Class 7 Machine Learning 1

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In this document we will start to explore some key achine learning methods. We will begin with clustering which involves finding groupings in data. We will then move on to dimensionality reduction.

Clustering

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

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# Make up some data
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                                                      3.6040341
                                                                  1.2304032
[817]
       3.1899993
                   3.9640734
                               1.8656499
                                          2.5938480
                                                      3.1979349
                                                                  3.1038426
[823]
       2.1777010
                   3.5673524
                               2.7769229
                                          3.5201537
                                                      3.3624201
                                                                  2.2335913
[829]
       4.1591496
                   3.7207027
                               2.7807845
                                          1.6784479
                                                      2.9628806
                                                                  3.5494105
       4.0700659
                   3.0036142
                                                      3.0739770
[835]
                              2.8586858
                                          1.4083141
                                                                  4.3497643
[841]
       3.1086893
                   3.4753190
                              3.0727431
                                          3.5989936
                                                      4.0430045
                                                                  2.6988640
[847]
       2.8965844
                   3.2317529
                              3.9520287
                                          3.6525173
                                                      3.1839338
                                                                  1.4305700
[853]
       3.3330191
                   2.4491811
                               4.5169294
                                          3.5786768
                                                      4.0925607
                                                                  3.0029641
[859]
       3.7799019
                   3.1535319
                              2.9859759
                                          3.3641246
                                                      2.1150829
                                                                  4.0240684
[865]
       3.7098629
                   3.5160591
                              3.8604727
                                          3.8926825
                                                      4.0145510
                                                                  3.3219419
[871]
       2.2868183
                   3.7783691
                              3.3879507
                                          2.3753322
                                                      2.4093828
                                                                  1.4197556
[877]
       3.7640038
                   2.0441836
                              4.3187793
                                          5.1221820
                                                      3.4442656
                                                                  2.9715264
[883]
       2.7011101
                   2.4402468
                               3.0597035
                                          3.9961661
                                                      2.4222638
                                                                  0.9062828
[889]
                   3.8182325
                                          2.6986061
                                                      2.9744847
       5.1630251
                              2.5504188
                                                                  4.0078090
```

```
[895]
       3.1760469 2.9532980 3.4613943 2.6661356 3.8131846 2.0630504
 [901]
       3.0902450 2.8878584 2.3271337 3.3710618 3.4324212
                                                        2.1803341
 [907]
      1.1691189 2.9008293 2.6694719 2.8638878 2.7280397 1.6636235
 [913]
       2.3666633 4.8146361 3.4381745
                                    1.3673203 2.8977594 3.8347500
 [919]
       1.0962643 3.6555622 3.6405139 4.0731440 3.0450765
                                                       1.9349989
 [925]
       3.5762594 3.3274452 3.0046418
                                    3.1160413 4.6239132
                                                        2.3495348
 [931]
       4.2567347 2.5787465 2.6537362 3.0748882 3.5245930 4.8465475
 [937]
       5.1013963 2.9234833 3.9482546 3.6306755 2.1225218 1.9306047
 [943]
       3.1541051 2.5870005 2.8147477 2.2334575 4.1329614 2.1661373
 [949]
       4.1642023 3.6473532 2.2754110 2.4147588 2.1122891 2.7641245
 [955]
       2.0693579 1.8536265 1.0719140 2.2821163 3.5028556 0.5178372
 [961]
       1.2615349 4.0135809 3.2147314 2.2918324 3.4975869 1.9345356
       3.8470178 1.4555513 5.2433358 3.1042070 3.2373087
 [967]
                                                        4.0517608
 [973]
       4.2213922 2.8805723 3.4679938 4.9471234 2.5739313 4.0314247
 [979]
      4.7675089 2.6119777 2.4815325 3.8434142 1.7118540
                                                        3.6701789
 [985]
       2.2693696 2.3911428 2.5876232 3.0127146 3.3399743 3.1089496
 [991]
       2.6933405 2.5268251 3.5271795 4.7483548 3.4081626 5.0255342
 [997]
       2.6615844 2.9119588 2.8773498 2.7818028
  library(ggplot2)
  tmp <- c(rnorm(30, -3), rnorm(30, +3))
  x \leftarrow cbind(x = tmp, y = rev(tmp))
Now let's try the kmeans() algorithm
  km \leftarrow kmeans(x, 2)
  km
K-means clustering with 2 clusters of sizes 30, 30
Cluster means:
         Х
                  У
1 3.138545 -2.680385
2 -2.680385 3.138545
Clustering vector:
 Within cluster sum of squares by cluster:
[1] 44.25586 44.25586
 (between_SS / total_SS = 92.0 %)
```

Available components:

```
[1] "cluster" "centers" "totss" "withinss" "tot.withinss"
```

[6] "betweenss" "size" "iter" "ifault"

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

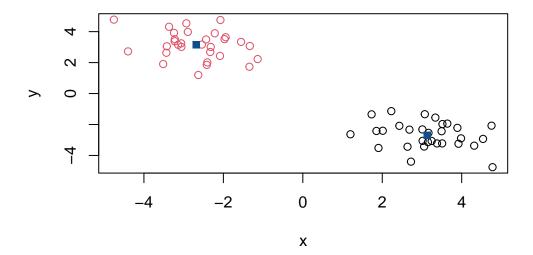
Q. What are center/mean values of each cluster?

km\$centers

```
x y
1 3.138545 -2.680385
2 -2.680385 3.138545
```

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

```
plot(x, col = km$cluster)
points(km$centers, col = "dodgerblue4", pch = 15, cex = 1)
```



Run kmeans() again and cluster in 4 groups and plot the results

First we run the kmeans() algorithm:

```
km2 <- kmeans(x,4)
km2</pre>
```

K-means clustering with 4 clusters of sizes 7, 9, 30, 14

Cluster means:

x y 1 -3.069348 4.310492 2 -3.386601 2.957190 3 3.138545 -2.680385 4 -2.031908 2.669157

Clustering vector:

Within cluster sum of squares by cluster:

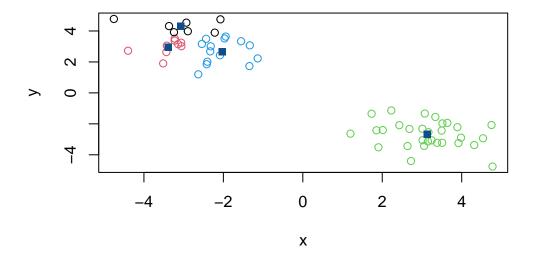
[1] 5.633583 3.257897 44.255864 10.934592 (between_SS / total_SS = 94.2 %)

Available components:

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

Then we plot the corresponding 4 clusters:

```
plot(x, col = km2$cluster)
points(km2$centers, col = "dodgerblue4", pch = 15, cex = 1)
```



```
nrow(x)
```

[1] 60

```
km3 <- data.frame(1:60)
z = NULL
for(y in 1:59){
   print(y)
   print(kmeans(x,y)$betweenss/kmeans(x,y)$totss)</pre>
```

```
z <- c(z, kmeans(x,y)$betweenss/kmeans(x,y)$totss)</pre>
[1] 1
[1] -2.058966e-16
[1] 2
[1] 0.9198489
[1] 3
[1] 0.9358667
[1] 4
[1] 0.9518846
[1] 5
[1] 0.9577638
[1] 6
[1] 0.9640619
[1] 7
[1] 0.9695948
[1] 8
[1] 0.9715731
[1] 9
[1] 0.979022
[1] 10
[1] 0.9708365
[1] 11
[1] 0.9820717
[1] 12
[1] 0.9838238
[1] 13
[1] 0.9850194
[1] 14
[1] 0.9852791
[1] 15
[1] 0.988944
[1] 16
[1] 0.9795359
[1] 17
[1] 0.9908828
[1] 18
[1] 0.9915034
[1] 19
[1] 0.9931303
[1] 20
```

- [1] 0.9936377
- [1] 21
- [1] 0.9935559
- [1] 22
- [1] 0.995907
- [1] 23
- [1] 0.9952164
- [1] 24
- [1] 0.9962257
- [1] 25
- [1] 0.9962368
- [1] 26
- [1] 0.9967546
- [1] 27
- [1] 0.9970368
- [1] 28
- [1] 0.9976029
- [1] 29
- [1] 0.9975595
- [1] 30
- [1] 0.9950355
- [1] 31
- [1] 0.9980786
- [1] 32
- [1] 0.9978351
- [1] 33
- [1] 0.9976357
- [1] 34
- [1] 0.9980894
- [1] 35
- [1] 0.9982578
- [1] 36
- [1] 0.9988097
- [1] 37
- [1] 0.9986888
- [1] 38
- [1] 0.9985501
- [1] 39
- [1] 0.9986367
- [1] 40
- [1] 0.9987816
- [1] 41
- [1] 0.9989192

- [1] 42
- [1] 0.999292
- [1] 43
- [1] 0.9993773
- [1] 44
- [1] 0.9992423
- [1] 45
- [1] 0.9993077
- [1] 46
- [1] 0.9994027
- [1] 47
- [1] 0.9993904
- [1] 48
- [1] 0.9994219
- [1] 49
- [1] 0.9995758
- [1] 50
- [1] 0.9995995
- [1] 51
- [1] 0.9996318
- [1] 52
- [1] 0.9997393
- [1] 53
- [1] 0.9997013
- [1] 54
- [1] 0.9998936
- [1] 55
- [1] 0.9998881
- [1] 56
- [1] 0.9999461
- [1] 57
- [1] 0.9998529
- [1] 58
- [1] 0.9999817
- [1] 59
- [1] 0.999943

print(z)

- [1] -2.058966e-16 9.198489e-01 9.358667e-01 9.517022e-01 9.591713e-01
- [6] 9.638958e-01 9.668447e-01 9.542347e-01 9.790220e-01 9.797125e-01

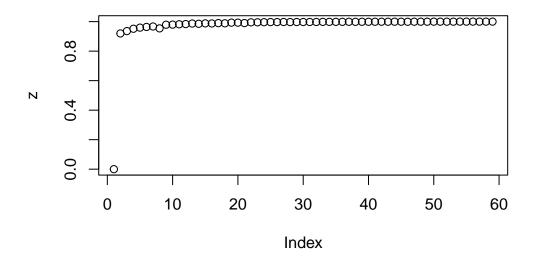
```
[11]
     9.819254e-01 9.832965e-01 9.870270e-01 9.852628e-01 9.881463e-01
[16]
     9.874566e-01 9.898328e-01 9.886068e-01 9.930429e-01 9.929749e-01
[21]
     9.901215e-01 9.951296e-01
                                9.952461e-01
                                              9.960932e-01 9.968172e-01
[26]
     9.967713e-01 9.973029e-01
                                9.969181e-01
                                              9.972800e-01 9.973819e-01
[31]
     9.975490e-01 9.976011e-01
                                9.983296e-01
                                              9.983711e-01
                                                           9.984599e-01
[36]
     9.985172e-01 9.988674e-01
                                9.986406e-01
                                              9.989819e-01
                                                           9.989819e-01
[41]
     9.990291e-01 9.992923e-01 9.992174e-01
                                              9.994097e-01
                                                           9.993418e-01
Γ46]
     9.990998e-01 9.993968e-01 9.994734e-01 9.994930e-01 9.997740e-01
[51]
     9.996360e-01 9.995908e-01 9.997260e-01 9.998648e-01 9.998884e-01
[56]
     9.999413e-01 9.998288e-01 9.998860e-01 9.999883e-01
  length(z)
```

[1] 59

Z

```
[1] -2.058966e-16 9.198489e-01 9.358667e-01 9.517022e-01 9.591713e-01
 [6]
    9.638958e-01 9.668447e-01 9.542347e-01 9.790220e-01 9.797125e-01
     9.819254e-01 9.832965e-01 9.870270e-01
[11]
                                             9.852628e-01 9.881463e-01
[16]
     9.874566e-01 9.898328e-01 9.886068e-01 9.930429e-01 9.929749e-01
[21]
     9.901215e-01 9.951296e-01 9.952461e-01 9.960932e-01 9.968172e-01
[26]
                                             9.972800e-01 9.973819e-01
     9.967713e-01 9.973029e-01
                                9.969181e-01
[31]
     9.975490e-01 9.976011e-01
                                9.983296e-01
                                             9.983711e-01 9.984599e-01
[36]
     9.985172e-01 9.988674e-01 9.986406e-01 9.989819e-01 9.989819e-01
[41]
     9.990291e-01 9.992923e-01
                                9.992174e-01
                                             9.994097e-01 9.993418e-01
                                9.994734e-01
[46]
     9.990998e-01 9.993968e-01
                                             9.994930e-01 9.997740e-01
[51]
     9.996360e-01 9.995908e-01
                                9.997260e-01 9.998648e-01
                                                          9.998884e-01
[56]
     9.999413e-01 9.998288e-01 9.998860e-01 9.999883e-01
```

plot(z)



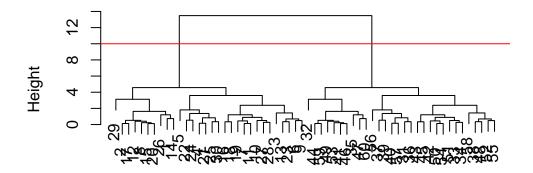
Hierarchical Clustering

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

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 dissimilar our input points are to each other.

```
hc <- hclust(dist(x))
plot(hc)
abline(h = 10, col = "red")</pre>
```

Cluster Dendrogram

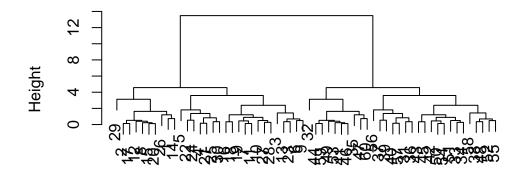


dist(x) hclust (*, "complete")

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

plot(hc)

Cluster Dendrogram

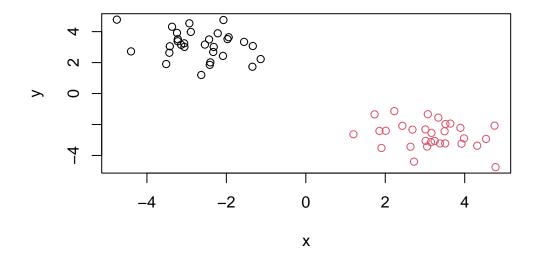


dist(x)
hclust (*, "complete")

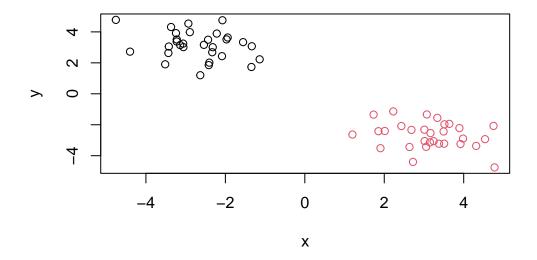
To get my main result (my cluster membership vector) I need to "cut" my tree using function cutree():

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

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



plot(x, col = cutree(hc, h=5))



Principal Component Analysis (PCA)

The goal of PCA is to reduce

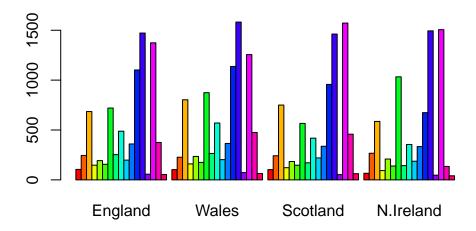
Data import

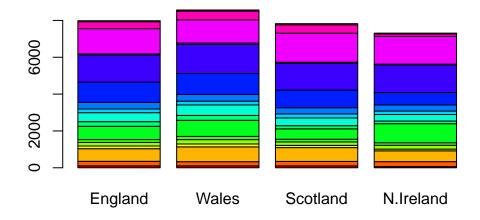
Read data about crazy eating trends in the UK and N. Ireland

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

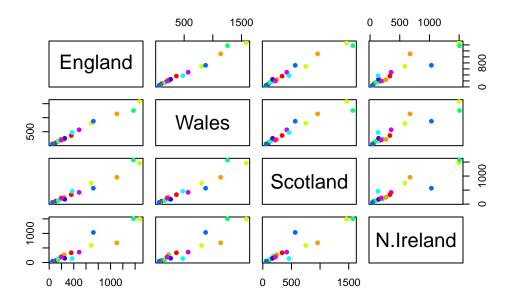
	England	Wales	${\tt Scotland}$	${\tt N.Ireland}$
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139

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





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



If there is a point on the diagonal that means that for that food the countries are very similar in consumption.

The paris plot is useful for small datasets but it can be a lot to interpret and gets intractable for larger datasets.

So PCA to the rescue...

The main dunction to do PCA in base R is called prcomp()

```
pca<- (prcomp(t(x)))
summary(pca)</pre>
```

Importance of components:

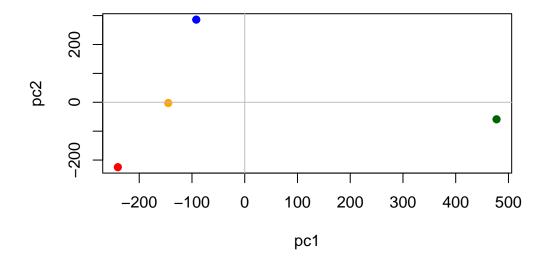
```
PC1 PC2 PC3 PC4
Standard deviation 324.1502 212.7478 73.87622 3.176e-14
Proportion of Variance 0.6744 0.2905 0.03503 0.000e+00
Cumulative Proportion 0.6744 0.9650 1.00000 1.000e+00
```

```
attributes(pca)
```

```
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 viz is called a "PCA plot" (a.k.a a score plot, screen plot, biplot, PC1 v PC2 plot, ordination plot)

```
mycols <- c("orange", "red","blue","darkgreen")
plot(pca$x[,1], pca$x[,2], col = mycols, xlab = "pc1", ylab = "pc2", pch = 19)
abline(h=0, col = "gray")
abline(v=0, col = "gray")</pre>
```



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 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