Class 7: Machine Learning!

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Today, we are going to learn how to apply different machine learning methods, beginning with clustering:

The goal here is to find groups/clusters in your input data.

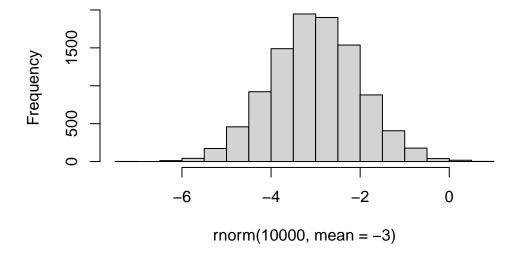
First I will make up some data with clear groups. For this I will use the rnorm() function:

rnorm(10)

```
[1] 1.2252965 1.8047302 0.7287003 0.2569677 -1.4240550 0.2942927 [7] -1.4488933 0.2363693 0.7787932 0.9650687
```

```
hist(rnorm(10000, mean = -3))
```

Histogram of rnorm(10000, mean = -3)

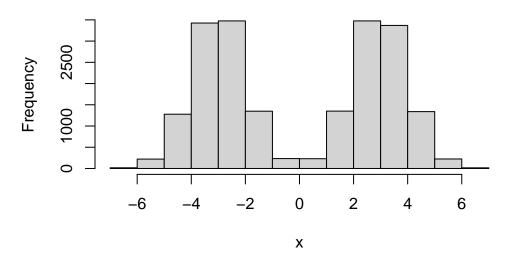


```
n <- 10000

x <- c(rnorm(n,-3), rnorm(n,+3))

hist(x)
```

Histogram of x

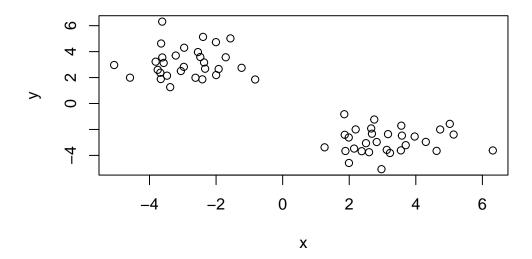


```
n <- 30
x <- c(rnorm(n,-3) , rnorm(n,+3))
y <- rev(x)

z <- cbind(x,y)
head(z)</pre>
```

```
x y
[1,] -2.329109 2.682196
[2,] -3.378416 1.259114
[3,] -1.234163 2.751841
[4,] -2.958812 4.300482
[5,] -2.412750 1.865115
[6,] -3.659845 1.885551
```

```
plot(z)
```



Use the kmeans() function setting k to 2 and nstart=20

Inspect/print the results

- Q. How many points are in each cluster?
- Q. What 'component' of your result object details cluster size? cluster assignment/membership? cluster center?
- Q. Plot x colored by the kmeans cluster assignment and add cluster centers as blue points

```
km <- kmeans(z, centers = 2)
km</pre>
```

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

Cluster means:

Clustering vector:

Within cluster sum of squares by cluster:

[1] 67.47189 67.47189

(between_SS / total_SS = 89.0 %)

Available components:

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

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

Results in kmeans object km

attributes(km)

\$names

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

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

\$class

[1] "kmeans"

cluster size?

km\$cluster

cluster assignment/membership

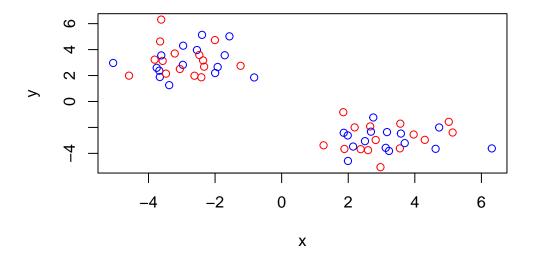
km\$cluster

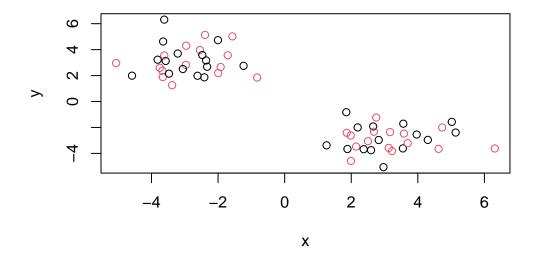
cluster center?

km\$centers

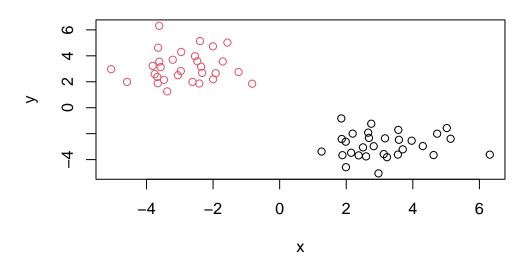
Q. Plot x colored by the kmeans cluster assignment and add cluster centers as blue points

R will re-cycle the shorter color vector to be the same length as the longer (number of data points) in z



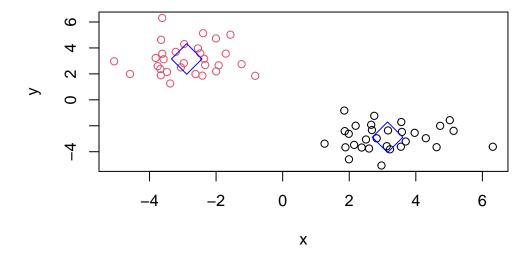


plot(z, col=km\$cluster)



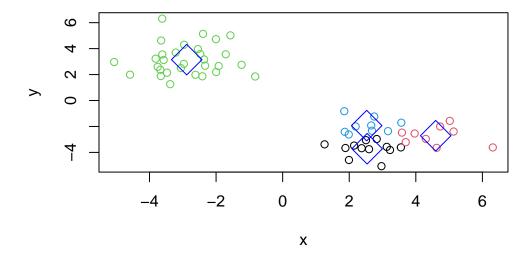
We can use the points() function to add new points to an existing plot... like the cluster centers.

```
plot(z, col=km$cluster)
points(km$centers, col="blue", pch=5, cex=3)
```



Q. Can you run kmeans and ask for 4 clusters please and plot the results like we have done above?

```
km4 <- kmeans(z, centers = 4)
plot(z, col=km4$cluster)
points(km4$centers, col="blue", pch=5, cex=3)</pre>
```



Hierarchical Clustering

Let's take our same made-up data ${\bf z}$ and see how helust works.

First we need a distance matrix of our data to be clustered.

```
d <- dist(z)
hc <- hclust(d)
hc</pre>
```

Call:
hclust(d = d)

Cluster method : complete
Distance : euclidean

Number of objects: 60

d 1 2 3 4 5 6 7

```
2
    1.7681087
3
    1.0971589
               2.6126719
4
    1.7364833
               3.0701776
                           2.3179091
5
    0.8213516
               1.1400643
                           1.4749074
                                       2.4958363
    1.5509683
                           2.5757318
6
               0.6867509
                                       2.5146253
                                                  1.2472627
7
    0.4834178
               2.1603997
                           1.1994550
                                       1.2838871
                                                  1.3005441
                                                              1.8233585
8
    1.0775499
               2.8454813
                           0.9411252
                                       1.4500436
                                                  1.8385550
                                                              2.5729231
                                                                         0.7634011
9
    2.3492511
               3.3762938
                           3.0572085
                                       0.7640314
                                                  3.0243003
                                                              2.7388677
                                                                         1.9483838
10
    2.7480296
               2.3991484
                           3.8341655
                                       2.4898856
                                                  2.8699008
                                                              1.7716151
                                                                         2.7089984
    2.0744130
11
               3.7339373
                           2.1237570
                                       1.0470897
                                                  2.8948683
                                                              3.2920291
                                                                         1.6063752
   0.4070812
12
               2.0196539
                           0.6947460
                                       1.9410872
                                                  0.9330135
                                                              1.9015891
                                                                         0.6686786
13
    1.3447013
               2.4438241
                           2.1913808
                                       0.6539199
                                                  1.9984954
                                                              1.8663952
                                                                         1.0037386
14
    0.6548548
               1.6188980
                           1.7355531
                                       1.4753439
                                                  1.1091391
                                                              1.1667476
                                                                         0.6961642
15
    1.3221134
               1.8783474
                           2.3698254
                                       1.3247741
                                                  1.7151162
                                                              1.2446520
                                                                         1.2142806
16
    1.3815166
               1.1529505
                           2.4706435
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17
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               5.0594850
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                                       2.1177657
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18
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               2.8317570
                           1.7862201
                                       0.5325956
                                                  2.1044349
                                                              2.3598783
                                                                         0.8217705
19
    1.2642287
               0.8923200
                           2.3203776
                                       2.2149758
                                                  1.0979913
                                                              0.3201131
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                           2.5240163
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                                       1.8812168
                                                                         1.5048153
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               2.4928863
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                                                  1.7182011
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                           0.9885762
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                                                  1.5868404
                                                              2.8340819
                                                                         2.0195703
23
    0.7544781
               1.0510026
                           1.5826240
                                       2.3396971
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                                                              1.0457132
                                                                         1.2070201
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    2.4589031
               4.1741062
                           2.2934373
                                       1.5652644
                                                  3.2664118
                                                              3.7683422
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                                       2.3161957
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    6.5080009
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45 7.9077454 7.5783519 7.3705108 9.5941274 7.3214730 8.2050551 8.3183001
46 8.3013615 8.1045189
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                                               1.7164644 0.6757018 0.6770257
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              2.2514371
                         1.5088927
                                    2.8901473
                                               1.7760899 1.4032019 0.8395422
              1.6888085
17
   3.3466039
                         3.6430905
                                    2.2600073
                                               4.0281639
                                                         2.6472162 3.5478352
                         2.7077338
                                               1.4469240 0.7182561 1.2162815
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   0.9265648
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   0.7646348
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   1.9270884
              3.9583698
                         4.3809537
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   1.8214876
             2.8333688
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   1.4635088
              2.1190823
                         4.0515546
                                    0.5228292
                                               2.3879565
                                                         2.1090209
24
25
   2.1328838
              1.4097359
                         1.2728576
                                    2.3558862
                                               1.9753318 0.7673175 0.9365622
   1.9064444 1.0735918
                         1.5592651
                                    1.9973843
                                               1.9141680 0.4304677
                                                                    0.9732698
26
27
   3.2772526 2.7937773 1.0869345 3.7637047
                                               2.7448460 2.1902651 1.8192133
```

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1.7132147 1.3588041 3.4393376 0.5601466
                                             2.5205360 1.6553566 2.3812033
28
29
   1.7148909 2.2024391 2.0580047
                                   2.4639727
                                             1.1453119
                                                       1.2036563 0.3338931
   1.4010410 2.9399682
                       3.1606444
                                   2.5381190
                                             0.4722089
                                                       1.9324345
30
                                                                  1.1578999
   6.7946678 8.8321342 8.7920759
                                  7.9308474
                                             6.2151040 7.8511498
31
                                                                  7.0640556
32
   7.8481044 9.8429542 9.6718872 8.9988304
                                             7.2296579
                                                        8.8476224
                                                                  8.0338315
   9.0735398 11.2439608 11.5205632 10.0852638
                                             8.6792789 10.3316599
                                                                  9.6377891
   8.9502310 10.8004874 10.3347154 10.1369226
                                             8.2340104
                                                       9.7808116
                                                                  8.9168696
35
   8.9013114 10.9442998 10.8418925 10.0270258
                                             8.3272793 9.9607593
                                                                  9.1648759
36 8.8769441 10.8856537 10.7090181 10.0190047
                                             8.2710616 9.8921455
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37
   8.4644505 10.6561561 11.0567347 9.4362262
                                             8.1294332 9.7722476
                                                                  9.1176358
38
   7.2030367 9.1779459 8.9937200 8.3631023
                                             6.5674894 8.1792242
                                                                  7.3605733
39
   5.6527663 7.7447627 7.8863381
                                  6.7636874
                                             5.1370923 6.7889000
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40 8.0289376 10.1343927 10.2149318 9.1172562
                                             7.5268833 9.1779908
                                                                  8.4255836
   8.4897446 10.4498521 10.1889651
                                  9.6509340
                                             7.8441428 9.4458854
                                                                  8.6155878
42
   8.0251914 9.9595288 9.6677400 9.1952306
                                             7.3602016 8.9515398
                                                                  8.1141098
43 8.3381442 10.4596436 10.5778377 9.4114760 7.8581216 9.5113496 8.7699064
44 10.7679910 12.9313285 13.1444338 11.7851546 10.3552794 12.0094088 11.2985925
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                                             7.6538747 9.2488974
                                                                  8.4136323
46 8.6225220 10.6375041 10.4817734
                                   9.7625647
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                                                                  8.8376590
   7.9519887 9.9792289 9.8716992 9.0885467
                                             7.3625951 8.9924520
                                                                  8.1930120
47
48 8.6681662 10.7419093 10.7196481
                                   9.7767876
                                             8.1266498 9.7698754
                                                                  8.9924520
49
   7.0135416 9.0927700 9.1399248
                                   8.1252177
                                             6.4795689 8.1266498
                                                                  7.3625951
50 8.5140754 10.6861991 10.9833090 9.5252402 8.1252177 9.7767876
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                                             9.1399248 10.7196481 9.8716992
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                                             8.3838128 10.0362855
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    0.7609451
17
    3.1859677
               3.9402137
18
    1.3273381
               1.9529601
                           2.5813517
19
    0.9860356
               0.3033782
                           4.1691151
                                      2.0427366
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   0.5613585
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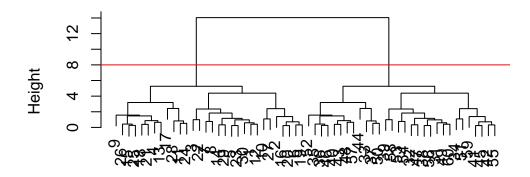
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51 3.5296645
52 1.6498937 2.1761092
53 1.2036738 3.4050135 2.2118193
54 1.6063752 2.7089984 1.9483838 0.7634011
```

```
56 2.8948683 2.8699008 3.0243003 1.8385550 1.3005441 1.2472627
57 1.0470897 2.4898856 0.7640314 1.4500436 1.2838871 2.5146253 2.4958363
58 2.1237570 3.8341655 3.0572085 0.9411252 1.1994550 2.5757318 1.4749074
59 3.7339373 2.3991484 3.3762938 2.8454813 2.1603997 0.6867509 1.1400643
60 \quad 2.0744130 \quad 2.7480296 \quad 2.3492511 \quad 1.0775499 \quad 0.4834178 \quad 1.5509683 \quad 0.8213516
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58 2.3179091
59 3.0701776 2.6126719
60 1.7364833 1.0971589 1.7681087
plot(hc)
abline(h=8, col="red")
```

Cluster Dendrogram



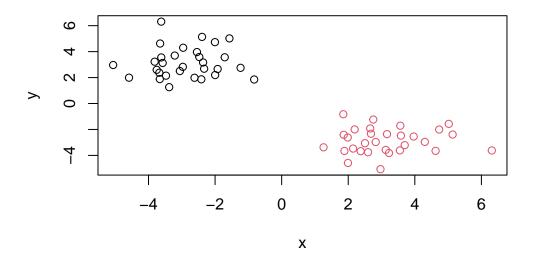
d hclust (*, "complete")

I can get my cluster membership vector by "cutting the tree" with the ${\tt cutree}$ () function like so:

```
grps <- cutree(hc, h=8)
grps</pre>
```

Can you plot ${\bf z}$ colored by our hclust results:

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



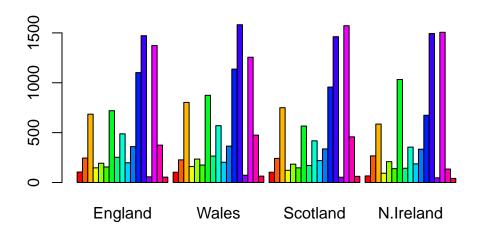
PCA of UK food data

Read data from the UK food

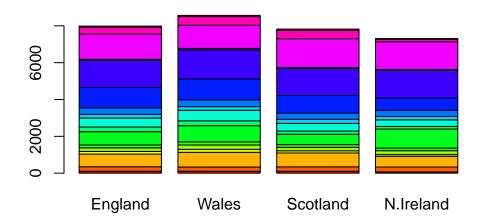
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names=1)
head(x)</pre>
```

	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

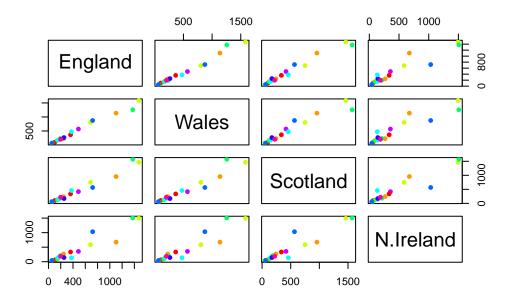
```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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



A so-called "Pairs" plot can be useful for small datasets like this



It is hard to see structure and trends in even this small data-set. How will we ever do this when we have big datasets with 1,000s or 10s of thousands of things we are measuring...

PCA to the rescue

Let's see how PCA deals with this dataset. So main function in base R to do PCA 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	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

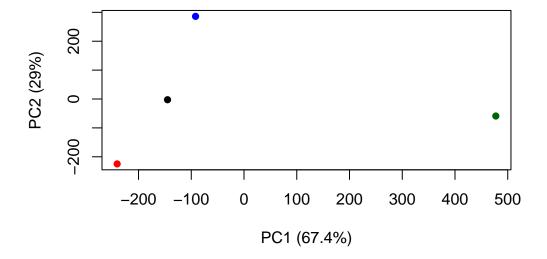
Let's see what is inside this pca object taht we created from running prcomp()

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
```



```
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```

