Data Mining and Machine Learning in Bioinformatics

Exercise Series 8

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Task 7-2:

A) GMM - cluster patients in one of two categories on the basis of expressions from 25 genes.

i) Degrees of freedom:

n(π*k) = 25, n(μ*k) = 25, n(∑) = 25 x 25, where n(p) is number of adjustable parameter p
totally, 25+25+(25x25) = **675**

ii) with diagonal covariance matrix

n(π*k) = 25, n(μ*k) = 25, n(∑) = 25 totally, 25+25+25 = **75**

iii) no correlation, the variation for each gene is same for each Gaussian.

n(π*k) = 25, n(μ*k) = 25 totally, 25+25 = **50**

B) GMM clustering

```
#install.packages("mclust")
library(mclust)
library(colonCA)

data(colonCA)
colon.ds <- log(exprs(colonCA))

pvalues <- apply(colon.ds, 1, function(x) {
  return (t.test(x[colonCA$class=='t'], x[colonCA$class=='n'])$p.value)
})
alpha = 0.0001
colon.signif = colon.ds[pvalues <= alpha,]
```

i) patients based on their gene expression profiles

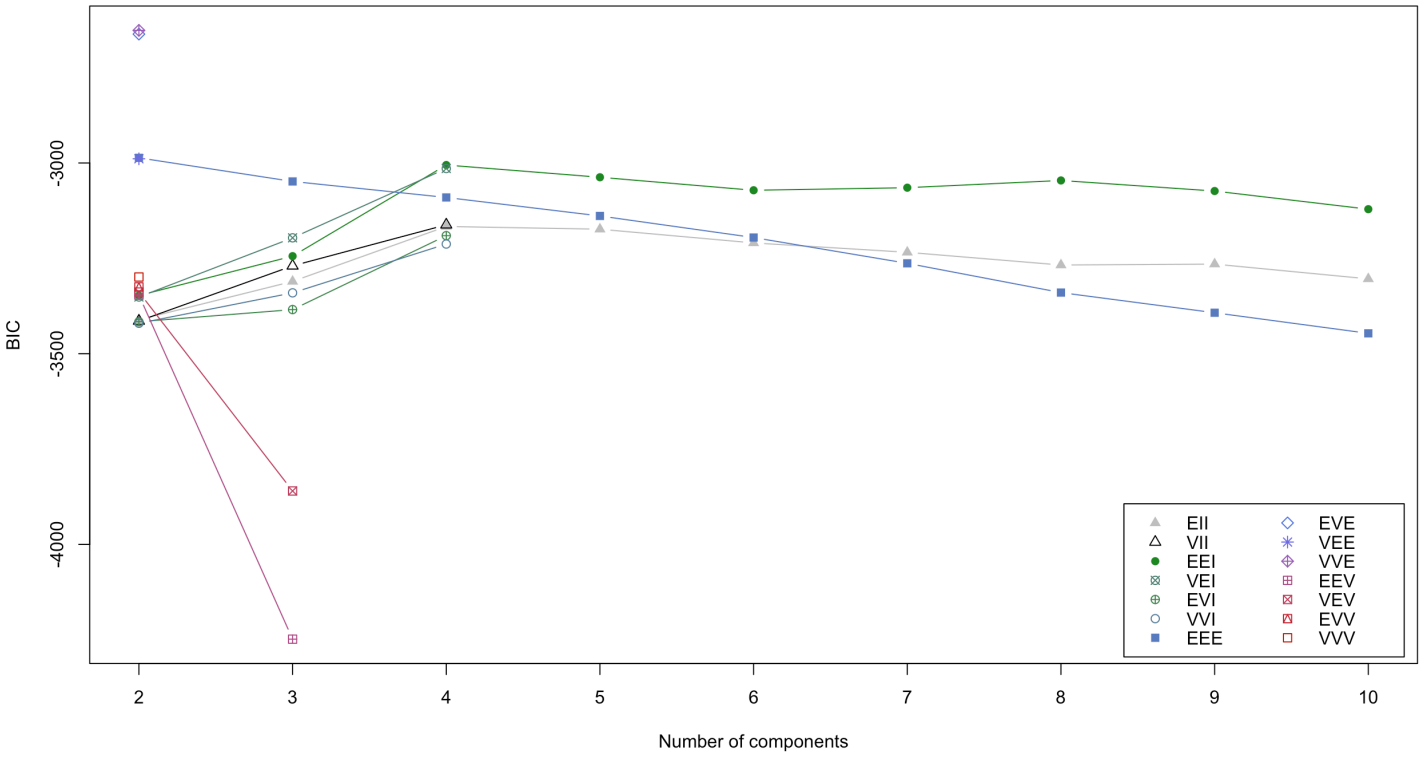
```
cl1 = Mclust(t(colon.signif), G=2:10)
summary(cl1)
plot(cl1,  what = "BIC")
```

ii) differentially expressed genes based on their profiles across patients

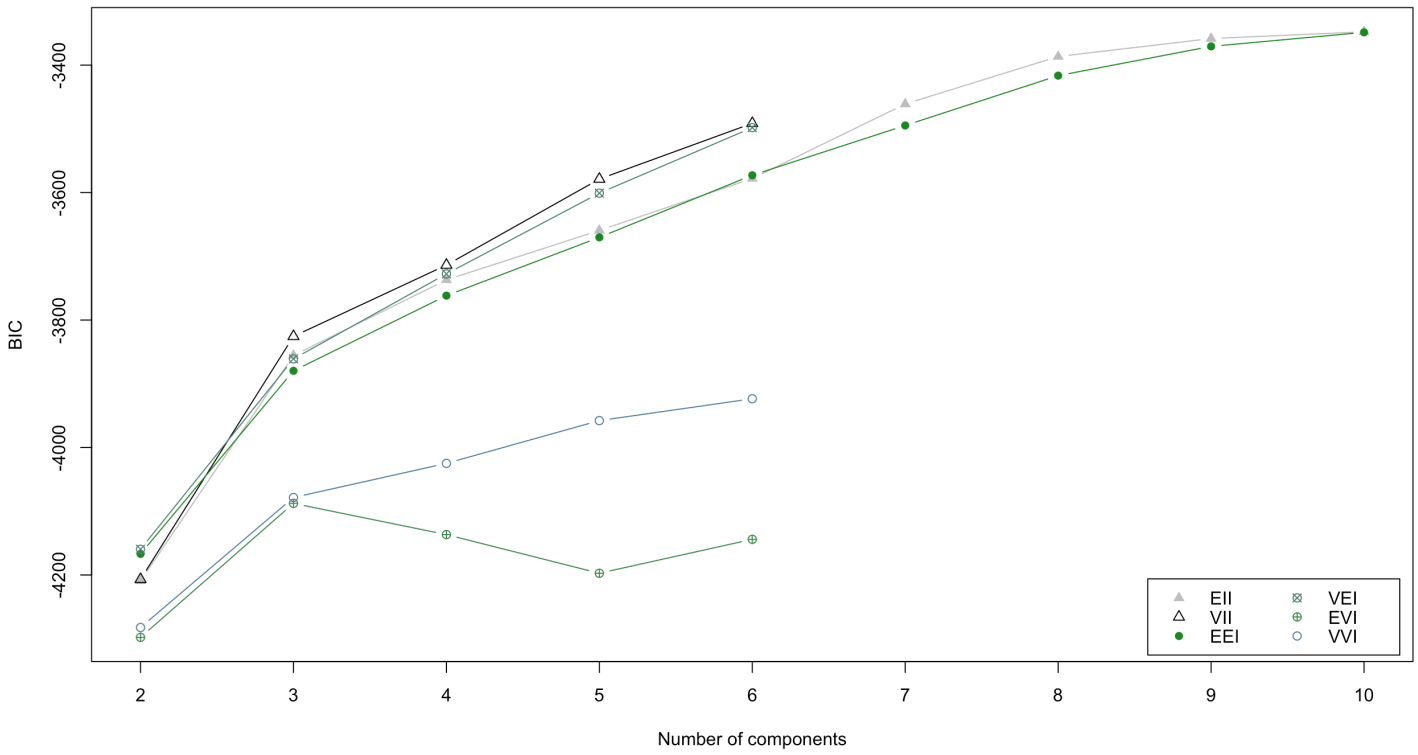
```
cl2 = Mclust(colon.signif, G=2:10)
summary(cl2)
plot(cl2,  what = "BIC")
```

RESULT

- GMM for patients: Mclust VVE (ellipsoidal, equal orientation) model with **2 components**, with BIC **-2652.285**



- GMM for genes: Mclust EII (spherical, equal volume) model with **10 components**, with BIC **-3347.762**



C) GMM clustering - Standardized gene expressions

```
scaled.colon.signif <- scale(colon.signif, center=TRUE, scale=TRUE)
```

i) GMM for patients

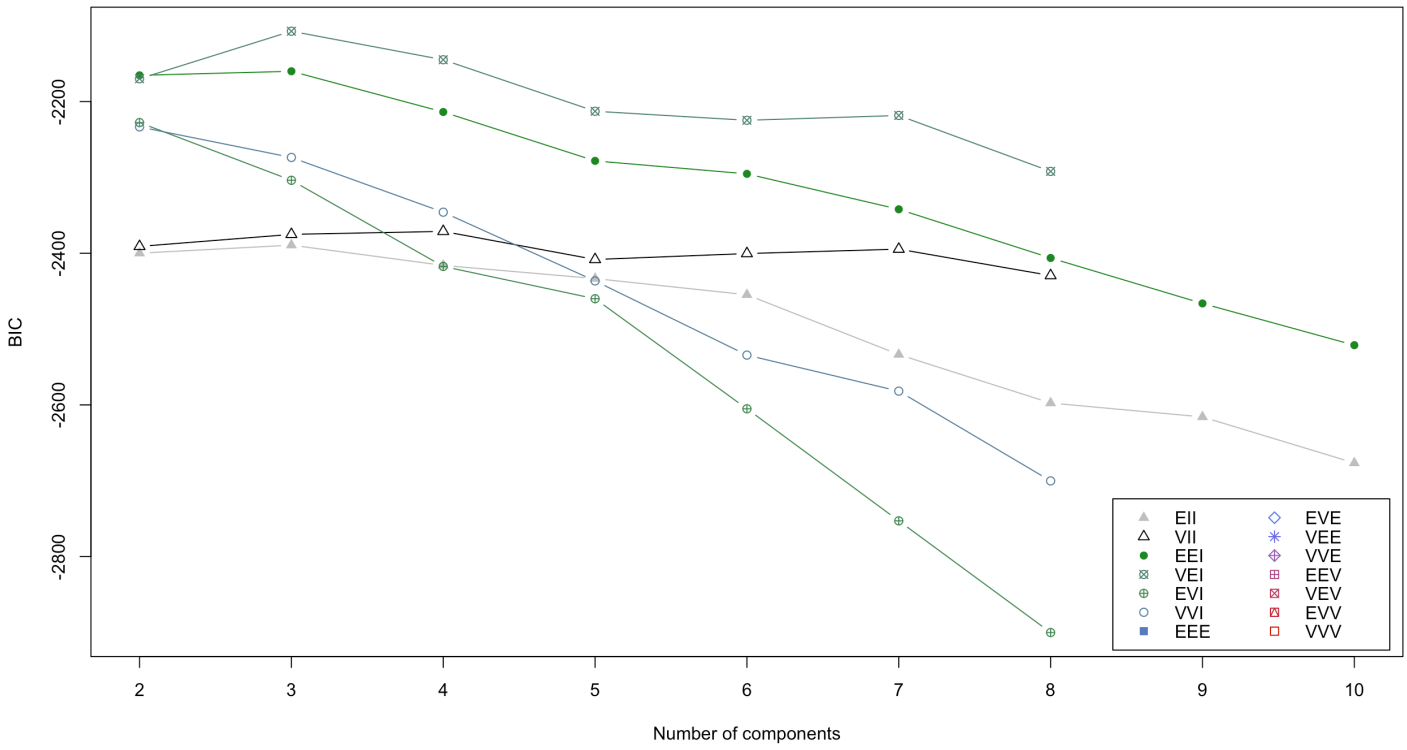
```
cl3 = Mclust(t(scaled.colon.signif), G=2:10)
summary(cl3)
plot(cl3,  what = "BIC")
plot(cl3,  what = "classification")
```

ii) GMM for genes

```
cl4 = Mclust(scaled.colon.signif, G=2:10)
summary(cl4)
plot(cl4,  what = "BIC")
plot(cl4,  what = "classification")
```

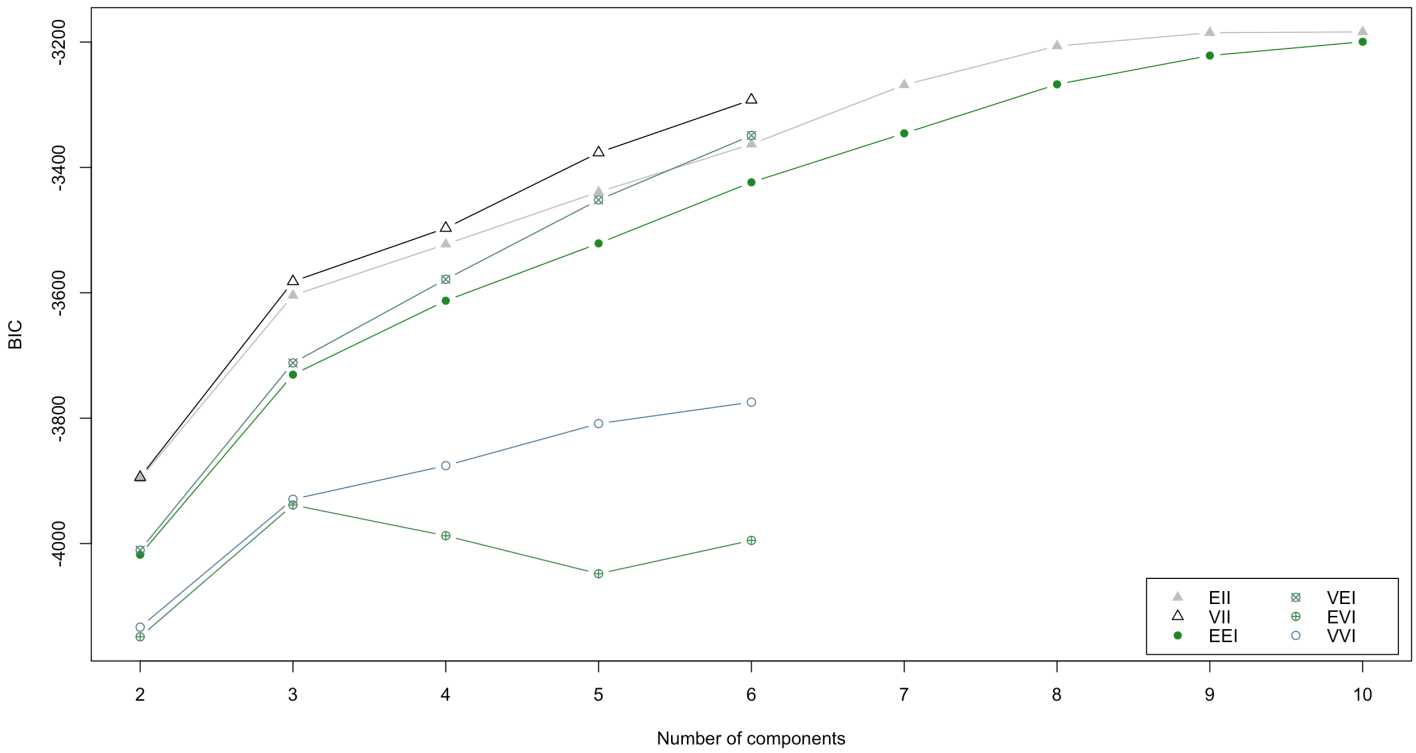
RESULT

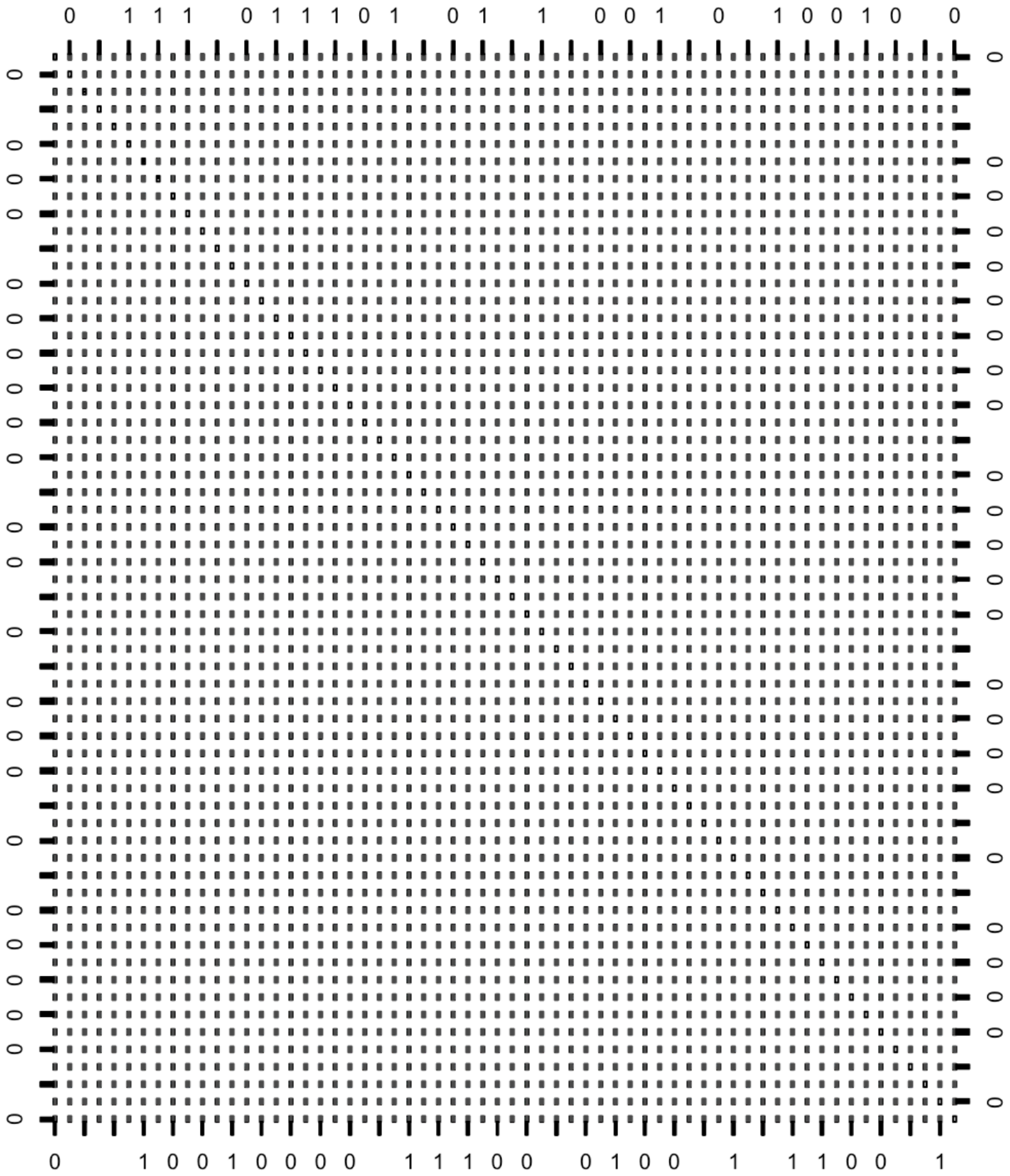
- GMM for patients: Mclust VEI (diagonal, equal shape) model with **3 components**, with BIC **-2107.218**



24 variables

- GMM for genes: Mclust EII (spherical, equal volume) model with **10 components**, with BIC **-3183.784**


BIC
-3200
-3400
-3600
-3800
-4000
2
3
4
5
6
7
8
9
10
Number of components
EII
VII
EEI
VEI
EVI
VVI



62 variables

D) Comparing above clusterings

- GMM for patients
  - b) **2 components**, with BIC **-2652.285**
  - c) **3 components**, with BIC **-2107.218**

- GMM for genes
  - b) **10 components**, with BIC **-3347.762**
  - c) **10 components**, with BIC **-3183.784**

For genes, it is difficult to say that using standardized data makes big difference. It probably over-fitted with 10 components.
For patients, standardizing made a bigger number of clusters than the clustering without standardizing.

Standardizing data is recommended because otherwise the range of values in each feature will act as a weight when determining how to cluster data, which is typically undesired.
If one of the features has a range of values much larger than the others, clustering will be completely dominated by that one feature.

E) silhouettes

Task 8:

1.a

```
library(GSVAdata)
data(gbm_VerhaakEtAl)

# gbm_eset
# head(pData(gbm_eset))

# get genes expressions, the matrix is already in the proper format.

data_gbm = exprs(gbm_eset)
# data_gbm[1:5,1:3]

# For the purpose of selecting the most informative genes for class detection,
# we reduce the dataset to the top 2,000 most variable genes, measured by median
# absolute deviation.

mads = apply(data_gbm,1,mad)
data_gbm = data_gbm[rev(order(mads))[1:2000],]
```

result

```
GABRB1                     0.88844            -0.07679
CHI3L2                     0.26796             0.25706
AQP1                      -0.58220            -0.50364
SNAP25                    -0.27376            -2.00055
FCGR2B                     1.16052            -0.03571
CXCL10                     0.06882            -0.40070
CXCL14                     0.27617             0.86518
PLA2G5                     0.16101             1.20059
MMP7                       0.68311            -0.28043
 [ reached getOption("max.print") -- omitted 1943 rows ]
```

2.a

```
data(leukemia)
leukemia_eset

# get gene expressions

data_leukemia = exprs(leukemia_eset)
# data_leukemia[1:5,1:3]

# Prioritize the gene expressions based on their median absolute deviation (MAD) a
nd
# select the 2000 top genes

mads = apply(data_leukemia,1,mad)
data_leukemia = data_leukemia[rev(order(mads))[1:2000],]
```

** result

```
33781_s_at                          9.281447
40790_at                           11.597086
39932_at                            9.952415
33500_i_at                         12.874146
1226_at                             7.853077
32434_at                            6.916666
 [ reached getOption("max.print") -- omitted 1730 rows ]
```