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:

$n(\pi k) = 25$, $n(\mu k) = 25$, $n(\sum) = 25$ x 25, where n(p) is number of adjustable parameter p
totally, 25+25+(25x25) = **675**

ii) with diagonal covariance matrix

$n(\pi k) = 25$, $n(\mu k) = 25$, $n(\sum) = 25$ totally, 25+25+25 = **75**

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

$n(\pi k) = 25$, $n(\mu k) = 25$ 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

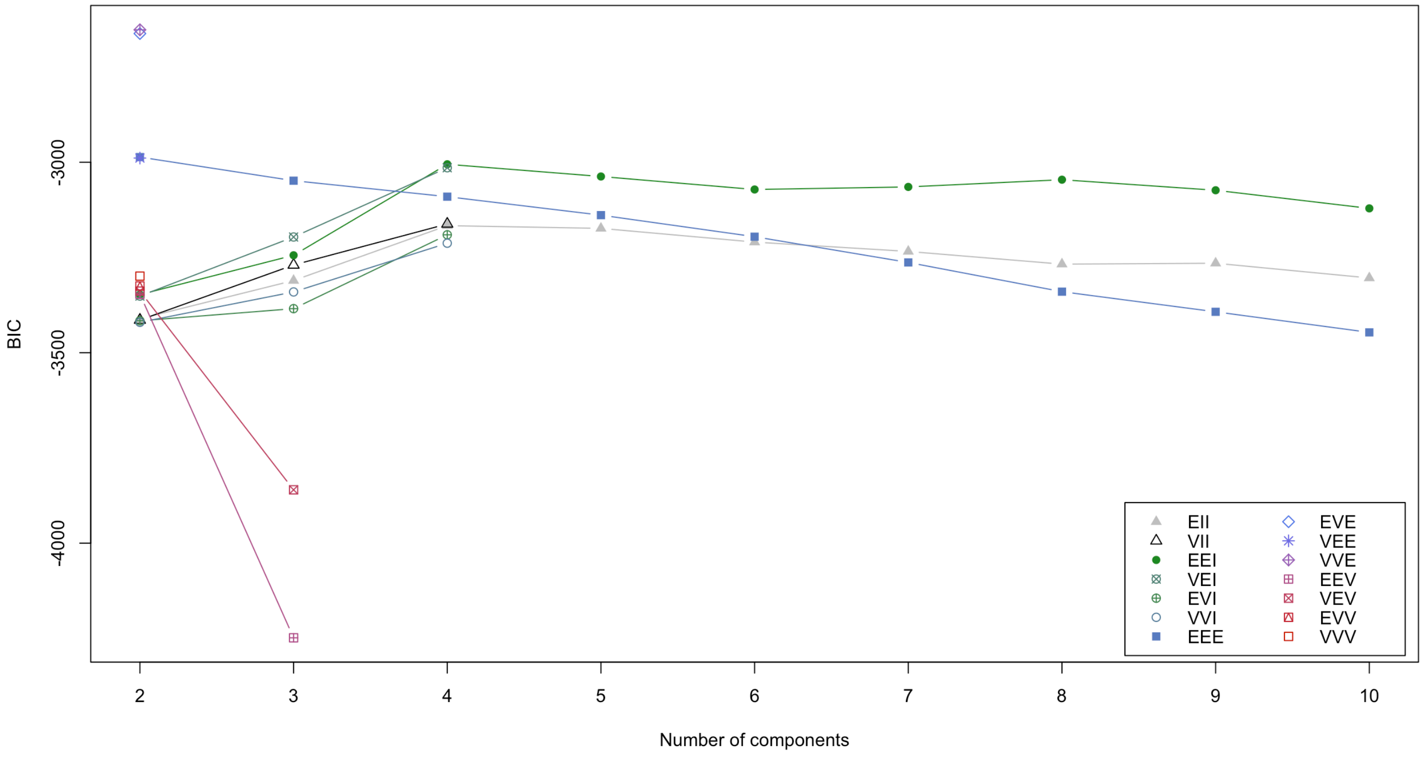
```
cl1 = Mclust(t(colon.signif), G=2:10)
summary(cl1)
plot(cl1,  what = "BIC")
```

ii) differentially expressed genes based on their profiles across patients

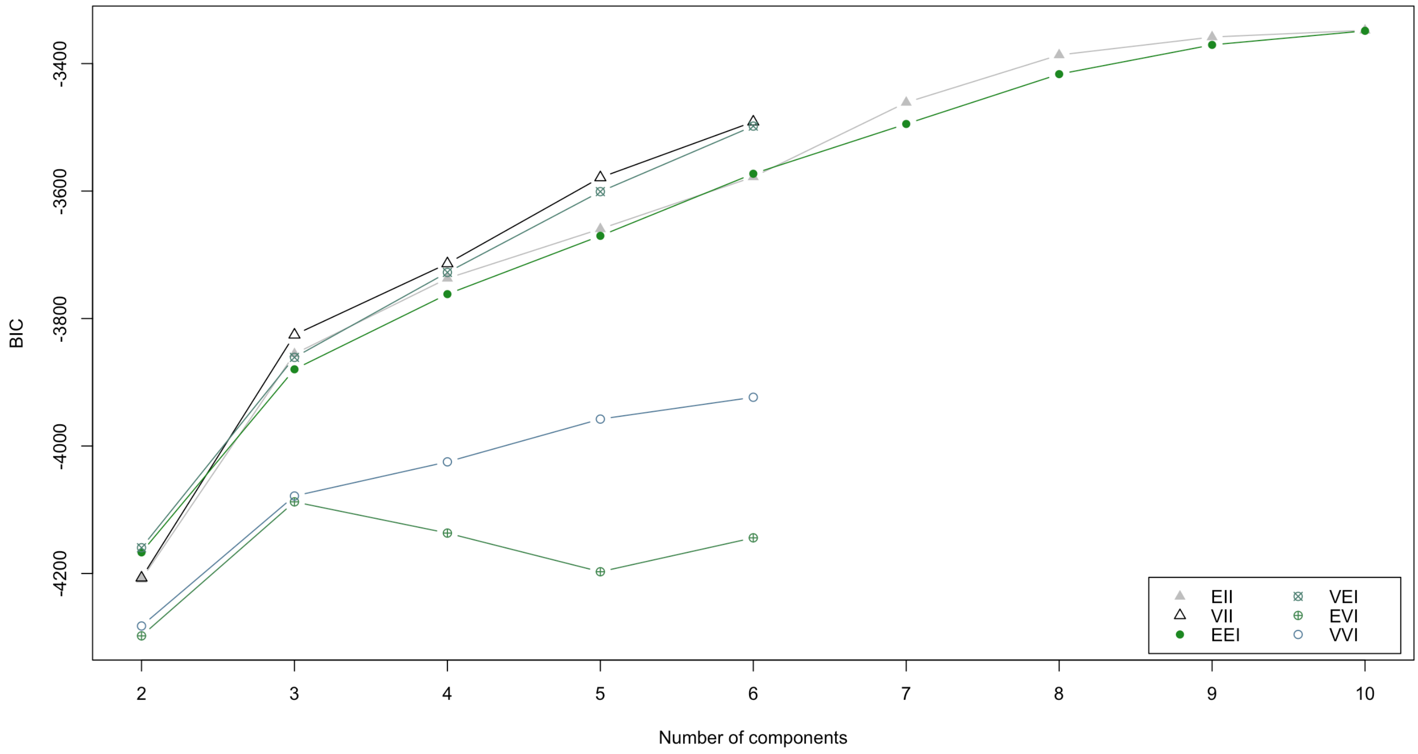
```
cl2 = Mclust(colon.signif, G=2:10)
summary(cl2)
plot(cl2,  what = "BIC")
```

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

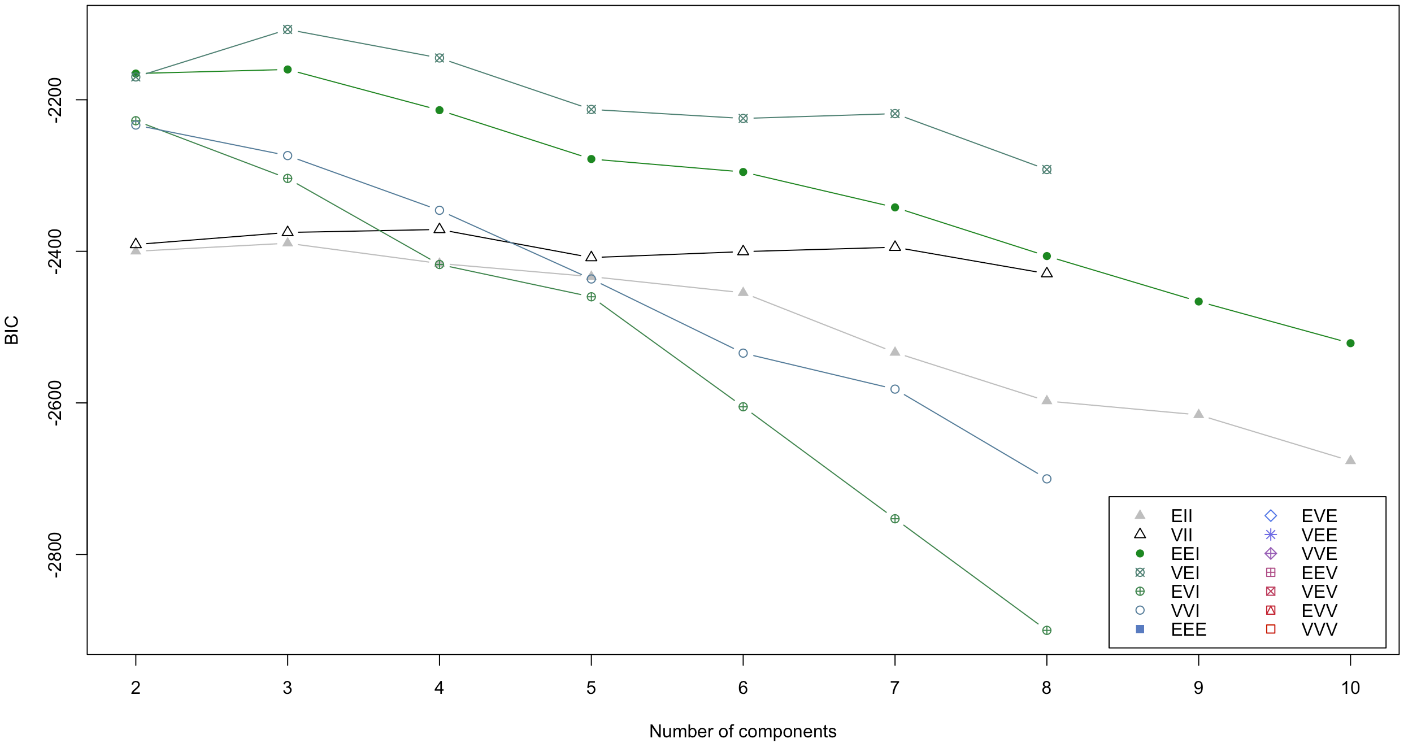
```
cl3 = Mclust(t(scaled.colon.signif), G=2:10)
summary(cl3)
plot(cl3,  what = "BIC")
plot(cl3,  what = "classification")
```

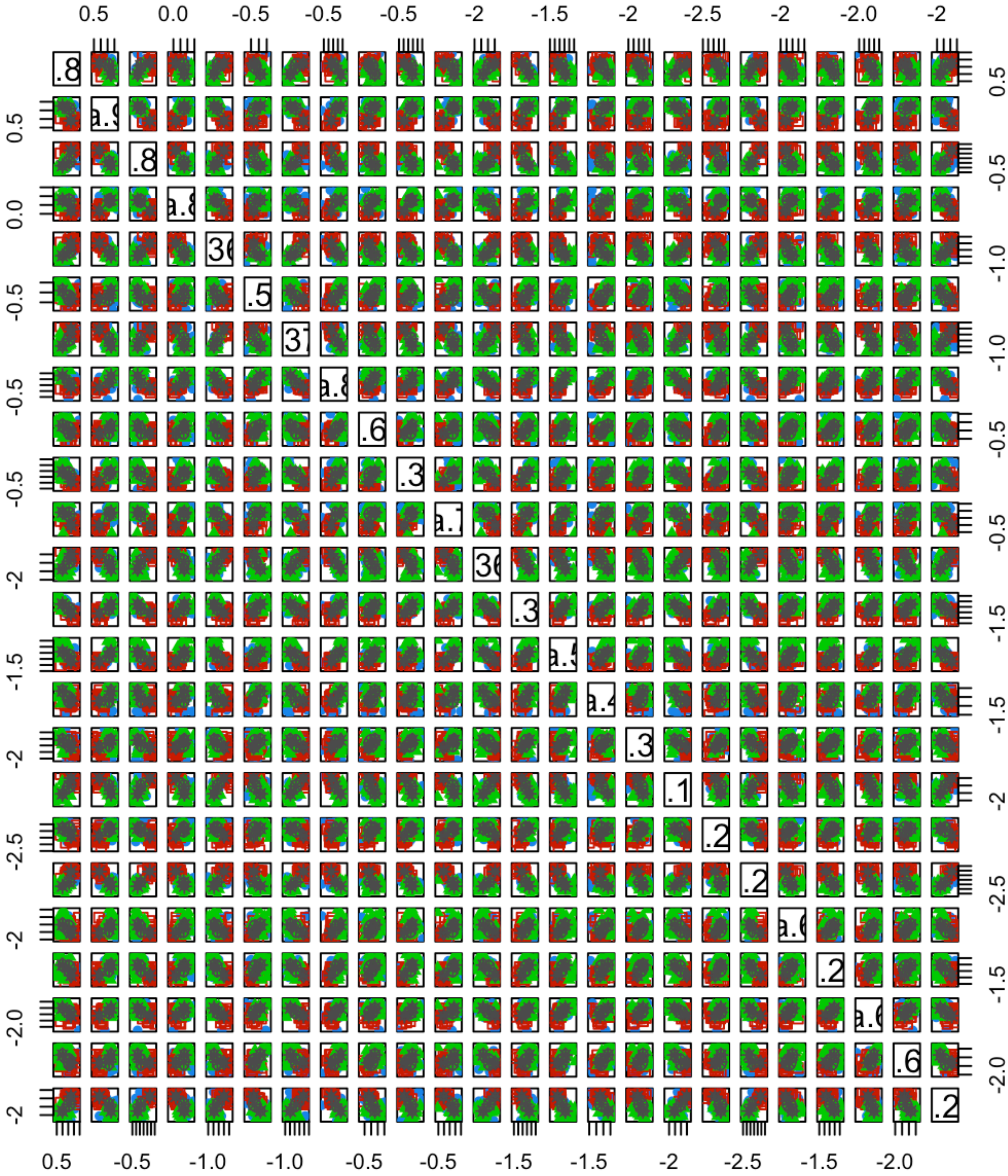
ii) GMM for genes

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

RESULT

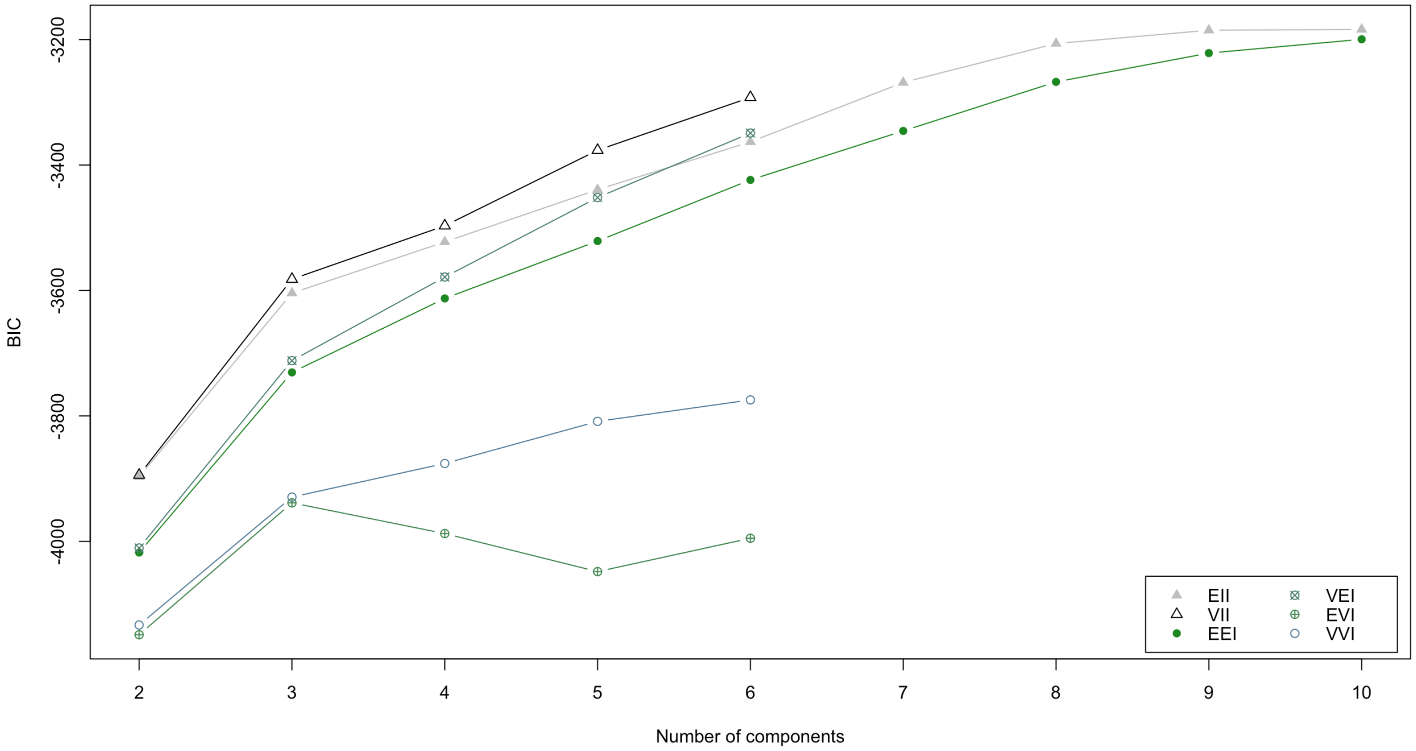
- GMM for patients: Mclust VEI (diagonal, equal shape) model with **3 components**, with BIC **-2107.218**

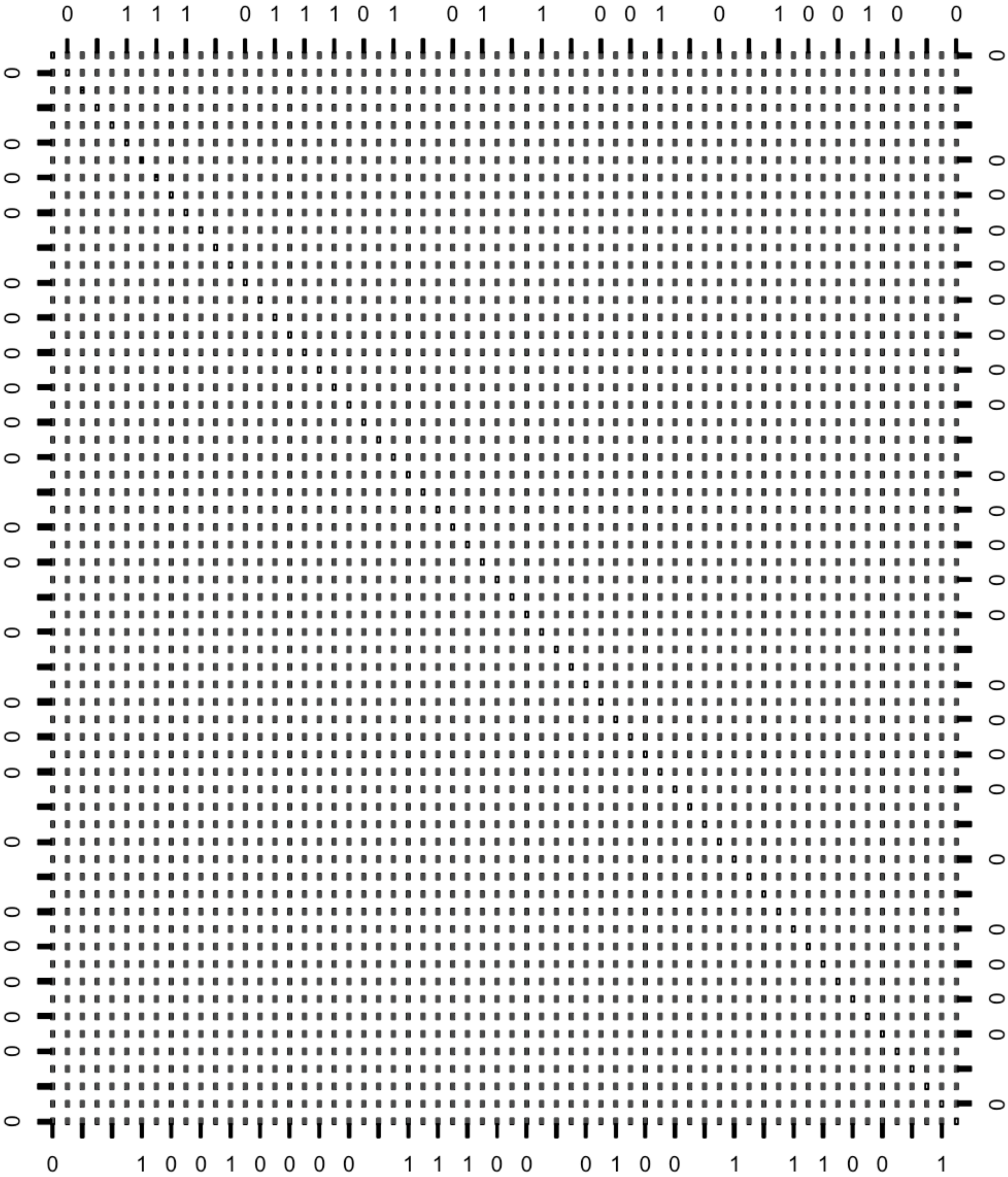




24 variables

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


BIC
-3200
-3400
-3600
-3800
-4000
Number of components
2
3
4
5
6
7
8
9
10
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