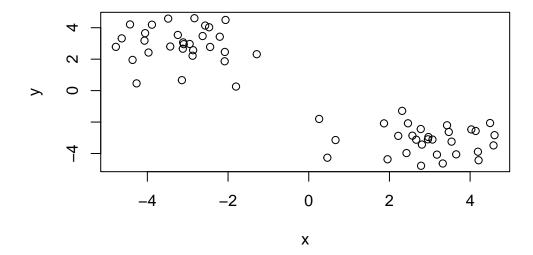
Class 7: Machine Learning

Mahsa Naeimi

Example of k-means clustering

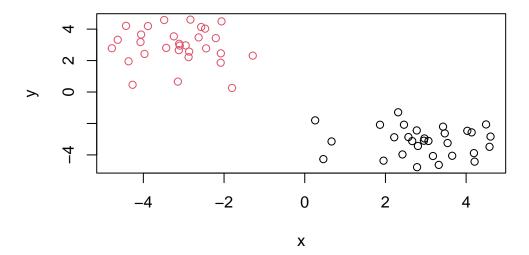
First step is to make up some data with a known structure, so we know what the answer should be.

```
tmp <- c(rnorm(30,mean= -3), rnorm(30, mean=3))
x <- cbind(x=tmp, y= rev(tmp))
plot(x)</pre>
```



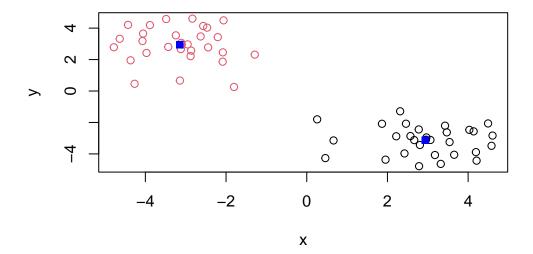
Now we have some structured data in x. Let's see if k-mean is able to identify the two groups.

```
k <- kmeans(x, centers= 2, nstart = 20)</pre>
  k
K-means clustering with 2 clusters of sizes 30, 30
Cluster means:
        X
1 2.934783 -3.142104
2 -3.142104 2.934783
Clustering vector:
Within cluster sum of squares by cluster:
[1] 61.45519 61.45519
(between_SS / total_SS = 90.0 %)
Available components:
[1] "cluster"
               "centers"
                           "totss"
                                       "withinss"
                                                    "tot.withinss"
[6] "betweenss"
               "size"
                           "iter"
                                       "ifault"
Let's explore k:
  k$size
[1] 30 30
  k$centers
        X
1 2.934783 -3.142104
2 -3.142104 2.934783
  plot(x, col= k$cluster)
```



Now we can add the clusters centers:

```
plot(x, col= k$cluster)
points(k$centers, col= 'blue', pch= 15)
```



Example of Hierarchical Clustering

Let's use the same data as before, which we stored in 'x'. We will use the 'hclust()' function.

dist(x)

```
3
                                                           5
                                                                      6
                                                                                  7
            1
                        2
                                               4
2
    0.5388040
3
    2.7626156
               2.2256934
4
    0.7790038
               0.6177529
                           2.3126622
5
    0.6813359
               0.1452447
                           2.0816574
                                      0.6174304
6
    1.6429408
               1.2323936
                           1.7861007
                                       1.7676931
                                                  1.1675051
7
    1.5479148
               1.5649991
                           3.0741154
                                       2.1624766
                                                  1.6300241
                                                              1.3007743
8
    1.9623455
               1.5741324
                           1.8657051
                                       2.1144623
                                                  1.5133386
                                                              0.3468048
                                                                          1.3616007
    1.6440675
                           3.6684278
                                      2.3839810
                                                  1.9687861
                                                              1.9315897
                                                                          0.6697024
9
               1.8643567
   0.6511228
               1.0189078
                           3.1545640
                                       1.4242917
                                                  1.1548227
                                                              1.6991725
10
                                                                          1.0873411
11
    1.1415501
               0.9035729
                           2.3084519
                                       1.5192976
                                                  0.9173073
                                                              0.6444822
                                                                          0.8184429
   2.6658125
12
               2.5947241
                           3.5236750
                                       3.2113236
                                                  2.6257584
                                                              1.8382394
                                                                          1.1329707
13
    1.5641852
               1.2023045
                           1.9728033
                                       1.7727960
                                                  1.1587487
                                                              0.1894812
                                                                          1.1112948
   2.8406916
               2.3226905
                           0.9136363
                                      2.6291747
                                                  2.1983737
                                                              1.4020829
                                                                          2.6626045
```

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15
    1.6718779
               1.2966574
                           1.9187678
                                      1.8555991
                                                  1.2455823
                                                            0.1465967
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16
    1.8694426
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                           1.2445468
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17
    1.8891468
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                                                             1.1394547
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    4.3848654
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                                      4.5963338
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34 11.1030807 10.5656272
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58 7.8256992 7.2983582 5.0959934 7.2527604 7.1531146 6.7704342 8.0630840
59 10.0012027 9.4804520 7.2983582 9.3963798 9.3353830 8.9922839 10.2867596
60 10.5199357 10.0012027 7.8256992 9.9073764 9.8562505 9.5258135 10.8211849
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10 1.9500426 1.0150466
11 0.8849645 1.3608377 1.0668674
12 1.6638584 1.4683490 2.2147304 1.7117577
13 0.4021596 1.7443394 1.5588104 0.4922940 1.6916400
14 1.3094040 3.3168087 3.0547146 2.0381971 2.8493659 1.5814255
15 0.2912104 1.8305843 1.6710456 0.6042555 1.6916629 0.1128316 1.4879616
16 0.6863472 2.4486675 2.0816721
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17 1.0800378 1.0926648 1.5200201 0.9022798 0.8113239 0.9649896 2.3818457
18 2.4830111 3.7523267 4.1924512 3.2442891 2.3791669 2.8491936 2.5959687
19 1.0615627 2.9303093 2.5434871 1.5893679
                                            2.7206466 1.1980432 0.5943214
20 0.3420840 1.7226512 1.7757229 0.7589544 1.3479719 0.4131601 1.6442479
21 1.9997287 3.7714380 3.9302855 2.8776354 2.6781133 2.4018726 1.6021298
22 0.5071798 2.5240465 2.4378928 1.3716002 1.9841147 0.8793075 0.8702479
23 0.2730339 2.2668756 2.1035431 1.0423542 1.9276994 0.5548081 1.0519791
24 2.7432663 4.7451099 4.6371918 3.5848034 3.9050333 3.0982601 1.6312285
25 1.7104049 0.5431308 0.5578393 0.9157531 1.6689397 1.3675721 2.9448021
                                            2.2579340 0.6303452 1.6962706
26 0.9450248 1.9454880 1.3998006 0.6189960
27 1.6510348 0.9111142 1.7047018 1.4072886 0.5574616 1.5439930 2.9384028
28  0.8840564  1.8450273  2.2116017  1.3330876  0.8861373  1.0732094  1.9686485
29 1.1929859 2.3579705 1.7214521 1.0459604
                                            2.6549352 0.9772156 1.5674927
30 1.4340562 2.2576792 2.7709749 1.9434843 0.9284690 1.6766012 2.2848002
31 8.6704112 10.6908534 10.4691974 9.4623655 9.8222523 8.9947271 7.4249606
32 8.1606832 10.1435040 9.6857010 8.8053230 9.6058693 8.4001489 6.8514974
33 8.6465526 10.6718499 10.3931852 9.4099485 9.8755639 8.9535657 7.3738425
34 9.7362581 11.7612234 11.4562817 10.4864022 10.9865534 10.0357625 8.4544840
35 8.4546182 10.4499197 10.0177693 9.1199054 9.8692383 8.7055833 7.1455416
36 9.8189801 11.8283138 11.4292744 10.5112315 11.1818290 10.0855056 8.5137475
37 5.6008088 7.6239231 7.3986850 6.3887441 6.8138282 5.9215654 4.3515485
38 7.9341988 9.9518669 9.5954659 8.6505847 9.2702190 8.2135586 6.6351379
39 7.6962513 9.7182610 9.3889445 8.4291750 9.0030729 7.9850198 6.4040901
40 6.9326238 8.9457700 8.7674614 7.7433798 8.0492451 7.2683621 5.7133870
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41 8.5021942 10.5236483 10.1860590 9.2315723 9.8076683 8.7892559 7.2087002
42 7.3241234 9.3281459 8.9260535 8.0074997 8.7220519 7.5844604 6.0165907
43 7.8018810 9.7864868 9.6866881 8.6420921 8.7860125 8.1574284 6.6391845
44 9.2214773 11.2447656 10.9188302 9.9589765 10.5037893 9.5134809 7.9322371
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46 8.3727669 10.3883145 10.0197498 9.0822463 9.7170559 8.6483979 7.0715645
47 6.8848803 8.9011565 8.5450137 7.5986131 8.2378062 7.1621377 5.5843478
48 8.4645486 10.4786316 10.1034556 9.1698796 9.8153596 8.7378708 7.1621377
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50 8.9043023 10.9128137 10.5151787 9.5955114 10.2754551 9.1698796 7.5986131
51 9.8541803 11.8477227 11.4043716 10.5151787 11.2654992 10.1034556 8.5450137
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53 8.1812666 10.2009996 9.8541803 8.9043023 9.5022834 8.4645486 6.8848803
54 9.5423661 11.5613418 11.2039092 10.2612171 10.8595340 9.8237768 8.2448332
55 8.2818900 10.2948433 9.9161960 8.9844684 9.6391409 8.5535712 6.9786476
56 8.8021905 10.7778935 10.3025875 9.4354207 10.2574131 9.0358413 7.4936458
57 8.9629348 10.9077088 10.3816696 9.5543458 10.4649427 9.1742757 7.6612728
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59 8.9465076 10.9228044 10.4478117 9.5805130 10.3998330 9.1806590 7.6378683
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18 2.7537169 2.9469883 2.7236306
19 1.1319072 0.4832951 2.1172306 2.9629547
20 0.3670246 0.9891170 0.7392164 2.4877783 1.3967604
21 2.2903225 2.2252939 2.6789167 1.1412090
                                             2.0871356 2.1599474
22 0.7676494 0.7077023 1.5302920 2.2392990 0.8350943 0.8067603 1.5764370
23 0.4494915 0.4690266 1.3508498 2.5320551 0.7931611 0.6147265 1.9255644
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2.9907374 2.5987491 3.6972082 2.4728887
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    1.4691828
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28
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33
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34
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   8.6213302
               8.0136963
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               9.1895289 10.5037893
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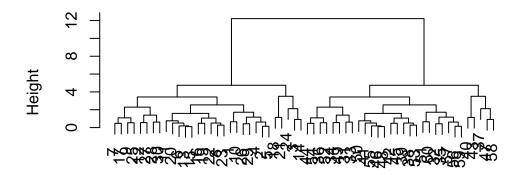
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58 2.3126622
59 0.6177529 2.2256934
60 0.7790038 2.7626156 0.5388040
  clustering <- hclust( dist(x))</pre>
  clustering
Call:
hclust(d = dist(x))
Cluster method : complete
Distance
              : euclidean
Number of objects: 60
  plot(clustering)
```

Cluster Dendrogram

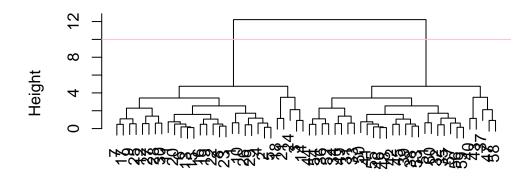


dist(x)
hclust (*, "complete")

group in the left from 1-30 and group to the right from 30-60 Let's add horizontal line:

```
plot(clustering)
abline(h = 10, col = 'pink')
```

Cluster Dendrogram



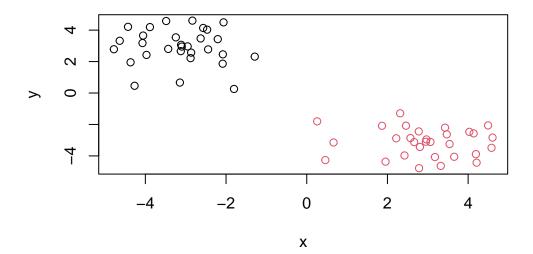
dist(x)
hclust (*, "complete")

to get our results (i.e., membership vector) we need to "cut" the tree. The function for doing that is cutree()

```
subgroups <- cutree(clustering, h =10)
subgroups</pre>
```

plotting this..

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



You can also "cut" your tree with the number of clusters you want:

```
cutree(clustering, h =2)

[1] 1 1 2 1 1 3 4 3 4 1 3 5 3 2 3 3 4 6 3 3 6 3 3 7 4

[26] 1 5 5 1 5 8 9 8 8 9 10 11 12 12 13 12 12 13 10 12 12 14 12 8 12

[51] 9 10 12 10 12 9 9 14 9 9
```

Principle Component Analysis (PCA)

PCA of UK food

First we read the data:

```
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

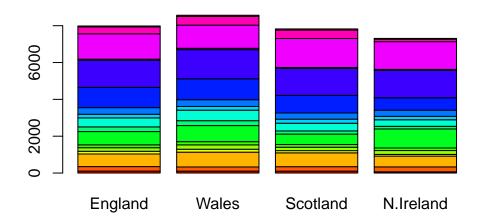
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139

Now we can generate some basic visualization

```
rainbow (nrow(x))

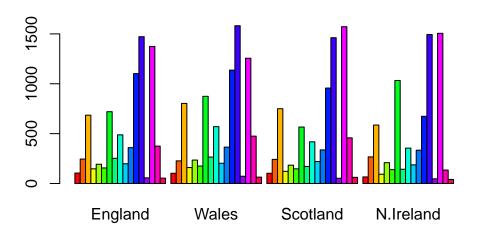
[1] "#FF0000" "#FF5A00" "#FFB400" "#F0FF00" "#96FF00" "#3CFF00" "#00FF1E"
[8] "#00FF78" "#00FFD2" "#00D2FF" "#0078FF" "#001EFF" "#3C00FF" "#9600FF"
[15] "#F000FF" "#FF00B4" "#FF005A"

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



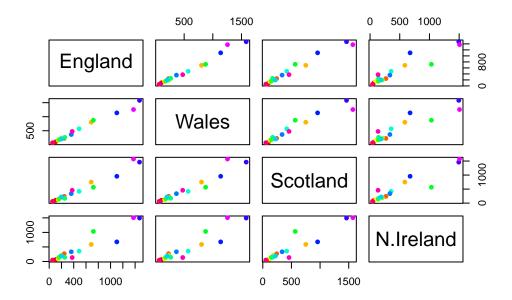
Let's refine our barplot

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



Other useful visualization:

```
pairs(x, col = rainbow(nrow(x)), pch =16)
```



Let's apply PCA. For that we need to use the command prcpm(). This function expects the transpose of our data

```
transpose_matrix <- t(x)
pca <- prcomp( transpose_matrix)

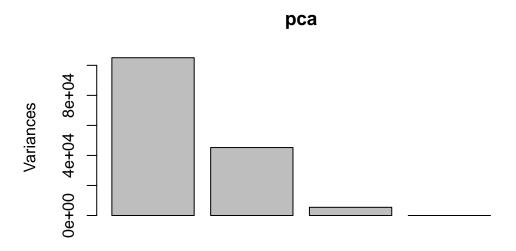
pca <- prcomp ( t(x))
summary(pca)</pre>
```

Importance of components:

```
PC1 PC2 PC3 PC4
Standard deviation 324.1502 212.7478 73.87622 4.189e-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 plot the PCA results:

```
plot(pca)
```



We need to access the results of PCA analysis

```
attributes(pca)
```

\$names

[1] "sdev" "rotation" "center" "scale" "x"

\$class

[1] "prcomp"

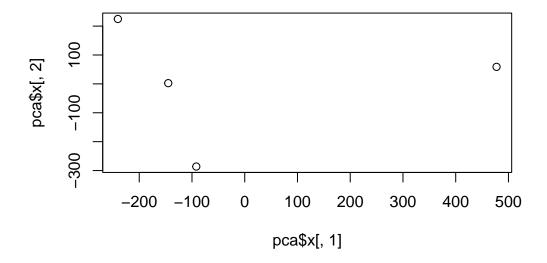
We can explore the pca\$x dataframe:

pca\$x

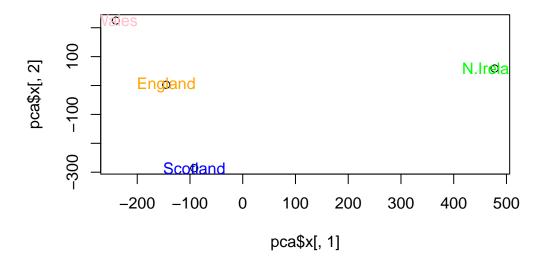
PC1 PC2 PC3 PC4 England -144.99315 2.532999 -105.768945 2.842865e-14 Wales 224.646925 -240.52915 56.475555 7.804382e-13 Scotland -91.86934 -286.081786 44.415495 -9.614462e-13 N.Ireland 477.39164 58.901862 4.877895 1.448078e-13

Plotting:

```
plot( x=pca$x[,1], y=pca$x[,2])
```



```
plot( x=pca$x[,1], y=pca$x[,2])
color_countries <- c('orange', 'pink', 'blue', 'green')
text( x=pca$x[,1], y=pca$x[,2], colnames(x), col = color_countries)</pre>
```



PCA of a RNA-seq data set

First step as always to load the data:

```
url2 <- "https://tinyurl.com/expression-CSV"
rna.data <- read.csv(url2, row.names=1)
head(rna.data)</pre>
```

```
wt1 wt2
                wt3
                     wt4 wt5 ko1 ko2 ko3 ko4 ko5
       439 458
                408
                     429 420
                               90
                                   88
                                       86
                                            90
gene1
                204
                     210 187 427 423 434 433 426
gene2
       219 200
gene3 1006 989 1030 1017 973 252 237 238 226 210
                     856 760 849 856 835 885 894
gene4
       783 792
                829
gene5
       181 249
                204
                     244 225 277 305 272 270 279
gene6
       460 502
                491
                     491 493 612 594 577 618 638
```

Q. How many genes and samples are in this data set?

```
dim(rna.data)
```

[1] 100 10

100 genes and 10 samples

Let's apply PCA:

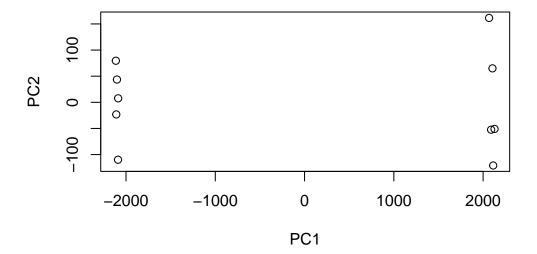
```
pca_rna = prcomp (t(rna.data))
summary(pca_rna)
```

Importance of components:

```
PC1
                                      PC2
                                               PC3
                                                        PC4
                                                                 PC5
                                                                           PC6
Standard deviation
                       2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
Proportion of Variance
                                          0.00144
                                                   0.00122
                          0.9917
                                  0.0016
                                                             0.00098
                                                                      0.00093
Cumulative Proportion
                          0.9917
                                  0.9933
                                           0.99471
                                                    0.99593
                                                             0.99691
                                                                      0.99784
                            PC7
                                      PC8
                                               PC9
                                                        PC10
Standard deviation
                       65.29428 59.90981 53.20803 3.142e-13
Proportion of Variance
                        0.00086
                                  0.00073
                                          0.00057 0.000e+00
Cumulative Proportion
                        0.99870
                                 0.99943 1.00000 1.000e+00
```

LEt's plot the principle component 1 and 2 :

```
plot(pca_rna$x[,1], pca_rna$x[,2], xlab ='PC1', ylab='PC2')
```



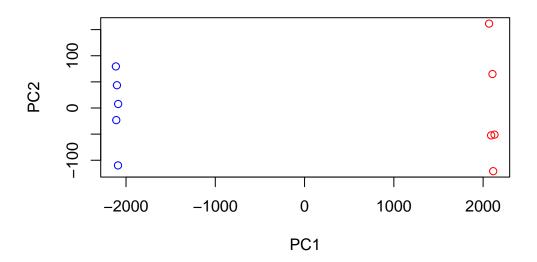
colnames(rna.data)

```
[1] "wt1" "wt2" "wt3" "wt4" "wt5" "ko1" "ko2" "ko3" "ko4" "ko5"

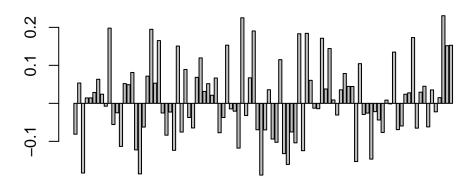
cols_samples <- c(rep('blue', 5), rep('red',5))
cols_samples

[1] "blue" "blue" "blue" "blue" "blue" "red" "red" "red" "red"

plot(pca_rna$x[,1], pca_rna$x[,2], xlab ='PC1', ylab='PC2', col = cols_samples)</pre>
```



barplot(pca_rna\$rotation[,1])



gene1 gene18 gene36 gene54 gene72 gene90

sort(pca_rna\$rotation[,1])

gene50	gene18	gene3	gene57	gene75	gene79
-0.188796985	-0.185668500	-0.183374164	-0.160771014	-0.153164404	-0.146803635
gene56	gene61	gene27	gene17	gene44	gene13
-0.132330117	-0.124572881	-0.123615228	-0.122536548	-0.117808971	-0.113357525
gene59	gene54	gene53	gene25	gene1	gene39
-0.103935563	-0.102503320	-0.093979884	-0.083761992	-0.081247810	-0.077306742
gene82	gene29	gene58	gene51	gene49	gene86
-0.076658760	-0.075605635	-0.075274651	-0.069855142	-0.069530208	-0.069165267
gene91	gene32	gene19	gene94	gene87	gene11
-0.065288752	-0.064721235	-0.062411218	-0.061938300	-0.059547317	-0.055698801
gene81	gene40	gene31	gene46	gene70	gene77
•	gene40 -0.037323670	•	•	•	_
-0.043780416	•	-0.037219970	-0.031990529	-0.030784982	-0.029225446
-0.043780416 gene78	-0.037323670	-0.037219970 gene12	-0.031990529 gene26	-0.030784982 gene96	-0.029225446 gene80
-0.043780416 gene78 -0.025639741	-0.037323670 gene24	-0.037219970 gene12 -0.024870802	-0.031990529 gene26 -0.022868107	-0.030784982 gene96 -0.022293151	-0.029225446 gene80 -0.021824860
-0.043780416 gene78 -0.025639741 gene43	-0.037323670 gene24 -0.025407507	-0.037219970 gene12 -0.024870802 gene65	-0.031990529 gene26 -0.022868107 gene64	-0.030784982 gene96 -0.022293151 gene9	-0.029225446 gene80 -0.021824860 gene84
-0.043780416 gene78 -0.025639741 gene43 -0.020617052	-0.037323670 gene24 -0.025407507 gene42	-0.037219970 gene12 -0.024870802 gene65 -0.014052839	-0.031990529 gene26 -0.022868107 gene64 -0.012639567	-0.030784982 gene96 -0.022293151 gene9 -0.007495075	-0.029225446 gene80 -0.021824860 gene84 -0.001289937
-0.043780416 gene78 -0.025639741 gene43 -0.020617052 gene83	-0.037323670 gene24 -0.025407507 gene42 -0.014550791	-0.037219970 gene12 -0.024870802 gene65 -0.014052839 gene4	-0.031990529 gene26 -0.022868107 gene64 -0.012639567 gene5	-0.030784982 gene96 -0.022293151 gene9 -0.007495075 gene97	-0.029225446 gene80 -0.021824860 gene84 -0.001289937 gene37
-0.043780416 gene78 -0.025639741 gene43 -0.020617052 gene83 0.008504287	-0.037323670 gene24 -0.025407507 gene42 -0.014550791 gene69	-0.037219970 gene12 -0.024870802 gene65 -0.014052839 gene4 0.014242602	-0.031990529 gene26 -0.022868107 gene64 -0.012639567 gene5 0.014303808	-0.030784982 gene96 -0.022293151 gene9 -0.007495075 gene97 0.014994546	-0.029225446 gene80 -0.021824860 gene84 -0.001289937 gene37 0.021280555

gene73	gene74	gene67	gene52	gene71	gene95
0.044581700	0.044286948	0.037840851	0.035802086	0.035589259	0.035342407
gene2	gene22	gene14	gene36	gene15	gene93
0.053465569	0.053013523	0.052004194	0.051765605	0.049090676	0.044940861
gene20	gene33	gene47	gene38	gene7	gene63
0.071571203	0.068437703	0.067141911	0.066665407	0.063389255	0.060529157
gene34	gene55	gene76	gene30	gene16	gene72
0.119604059	0.114988217	0.104435777	0.089150461	0.081254592	0.078551648
gene41	gene100	gene99	gene28	gene68	gene85
0.153077075	0.152877246	0.151678253	0.150812015	0.144227333	0.134907896
gene48	gene62	gene60	gene90	gene66	gene23
0.190495289	0.184203008	0.183139926	0.173156806	0.171311307	0.165155192
		gene98	gene45	gene10	gene21
		0.230633225	0.225149201	0.197905454	0.194884023