Class 7: Machine Learning 1

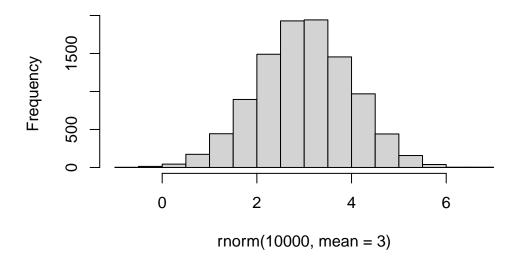
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Clustering

We will start with k-means clustering, one of the most prevalent of all clustering methods. To get started let's make up some data:

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

Histogram of rnorm(10000, mean = 3)

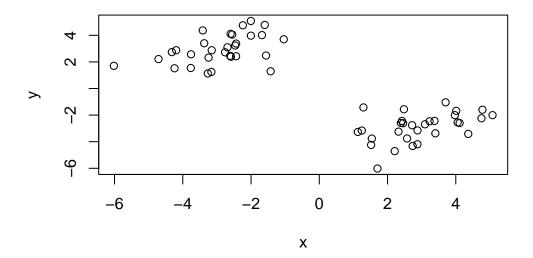


```
tmp <- c( rnorm(30,3), rnorm(30, -3))
tmp</pre>
```

```
[1]
     2.879270 1.539834 5.077270 2.210861 3.376840 4.365716 4.054800
 [8]
    1.130313 3.231119 2.455928 2.572094 4.013586 2.480226 3.401627
[15]
     3.098684 4.780768 3.702022 2.877222 2.321431 1.293929 2.721148
[22]
     2.391724 4.752520 1.705171 4.112709 2.424112 1.245857 1.518727
[29] 2.736345 3.973897 -2.003955 -4.320436 -4.243024 -3.162015 -2.438352
[36] -2.598156 -6.019735 -2.239794 -2.590143 -2.760598 -1.425068 -3.244289
[43] -4.194173 -1.040783 -1.598070 -2.691046 -3.372093 -1.560717 -1.679061
[50] -3.758887 -2.610714 -2.464274 -3.267200 -2.552296 -3.414925 -2.436652
[57] -4.711054 -2.005091 -3.765200 -3.152162
  x \leftarrow cbind(x = tmp, y = rev(tmp))
  head(x)
[1,] 2.879270 -3.152162
[2,] 1.539834 -3.765200
[3,] 5.077270 -2.005091
```

plot(x)

[4,] 2.210861 -4.711054 [5,] 3.376840 -2.436652 [6,] 4.365716 -3.414925



The main function in R for K-means clustering is called kmeans().

```
k <- kmeans(x, centers = 2, nstart = 20)
k</pre>
```

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

Cluster means:

```
x y
1 -2.910665 2.948192
2 2.948192 -2.910665
```

Clustering vector:

Within cluster sum of squares by cluster:

```
[1] 70.31432 70.31432 (between_SS / total_SS = 88.0 %)
```

Available components:

- [1] "cluster" "centers" "totss" "withinss" "tot.withinss"
- [6] "betweenss" "size" "iter" "ifault"
 - Q1. How many points are in each cluster?

k\$size

[1] 30 30

Q2. The clustering result i.e. membership vector?

k\$cluster

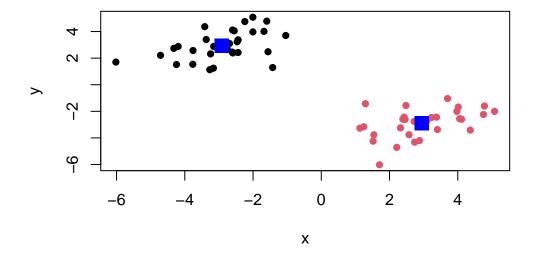
Q3. Cluster centers

k\$centers

```
x y
1 -2.910665 2.948192
2 2.948192 -2.910665
```

Q4. Make a plot of our data colored by clustering results with optionally the cluster centers shown.

```
plot(x, col = k$cluster, pch = 16)
points(k$centers, col = "blue", pch = 15, cex = 2)
```



Q5. Run kmeans again but cluster into 3 groups and plot the results like we did above.

```
k <- kmeans(x, centers = 3, nstart = 20)
k</pre>
```

K-means clustering with 3 clusters of sizes 13, 17, 30

Cluster means:

x y 1 3.924628 -2.175755 2 2.201505 -3.472655

3 -2.910665 2.948192

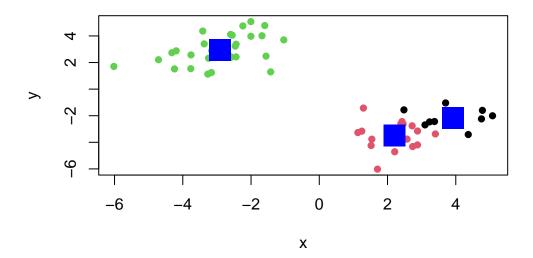
```
Clustering vector:
```

Within cluster sum of squares by cluster:

points(k\$centers, col = "blue", pch = 15, cex = 3)

```
[1] 11.18543 24.86579 70.31432 (between_SS / total_SS = 90.9 %)
```

Available components:



K-means will always return a clustering result - even if there is no clear groupings.

Hierarchical Clustering (bottom up)

Hierarchical clustering has an advantage in that it can reveal the structure in your data rather than imposing a structure as k-means will.

The main function for this in base R is called hclust()

It requires a distance matrix as input, not the raw data itself.

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                        у
 [1,]
      2.879270 -3.152162
 [2,]
      1.539834 -3.765200
 [3,]
      5.077270 -2.005091
 [4,]
      2.210861 -4.711054
 [5,]
      3.376840 -2.436652
 [6,]
      4.365716 -3.414925
 [7,]
      4.054800 -2.552296
 [8,]
      1.130313 -3.267200
 [9,]
      3.231119 -2.464274
[10,]
      2.455928 -2.610714
[11,]
      2.572094 -3.758887
[12,]
      4.013586 -1.679061
[13,]
      2.480226 -1.560717
[14,]
      3.401627 -3.372093
[15,]
      3.098684 -2.691046
[16,]
      4.780768 -1.598070
[17,]
      3.702022 -1.040783
[18,]
      2.877222 -4.194173
      2.321431 -3.244289
[19,]
[20,]
      1.293929 -1.425068
      2.721148 -2.760598
[21,]
[22,]
      2.391724 -2.590143
[23,]
      4.752520 -2.239794
[24,]
      1.705171 -6.019735
[25,]
      4.112709 -2.598156
[26,]
      2.424112 -2.438352
[27,]
      1.245857 -3.162015
[28,]
      1.518727 -4.243024
[29,]
      2.736345 -4.320436
[30,]
      3.973897 -2.003955
[31,] -2.003955
                3.973897
[32,] -4.320436
                 2.736345
[33,] -4.243024
                1.518727
```

```
[34,] -3.162015 1.245857
[35,] -2.438352 2.424112
[36,] -2.598156 4.112709
[37,] -6.019735 1.705171
[38,] -2.239794 4.752520
[39,] -2.590143 2.391724
[40,] -2.760598 2.721148
[41,] -1.425068 1.293929
[42,] -3.244289 2.321431
[43,] -4.194173 2.877222
[44,] -1.040783 3.702022
[45,] -1.598070 4.780768
[46,] -2.691046 3.098684
[47,] -3.372093 3.401627
[48,] -1.560717
                2.480226
[49,] -1.679061 4.013586
[50,] -3.758887 2.572094
[51,] -2.610714 2.455928
[52,] -2.464274 3.231119
[53,] -3.267200 1.130313
[54,] -2.552296 4.054800
[55,] -3.414925 4.365716
[56,] -2.436652 3.376840
[57,] -4.711054 2.210861
[58,] -2.005091 5.077270
[59,] -3.765200 1.539834
[60,] -3.152162 2.879270
            1
                        2
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2
   1.47306003
   2.47930953 3.95113158
3
4
   1.69614716 1.15970528
                          3.94189536
   0.87151031 2.26707570
                          1.75433961 2.55585828
5
6
   1.50949194 2.84750829
                          1.57922215 2.51462740 1.39100489
                          1.15968917
7
   1.31973826 2.79216599
                                      2.83907496 0.68775230 0.91695034
8
   1.75273713 0.64475695 4.14383832 1.80341272 2.39514033 3.23877446
9
   0.77264920 2.13374142 1.90239981 2.46757873 0.14831637 1.48021932
10 0.68730212 1.47379330 2.69039278 2.11458852 0.93721735 2.07220790
11 0.68005364 1.03227962 3.05805649 1.01838620 1.54787679 1.82630497
12 1.85921990 3.23595817 1.11252915 3.52743529 0.98964106 1.77122074
13 1.64071104 2.39668150
                          2.63478773 3.16183148 1.25346664 2.64445855
14 0.56676749 1.90284127 2.16251623 1.79185369 0.93576904 0.96504083
```

```
2.09411966
15
   0.51065674
                1.89309835
                                         2.20650441
                                                      0.37694438
                                                                  1.45923651
16
    2.45578846
                3.89873181
                             0.50356685
                                         4.03671827
                                                      1.63530862
                                                                  1.86366107
                3.47814724
17
    2.26601922
                             1.67964228
                                         3.96162248
                                                      1.43324619
                                                                  2.46516613
18
    1.04201327
                1.40450167
                             3.10359373
                                         0.84332843
                                                      1.82715603
                                                                  1.68013162
    0.56539568
19
                0.93927761
                             3.02163241
                                         1.47092672
                                                      1.32897179
                                                                   2.05139454
20
    2.34438961
                2.35301667
                             3.82754523
                                         3.41151981
                                                      2.31556124
                                                                  3.65997445
21
    0.42228596
                1.55071881
                             2.47428848
                                         2.01610328
                                                      0.73135029
                                                                   1.76995770
22
    0.74402104
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                             2.74853561
                                         2.12860841
                                                      0.99700280
                                                                  2.13937224
23
    2.08362142
                3.55643271
                             0.40068502
                                         3.54501845
                                                      1.38969304
                                                                  1.23715452
24
   3.09862633
                2.26058926
                             5.24294033
                                         1.40298571
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25
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                                         2.84277335
    1.35214336
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                                                      0.75338281
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                1.59451304
                             2.68830173
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                9.33123992 11.70083628 10.43602624 10.26890076 11.57898886
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   9.41747367
                9.31864447
                             9.96015707 10.45789409
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                7.41379919
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    8.14271950
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                7.74176386
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   9.29446493
                8.77499918 10.47838957
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   7.89598994
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    9.05713455
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   7.17197937
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   8.49272165
                8.41847903
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                                                      8.19559029
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                8.06110170
                             9.18111042
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   8.32464678
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53
   7.49124098
                6.86102198
                             8.91408698
                                         8.00816553
                                                      7.54098883 8.88372699
   9.02453444
                8.82598067
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                                         9.97636521
                                                      8.79167866 10.18114436
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   9.80486598
                9.52163025 10.61624114 10.67882145
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   8.41943606
                8.17442243
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56
                8.64794205 10.65765173 9.78906555
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   9.29381711
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58 9.56977241 9.52658264 10.01597147 10.65765173 9.24252211 10.61624114
59 8.13411426 7.50245108 9.52658264 8.64794205 8.17442243 9.52163025
               8.13411426
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                                      9.29381711 8.41943606
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10 1.59993865
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              1.52331568
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11
12 0.87420778
               3.29172464
                           1.10851921
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                           1.17484251
13 1.86078269
               2.17585645
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                                                 2.20008907 1.53791942
14
   1.04818995
               2.27373467
                           0.92369223
                                       1.21410140 0.91527801 1.80023663
                           0.26261066
                                      0.64775648
15 0.96613094
               2.05096103
                                                 1.19062259
                                                              1.36424302
16 1.19899039
               4.01395371
                           1.77530957
                                       2.53580948
                                                  3.08988254
                                                              0.77144603
   1.55213590
               3.40156225
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                                       2.00435394 2.94360844
                                                              0.71026088
17
18 2.02050743
              1.97761765
                           1.76572746
                                       1.63854536
                                                 0.53157946
                                                              2.75991193
19
   1.86639295
               1.19133869
                           1.19831326
                                       0.64769308
                                                  0.57240184
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20
   2.98212276 1.84938407
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                                       1.66012067
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                                                              2.73149173
21 1.34982144
               1.66955183
                           0.58981169
                                       0.30464143
                                                  1.00935603
                                                              1.68526482
22 1.66350728 1.43162986
                           0.84877994
                                      0.06741988 1.18258066
                                                              1.86024405
   0.76450651
               3.76509602
                           1.53787254
                                       2.32635190 2.65742361
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23
24 4.18854272
               2.81192264
                           3.86908499
                                       3.49071050 2.42136081
                                                              4.91632319
25 0.07386826
               3.05651849
                           0.89169774
                                      1.65682770
                                                 1.92893463
                                                              0.92442546
26
   1.63466448
               1.53652370
                           0.80742322
                                       0.17527368
                                                  1.32880072
                                                              1.76151958
   2.87435494
              0.15625181
                           2.10430619
                                       1.32973834
                                                  1.45435947
                                                              3.13997966
27
                           2.46905588
28
   3.04798750
               1.05028495
                                       1.88222808
                                                  1.15929754
                                                              3.57746122
29 2.20559336
               1.92058455
                           1.92097299
                                       1.73256505
                                                  0.58507687
                                                              2.93397467
30 0.55427705
                                                  2.24607182
               3.11155307
                           0.87384985
                                       1.63474347
                                                              0.32730989
               7.89031887
                           8.29795494
                                       7.95284060
                                                              8.25631478
31 8.90503923
                                                  8.98533204
32 9.90526656
               8.10883555
                           9.16910127
                                       8.63192646
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                                       7.86945071
33 9.24267953
               7.19568286
                           8.46918630
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34 8.15526748
               6.22830334 7.39170019
                                       6.81428121
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35 8.18081105
               6.71761890
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                                       7.02164214
                                                  7.95826967
                                                              7.64614471
36 9.41722469
               8.26828490 8.78846698 8.41119412 9.41772344 8.78975096
37 10.93719728
               8.70905581 10.14704719
                                       9.51124241 10.18211475 10.58869885
38 9.64273038 8.69905309
                           9.05610283 8.73309908 9.77743917
                                                              8.97050601
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                                      7.10543599 8.02986360
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40 8.61735812 7.14139316 7.92396797 7.45928261 8.39216661 8.07783343
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41 6.69495343 5.22818001 5.98365808 5.50530365 6.44269008 6.19819473
42 8.77666894 7.09717806 8.05194870 7.53780684 8.41430826 8.28738038
43 9.87548647 8.13044130
                          9.14694185
                                     8.62213992 9.47735858 9.38759914
                                     7.21648314 8.28963520 7.38259374
44 8.06730837 7.29956961
                          7.50149011
45 9.25898367
              8.49787454
                          8.70699185
                                      8.43023830
                                                9.50347260
                                                            8.55687259
46 8.80000147
              7.42477411
                          8.12517980
                                      7.68690962
                                                8.64447444 8.23279626
47 9.51882012 8.04642189
                          8.83239464
                                      8.37341460
                                                 9.30625165
                                                            8.96446468
                                      6.48468326
48
   7.54057819
              6.34622356
                          6.88547587
                                                7.48376045
                                                            6.95503554
49 8.71710762 7.80400034 8.12850112
                                     7.80893606 8.85910013
                                                            8.05061748
                          8.61540453
50 9.34414755 7.61588065
                                     8.09230745 8.95336019
                                                            8.85910013
51 8.33734954 6.83735942
                          7.63776194
                                     7.16531472 8.09230745
                                                            7.80893606
52 8.71471298 7.42625113
                          8.05450212
                                     7.63776194 8.61540453
                                                            8.12850112
                          7.42625113
53 8.19593191
              6.21902237
                                      6.83735942
                                                7.61588065
                                                            7.80400034
54 9.34384550 8.19593191
                          8.71471298
                                     8.33734954 9.34414755
                                                            8.71710762
55 10.18114436
              8.88372699
                          9.52988331
                                      9.11797721 10.09225404
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                                      7.73227993 8.71815063
56 8.79167866 7.54098883
                          8.13893397
                                                            8.19559029
57 9.97636521
              8.00816553
                          9.21601834
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59 \quad 3.00443804 \quad 1.31906226 \quad 0.47829022 \quad 0.67101038 \quad 1.59451304 \quad 2.82518575
60 \quad 1.58637532 \quad 1.17698411 \quad 1.74386315 \quad 1.63344280 \quad 0.84657749 \quad 1.35214336
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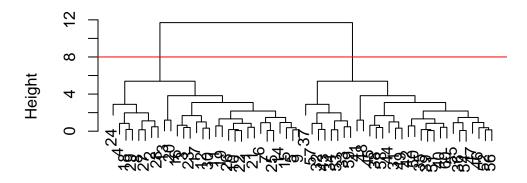
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54 0.87420778 1.91161688 1.59993865 0.82837126 3.01060055
55 1.77122074 1.82630497 2.07220790 1.48021932 3.23877446 0.91695034
56 0.98964106 1.54787679 0.93721735 0.14831637 2.39514033 0.68775230
57 3.52743529 1.01838620 2.11458852 2.46757873 1.80341272 2.83907496
58 1.11252915 3.05805649 2.69039278 1.90239981 4.14383832 1.15968917
59 3.23595817 1.03227962 1.47379330 2.13374142 0.64475695 2.79216599
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56 1.39100489
57 2.51462740 2.55585828
58 1.57922215 1.75433961 3.94189536
59 2.84750829 2.26707570 1.15970528 3.95113158
60 \quad 1.50949194 \quad 0.87151031 \quad 1.69614716 \quad 2.47930953 \quad 1.47306003
```

Cluster Dendrogram



d hclust (*, "complete")

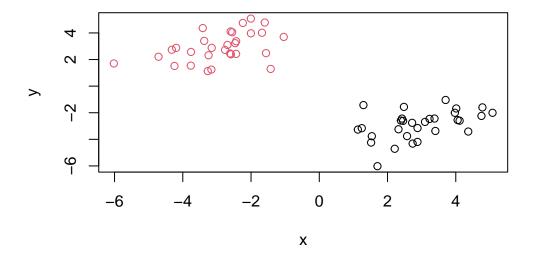
The function to get our clusters/groups from a hclust object is called cutree()

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

We can now see the 2 clusters in the original matrix 'x' and that there is instric hierarchy within.

Q6. Plot our helust results in terms of our data colored by cluster membership

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



PCA of UK Food Data

```
#Importing UK Food Data
url <- "https://tinyurl.com/UK-foods"
uk_food_data <- read.csv(url)</pre>
```

Q1: How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?

Observing dimensions and first 6 rows

```
dim(uk_food_data)
[1] 17 5
head(uk_food_data)
```

	Х	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

Assigning row names the wrong way...

```
rownames(x) <- x[,1]
x <- x[,-1]
head(x)
```

```
2.879270479694 1.53983397008687 5.0772704170472 2.21086082389677

-3.152162 -3.765200 -2.005091 -4.711054

3.37684033250668 4.36571633499587

-2.436652 -3.414925
```

Assigning it the right way...

```
x <- read.csv(url, row.names=1) #rownames = first column of df
head(x)</pre>
```

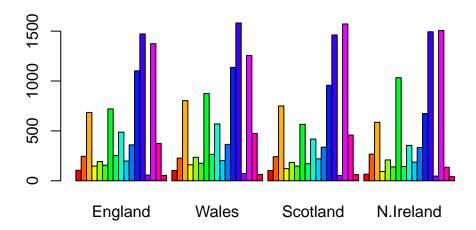
	England	Wales	Scotland	N.Ireland
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139

Q2: Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

Second one, since it does not iteratively remove columns and also assigns the row names correctly as you are importing the dataset into R.

Spotting Major Differences and Trends in Dataset

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



Q3: Changing what optional argument in the above barplot() function results in the following plot?

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



#changing beside = T to F results in the shown plot

Q4: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

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



at the y=x line for each plot implies the different foods are equally favored by both corresponsind countries. Above that line implies the country above favors it more by consumption, and vice versa.

Q5: What is the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

PCA to the rescue

The main function for PCA in base R is called prcomp() It wants the transpose (with the t()) of our food data for analysis

```
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

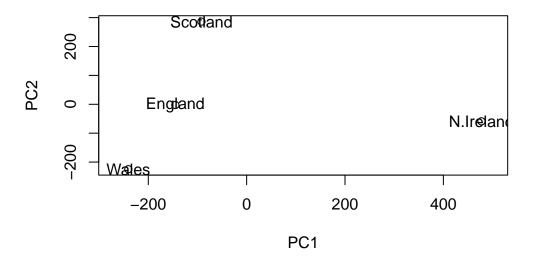
One of the main results that folks look for is called the "score plot" a.k.a PC plot, PC1 vs PC2, etc...

Q6: Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

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
```

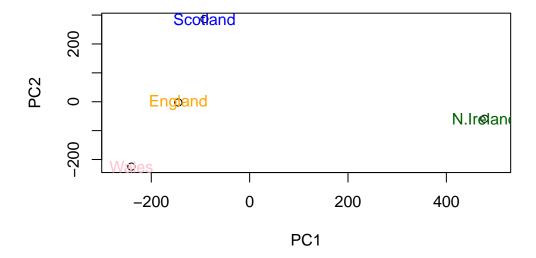
```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x))
```



Q7: Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

```
colors <- c("orange", "pink", "blue", "#006400")

plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x), col = colors)</pre>
```

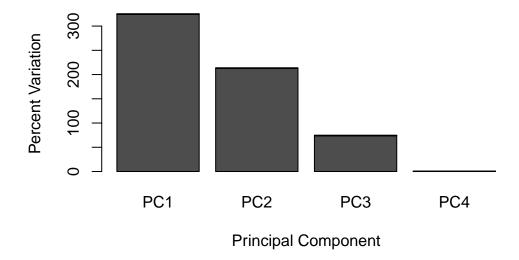


How much variation does each PC account for?

```
z <- summary(pca)
z$importance</pre>
```

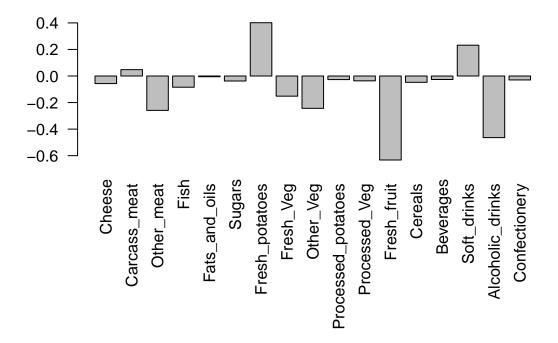
```
PC1 PC2 PC3 PC4
Standard deviation 324.15019 212.74780 73.87622 2.921348e-14
Proportion of Variance 0.67444 0.29052 0.03503 0.000000e+00
Cumulative Proportion 0.67444 0.96497 1.00000 1.000000e+00
```

```
#visualizing the above
barplot(z$importance, xlab="Principal Component", ylab="Percent Variation")
```



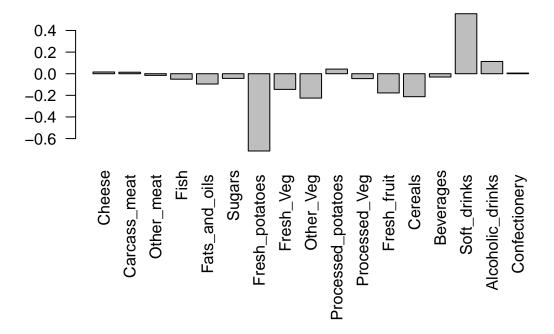
Digging Deeper: Variable Loadings

```
## 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 )
```



Q8: Generate a similar 'loadings plot' for PC2. What two food groups feature prominantely and what does PC2 maniply tell us about?

```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las = 2)
```



Fresh potatoes and soft drinks contribute to the PC2 loadings the most. The negative PC loading of fresh potatoes implies that Wales consume more of these than the others. And vice versa with soft drinks (Scotland consumes more of these than the rest)

Using ggplot for these figures

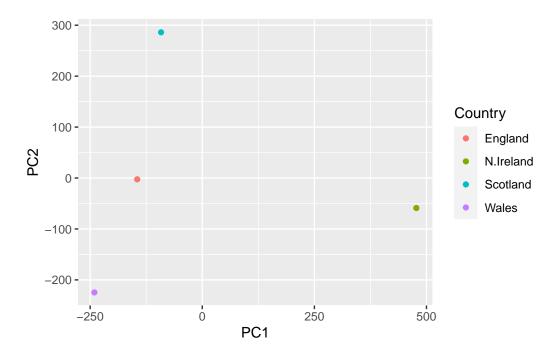
```
library(ggplot2)

df <- as.data.frame(pca$x)

df_lab <- tibble::rownames_to_column(df, "Country")

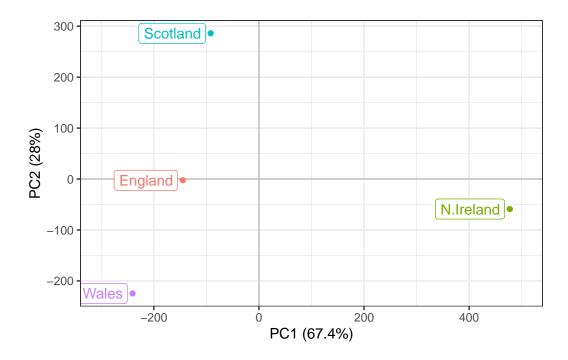
# Our first basic plot

ggplot(df_lab) +
   aes(PC1, PC2, col=Country) +
   geom_point()</pre>
```



Make it look nicer!

```
ggplot(df_lab) +
  aes(PC1, PC2, col=Country, label=Country) +
  geom_hline(yintercept = 0, col="gray") +
  geom_vline(xintercept = 0, col="gray") +
  geom_point(show.legend = FALSE) +
  geom_label(hjust=1, nudge_x = -10, show.legend = FALSE) +
  expand_limits(x = c(-300,500)) +
  xlab("PC1 (67.4%)") +
  ylab("PC2 (28%)") +
  theme_bw()
```



Looking at loadings...

```
ld <- as.data.frame(pca$rotation)
ld_lab <- tibble::rownames_to_column(ld, "Food")

ggplot(ld_lab) +
  aes(PC1, Food) +
  geom_col()</pre>
```

