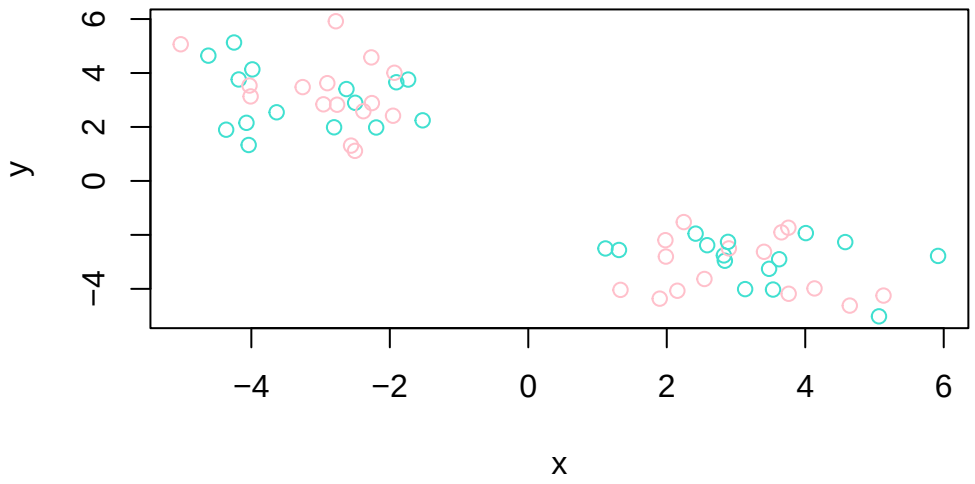
Q. what are centers/mean values of each cluster?

```
km$centers
```

```
          x         y
1  3.161081 -3.067238
2 -3.067238  3.161081
```

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

```
plot(x, col=c("turquoise", "pink"))
```

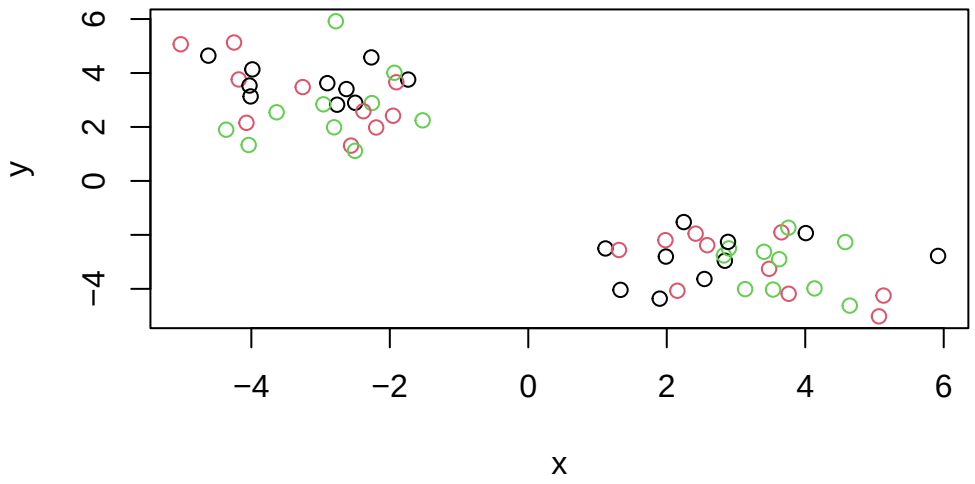



```
c(1:5) + c(100,1)
```

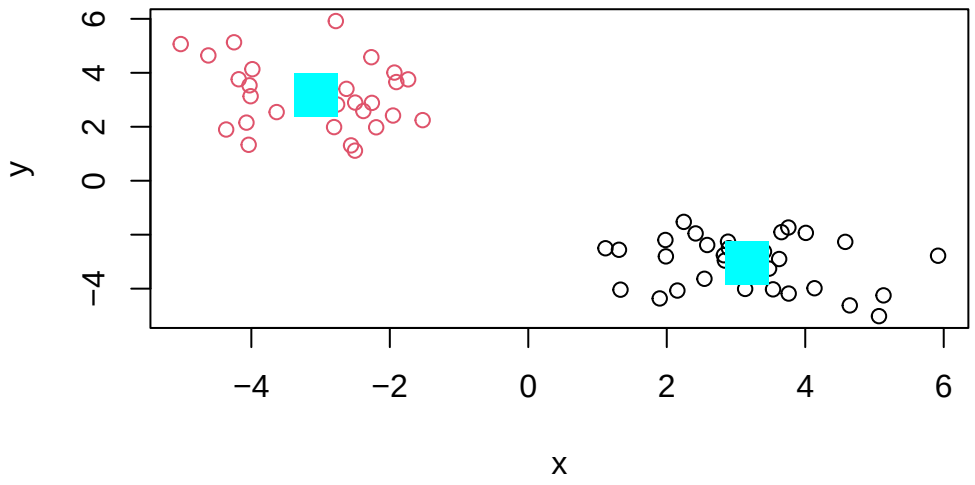
```
Warning in c(1:5) + c(100, 1): longer object length is not a multiple of
shorter object length
```

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

```
plot(x, col=c(1,2,3))
```

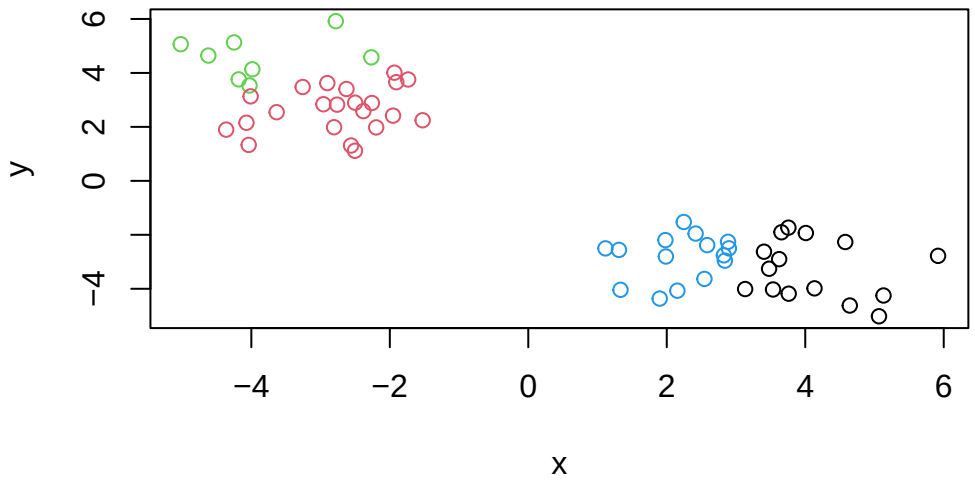



```
plot(x, col=km$cluster)
points(km$centers, col="cyan", pch=15, cex=3)
```



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 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.

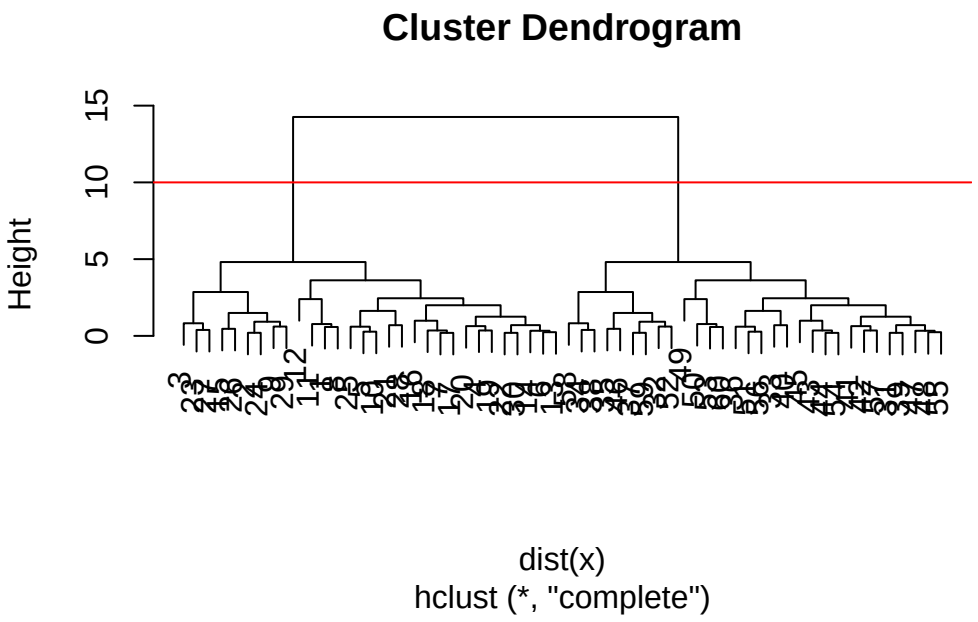
```
hc <- hclust(dist(x))
hc
```

```
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's a useful `plot()` method.

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

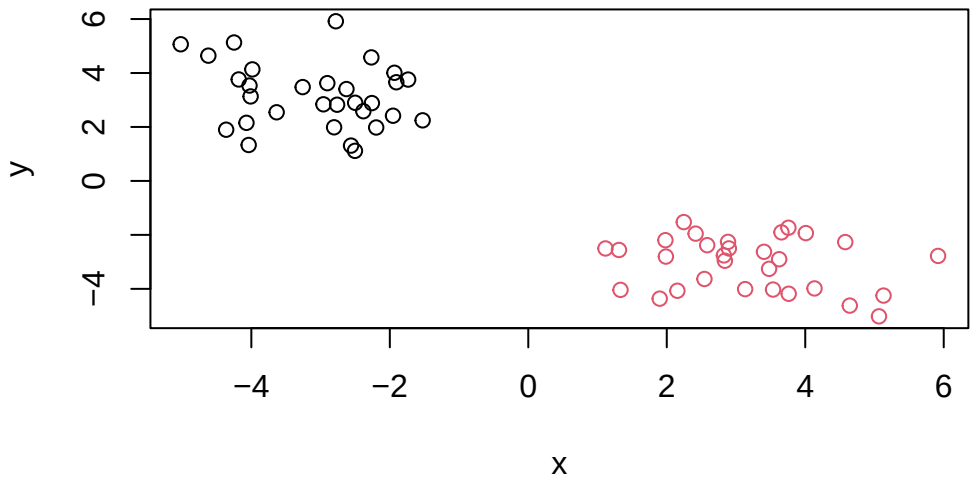


To get my main result (my cluster membership vector) I need to "cut" my tree using the function `cutree()`

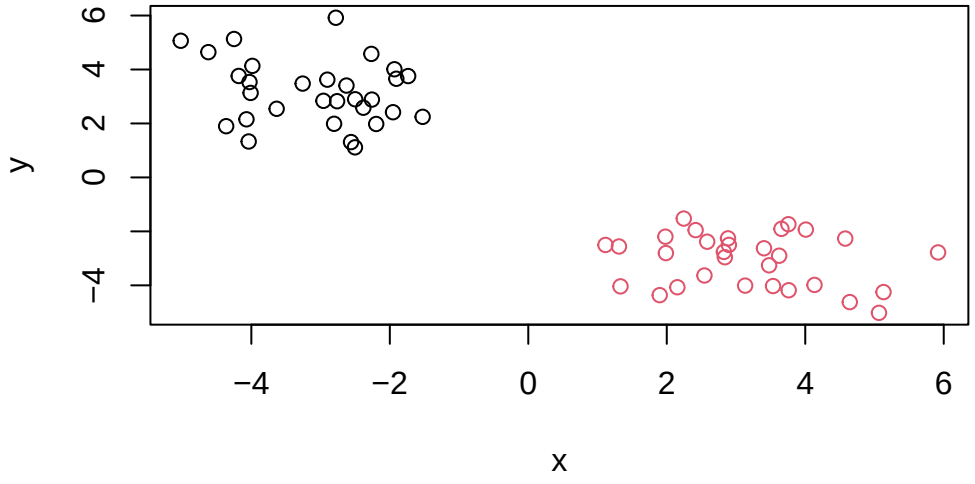
```
grps <- cutree(hc, h=10)
grps
```

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

Data import

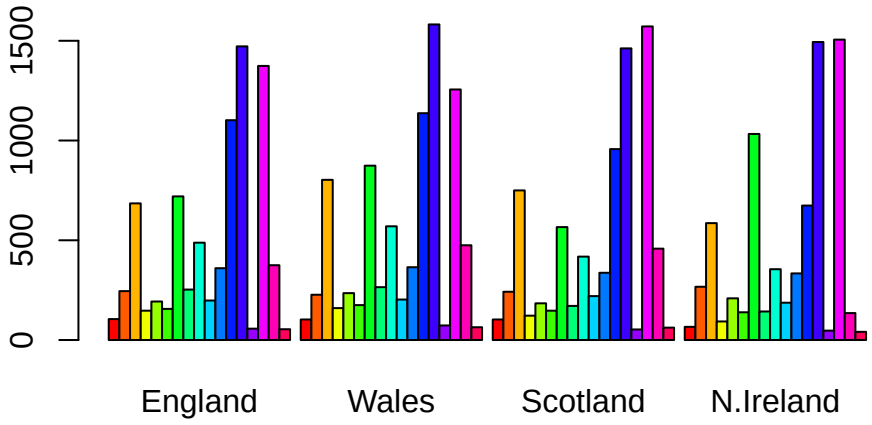
Read data about crazy eating trends in the UK and N. Ireland

```
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

stacked barplot

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



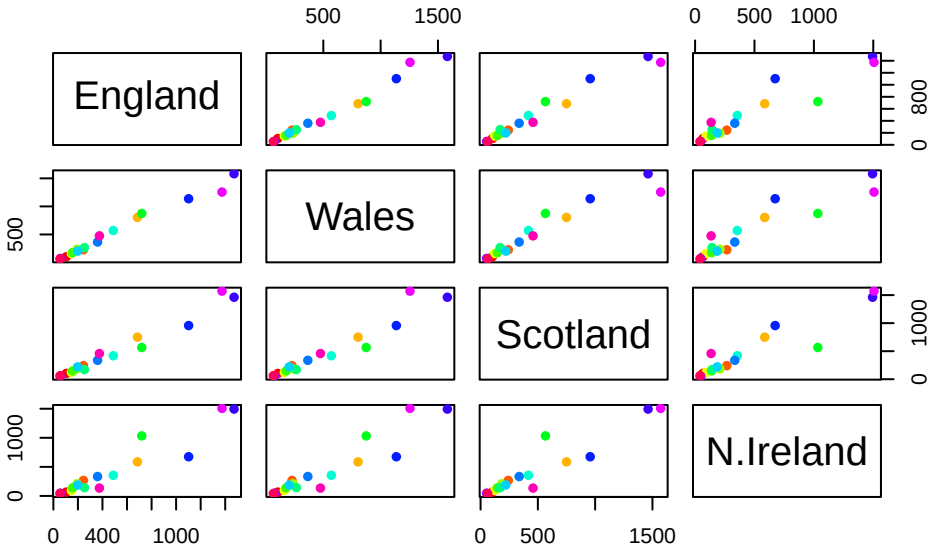
The so-called "pairs" plot can be useful for small datasets:

```
rainbow(nrow(x))
```

```
 [1] "#FF0000" "#FF5A00" "#FFB400" "#F0FF00" "#96FF00" "#3CFF00" "#00FF1E"
 [8] "#00FF78" "#00FFD2" "#00D2FF" "#0078FF" "#001EFF" "#3C00FF" "#9600FF"
[15] "#F000FF" "#FF00B4" "#FF005A"
```

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

```
#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.

```
t(x)
```

```
           Cheese Carcass_meat  Other_meat  Fish Fats_and_oils  Sugars
England       105           245         685  147            193    156
Wales         103           227         803  160            235    175
Scotland      103           242         750  122            184    147
N.Ireland      66           267         586   93            209    139
           Fresh_potatoes  Fresh_Veg  Other_Veg  Processed_potatoes
England               720        253        488                 198
Wales                 874        265        570                 203
Scotland              566        171        418                 220
N.Ireland            1033        143        355                 187
           Processed_Veg  Fresh_fruit  Cereals  Beverages Soft_drinks
England              360         1102     1472         57         1374
Wales                365         1137     1582         73         1256
```

```
Scotland             337          957     1462        53         1572
N.Ireland            334          674     1494        47         1506
          Alcoholic_drinks  Confectionery
England                375             54
Wales                  475             64
Scotland               458             62
N.Ireland              135             41
```

```
#prcomp()
```

```
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)
```

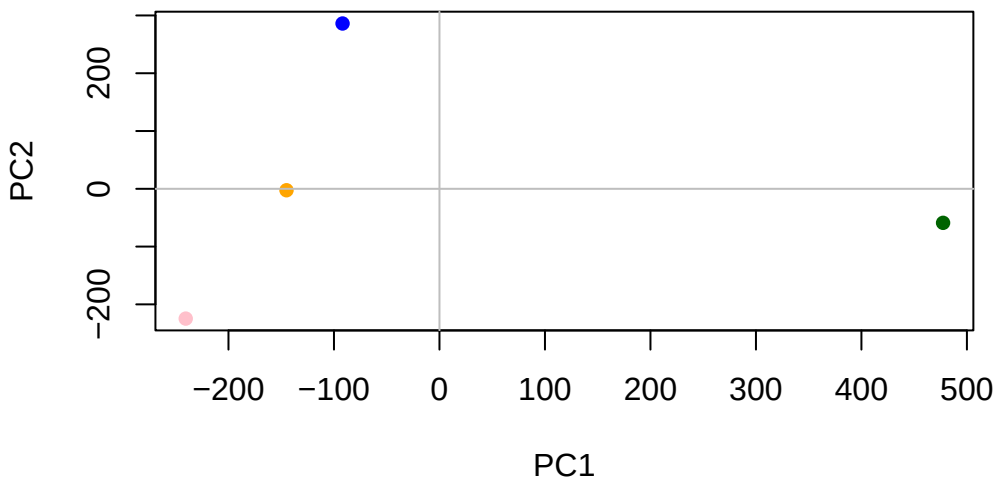
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$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" (aka. a score plot, biplot, PC1 vs PC2 plot, ordination plot)

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



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) contributes 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.