

A quick tour of mclust

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Introduction

mclust is a contributed R package for model-based clustering, classification, and density estimation based on finite normal mixture modelling. It provides functions for parameter estimation via the EM algorithm for normal mixture models with a variety of covariance structures, and functions for simulation from these models. Also included are functions that combine model-based hierarchical clustering, EM for mixture estimation and the Bayesian Information Criterion (BIC) in comprehensive strategies for clustering, density estimation and discriminant analysis. Additional functionalities are available for displaying and visualizing fitted models along with clustering, classification, and density estimation results.

This document gives a quick tour of **mclust** (version 5.4.2) functionalities. It was written in R Markdown, using the [knitr](#) package for production. See `help(package="mclust")` for further details and references provided by `citation("mclust")`.

```
library(mclust)
##
##  _ _ _ _ _
##  / | / _ / / / / / _ /
##  / | / _ / / / / / \ _ \ /
##  / / / _ / _ / _ / _ / /
##  / / / _ \ _ \ _ \ _ \ _ / / version 5.4.2
## Type 'citation("mclust")' for citing this R package in publications.
```

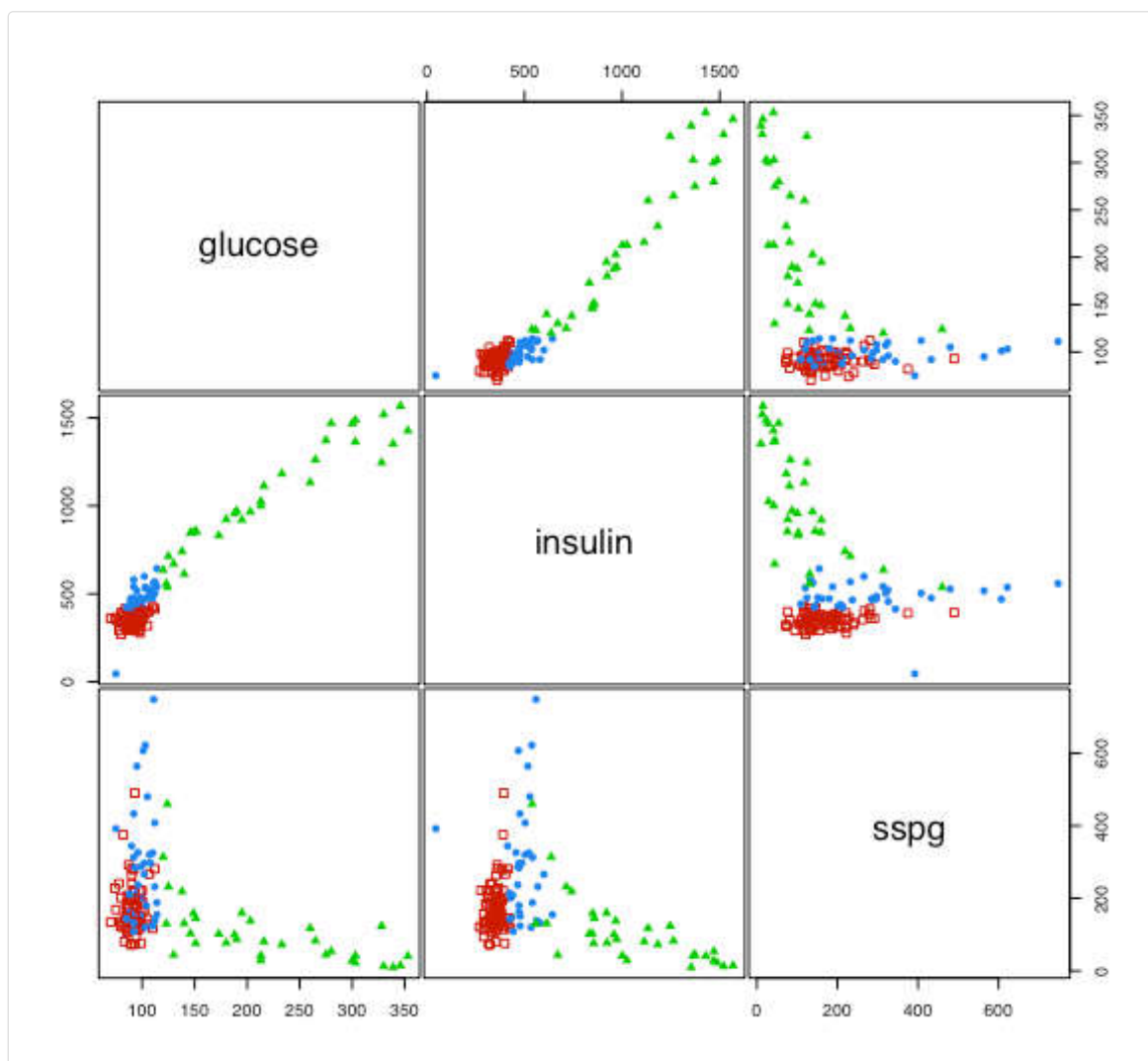
Clustering

```
data(diabetes)
```

```

class <- diabetes$class
table(class)
## class
## Chemical    Normal    Overt
##          36         76         33
X <- diabetes[,-1]
head(X)
##   glucose insulin sspg
## 1      80      356  124
## 2      97      289  117
## 3     105      319  143
## 4      90      356  199
## 5      90      323  240
## 6      86      381  157
clPairs(X, class)

```

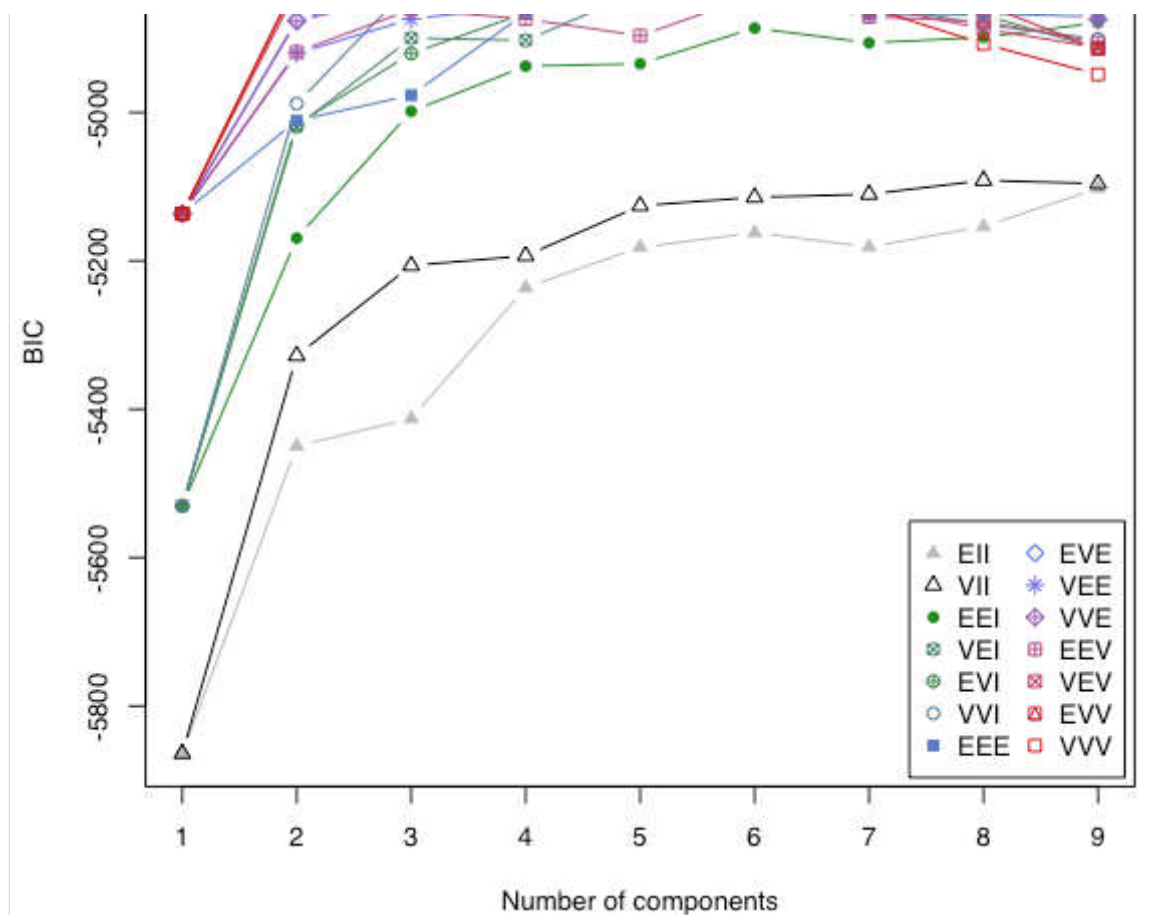


```

BIC <- mclustBIC(X)
plot(BIC)

```





```
summary(BIC)
```

```
## Best BIC values:
```

```
##           VVV,3      VVV,4      EVE,6
## BIC      -4751.316 -4784.32213 -4785.24591
## BIC diff      0.000   -33.00573   -33.92951
```

```
mod1 <- Mclust(X, x = BIC)
```

```
summary(mod1, parameters = TRUE)
```

```
## -----
```

```
## Gaussian finite mixture model fitted by EM algorithm
```

```
## -----
```

```
##
```

```
## Mclust VVV (ellipsoidal, varying volume, shape, and orientation) model
```

```
## with 3 components:
```

```
##
```

```
## log.likelihood  n df      BIC      ICL
```

```
##      -2303.496 145 29 -4751.316 -4770.169
```

```
##
```

```
## Clustering table:
```

```
##  1  2  3
```

```
## 81 36 28
```

```
##
```

```
## Mixing probabilities:
```

```
##      1      2      3
```

```
## 0.5368974 0.2650129 0.1980897
```

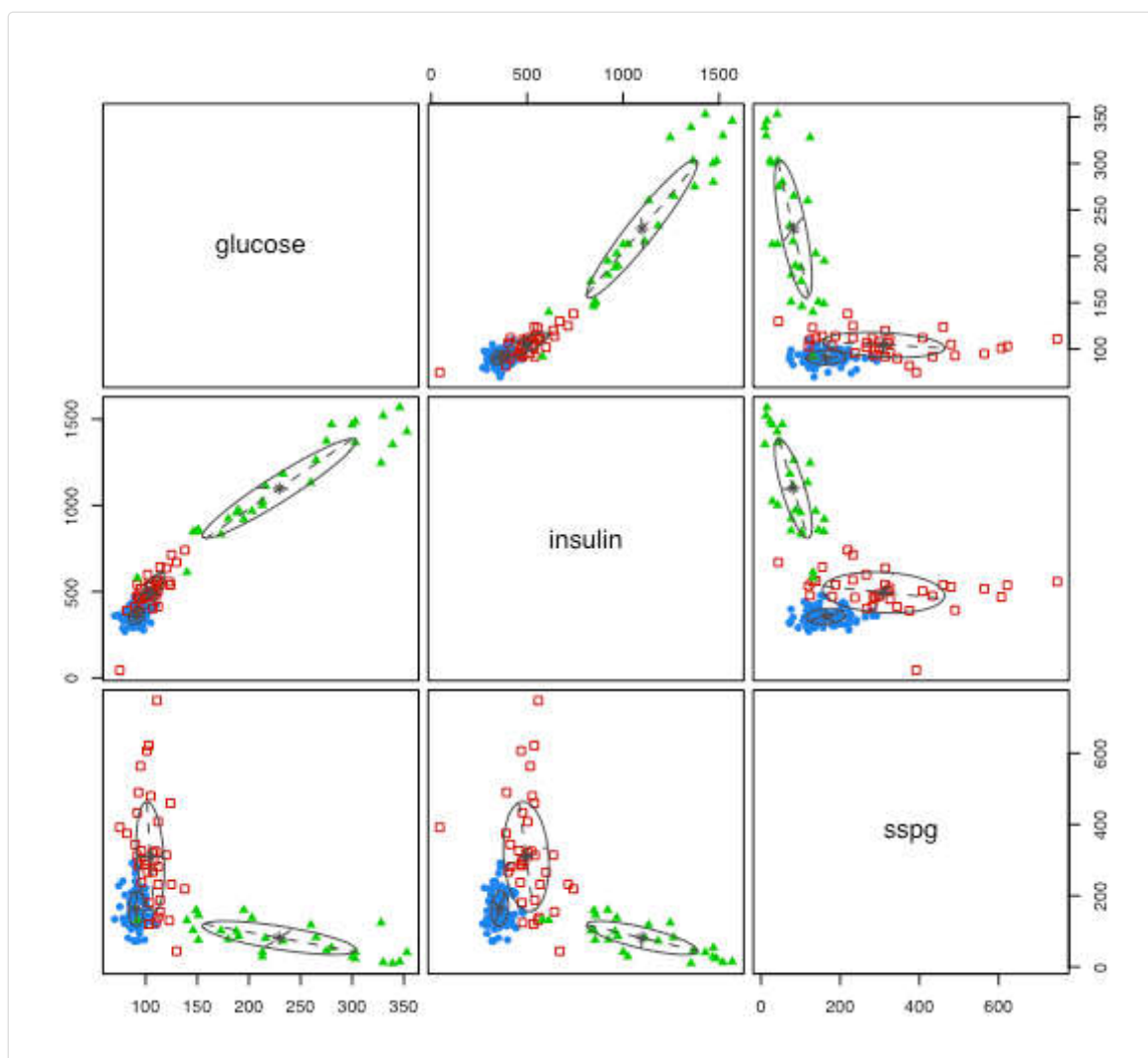
```
##
```

```
## Means:
```

```
##      [,1]      [,2]      [,3]
```

```
## glucose  90.96239 104.5335 229.42136
## insulin 357.79083 494.8259 1098.25990
## sspg     163.74858 309.5583  81.60001
##
## Variances:
## [,1]
##      glucose    insulin    sspg
## glucose 57.18044  75.83206  14.73199
## insulin 75.83206 2101.76553  322.82294
## sspg     14.73199  322.82294 2416.99074
## [,2]
##      glucose    insulin    sspg
## glucose 185.0290 1282.340 -509.7313
## insulin 1282.3398 14039.283 -2559.0251
## sspg     -509.7313 -2559.025 23835.7278
## [,3]
##      glucose    insulin    sspg
## glucose 5529.250 20389.09 -2486.208
## insulin 20389.088 83132.48 -10393.004
## sspg     -2486.208 -10393.00 2217.533
```

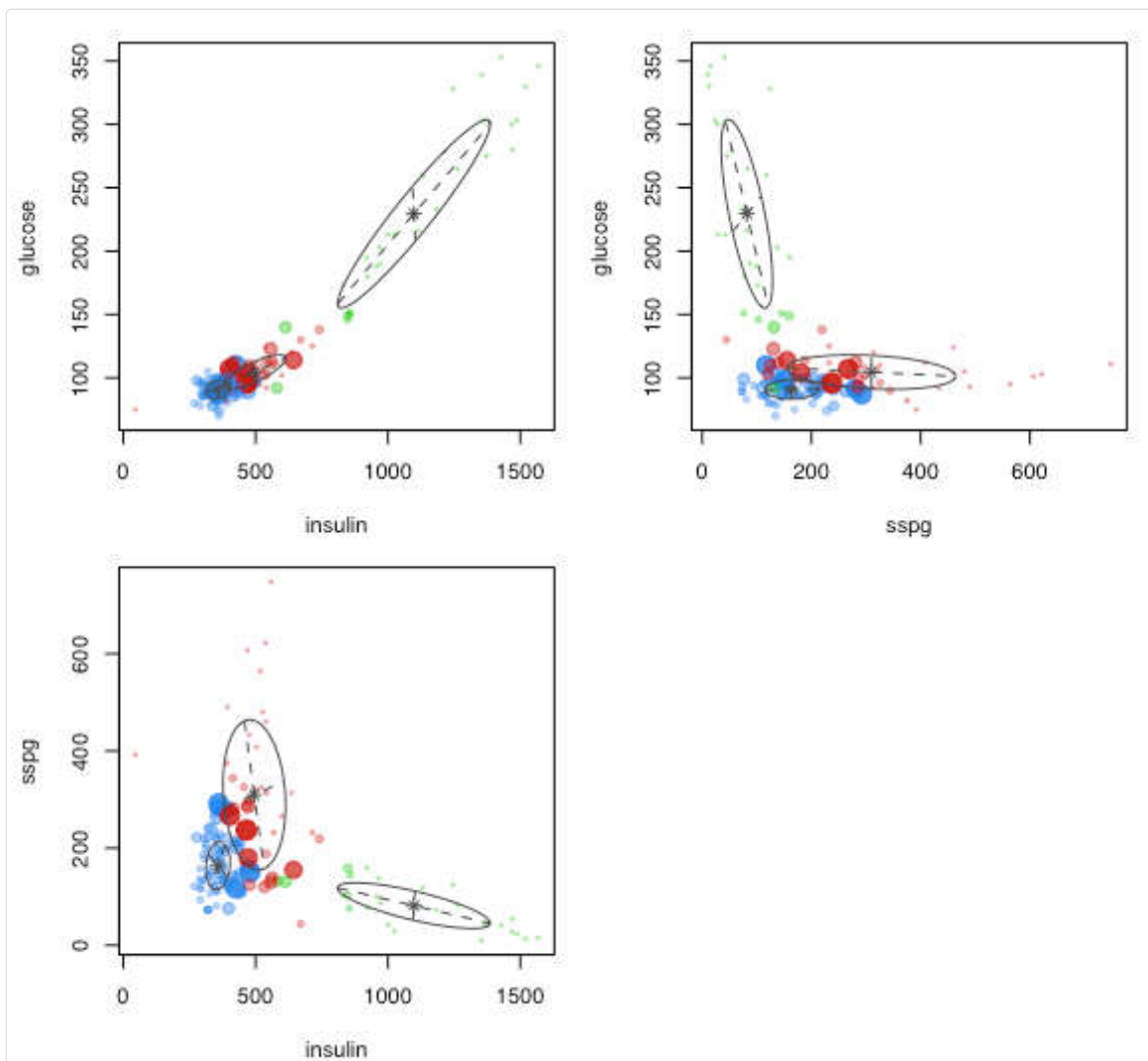
```
plot(mod1, what = "classification")
```



```
table(class, mod1$classification)
```

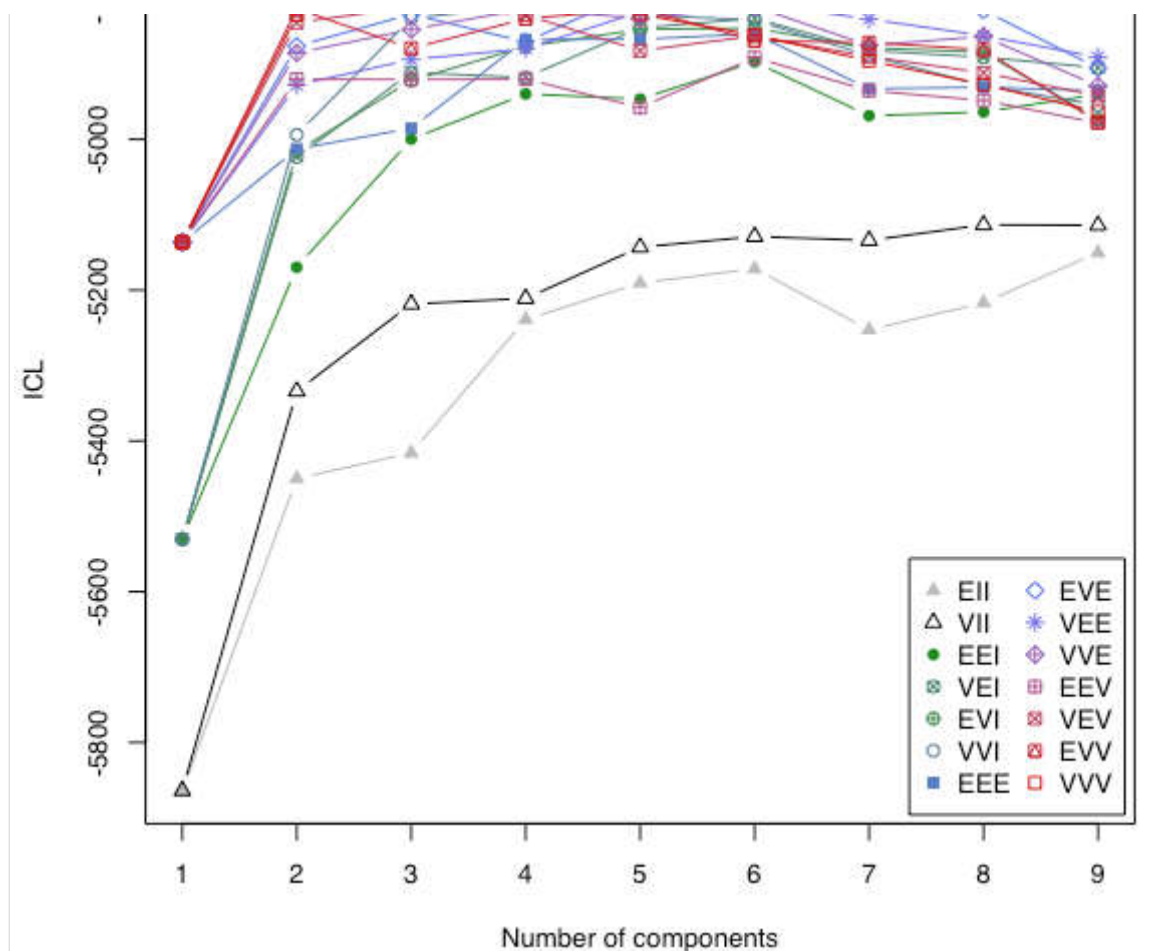
```
##
## class      1  2  3
## Chemical   9 26  1
## Normal    72  4  0
## Overt      0  6 27

par(mfrow = c(2,2))
plot(mod1, what = "uncertainty", dims = c(2,1), main = "")
plot(mod1, what = "uncertainty", dims = c(3,1), main = "")
plot(mod1, what = "uncertainty", dims = c(2,3), main = "")
par(mfrow = c(1,1))
```



```
ICL <- mclustICL(X)
summary(ICL)
## Best ICL values:
##          VVV,3      EVE,6      EVE,7
## ICL      -4770.169 -4797.38232 -4797.50566
## ICL diff    0.000   -27.21342   -27.33677
plot(ICL)
```





```
LRT <- mclustBootstrapLRT(X, modelName = "VVV")
LRT
## -----
## Bootstrap sequential LRT for the number of mixture components
## -----
## Model          = VVV
## Replications = 999
##               LRTS bootstrap p-value
## 1 vs 2    361.16739          0.001
## 2 vs 3    123.49685          0.001
## 3 vs 4     16.76161          0.498
```

Initialisation

EM algorithm is used by **mclust** for maximum likelihood estimation. Initialisation of EM is performed using the partitions obtained from agglomerative hierarchical clustering. For details see `help(mclustBIC)` or `help(Mclust)`, and `help(hc)`.

```
(hc1 <- hc(X, modelName = "VVV", use = "SVD"))
## Call:
## hc(data = X, modelName = "VVV", use = "SVD")
##
## Model-Based Agglomerative Hierarchical Clustering:
## Model name = VVV
## Use = SVD
```

```
## Number of objects = 145
BIC1 <- mclustBIC(X, initialization = list(hcPairs = hc1)) # default
summary(BIC1)
## Best BIC values:
##           VVV,3      VVV,4      EVE,6
## BIC      -4751.316 -4784.32213 -4785.24591
## BIC diff    0.000   -33.00573   -33.92951

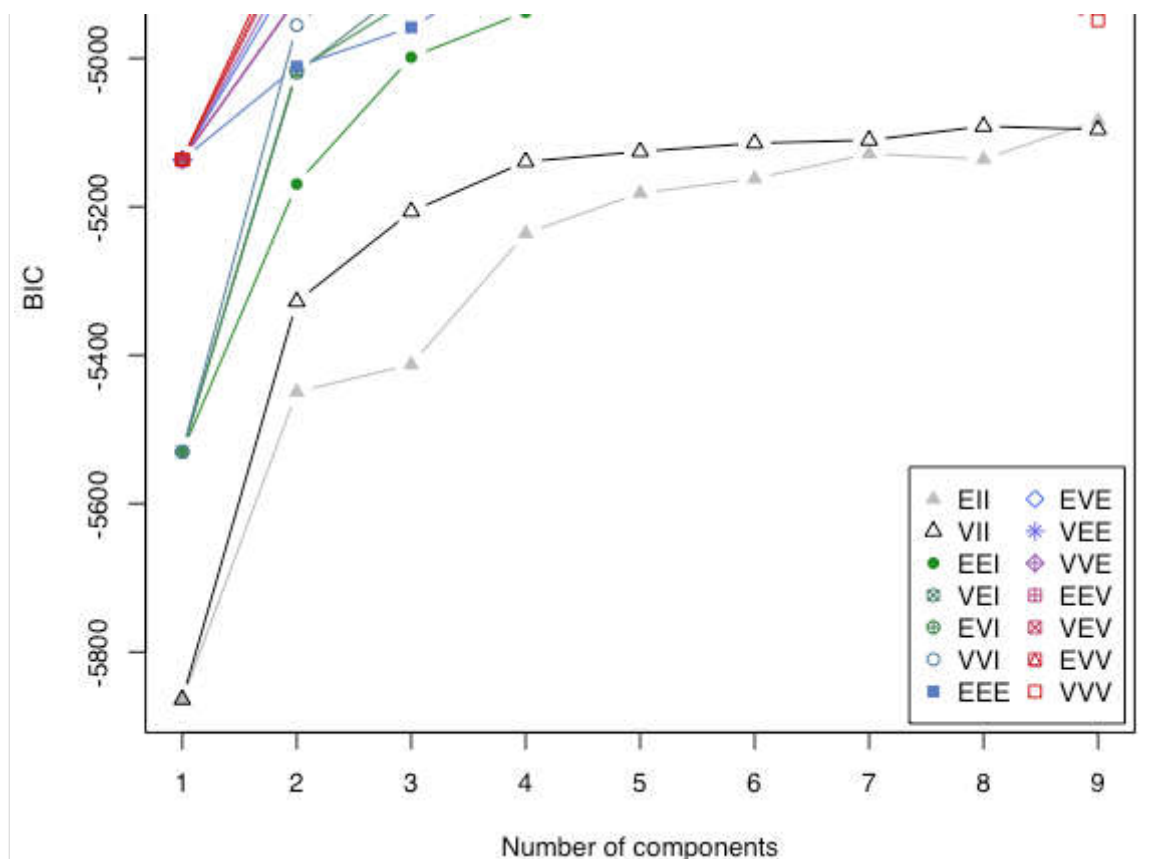
(hc2 <- hc(X, modelName = "VVV", use = "VARS"))
## Call:
## hc(data = X, modelName = "VVV", use = "VARS")
##
## Model-Based Agglomerative Hierarchical Clustering:
## Model name = VVV
## Use = VARS
## Number of objects = 145
BIC2 <- mclustBIC(X, initialization = list(hcPairs = hc2))
summary(BIC2)
## Best BIC values:
##           VVV,3      VVE,3      EVE,4
## BIC      -4760.091 -4775.53693 -4793.26143
## BIC diff    0.000   -15.44628   -33.17079

(hc3 <- hc(X, modelName = "EEE", use = "SVD"))
## Call:
## hc(data = X, modelName = "EEE", use = "SVD")
##
## Model-Based Agglomerative Hierarchical Clustering:
## Model name = EEE
## Use = SVD
## Number of objects = 145
BIC3 <- mclustBIC(X, initialization = list(hcPairs = hc3))
summary(BIC3)
## Best BIC values:
##           VVV,3      VVE,4      VVE,3
## BIC      -4751.354 -4757.091572 -4775.69587
## BIC diff    0.000   -5.737822   -24.34212
```

Update BIC by merging the best results:

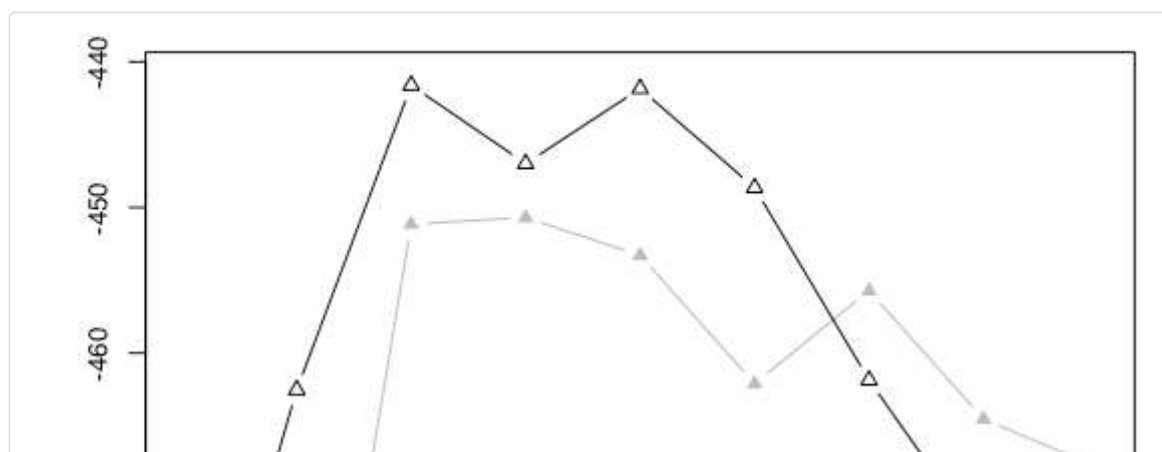
```
BIC <- mclustBICupdate(BIC1, BIC2, BIC3)
summary(BIC)
## Best BIC values:
##           VVV,3      VVE,4      VVE,3
## BIC      -4751.316 -4757.091572 -4775.53693
## BIC diff    0.000   -5.775172   -24.22053
plot(BIC)
```

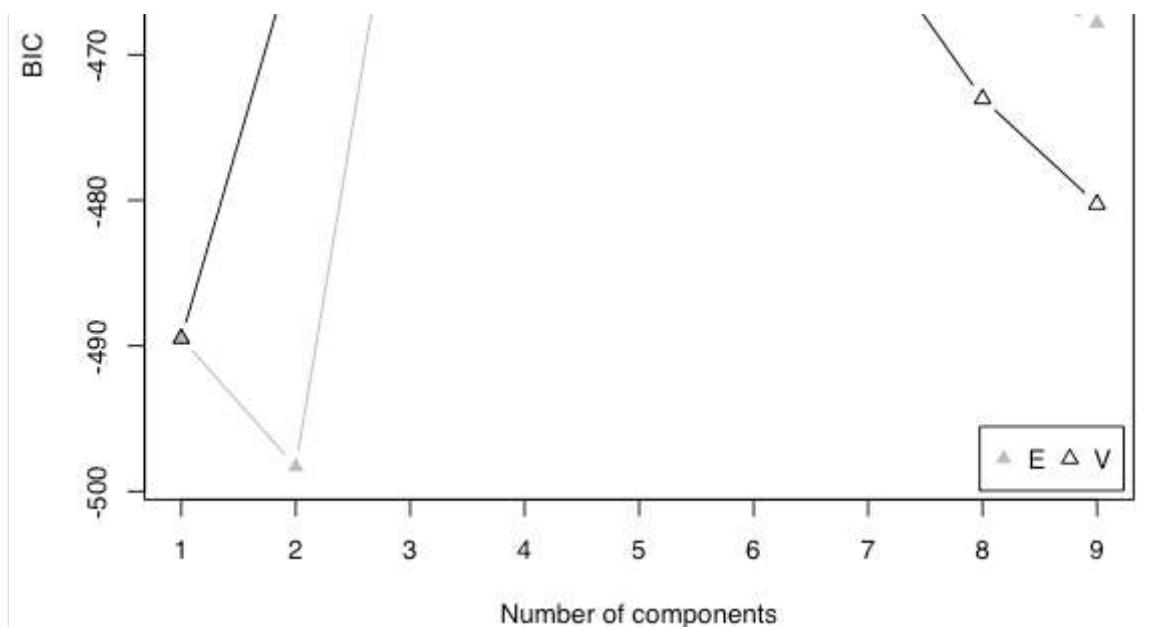




Univariate fit using random starting points obtained by creating random agglomerations (see `help(randomPairs)`) and merging best results:

```
data(galaxies, package = "MASS")
galaxies <- galaxies / 1000
BIC <- NULL
for(j in 1:20)
{
  rBIC <- mclustBIC(galaxies, verbose = FALSE,
                    initialization = list(hcPairs = randomPairs(galaxies)))
  BIC <- mclustBICupdate(BIC, rBIC)
}
summary(BIC)
## Best BIC values:
##           V,3           V,5           V,4
## BIC      -441.6122 -441.8384995 -446.98899
## BIC diff    0.0000   -0.2262896   -5.37678
plot(BIC)
```





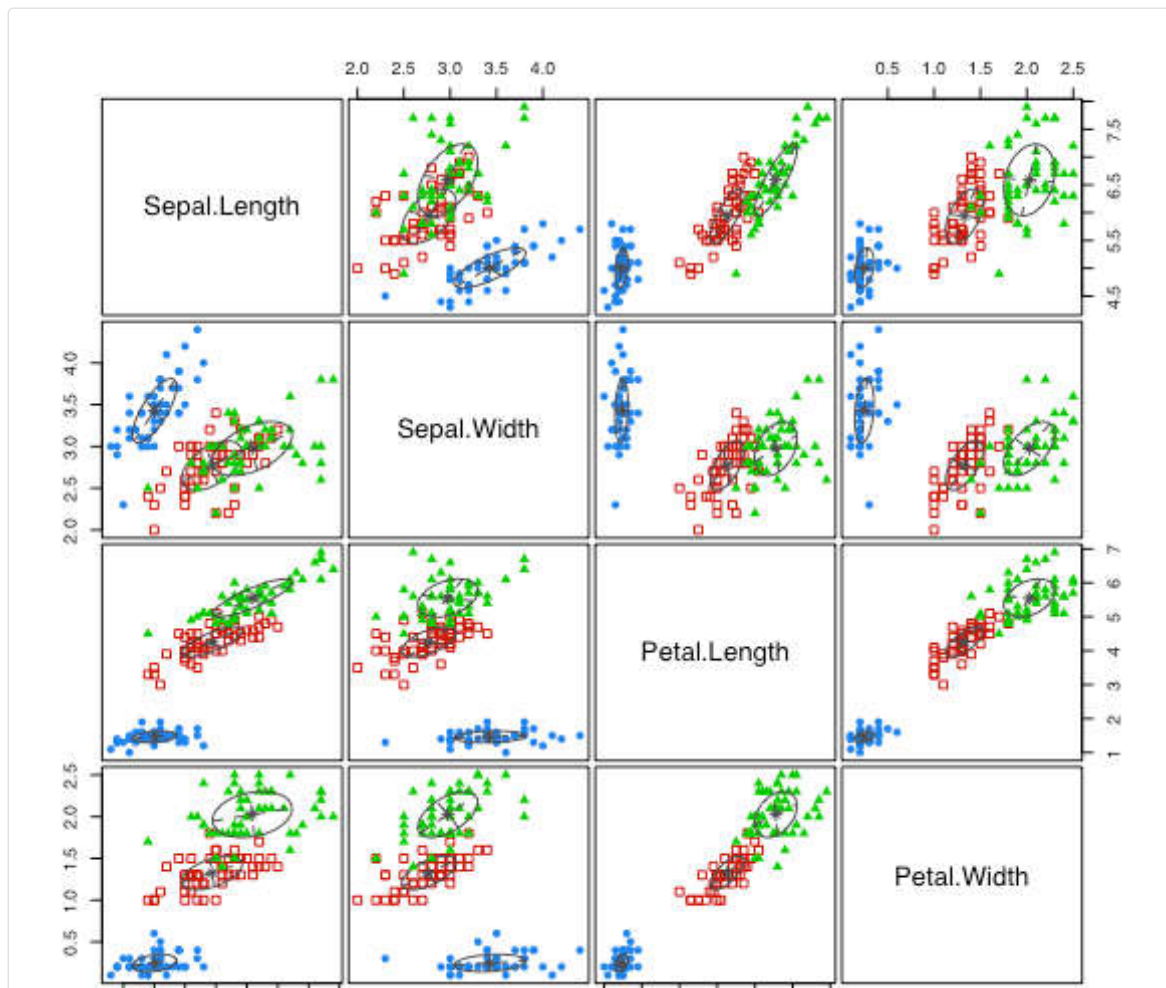
```
mod <- Mclust(galaxies, x = BIC)
summary(mod)
## -----
## Gaussian finite mixture model fitted by EM algorithm
## -----
##
## Mclust V (univariate, unequal variance) model with 3 components:
##
## log.likelihood n df      BIC      ICL
##      -203.1792 82  8 -441.6122 -441.6126
##
## Clustering table:
##  1  2  3
## 72  7  3
```

Classification

EDDA

```
data(iris)
class <- iris$Species
table(class)
## class
##      setosa versicolor virginica
##       50       50       50
X <- iris[,1:4]
head(X)
##      Sepal.Length Sepal.Width Petal.Length Petal.Width
## 1         5.1         3.5         1.4         0.2
## 2         4.9         3.0         1.4         0.2
## 3         4.7         3.2         1.3         0.2
## 4         4.6         3.1         1.5         0.2
## 5         5.0         3.6         1.4         0.2
```

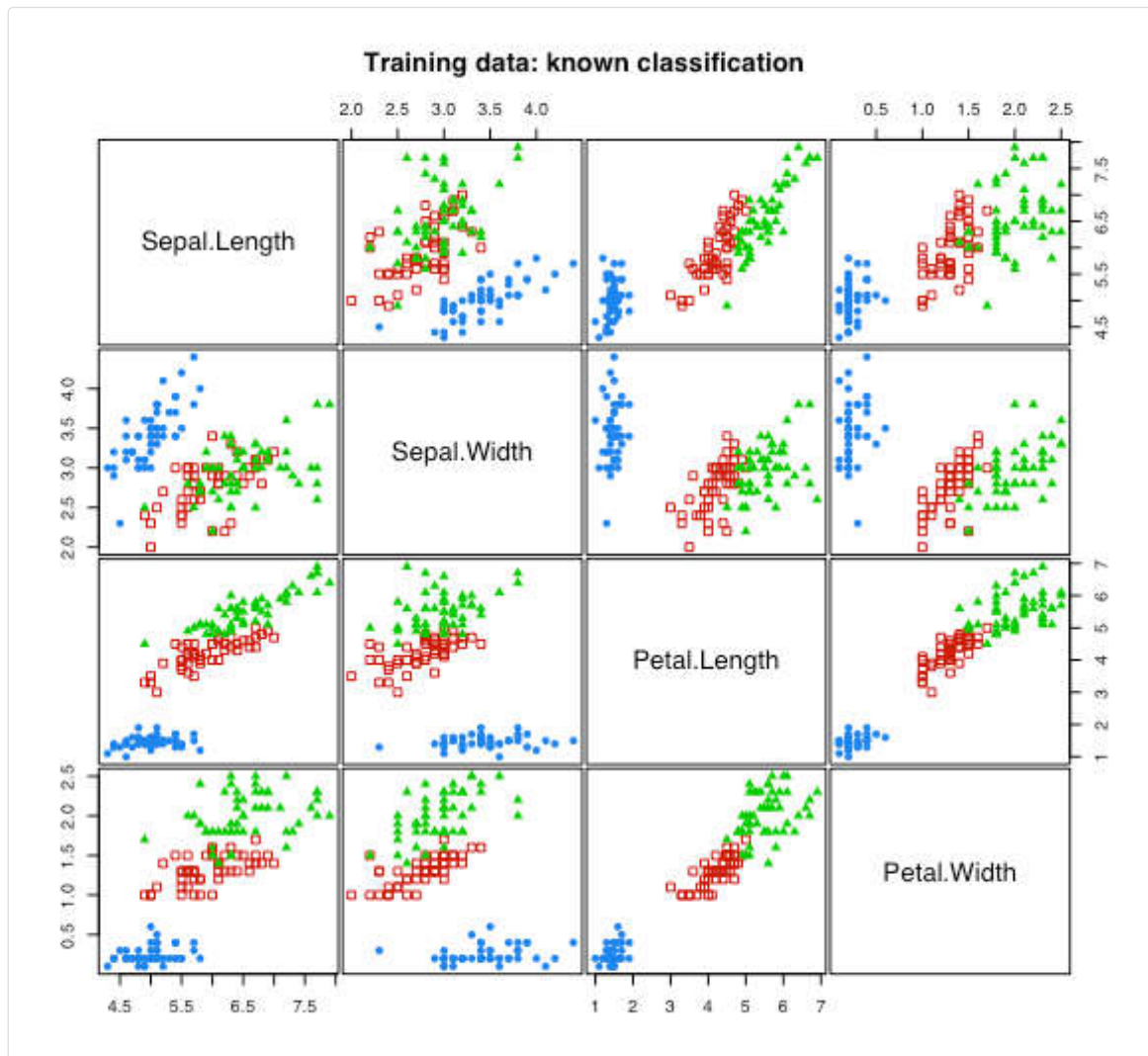
```
## 6          5.4          3.9          1.7          0.4
mod2 <- MclustDA(X, class, modelType = "EDDA")
summary(mod2)
## -----
## Gaussian finite mixture model for classification
## -----
##
## EDDA model summary:
##
## log.likelihood   n df      BIC
##      -187.7097 150 36 -555.8024
##
## Classes      n Model G
## setosa       50  VEV 1
## versicolor   50  VEV 1
## virginica    50  VEV 1
##
## Training classification summary:
##
##           Predicted
## Class      setosa versicolor virginica
## setosa       50         0         0
## versicolor    0        47         3
## virginica     0         0        50
##
## Training error = 0.02
plot(mod2, what = "scatterplot")
```



4.5 5.5 6.5 7.5

1 2 3 4 5 6 7

```
plot(mod2, what = "classification")
```



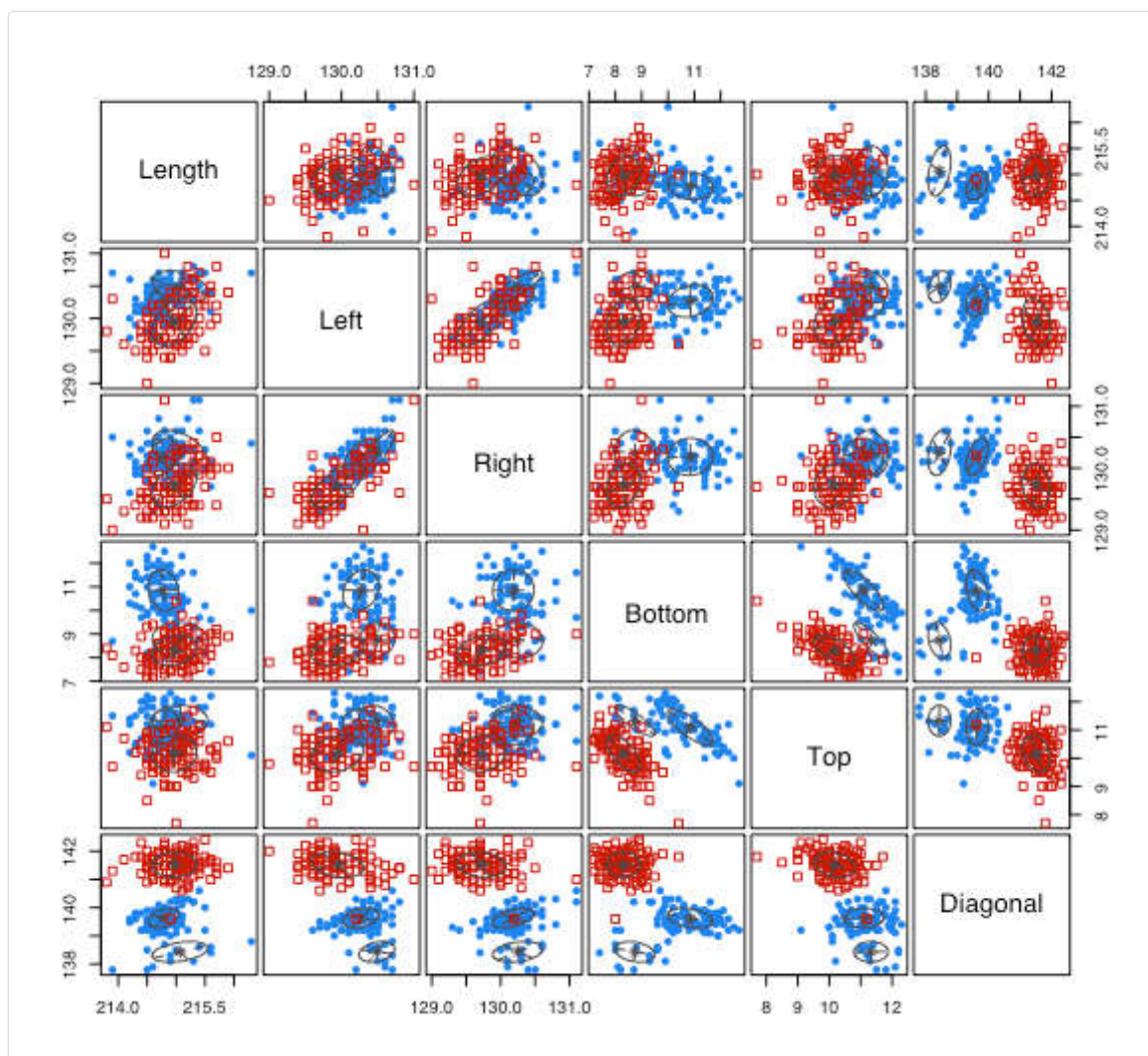
MclustDA

```
data(banknote)
class <- banknote$Status
table(class)
## class
## counterfeit    genuine
##           100         100
X <- banknote[,-1]
head(X)
##   Length Left Right Bottom Top Diagonal
## 1  214.8 131.0 131.1    9.0  9.7   141.0
## 2  214.6 129.7 129.7    8.1  9.5   141.7
## 3  214.8 129.7 129.7    8.7  9.6   142.2
## 4  214.8 129.7 129.6    7.5 10.4   142.0
## 5  215.0 129.6 129.7   10.4  7.7   141.8
## 6  215.7 130.8 130.5    9.0 10.1   141.4
```

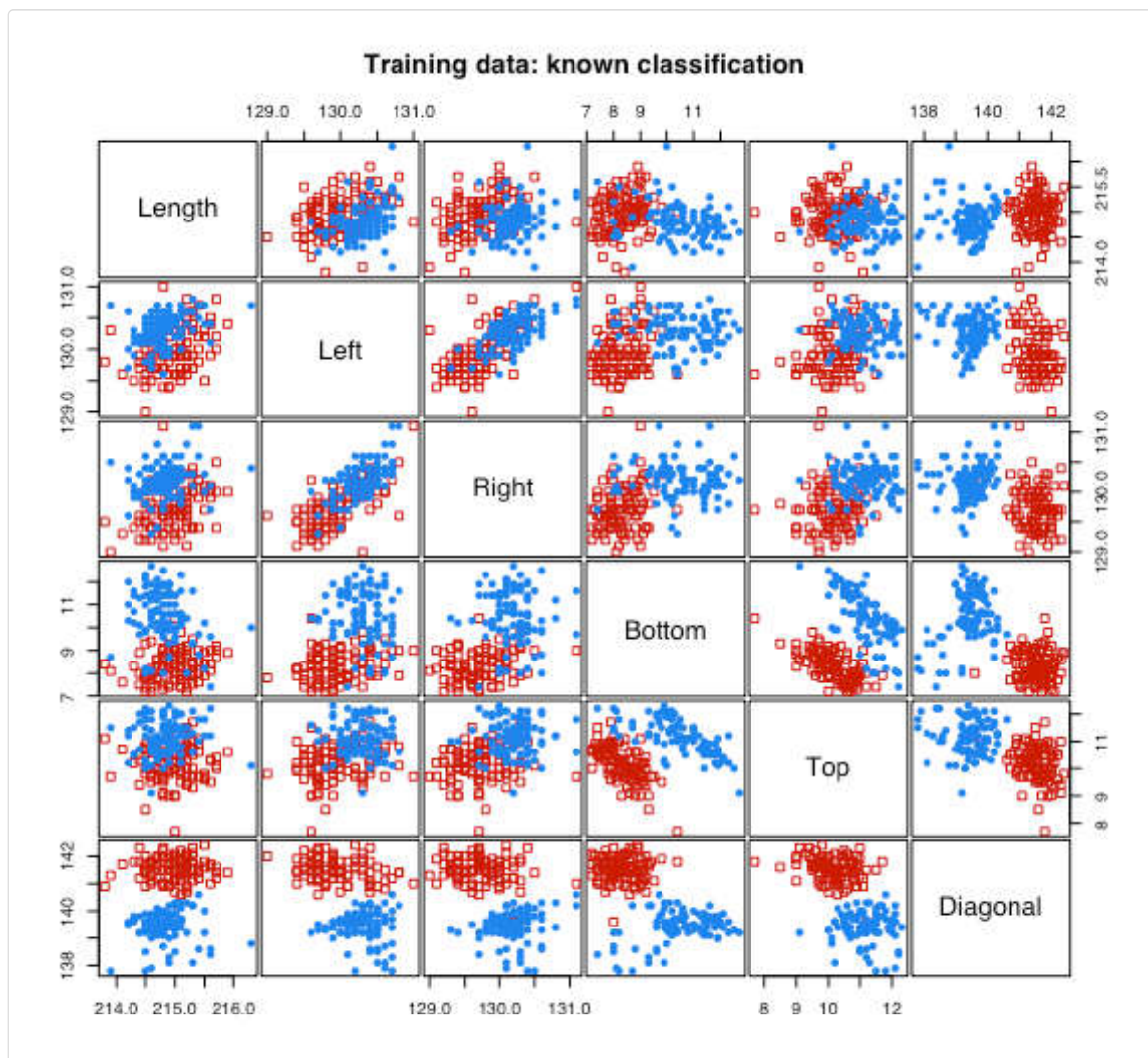
```

mod3 <- MclustDA(X, class)
summary(mod3)
## -----
## Gaussian finite mixture model for classification
## -----
##
## MclustDA model summary:
##
## log.likelihood   n df      BIC
##      -646.0798 200 66 -1641.849
##
## Classes          n Model G
## counterfeit 100   EVE 2
## genuine      100   XXX 1
##
## Training classification summary:
##
##           Predicted
## Class      counterfeit genuine
## counterfeit      100       0
## genuine           0      100
##
## Training error = 0
plot(mod3, what = "scatterplot")

```




```
plot(mod3, what = "classification")
```



Cross-validation error

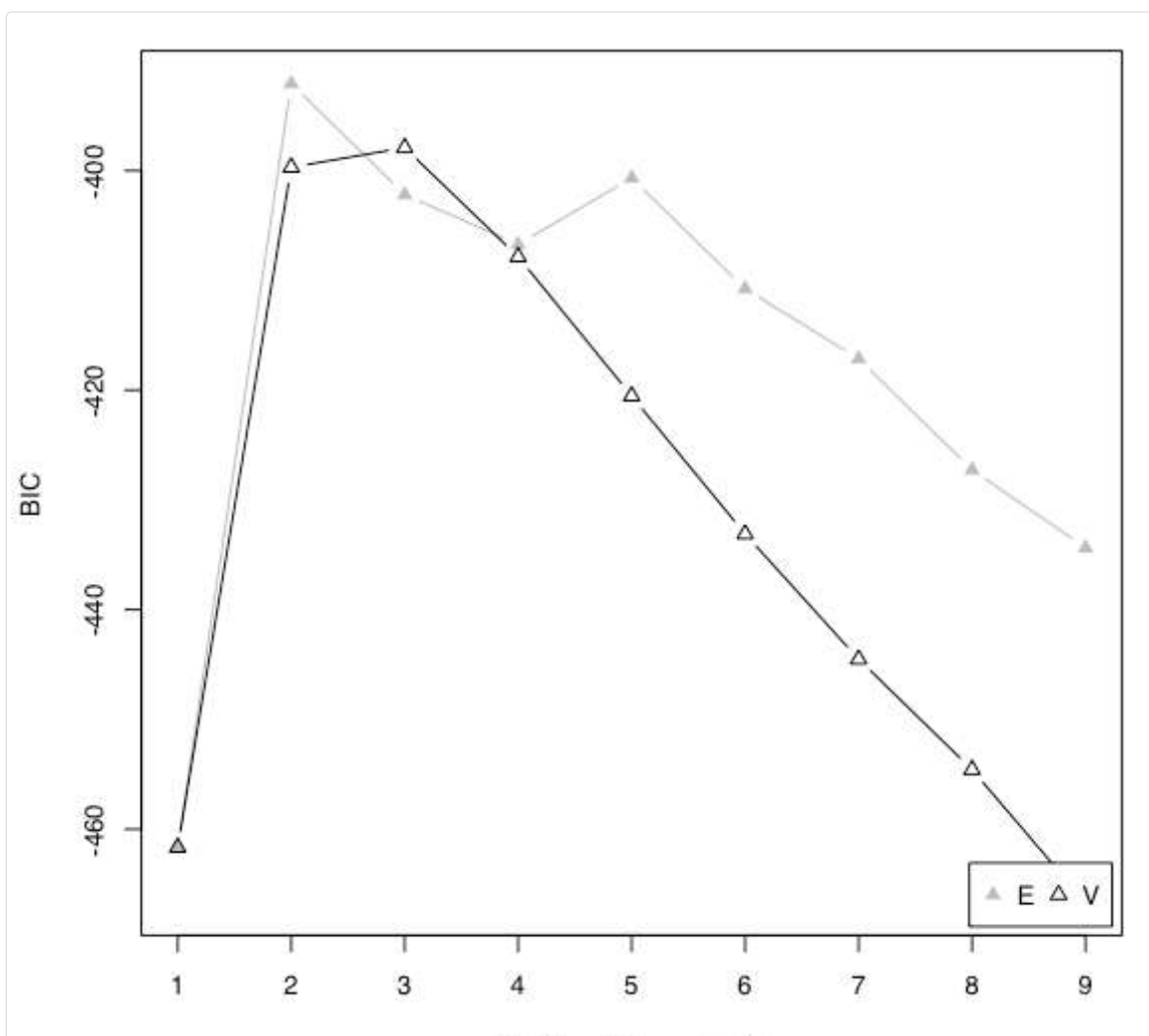
```
cv <- cvMclustDA(mod2, nfold = 10)
str(cv)
## List of 4
## $ classification: Factor w/ 3 levels "setosa","versicolor",...: 1 1 1 1 1 1 1 1 1 ...
## $ z              : num [1:150, 1:3] 1 1 1 1 1 1 1 1 1 1 ...
## $ error          : num 0.0267
## $ se             : num 0.0147
unlist(cv[3:4])
##      error      se
## 0.02666667 0.01474055
cv <- cvMclustDA(mod3, nfold = 10)
str(cv)
## List of 4
## $ classification: Factor w/ 2 levels "counterfeit",...: 2 2 2 2 2 2 2 2 2 ...
## $ z              : num [1:200, 1:2] 9.13e-05 3.21e-21 2.27e-26 1.07e-22 9.30e-21 ...
## $ error          : num 0
## $ se             : num 0
unlist(cv[3:4])
```

```
## error      se
##      0      0
```

Density estimation

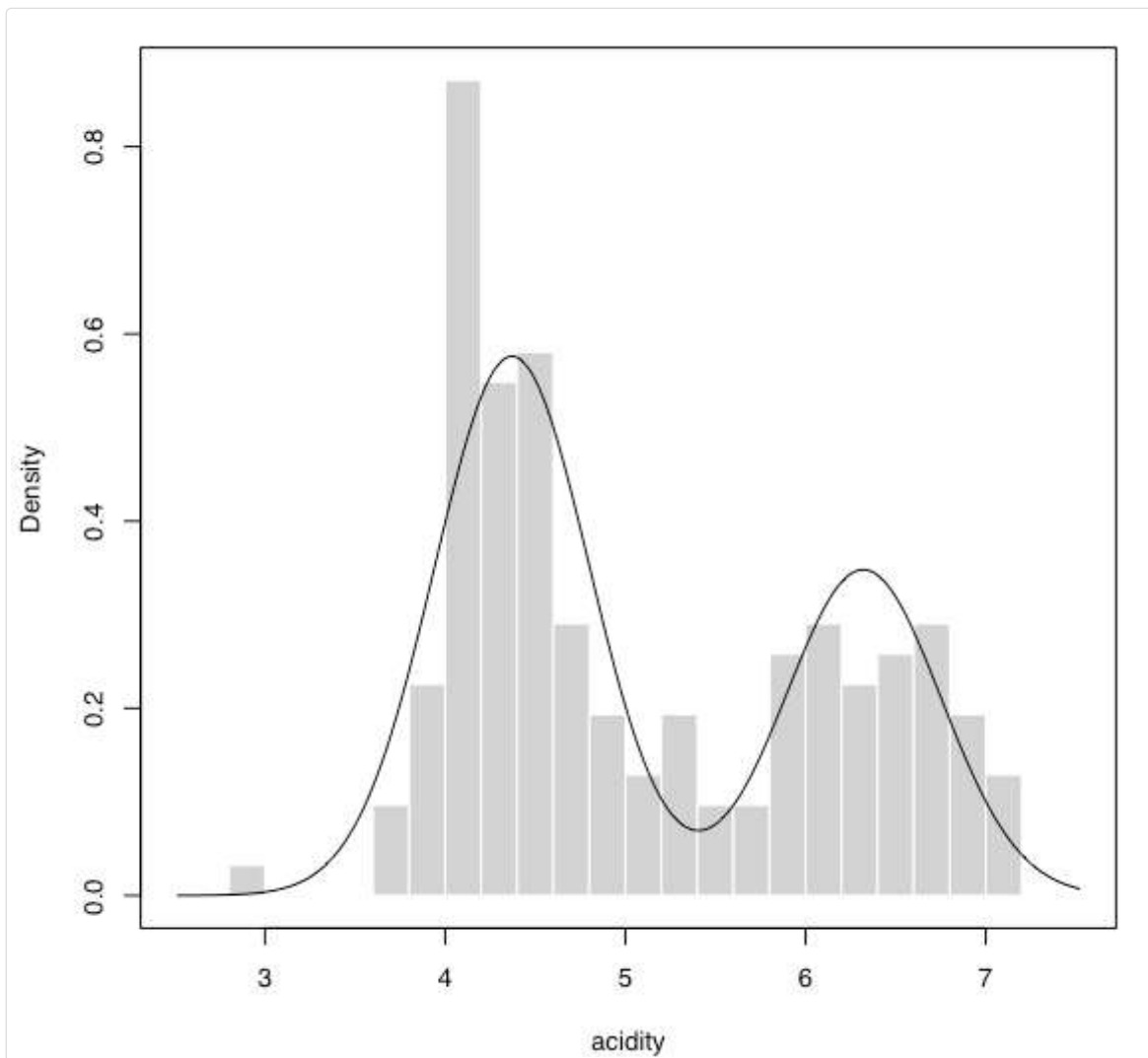
Univariate

```
data(acidity)
mod4 <- densityMclust(acidity)
summary(mod4)
## -----
## Density estimation via Gaussian finite mixture modeling
## -----
##
## Mclust E (univariate, equal variance) model with 2 components:
##
## log.likelihood  n df      BIC      ICL
##      -185.9493 155  4 -392.0723 -398.5554
##
## Clustering table:
##  1  2
## 98 57
plot(mod4, what = "BIC")
```

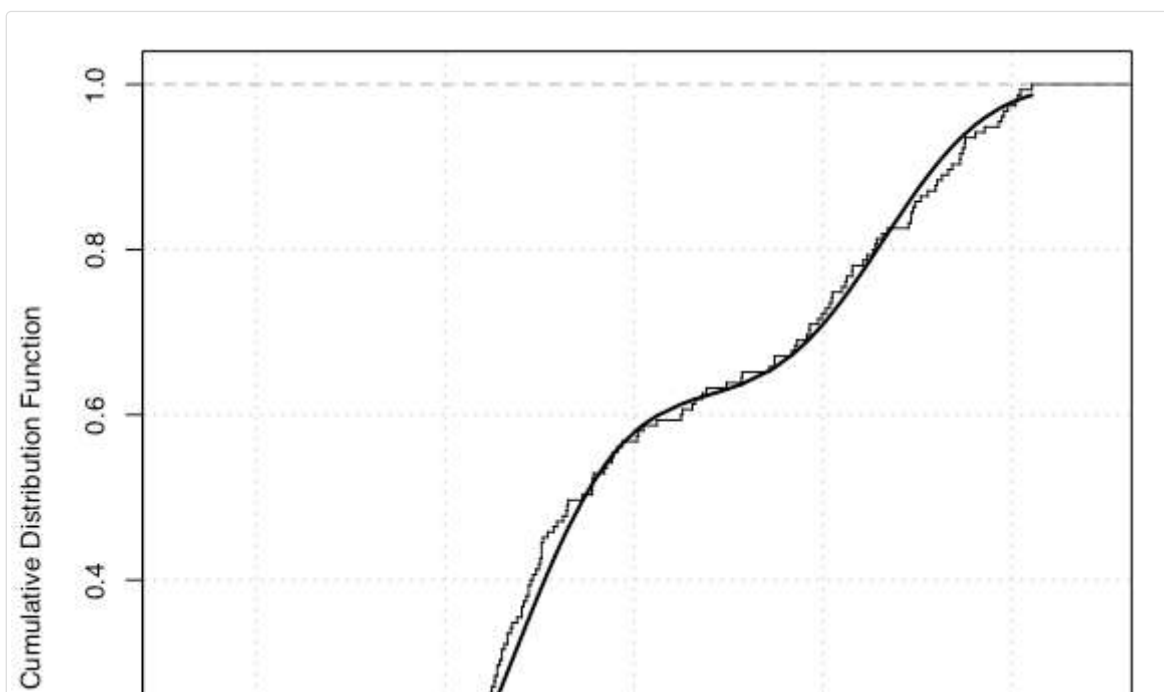


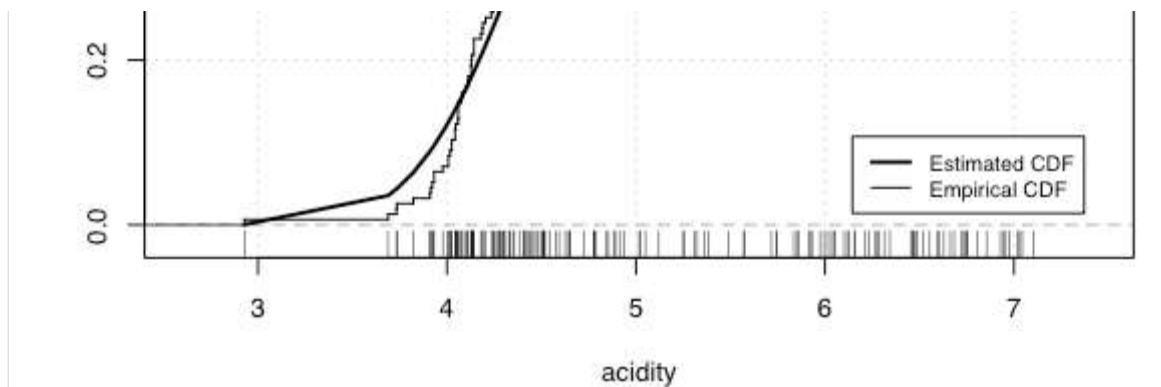
Number of components

```
plot(mod4, what = "density", data = acidity, breaks = 15)
```

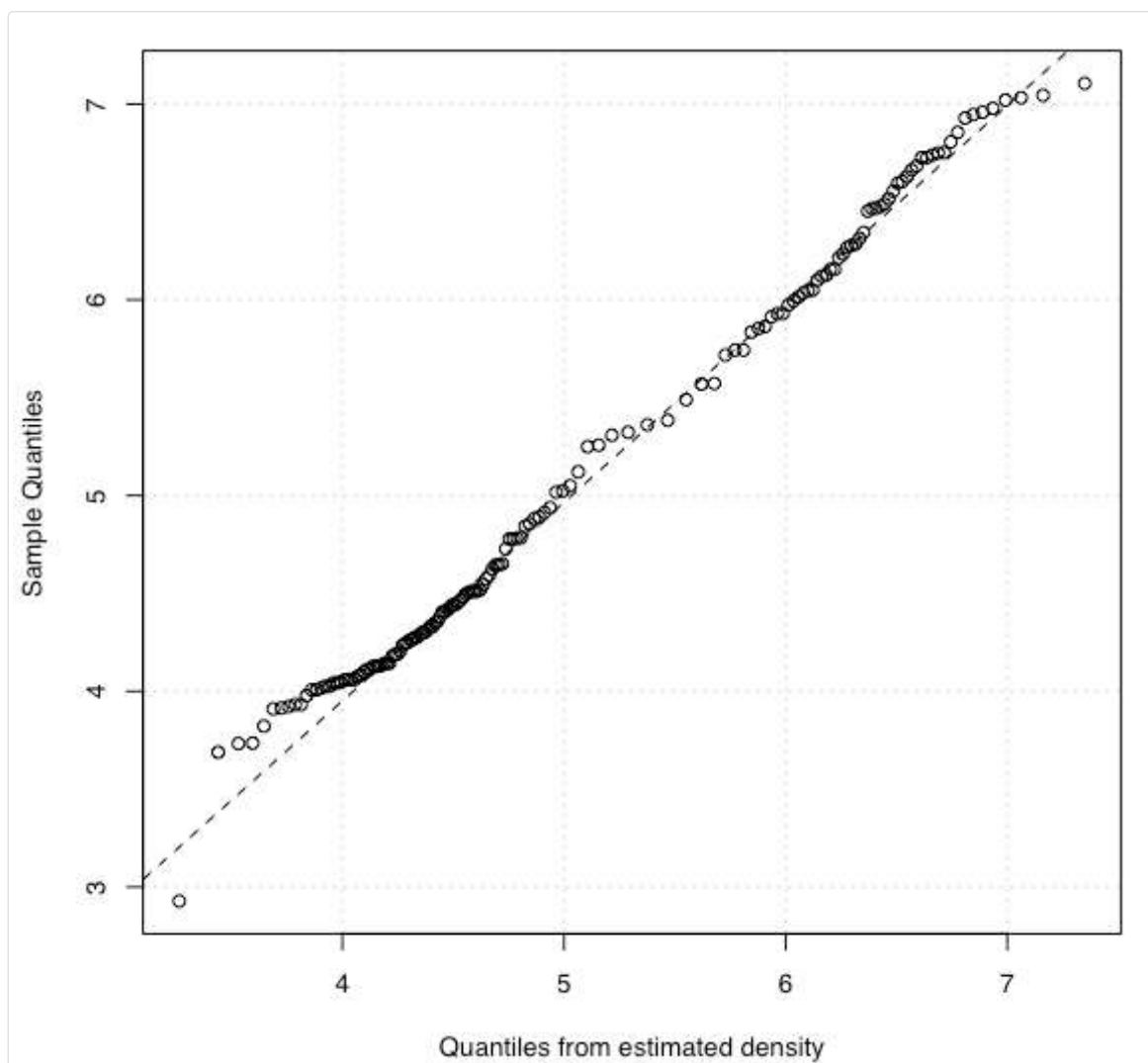


```
plot(mod4, what = "diagnostic", type = "cdf")
```





```
plot(mod4, what = "diagnostic", type = "qq")
```

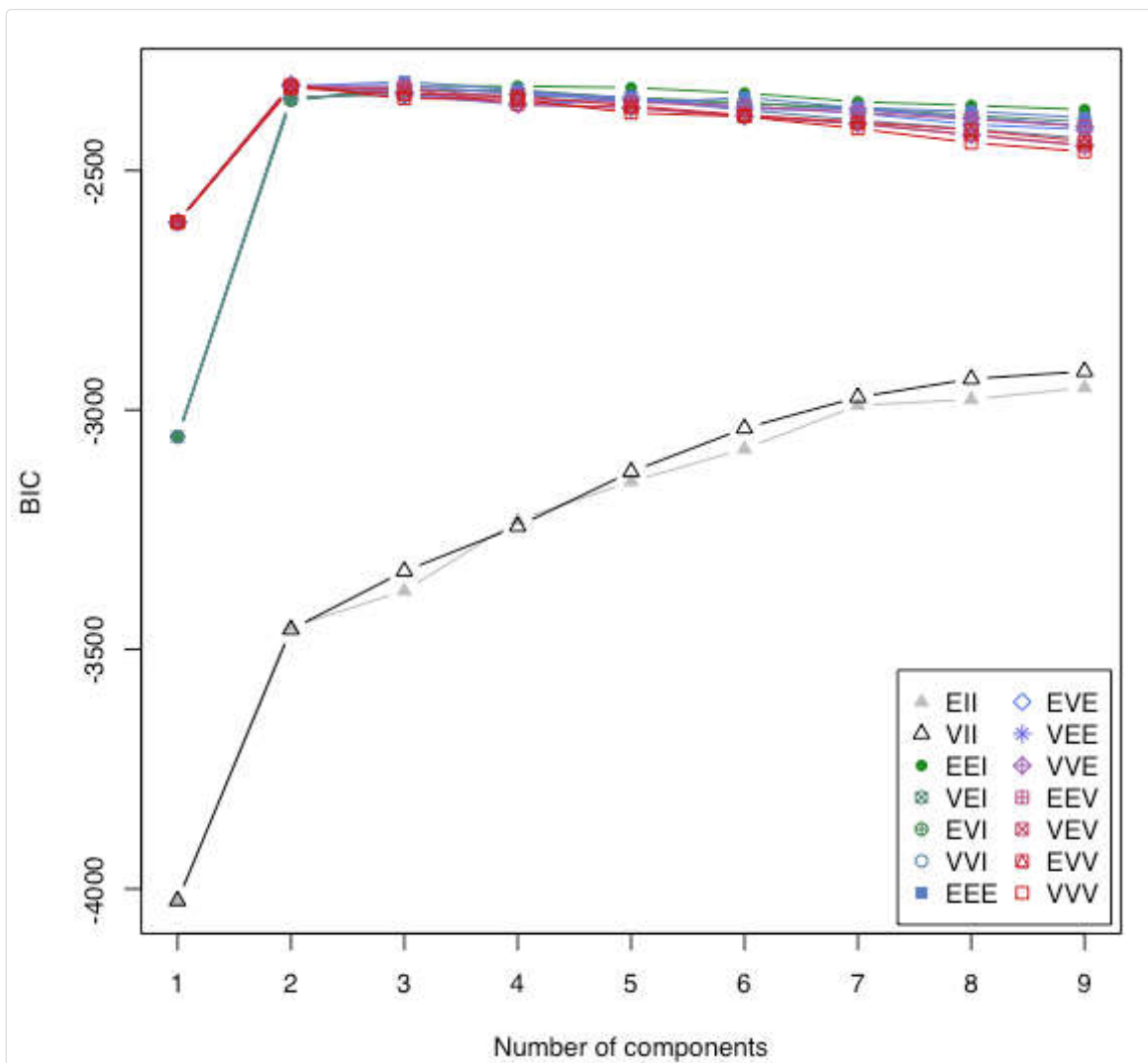


Multivariate

```
data(faithful)
mod5 <- densityMclust(faithful)
summary(mod5)
## -----
## Density estimation via Gaussian finite mixture modeling
## -----
##
```

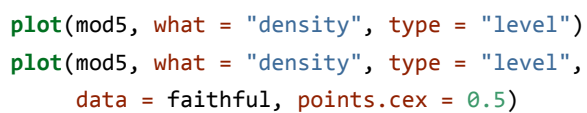


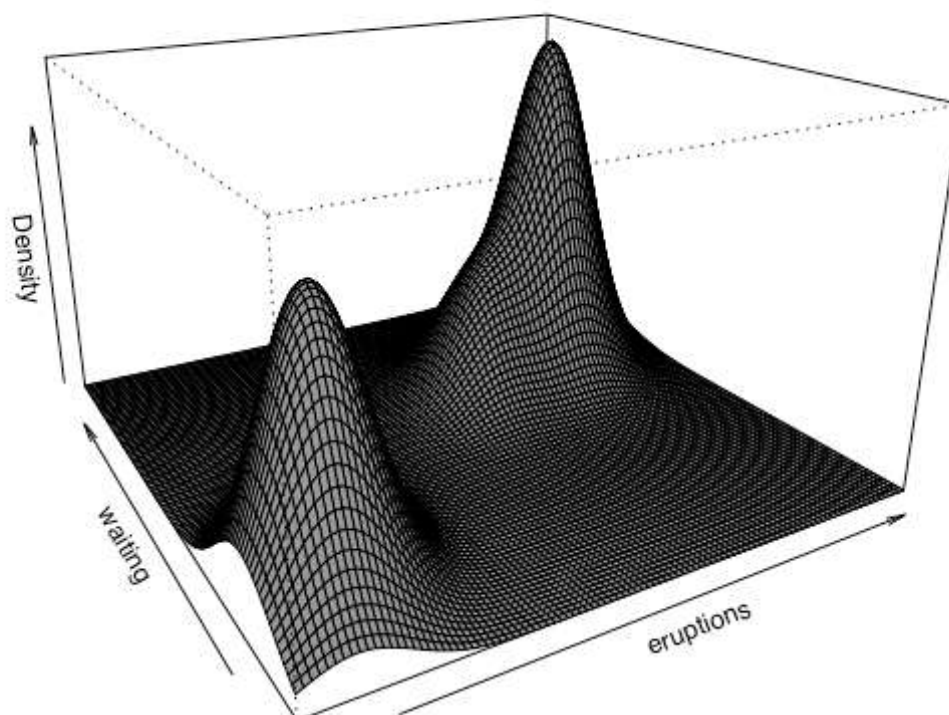
```
## Mclust EEE (ellipsoidal, equal volume, shape and orientation) model with 3
## components:
##
## log.likelihood  n df      BIC      ICL
##      -1126.326 272 11 -2314.316 -2357.824
##
## Clustering table:
##   1  2  3
## 40 97 135
plot(mod5, what = "BIC")
```



```
plot(mod5, what = "density")
```







Bootstrap inference

```
boot1 <- MclustBootstrap(mod1, nboot = 999, type = "bs")
summary(boot1, what = "se")
## -----
## Resampling standard errors
## -----
## Model                      = VVV
## Num. of mixture components = 3
## Replications                = 999
## Type                        = nonparametric bootstrap
##
## Mixing probabilities:
##      1      2      3
## 0.05561571 0.05096443 0.03637319
##
## Means:
##      1      2      3
## glucose 0.965088 3.379977 16.569600
## insulin 7.693082 28.802030 65.214885
## sspg     8.389342 29.982110 9.838989
##
## Variances:
```

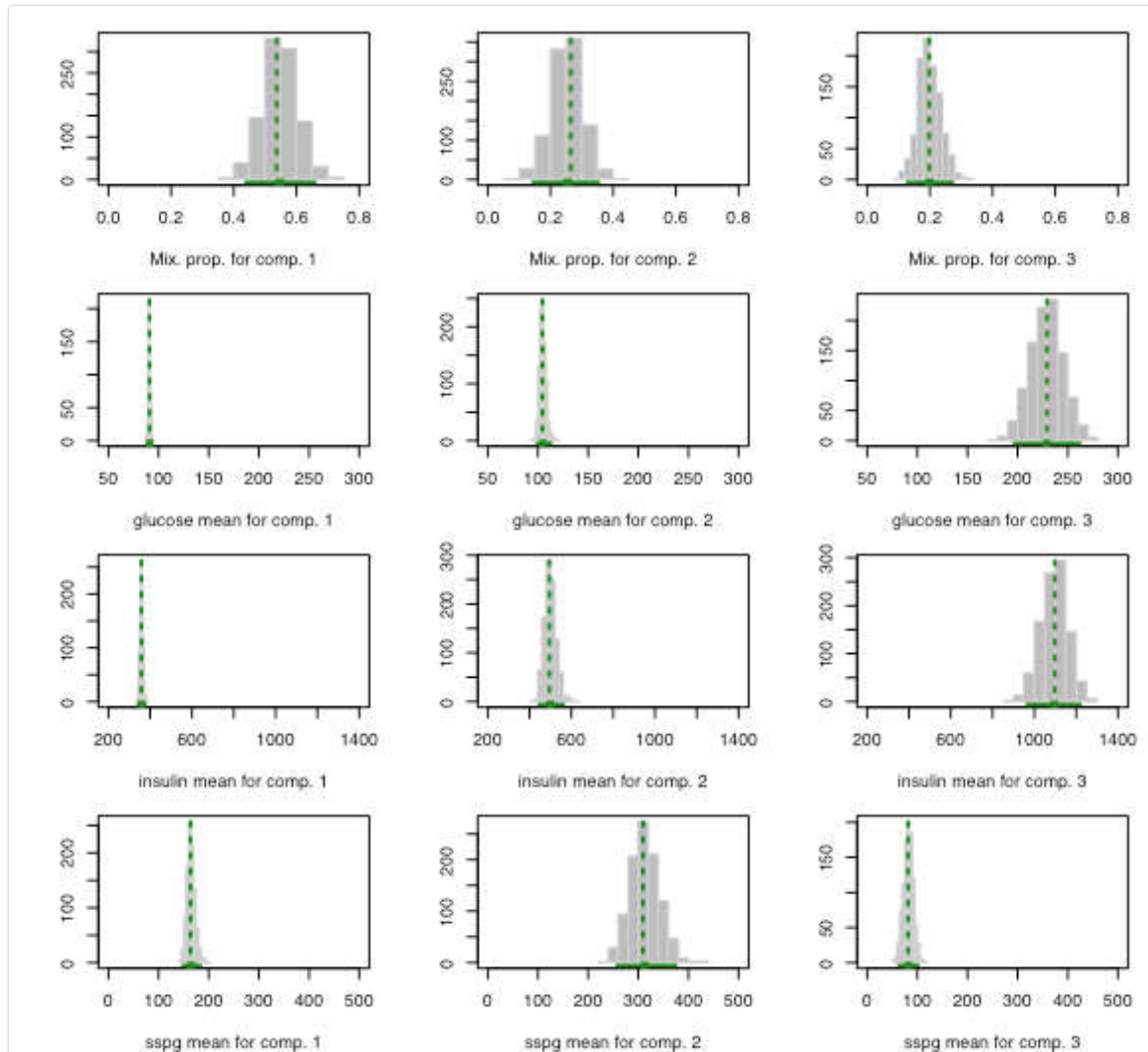
```

## [,1]
##          glucose  insulin      sspg
## glucose 11.38885  53.00902  51.77266
## insulin 53.00902  524.72305  437.21126
## sspg    51.77266  437.21126  683.20260
## [,2]
##          glucose  insulin      sspg
## glucose 65.58419  638.4846  438.0692
## insulin 638.48459 7635.8741 3083.3778
## sspg    438.06916 3083.3778 6875.7911
## [,3]
##          glucose  insulin      sspg
## glucose 1020.9246 4246.954  647.6164
## insulin 4246.9540 19742.656 2491.2115
## sspg     647.6164 2491.211  484.1560
summary(boot1, what = "ci")
## -----
## Resampling confidence intervals
## -----
## Model                      = VVV
## Num. of mixture components = 3
## Replications                = 999
## Type                        = nonparametric bootstrap
## Confidence level            = 0.95
##
## Mixing probabilities:
##           1          2          3
## 2.5%  0.4388552 0.1448245 0.1284124
## 97.5% 0.6586360 0.3526105 0.2725898
##
## Means:
## [,1]
##          glucose  insulin      sspg
## 2.5%  89.25108 343.8573 149.3941
## 97.5% 93.04648 374.6513 183.2884
## [,2]
##          glucose  insulin      sspg
## 2.5%  99.28085 446.3719 258.0851
## 97.5% 112.82028 561.8197 374.9310
## [,3]
##          glucose  insulin      sspg
## 2.5%  196.6521  965.780  63.3021
## 97.5% 261.6904 1218.499 101.1608
##
## Variances:
## [,1]
##          glucose  insulin      sspg
## 2.5%  36.68223 1241.731 1515.547
## 97.5% 81.05742 3284.257 4250.538
## [,2]
##          glucose  insulin      sspg
## 2.5%   86.49502 3463.088 12227.24
## 97.5% 357.64427 32098.298 38406.29

```

```
## [,3]
##      glucose  insulin  sspg
## 2.5% 3354.110 48397.29 1298.067
## 97.5% 7414.512 122881.85 3211.125
```

```
par(mfrow=c(4,3))
plot(boot1, what = "pro")
plot(boot1, what = "mean")
```

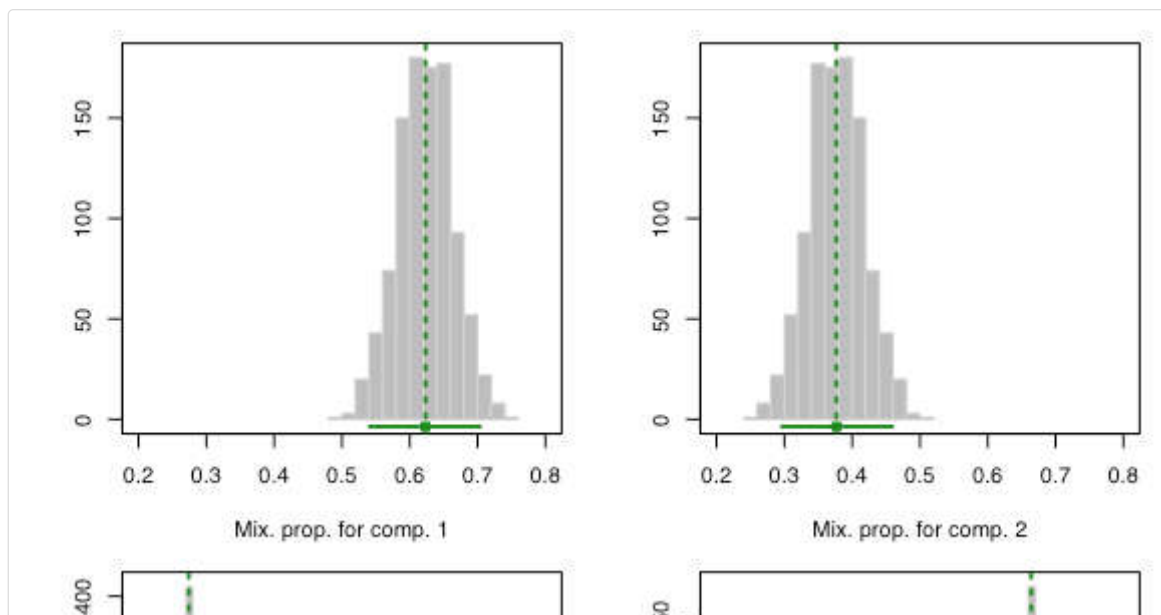


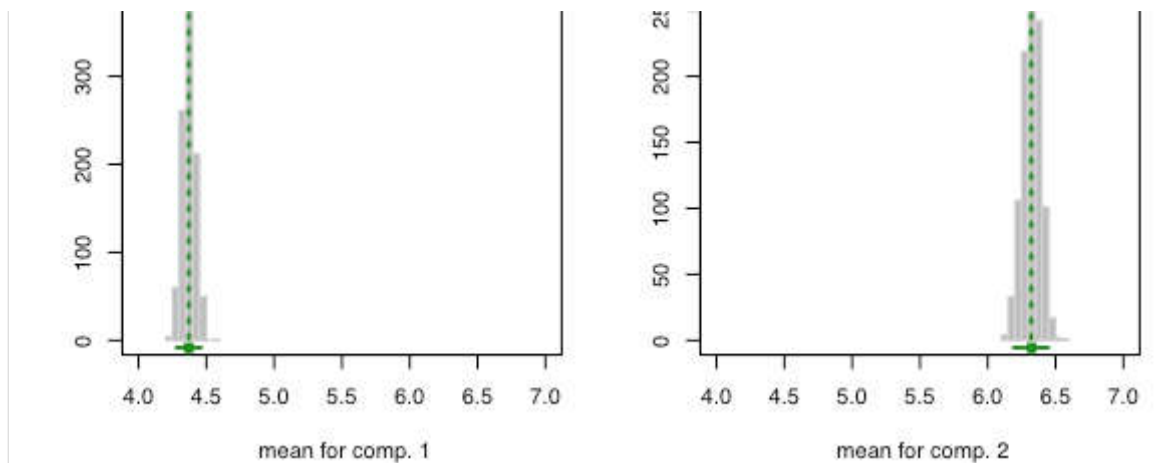
```
par(mfrow=c(1,1))
```

```
boot4 <- MclustBootstrap(mod4, nboot = 999, type = "bs")
summary(boot4, what = "se")
## -----
## Resampling standard errors
## -----
## Model = E
## Num. of mixture components = 2
## Replications = 999
## Type = nonparametric bootstrap
##
## Mixing probabilities:
##      1      2
```

```
## 0.04087099 0.04087099
##
## Means:
##      1      2
## 0.04630168 0.06691267
##
## Variances:
##      1      2
## 0.02440752 0.02440752
summary(boot4, what = "ci")
## -----
## Resampling confidence intervals
## -----
## Model = E
## Num. of mixture components = 2
## Replications = 999
## Type = nonparametric bootstrap
## Confidence level = 0.95
##
## Mixing probabilities:
##      1      2
## 2.5% 0.5407673 0.2963491
## 97.5% 0.7036509 0.4592327
##
## Means:
##      1      2
## 2.5% 4.279990 6.191580
## 97.5% 4.462024 6.446309
##
## Variances:
##      1      2
## 2.5% 0.1405255 0.1405255
## 97.5% 0.2373633 0.2373633

par(mfrow=c(2,2))
plot(boot4, what = "pro")
plot(boot4, what = "mean")
```



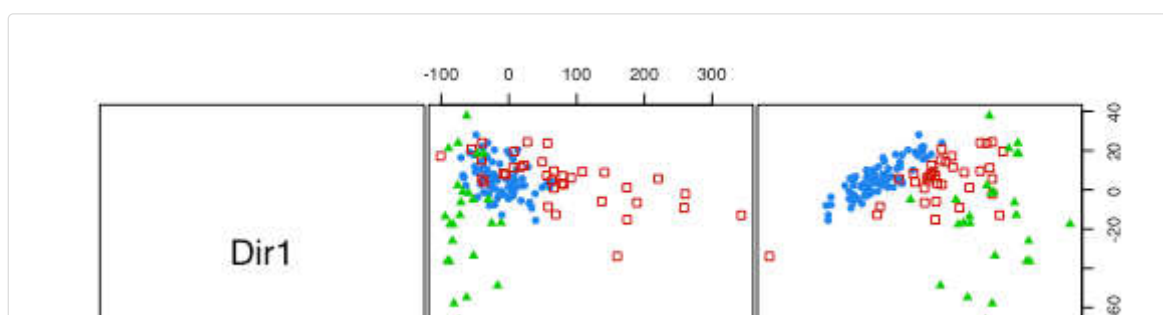


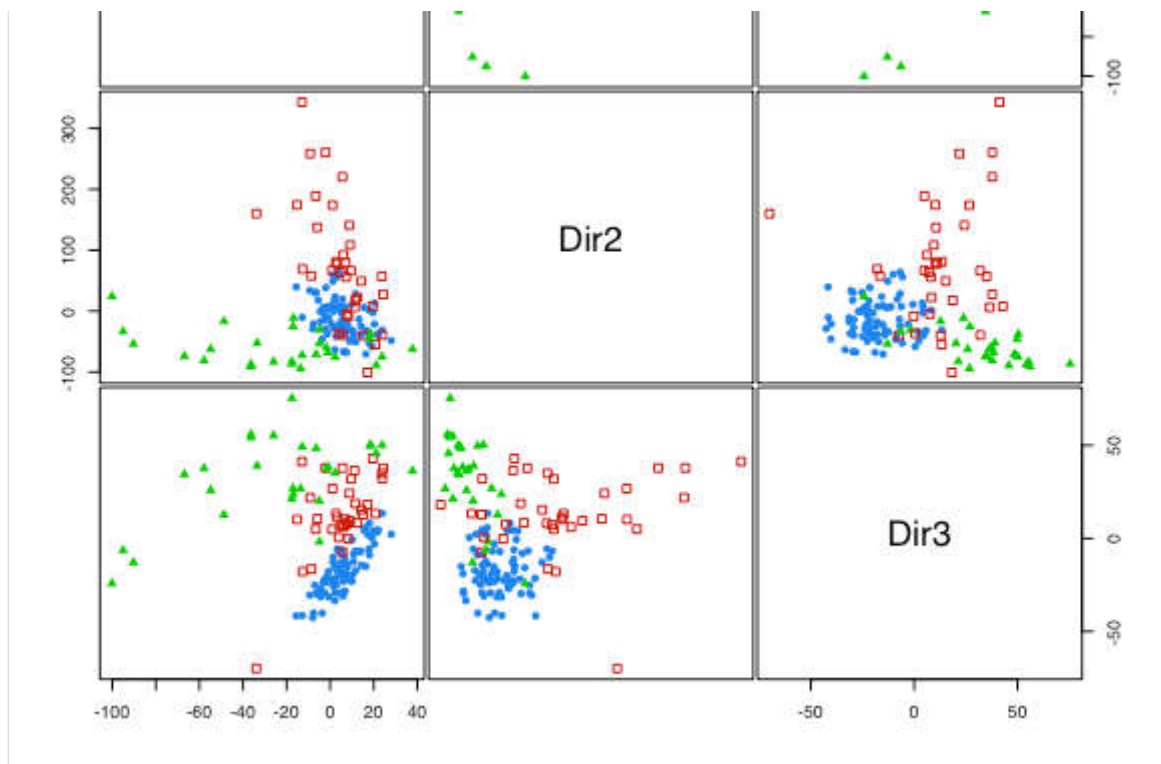
```
par(mfrow=c(1,1))
```

Dimension reduction

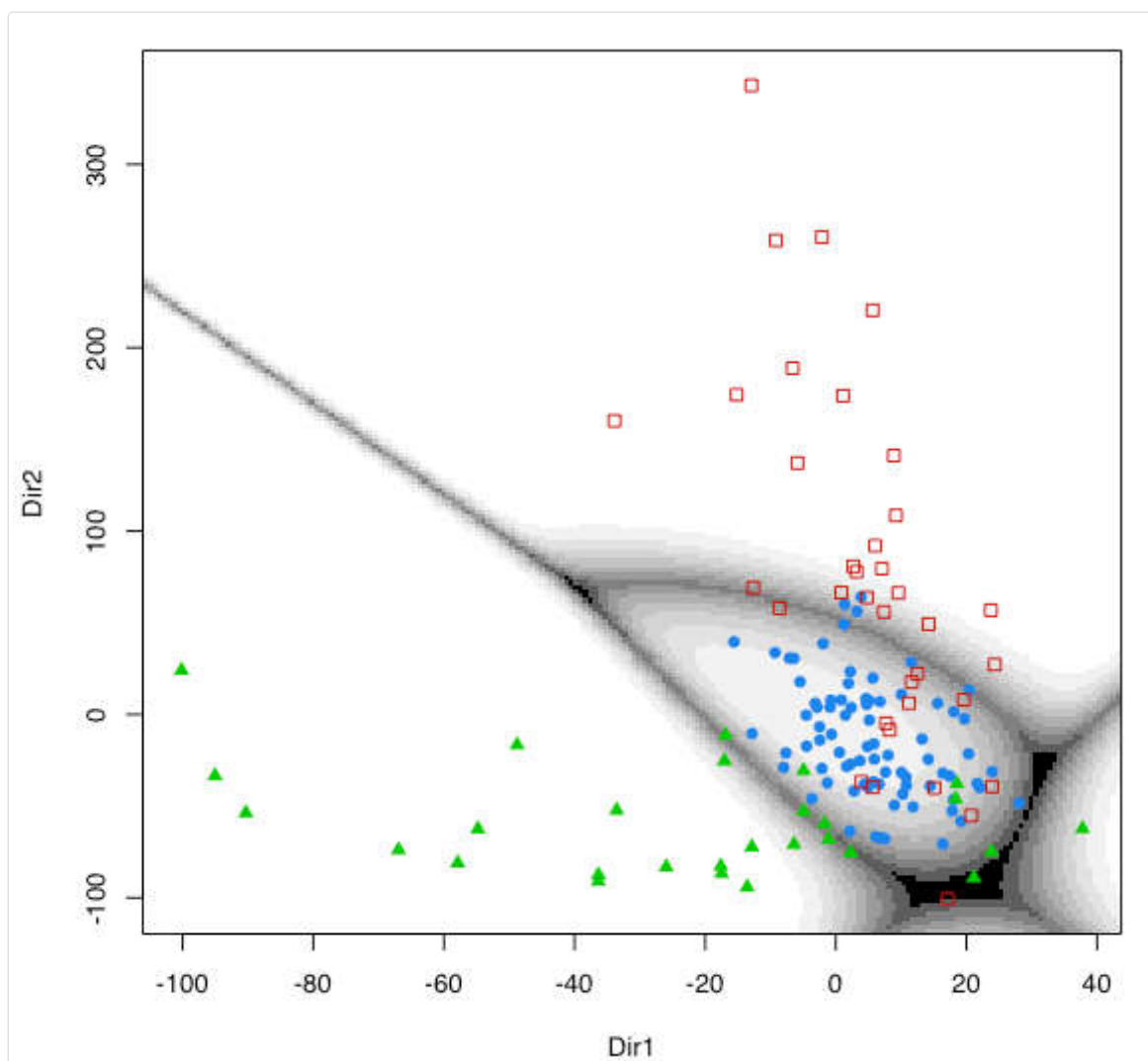
Clustering

```
mod1dr <- MclustDR(mod1)
summary(mod1dr)
## -----
## Dimension reduction for model-based clustering and classification
## -----
##
## Mixture model type: Mclust (VWV, 3)
##
## Clusters  n
##      1 81
##      2 36
##      3 28
##
## Estimated basis vectors:
##           Dir1    Dir2    Dir3
## glucose -0.988671  0.76532 -0.966565
## insulin  0.142656 -0.13395  0.252109
## sspg     -0.046689  0.62955  0.046837
##
##           Dir1    Dir2    Dir3
## Eigenvalues 1.3506  0.75608  0.53412
## Cum. %      51.1440 79.77436 100.00000
plot(mod1dr, what = "pairs")
```





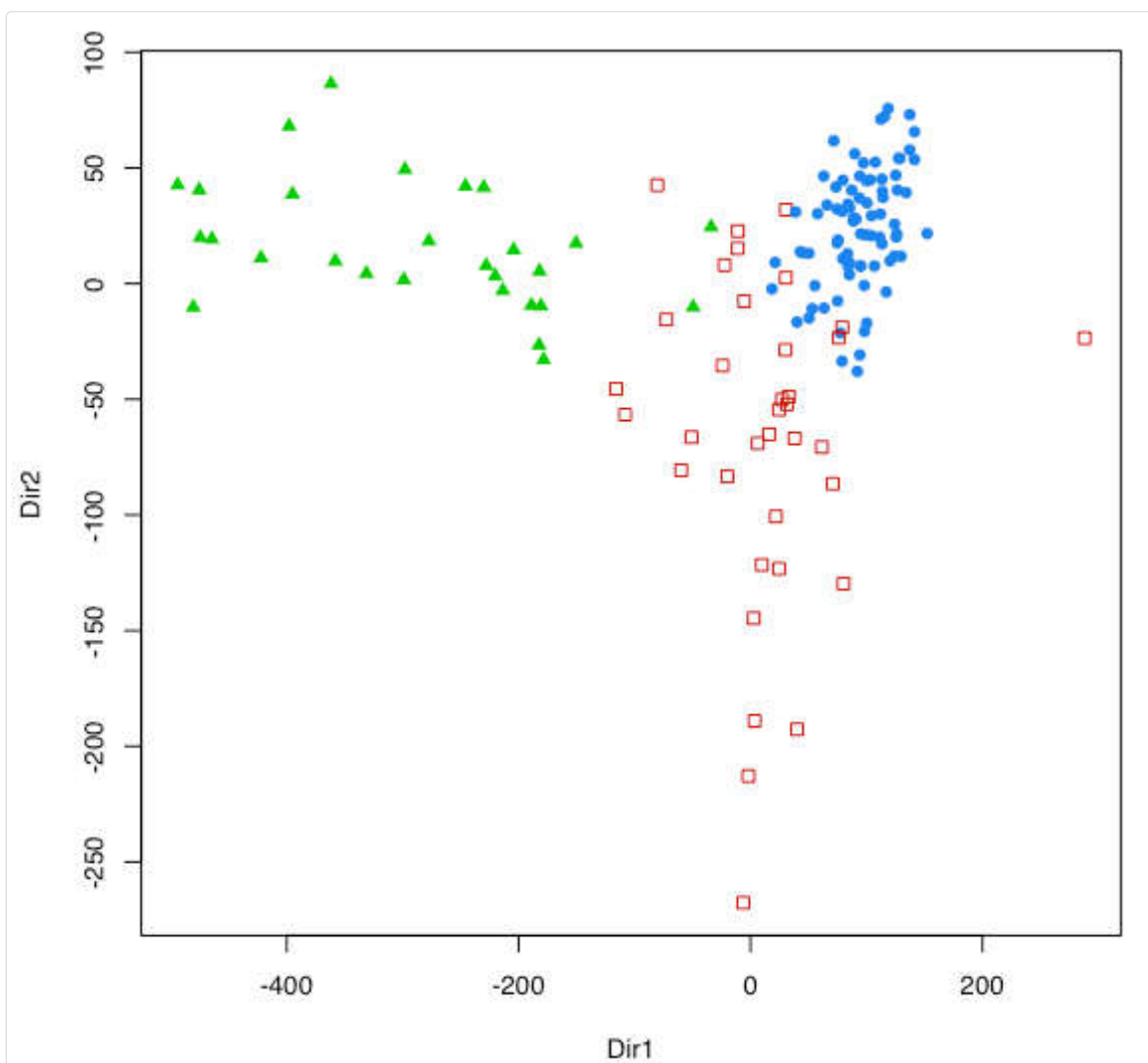
```
plot(mod1dr, what = "boundaries", ngrid = 200)
```



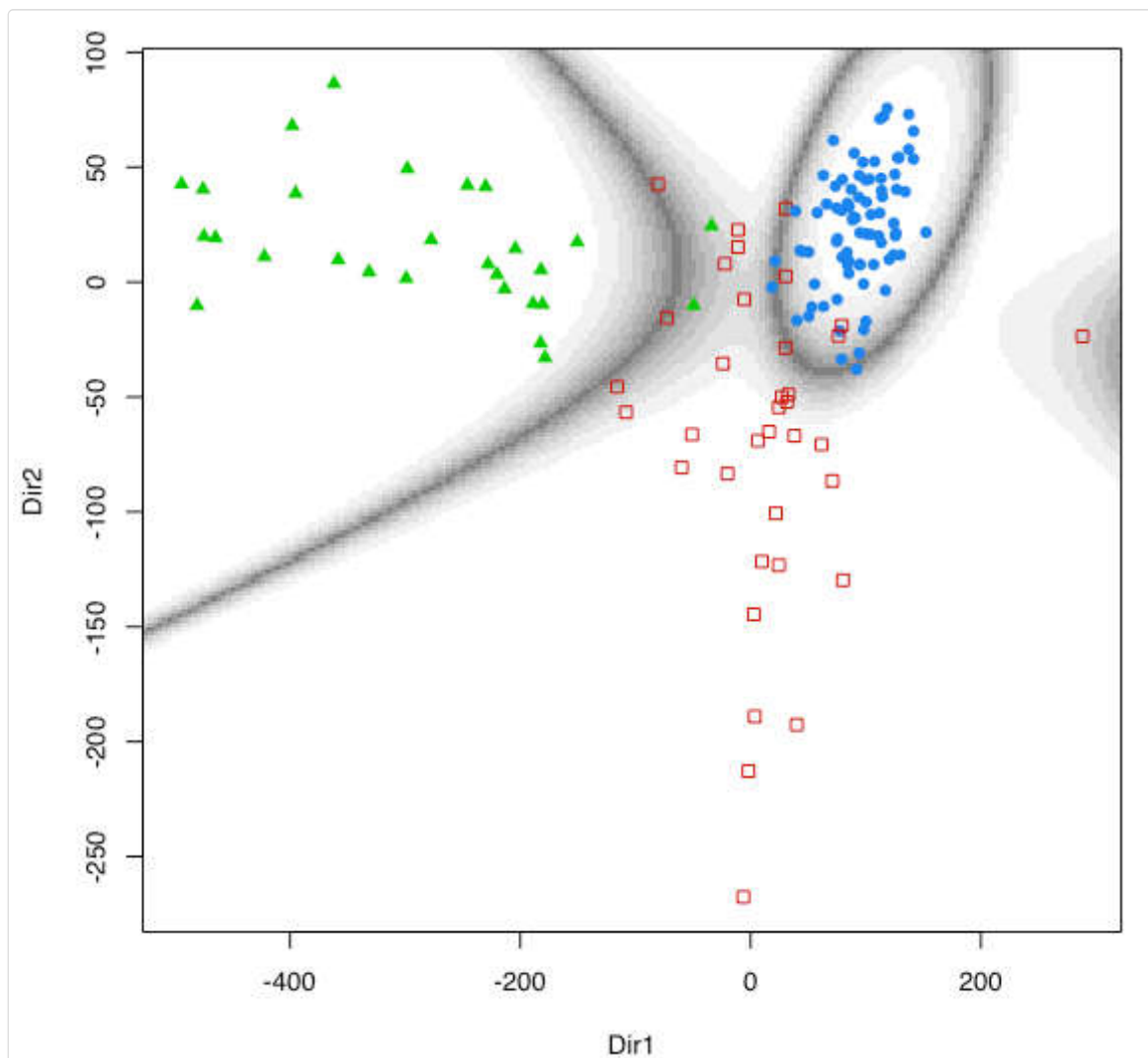

```

mod1dr <- MclustDR(mod1, lambda = 1)
summary(mod1dr)
## -----
## Dimension reduction for model-based clustering and classification
## -----
##
## Mixture model type: Mclust (VVV, 3)
##
## Clusters  n
##      1 81
##      2 36
##      3 28
##
## Estimated basis vectors:
##           Dir1    Dir2
## glucose  0.764699  0.86359
## insulin -0.643961 -0.22219
## sspg      0.023438 -0.45260
##
##           Dir1    Dir2
## Eigenvalues 1.2629  0.35218
## Cum. %      78.1939 100.00000
plot(mod1dr, what = "scatterplot")

```



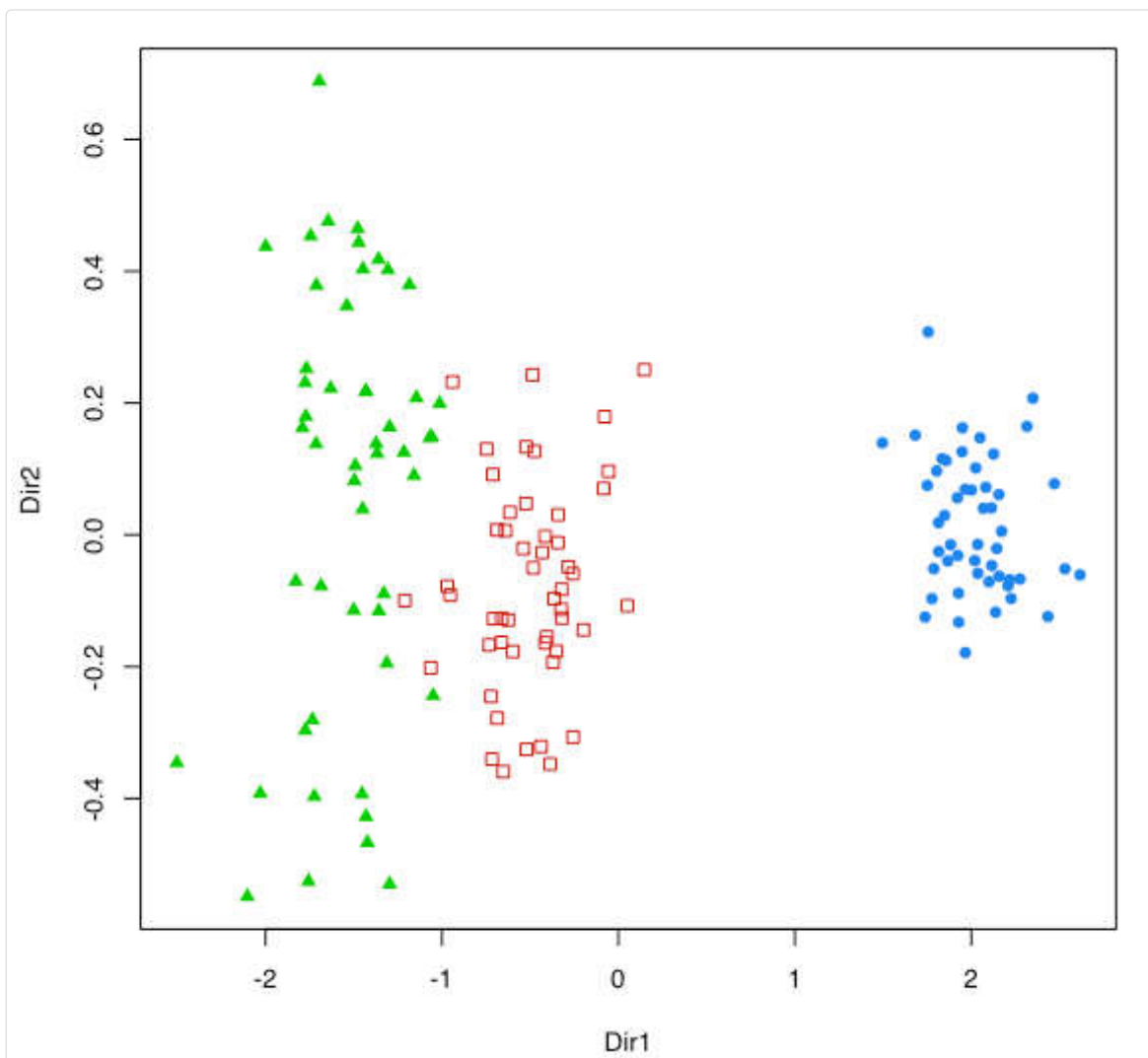
```
plot(mod1dr, what = "boundaries", ngrid = 200)
```



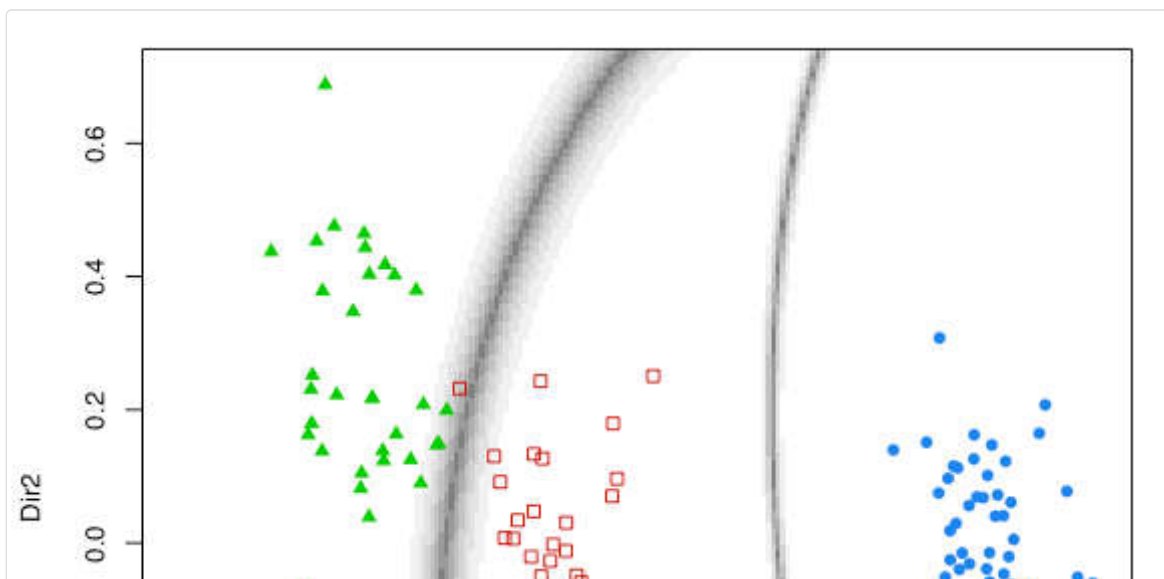
Classification

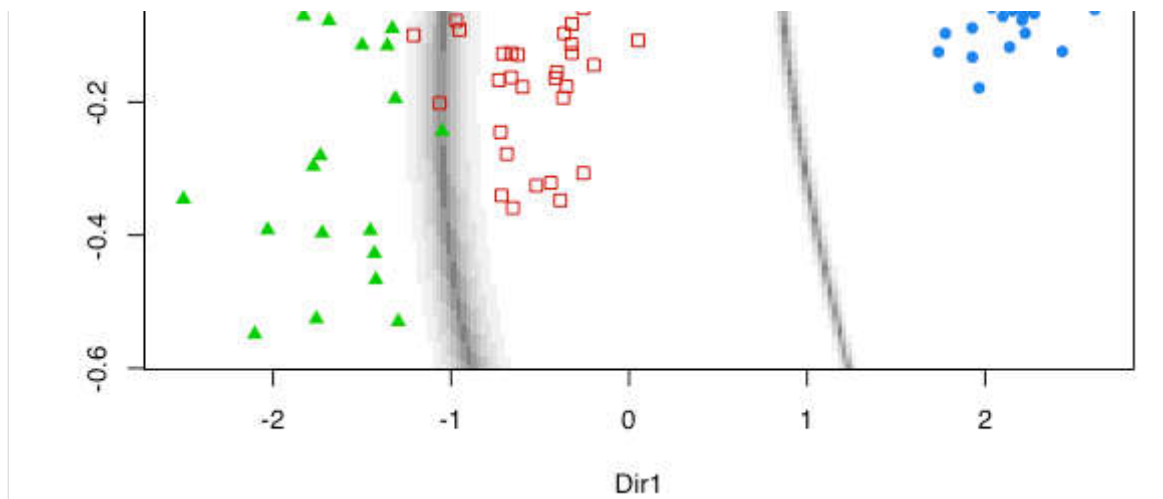
```
mod2dr <- MclustDR(mod2)
summary(mod2dr)
## -----
## Dimension reduction for model-based clustering and classification
## -----
##
## Mixture model type: EDDA
##
## Classes      n Model G
## setosa      50  VEV 1
## versicolor  50  VEV 1
## virginica   50  VEV 1
##
## Estimated basis vectors:
##           Dir1      Dir2      Dir3      Dir4
## Sepal.Length 0.17425 -0.193663 0.64081 -0.46231
## Sepal.Width  0.45292 0.066561 0.34852 0.57110
## Petal.Length -0.61629 -0.311030 -0.42366 0.46256
```

```
## Petal.Width  -0.62024  0.928076  0.53703 -0.49613
##
##              Dir1      Dir2      Dir3      Dir4
## Eigenvalues  0.94747  0.68835  0.076141  0.052607
## Cum. %       53.69408 92.70374 97.018700 100.000000
plot(mod2dr, what = "scatterplot")
```

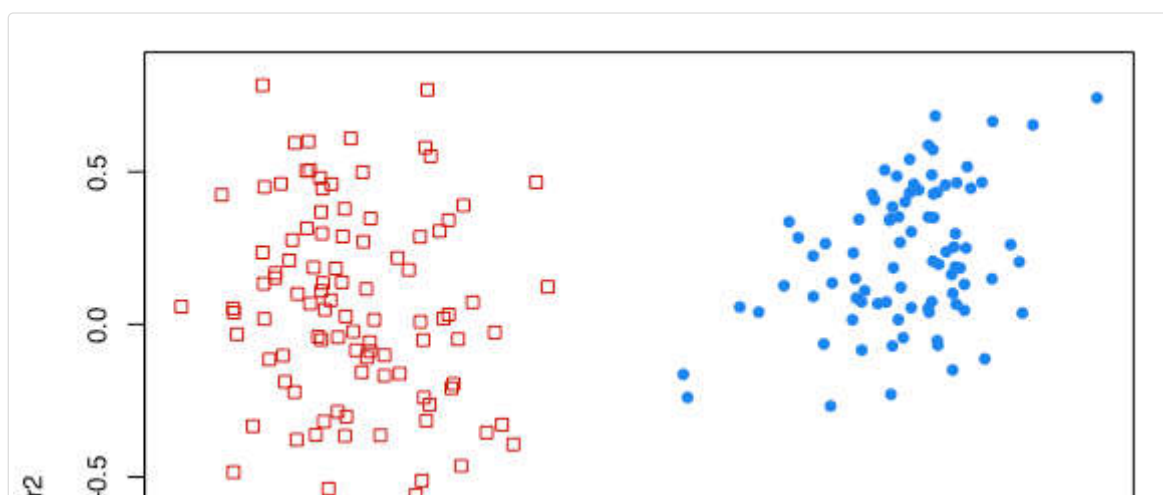


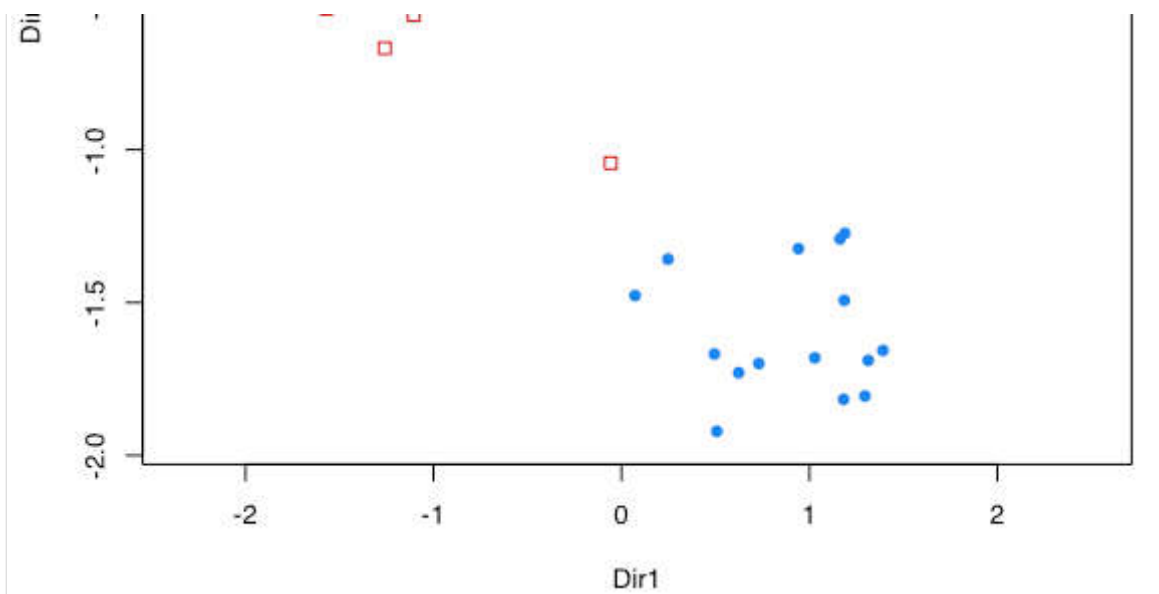
```
plot(mod2dr, what = "boundaries", ngrid = 200)
```



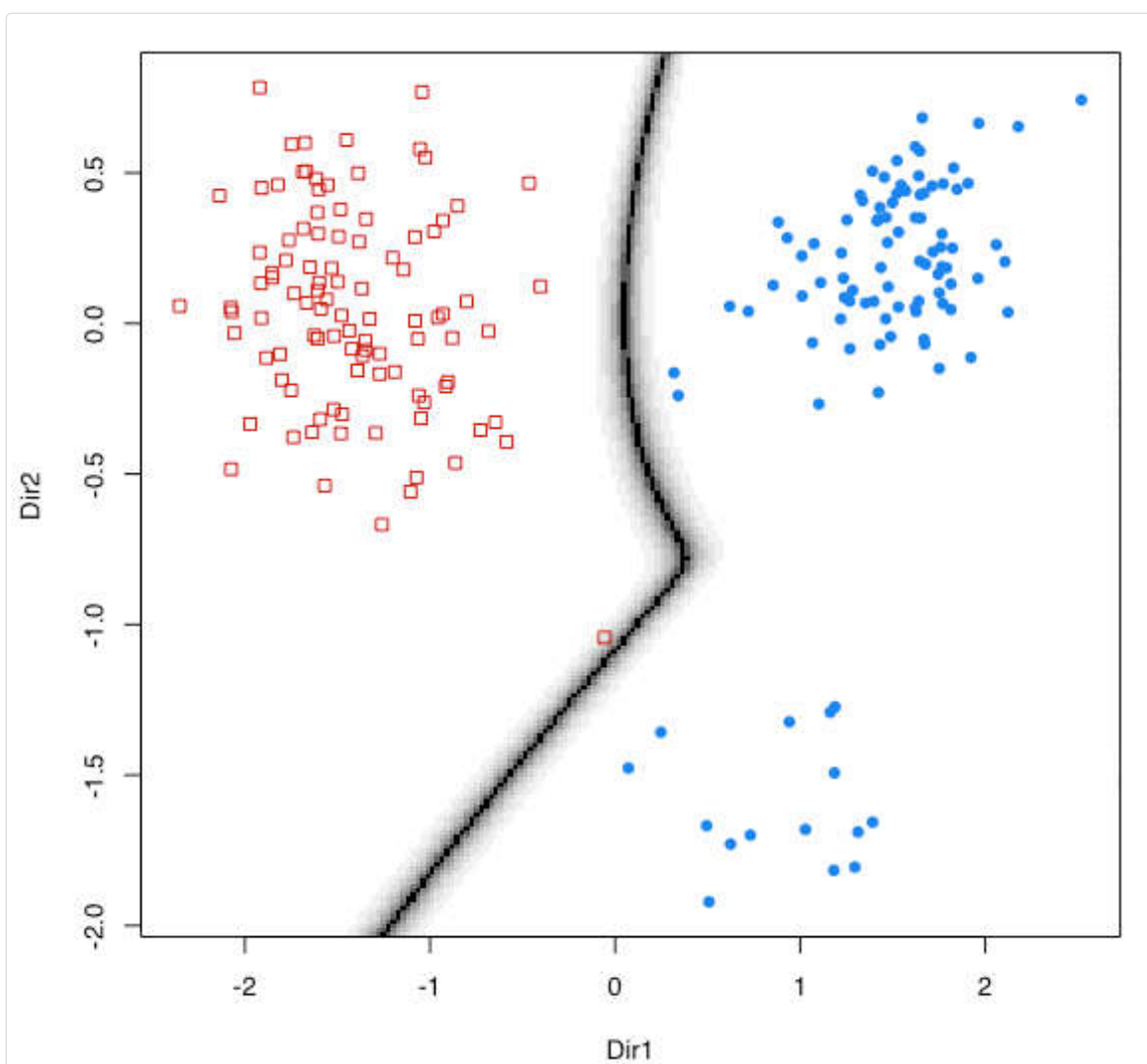


```
mod3dr <- MclustDR(mod3)
summary(mod3dr)
## -----
## Dimension reduction for model-based clustering and classification
## -----
##
## Mixture model type: MclustDA
##
## Classes          n Model G
## counterfeit 100   EVE 2
## genuine      100   XXX 1
##
## Estimated basis vectors:
##          Dir1    Dir2    Dir3    Dir4    Dir5    Dir6
## Length -0.10027 -0.327553 0.79718 -0.033721 -0.317043 0.084618
## Left   -0.21760 -0.305350 -0.30266 -0.893676 0.371043 -0.565611
## Right   0.29180 -0.018877 -0.49600 0.406605 -0.861020 0.481331
## Bottom  0.57603 0.445501 0.12002 -0.034570 0.004359 -0.078688
## Top     0.57555 0.385645 0.10093 -0.103629 0.136005 0.625416
## Diagonal -0.44088 0.672251 -0.04781 -0.151473 -0.044035 0.209542
##
##          Dir1    Dir2    Dir3    Dir4    Dir5    Dir6
## Eigenvalues 0.87241 0.55372 0.48603 0.13301 0.053113 0.027239
## Cum. %     41.04429 67.09530 89.96182 96.21965 98.718473 100.000000
plot(mod3dr, what = "scatterplot")
```





```
plot(mod3dr, what = "boundaries", ngrid = 200)
```



Using colorblind-friendly palettes

Most of the graphs produced by **mclust** use colors that by default are defined in the following options:

```
mclust.options("bicPlotColors")
```

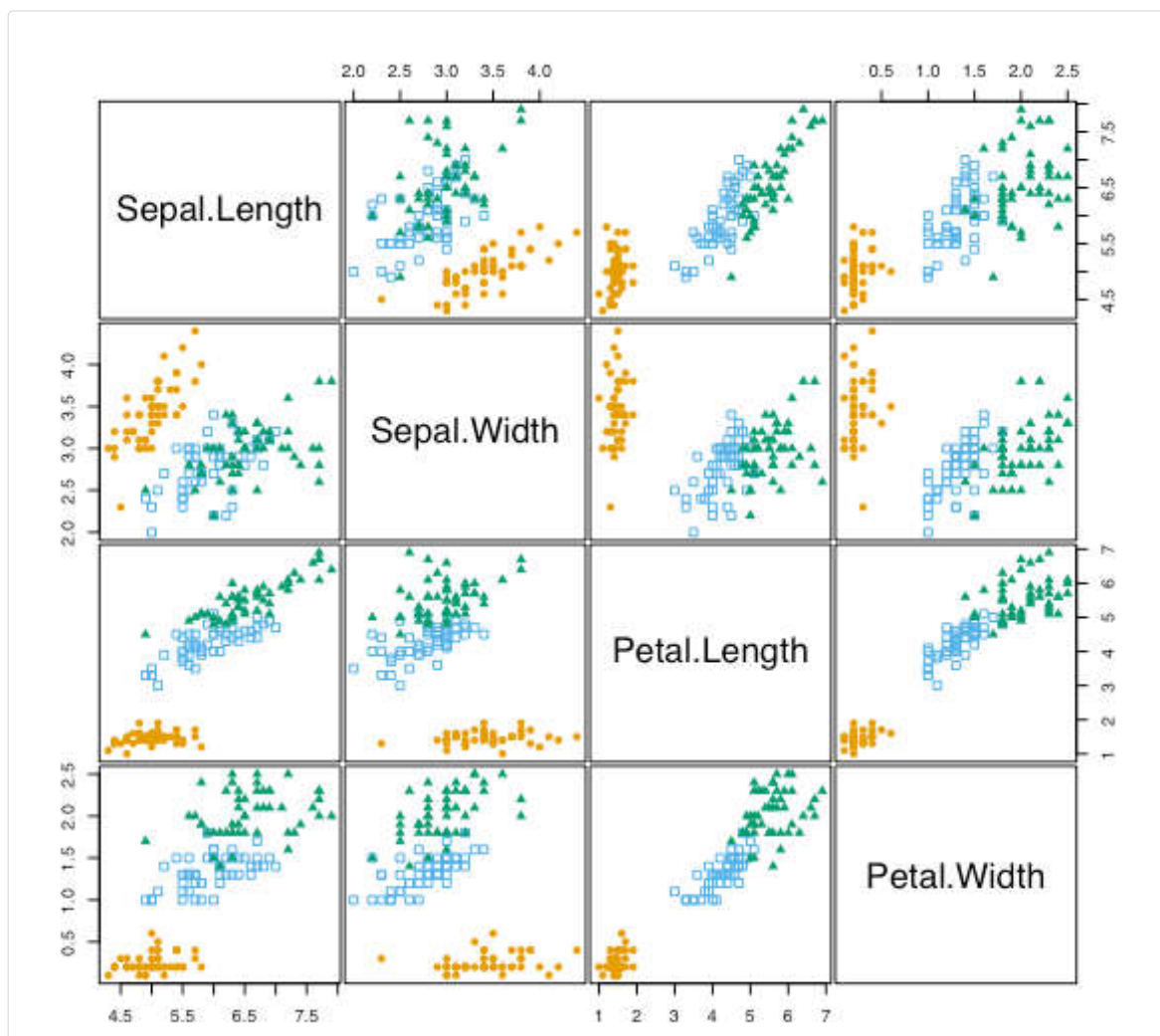
```
##      EII      VII      EEI      EVI      VEI      VVI      EEE
##    "gray"  "black" "#218B21" "#41884F" "#508476" "#58819C" "#597DC3"
##      EVE      VEE      VVE      EEV      VEV      EVV      VVV
##    "#5178EA" "#716EE7" "#9B60B8" "#B2508B" "#C03F60" "#C82A36" "#CC0000"
##      E      V
##    "gray"  "black"
mclust.options("classPlotColors")
## [1] "dodgerblue2"  "red3"          "green3"        "slateblue"
## [5] "darkorange"   "skyblue1"      "violetred4"    "forestgreen"
## [9] "steelblue4"   "slategrey"     "brown"         "black"
## [13] "darkseagreen" "darkgoldenrod3" "olivedrab"     "royalblue"
## [17] "tomato4"      "cyan2"         "springgreen2"
```

The first option controls colors used for plotting BIC, ICL, etc. curves, whereas the second option is used to assign colors for indicating clusters or classes when plotting data.

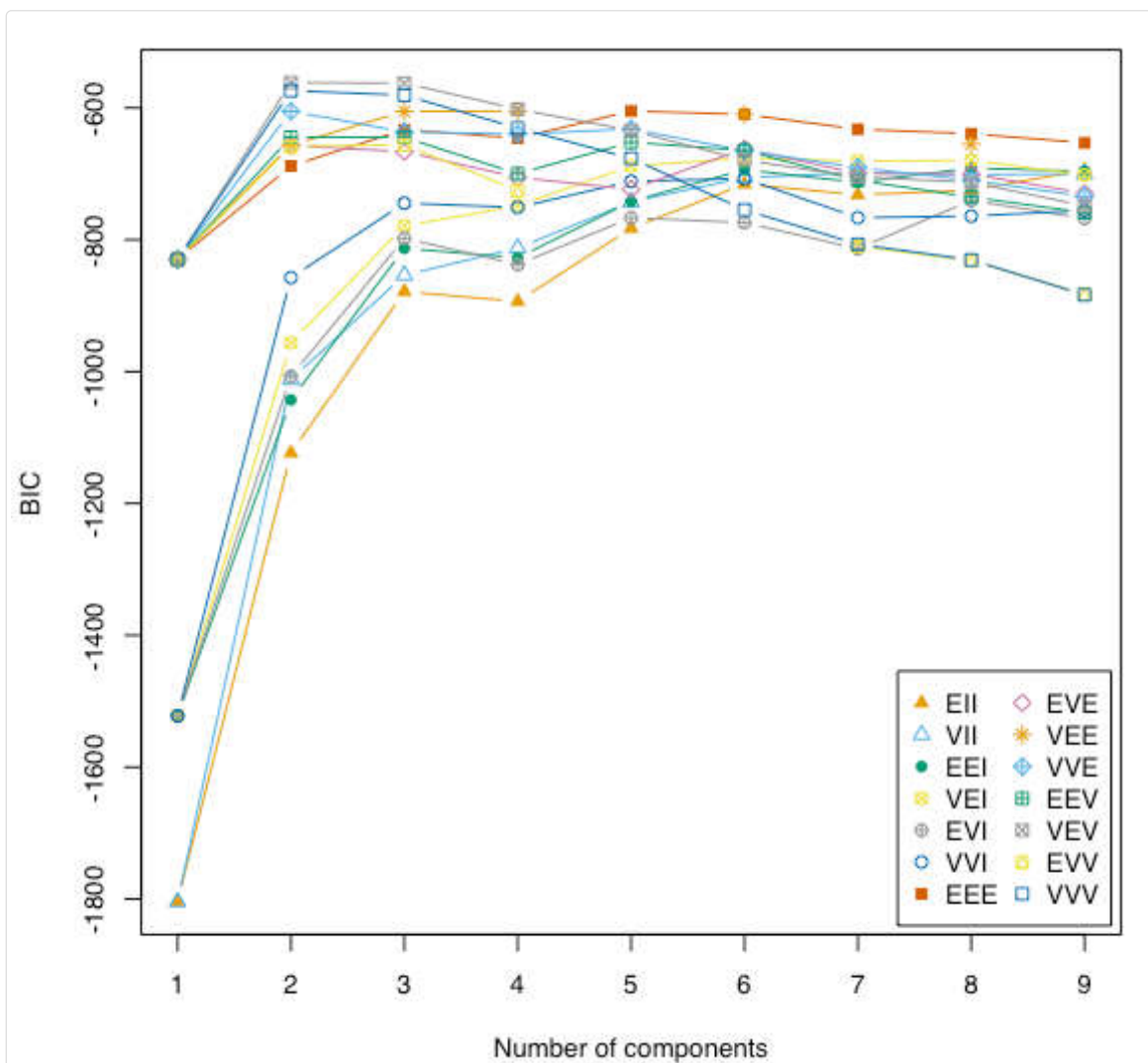
Color-blind-friendly palettes can be defined and assigned to the above options as follows:

```
cbPalette <- c("#E69F00", "#56B4E9", "#009E73", "#999999", "#F0E442", "#0072B2", "#D55E00",
               "#CC79A7")
bicPlotColors <- mclust.options("bicPlotColors")
bicPlotColors[1:14] <- c(cbPalette, cbPalette[1:6])
mclust.options("bicPlotColors" = bicPlotColors)
mclust.options("classPlotColors" = cbPalette)

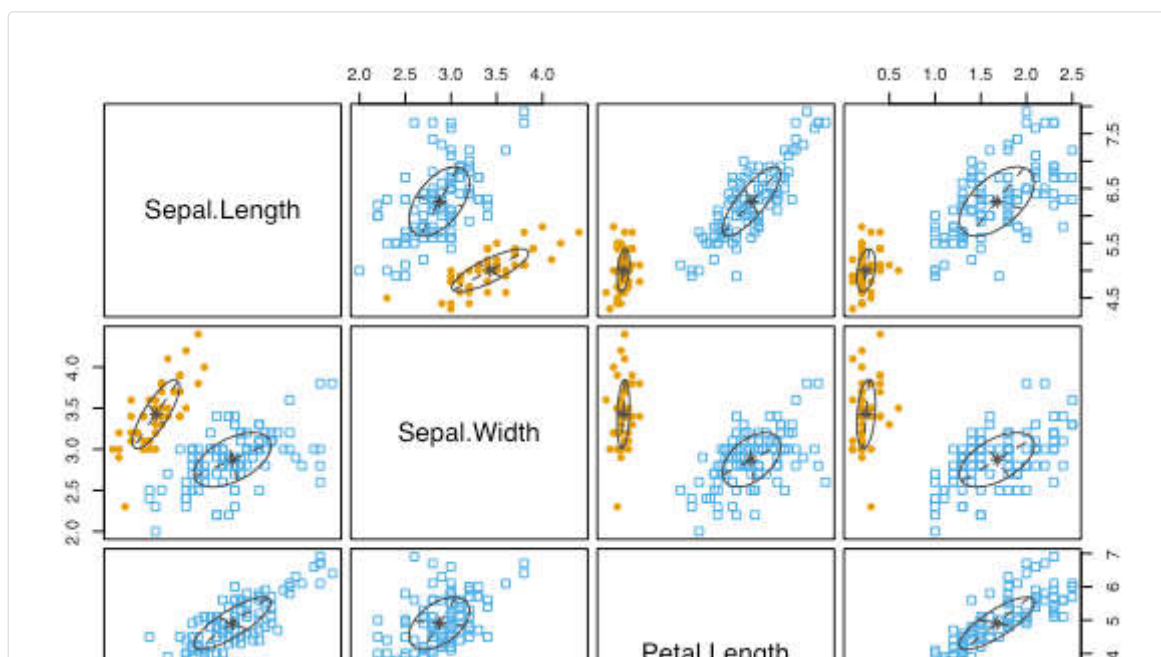
clPairs(iris[, -5], iris$Species)
```

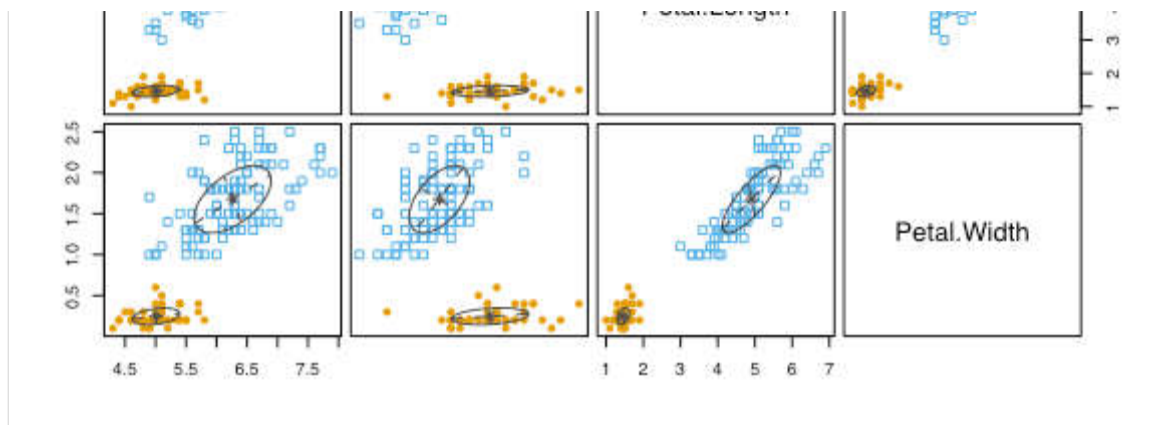


```
mod <- Mclust(iris[,-5])
plot(mod, what = "BIC")
```



```
plot(mod, what = "classification")
```





The above color definitions are adapted from [http://www.cookbook-r.com/Graphs/Colors_\(ggplot2\)/](http://www.cookbook-r.com/Graphs/Colors_(ggplot2)/), but users can easily define their own palettes if needed.

References

- Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 205-233. <https://journal.r-project.org/archive/2016/RJ-2016-021/RJ-2016-021.pdf>
- Fraley C. and Raftery A. E. (2002) Model-based clustering, discriminant analysis and density estimation, *Journal of the American Statistical Association*, 97/458, pp. 611-631.
- Fraley C., Raftery A. E., Murphy T. B. and Scrucca L. (2012) mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. *Technical Report No. 597*, Department of Statistics, University of Washington.