

# rebmix: Finite Mixture Modeling, Clustering & Classification

Marko Nagode, Branislav Panić, Jernej Klemenc & Simon Oman

March 17, 2023

## Abstract

The **rebmix** package provides R functions for random univariate and multivariate finite mixture model generation, estimation, clustering, latent class analysis and classification. Variables can be continuous, discrete, independent or dependent and may follow normal, lognormal, Weibull, gamma, binomial, Poisson, Dirac or von Mises parametric families.

## 1 Introduction

To cite the REBMIX algorithm please refer to (Nagode and Fajdiga, 2011a,b; Nagode, 2015, 2018; Panić et al., 2020a,b,c). For theoretical backgrounds please upload <http://doi.org/10.5963/JA00302001>.

## 2 What's new in version 2.14.2

Version 2.14.2 introduces several important improvements to the package. Estimation of mixture parameters can now be performed using the object of class "Histogram". Objects of class "Histogram" represent the data with bins and bin counts. The object "Histogram" is best suited for discrete datasets, such as digital images. The image resolution can be quite high, but there is a finite number of realizations of the image pixel intensity. Often the number of realizations is much smaller than the number of observations. Therefore, it is more useful to represent the original dataset as an ordered pair  $(\bar{y}_j, k_j)$ , where  $\bar{y}_j$  is the  $j$ th possible realization and  $k_j$  is its count. The continuous datasets can also be shrunk, but some bias may occur. When the number of observations is large, the bias is usually small and vice versa, and when time and memory efficiency is desired, shrinking the dataset is recommended. The original dataset (object of class `data.frame`) is transformed with the newly added methods "chistogram", "fhistogram" into a "Histogram". The method "fhistogram" is memory intensive, but very fast. It is best suited for one-dimensional datasets. Since it precomputes all possible realizations, even if some of them are not in the dataset, the argument `shrink= TRUE` should be added. The method "chistogram" is slower, but memory efficient. When a new realization  $y_j$  is found, it is appended. The two methods "chistogram" and "fhistogram" can be chained in a for loop so that multiple datasets can be shrunk into one "Histogram" object. This can be used when, for example, multiple images are to be loaded. Also, if for example a large dataset is to be processed, only parts of it can be loaded at a time to avoid large memory overhead.

The `mapclusters` method is added for maximum a posteriori estimation of cluster membership. This method was added to complement the `RCLRMIX` method. The `RCLRMIX` method performs clustering and cluster membership prediction as well as cluster merging using different estimators. For large datasets, this can be very time consuming. Using objects of class "histogram" speeds up the `RCLRMIX` method enormously, but the cluster membership is only determined of the realizations  $\bar{y}_j$  and the order is often not preserved either. Thus, we can use the `mapclusters` method to get the cluster membership on the original dataset of the object of the "data.frame" class.

Finally, all density estimation methods ("demix", "dfmix", "pemix", "pfmix") are modified to include estimation for objects of class "Histogram".

### 3 Previous versions

Version 2.14.0 introduces three parametric variant of the Gumbel parametric family

$$f(y) = \frac{1}{\sigma} \exp \left( \frac{y - \mu}{\xi \sigma} - \exp \left( \frac{y - \mu}{\xi \sigma} \right) \right), \quad (1)$$

where  $\xi \in \{-1, \text{NA}, 1\}$ . If initially  $\xi$  is set to NA, the package estimates  $\xi$ . Otherwise the estimated  $\xi$  equals initial  $\xi$ . The package was extended to handle three parameter parametric families. Class "EMMIX.Theta" and method **EMMIX** are added. They enable parameter estimation for all parametric families available in the package by using the EM algorithm only.

Version 2.13.1 introduces Gumbel probability density

$$f(y) = \frac{1}{\sigma} \exp \left( -\frac{y - \mu}{\sigma} - \exp \left( -\frac{y - \mu}{\sigma} \right) \right). \quad (2)$$

The Gumbel mixture models can now be estimated. In the mixture model the parameters  $\mu$  and  $\sigma$  are estimated for all components. The corresponding equations for the REBMIX and the EM algorithms have been derived. The EM algorithm has been implemented for all other parametric family types (normal, lognormal, Weibull, gamma, binomial, Poisson and von Mises parametric families), too. Therefore the EM algorithm can now be used with all parametric family types. Additionally, the histogram based EM algorithm has been added to speed up the calculations when the datasets contain large numbers of observations. Finally, the package has been debugged further and some core functions have been improved.

Version 2.12.0 introduces the Knuth algorithm (Knuth, 2019) as an effective way of optimal number of bins search. This affects the time efficiency of the REBMIX method considerably. The user can now enter different numbers of bins for different random variables. Two accompanied methods are added **optbins** and **bins**. The C++ code is optimized regarding memory allocation and efficiency. The R code is debugged and further improved regarding wrong user input messaging. Further debugging has been done. Outlier detection has been simplified. The REBMIX method now delivers some more components, but identifies also components with very low probability of occurrence, which is important regarding our future plans. The **plot** method is improved. The RCLRMIX method has been debugged and improved. The same holds for the REBMIX method.

Version 2.11.0 introduces the Expectation-Maximization (EM) algorithm for the improved estimation of Gaussian mixture model parameters (with diagonal and unrestriced covariance matrices). Here the REBMIX algorithm is used to assess the initial parameters of the EM algorithm. Two different variants of the EM algorithm are implemented, namely the original EM algorithm from (Dempster et al., 1977) and a  $k$ -means like variant of the EM algorithm (Classification EM) as described in (Celeux and Govaert, 1992). As the REBMIX algorithm estimates a wide range of parameters for the Gaussian mixture model for different numbers of components, three different strategies, named **exhaustive**, **best** and **single**, have been implemented. The **exhaustive** strategy is used to run the EM algorithm (or variant) on each solution of Gaussian mixture model parameters provided by the REBMIX algorithm. The **best** strategy utilizes a voting scheme for the estimated parameters from the REBMIX algorithm and runs the EM algorithm only on selected optimal parameters. The best candidates are chosen based on the value of the likelihood function (the highest one) for each number of components  $c$  from a minimum specified **cmin** to a maximum specified **cmax**. The **single** strategy is useful when the single value of, for example, the number of bins in histogram preprocessing is supplied as input for the REBMIX algorithm. Otherwise, when multiple numbers of bins  $k$  are supplied, this strategy is the same as the **exhaustive** strategy. To tackle the slow linear convergence of the EM algorithm, simple acceleration methods are implemented, which can be controlled with parameter **acceleration** and **acceleration.multiplier**. The increment of the EM algorithm in each iteration can be written as

$$\Delta \Theta = \Theta^{(i+1)} - \Theta^{(i)} \quad (3)$$

Instead of using a standard EM increment  $\Delta \Theta$  to reduce the number of iterations needed for the EM algorithm, this increment can be multiplied with some multiplier  $a_{\text{EM}}$ , which is referred to as

`acceleration.multiplier`. Therefore the update in each EM iteration now becomes

$$\Theta^{i+1} = \Theta^{(i)} + a_{\text{EM}} \Delta \Theta \quad (4)$$

The safe range for the  $a_{\text{EM}}$  multiplier lies between 1.0 and 2.0, where 1.0 gives a standard EM increment and 2.0 doubles the EM increment. However, this does not necessarily mean that multiplication by a value of 2.0 will double the speed of the EM algorithm (i.e. by reducing the required number of iterations by 2). Here, 1.5 is a safe value which mostly speeds up the EM algorithm whilst retaining good results for the estimated parameters. A value of 1.9 can significantly speed up the estimation process, yet it can also deteriorate the quality of the resulting estimated parameters. Therefore, the value of the multiplier needs to be set carefully. This value is set with `acceleration.multiplier` parameter. The other parameter `acceleration` controls how the  $a_{\text{EM}}$  multiplier is handled and can be one of **fixed**, **line** and **golden**. Selecting the **fixed** option means that the  $a_{\text{EM}}$  multiplier is specified via the `acceleration.multiplier` parameter and for each iteration of the EM algorithm the increment is increased by a specified value of  $a_{\text{EM}}$ . The **line** and **golden** options perform a, line and golden search (respectively) for the optimal value of  $a_{\text{EM}}$  for which the highest increase in the likelihood function of each EM iteration is achieved.

EM handling is carried out using the newly introduced class "EM.Control". Classes "REBMIX" and "REBMVNORM" and its signature method REBMIX now accept the "EM.Control" object via the argument called "EMcontrol". The class EM.Control has the same name convention for slots as the input argument EMcontrol (`strategy`, `variant`, `acceleration`, `tolerance`, `acceleration.multiplier` and `maximum.iterations`) as well as all accessor functions with the same name convention as `a.slot name` and setter function `a.slot name<-`.

Methods `Zp` and `coef` have been replaced by `a.Zp`, `a.theta1.all` and `a.theta2.all` getters. All slots can be accessed via accessors. Their names are generally composed of `a.` followed by the slot name and are used to read the slots. Class "RNGMIX.Theta" has been added to simplify random finite mixture model generation. Method `show` has been added for "RCLS.chunk" class. The minimum number of components `cmin` was added to REBMIX arguments and to the "REBMIX" class. The "Parzen window" preprocessing has been renamed to more commonly known "kernel density estimation". Rough parameter estimation for binomial and Poisson parametric families has also been improved and the package is now broadened to latent class analysis in version 2.10.3. Method `split` has been improved and examples for its proper use are added.

GCC 8.1 notes and warnings in C++ functions have been eliminated in version 2.10.2. Cholesky decomposition is now used to calculate the logarithm of the determinant and inverse of variance-covariance matrices instead of LU decomposition. Special attention has been paid to resolving numerical problems related to high dimensional datasets.

Version 2.10.1 is the further debugged version of 2.10.0. Large  $K$  in combination with large dimension  $d$  can lead to histograms with numerous nonempty bins  $v$ . In order to restrain  $v$ , the well known RootN rule (Velleman, 1976) may intuitively be extended to multidimensions

$$v_{\max} = \frac{1+d}{d} n^{\frac{d}{1+d}}. \quad (5)$$

If  $d = \infty$ , then  $v_{\max} = n$ . If  $d = 1$ , then  $v_{\max} = 2\sqrt{n}$ . Minor debugging and function improvements have also been carried out in version 2.10.0. The acceleration rate is now progressively increasing. Each time the inner loop starts, the counter  $I_2$  (see Nagode, 2015, for details) is initiated and constant

$$A = \frac{1 - a_r}{a_r(D_l w_l - D_{\min})} \Big|_{I_2=1} \quad (6)$$

is calculated. The acceleration rate  $a_r$  at  $I_2 = 1$  always equals the value stored in the input argument `ar`. Otherwise

$$a_r = \frac{1}{A(D_l w_l - D_{\min}) + 1} \Big|_{I_2 > 1}. \quad (7)$$

The Newton-Raphson root finding in C++ functions was improved in version 2.9.3. This affects only Weibull, gamma and von Mises parametric families. A circular von Mises parametric family has been

added and further debugging carried out in version 2.9.2. Version 2.9.1 is a further debugged version 2.8.4. The R code has been extended and rewritten in S4 class system. The background C code has also been extended and rewritten as object-oriented C++ code. The package can now more easily be extended to other parametric families. Multivariate normal mixtures with unrestricted variance-covariance matrices have been added. Clustering has also been added and classification improved.

## 4 Examples

To illustrate the use of the REBMIX algorithm, univariate and multivariate datasets are considered. The **rebmix** is loaded and the prompt before starting new page is set to **TRUE**.

```
R> library(rebmix)
R> devAskNewPage(ask = TRUE)
```

### 4.1 Gamma datasets

Three gamma mixtures are considered (Wiper et al., 2001). The first has four well-separated components with means 2, 4, 6 and 8, respectively

$$\begin{array}{lll} \theta_1 = 1/100 & \beta_1 = 200 & n_1 = 100 \\ \theta_2 = 1/100 & \beta_2 = 400 & n_2 = 100 \\ \theta_3 = 1/100 & \beta_3 = 600 & n_3 = 100 \\ \theta_4 = 1/100 & \beta_4 = 800 & n_4 = 100. \end{array}$$

The second has equal means but different variances and weights

$$\begin{array}{lll} \theta_1 = 1/27 & \beta_1 = 9 & n_1 = 40 \\ \theta_2 = 1/270 & \beta_2 = 90 & n_2 = 360. \end{array}$$

The third is a mixture of a rather diffuse component with mean 6 and two lower weighted components with smaller variances and means of 2 and 10, respectively

$$\begin{array}{lll} \theta_1 = 1/20 & \beta_1 = 40 & n_1 = 80 \\ \theta_2 = 1 & \beta_2 = 6 & n_2 = 240 \\ \theta_3 = 1/20 & \beta_3 = 200 & n_3 = 80. \end{array}$$

#### 4.1.1 Finite mixture generation

```
R> n <- c(100, 100, 100, 100)
R> Theta <- new("RNGMIX.Theta", c = 4, pdf = "gamma")
R> a.theta1(Theta) <- rep(1/100, 4)
R> a.theta2(Theta) <- c(200, 400, 600, 800)
R> gamma1 <- RNGMIX(Dataset.name = "gamma1", n = n, Theta = a.Theta(Theta))
R> n <- c(40, 360)
R> Theta <- new("RNGMIX.Theta", c = 2, pdf = "gamma")
R> a.theta1(Theta) <- c(1/27, 1/270)
R> a.theta2(Theta) <- c(9, 90)
R> gamma2 <- RNGMIX(Dataset.name = "gamma2", n = n, Theta = a.Theta(Theta))
R> n <- c(80, 240, 80)
R> Theta <- new("RNGMIX.Theta", c = 3, pdf = "gamma")
R> a.theta1(Theta) <- c(1/20, 1, 1/20)
R> a.theta2(Theta) <- c(40, 6, 200)
R> gamma3 <- RNGMIX(Dataset.name = "gamma3", rseed = -4, n = n,
+   Theta = a.Theta(Theta))
```

#### 4.1.2 Finite mixture estimation

```
R> gamma1est <- REBMIX(Dataset = a.Dataset(gamma1), Preprocessing = "kernel density estimation",
+   cmax = 8, Criterion = "BIC", pdf = "gamma")
R> gamma2est <- REBMIX(Dataset = a.Dataset(gamma2), Preprocessing = "histogram",
+   cmax = 8, Criterion = "BIC", pdf = "gamma")
R> gamma3est <- REBMIX(Dataset = a.Dataset(gamma3), Preprocessing = "histogram",
+   cmax = 8, Criterion = "BIC", pdf = "gamma", K = 23:27)
```

#### 4.1.3 Plot method

```
R> plot(gamma3est, pos = 1, what = c("pdf", "marginal cdf"), ncol = 2,
+   npts = 1000)
```

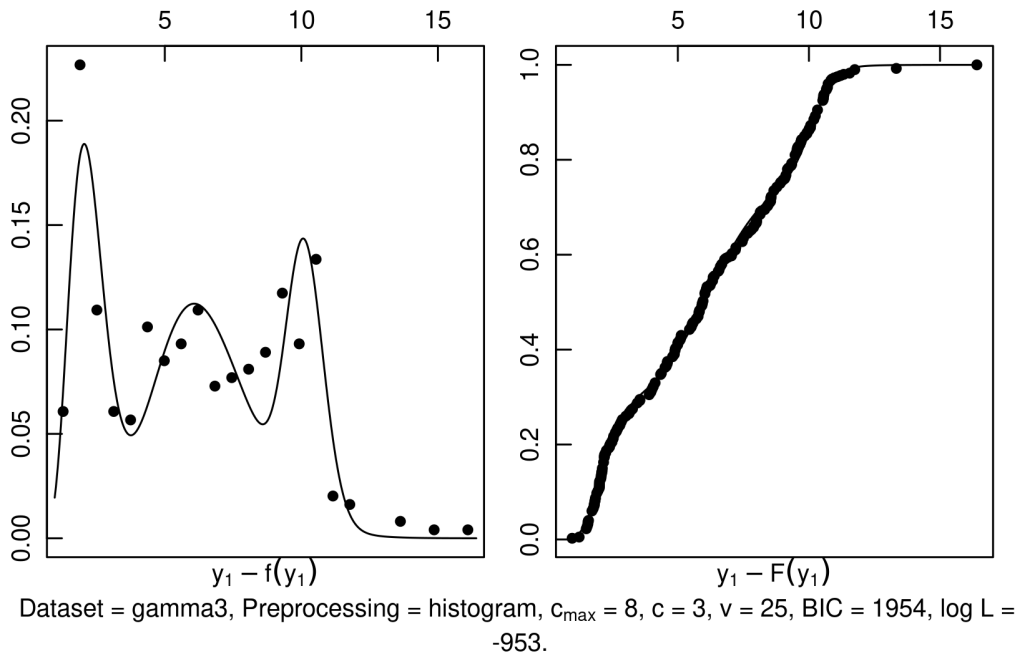


Figure 1: Gamma 3 dataset. Empirical density (circles) and predictive gamma mixture density in black solid line.

#### 4.1.4 Summary, a.theta1.all and a.theta2.all methods

```
R> summary(gamma2est)
```

```
Dataset Preprocessing Criterion c v/k IC logL M
1 gamma2 histogram BIC 2 27 -1346 688 5
Maximum logL = 688 at pos = 1.
```

```
R> a.theta1.all(gamma1est, pos = 1)
```

```
      [,1]
theta1.1 0.01021
theta1.2 0.00758
theta1.3 0.00927
theta1.4 0.01110
```

```
R> a.theta2.all(gamma1est, pos = 1)
```

```

      [,1]
theta2.1 196
theta2.2 1056
theta2.3 434
theta2.4 539

```

#### 4.1.5 Bootstrap methods

```

R> gamma3boot <- boot(x = gamma3est, pos = 1, Bootstrap = "p", B = 10)
R> gamma3boot

```

An object of class "REBMIX.boot"

Slot "c":

```
[1] 4 3 3 3 3 3 3 4 3
```

Slot "c.se":

```
[1] 0.422
```

Slot "c.cv":

```
[1] 0.132
```

Slot "c.mode":

```
[1] 3
```

Slot "c.prob":

```
[1] 0.8
```

```

R> summary(gamma3boot)

```

w.cv

```
[1] 0.142 0.105 0.239
```

```
      [,1]
```

```
theta1.1.cv 0.479
```

```
theta1.2.cv 1.018
```

```
theta1.3.cv 0.494
```

```
      [,1]
```

```
theta2.1.cv 0.464
```

```
theta2.2.cv 0.599
```

```
theta2.3.cv 1.318
```

```
      [,1]
```

```
theta3.1.cv NA
```

```
theta3.2.cv NA
```

```
theta3.3.cv NA
```

Mode probability = 0.8 at c = 3 components.

#### 4.1.6 Estimation of the mixture parameters using the Best REBMIX&EM strategy

```

R> EM <- new("EM.Control", strategy = "best", variant = "EM", acceleration = "fixed",
+           acceleration.multiplier = 1, tolerance = 1e-04, maximum.iterations = 1000,
+           K = 0)

```

```

R> gamma1est.em <- REBMIX(Dataset = a.Dataset(gamma1), Preprocessing = "kernel density estimation",
+                         cmax = 8, Criterion = "BIC", pdf = "gamma", EMcontrol = EM)

```

```

R> gamma2est.em <- REBMIX(Dataset = a.Dataset(gamma2), Preprocessing = "histogram",
+                         cmax = 8, Criterion = "BIC", pdf = "gamma", EMcontrol = EM)

```

```

R> gamma3est.em <- REBMIX(Dataset = a.Dataset(gamma3), Preprocessing = "histogram",
+                         cmax = 8, Criterion = "BIC", pdf = "gamma", K = 23:27, EMcontrol = EM)

```

```

R> summary(gamma1est.em)

```

	Dataset	Preprocessing	Criterion	c	v/k	IC	logL	M
1	gamma1	kernel density estimation	BIC	4	35	1054	-494	11

Maximum logL = -494 at pos = 1.

```
R> summary(gamma2est.em)
```

```
Dataset Preprocessing Criterion c v/k    IC logL M
1 gamma2      histogram      BIC 2  27 -1354  692 5
Maximum logL = 692 at pos = 1.
```

```
R> summary(gamma3est.em)
```

```
Dataset Preprocessing Criterion c v/k    IC logL M
1 gamma3      histogram      BIC 3  25 1926 -939 8
Maximum logL = -939 at pos = 1.
```

## 4.2 Poisson dataset

Dataset consists of  $n = 600$  two dimensional observations obtained by generating data points separately from each of three Poisson distributions. The component dataset sizes and parameters, which are those studied in Ma et al. (2009), are displayed below

$$\begin{aligned}\theta_1 &= (3, 2)^\top & n_1 &= 200 \\ \theta_2 &= (9, 10)^\top & n_2 &= 200 \\ \theta_3 &= (15, 16)^\top & n_3 &= 200\end{aligned}$$

For the dataset Ma et al. (2009) conduct 100 experiments by selecting different initial values of the mixing proportions. In all the cases, the adaptive gradient BYY learning algorithm leads to the correct model selection, i.e., finally allocating the correct number of Poissons for the dataset. In the meantime, it also results in an estimate for each parameter in the original or true Poisson mixture which generated the dataset. As the dataset of Ma et al. (2009) can not exactly be reproduced, 10 datasets are generated with random seeds  $r_{\text{seed}}$  ranging from  $-1$  to  $-10$ .

### 4.2.1 Finite mixture generation

```
R> n <- c(200, 200, 200)
R> Theta <- new("RNGMIX.Theta", c = 3, pdf = rep("Poisson", 2))
R> a.theta1(Theta, 1) <- c(3, 2)
R> a.theta1(Theta, 2) <- c(9, 10)
R> a.theta1(Theta, 3) <- c(15, 16)
R> poisson <- RNGMIX(Dataset.name = paste("Poisson_", 1:10, sep = ""),
+   n = n, Theta = a.Theta(Theta))
```

### 4.2.2 Finite mixture estimation

```
R> poissonest <- REBMIX(Dataset = a.Dataset(poisson), Preprocessing = "histogram",
+   cmax = 10, Criterion = "MDL5", pdf = rep("Poisson", 2), K = 1)
```

### 4.2.3 Plot method

### 4.2.4 Clustering

### 4.2.5 Summary, a.theta1.all and a.theta2.all methods

```
R> summary(poissonest)
```

	Dataset	Preprocessing	Criterion	c	v/k	IC	logL	M
1	Poisson_1	histogram	MDL5	3	1	7062	-3403	8
2	Poisson_2	histogram	MDL5	3	1	7116	-3430	8
3	Poisson_3	histogram	MDL5	3	1	7068	-3406	8
4	Poisson_4	histogram	MDL5	3	1	6992	-3368	8
5	Poisson_5	histogram	MDL5	3	1	6993	-3368	8
6	Poisson_6	histogram	MDL5	3	1	7052	-3398	8
7	Poisson_7	histogram	MDL5	2	1	7304	-3572	5
8	Poisson_8	histogram	MDL5	3	1	7123	-3434	8
9	Poisson_9	histogram	MDL5	3	1	7091	-3418	8
10	Poisson_10	histogram	MDL5	3	1	7042	-3393	8

Maximum logL = -3368 at pos = 4.

```
R> a.theta1.all(poissonest, pos = 1)
```

```
      [,1] [,2]
theta1.1 3.55 2.59
theta1.2 14.35 15.06
theta1.3 7.89 10.09
```

```
R> a.theta2.all(poissonest, pos = 1)
```

```
      [,1] [,2]
theta2.1 NA NA
theta2.2 NA NA
theta2.3 NA NA
```

#### 4.2.6 Estimation of the mixture parameters using the Exhaustive REBMIX&EM strategy

```
R> EM <- new("EM.Control", strategy = "exhaustive", variant = "EM",
+   acceleration = "fixed", acceleration.multiplier = 1, tolerance = 1e-04,
+   maximum.iterations = 1000, K = 0)
R> poissonest.em <- REBMIX(Dataset = a.Dataset(poisson), Preprocessing = "histogram",
+   cmax = 10, Criterion = "MDL5", pdf = rep("Poisson", 2), K = 1,
+   EMcontrol = EM)
R> summary(poissonest.em)
```

	Dataset	Preprocessing	Criterion	c	v/k	IC	logL	M
1	Poisson_1	histogram	MDL5	3	1	6987	-3365	8
2	Poisson_2	histogram	MDL5	3	1	7039	-3392	8
3	Poisson_3	histogram	MDL5	3	1	6992	-3368	8
4	Poisson_4	histogram	MDL5	3	1	6974	-3359	8
5	Poisson_5	histogram	MDL5	3	1	6989	-3367	8
6	Poisson_6	histogram	MDL5	3	1	7034	-3389	8
7	Poisson_7	histogram	MDL5	2	1	7239	-3539	5
8	Poisson_8	histogram	MDL5	3	1	7031	-3387	8
9	Poisson_9	histogram	MDL5	3	1	7006	-3375	8
10	Poisson_10	histogram	MDL5	3	1	6994	-3369	8

Maximum logL = -3359 at pos = 4.

### 4.3 Multivariate normal dataset

The `mvnorm` dataset from (Panić et al., 2020c) consists of 250 observations drawn from the 5-component normal mixture.

### 4.3.1 Finite mixture generation

```
R> n <- c(50, 50, 50, 50, 50)
R> Theta <- new("RNGMVNORM.Theta", c = 5, d = 2)
R> a.theta1(Theta, 1) <- c(2.7, 3.7)
R> a.theta1(Theta, 2) <- c(5.7, 9.1)
R> a.theta1(Theta, 3) <- c(2, 9)
R> a.theta1(Theta, 4) <- c(9.5, 6.6)
R> a.theta1(Theta, 5) <- c(6.3, 0.6)
R> a.theta2(Theta, 1) <- c(0.9, -0.1, -0.1, 0.4)
R> a.theta2(Theta, 2) <- c(2.8, -1.3, -1.3, 1.5)
R> a.theta2(Theta, 3) <- c(0.1, 0, 0, 0.3)
R> a.theta2(Theta, 4) <- c(1.3, -0.4, -0.4, 0.4)
R> a.theta2(Theta, 5) <- c(0.5, 0.3, 0.3, 2.5)
R> mvnrm.simulated <- RNGMIX(model = "RNGMVNORM", Dataset.name = "mvnrmdataset",
+   rseed = -1, n = n, Theta = a.Theta(Theta))
```

### 4.3.2 Finite mixture estimation

```
R> mvnrmest <- REBMIX(model = "REBMVNORM", Dataset = a.Dataset(mvnrm.simulated),
+   Preprocessing = "histogram", cmax = 20, Criterion = "BIC")
```

### 4.3.3 Plot method

### 4.3.4 Clustering

### 4.3.5 Summary method of estimation

```
R> summary(mvnrmest)
```

```
      Dataset Preprocessing Criterion c v/k   IC  logL  M
1 mvnrmdataset    histogram      BIC 5  10 2168 -1004 29
Maximum logL = -1004 at pos = 1.
```

### 4.3.6 Summary method of clustering

```
R> summary(mvnrmclu)
```

Number of clusters	1	2	3	4
From cluster	3	5	2	4
To cluster	1	3	1	2
Entropy	5.55e-15	3.55e-02	6.13e+00	1.26e+01
Entropy decrease	0.0355	6.0899	6.4933	7.6007

### 4.3.7 Estimation of the mixture parameters using the Single REBMIX&EM strategy

The strategy requires the preprocessing parameter K to be known. It can be estimated using the `optbins` method. To estimate the optimal parameter K, different rules are implemented. More information can be found in (Panić et al., 2020c).

```
R> EM <- new("EM.Control", strategy = "single", variant = "EM",
+   acceleration = "fixed", acceleration.multiplier = 1, tolerance = 1e-04,
+   maximum.iterations = 1000, K = 0)
R> K <- optbins(Dataset = a.Dataset(mvnrm.simulated), Rule = "Knuth equal",
+   kmin = 2, kmax = 100)
```

```
R> mvnormest.em <- REBMIX(model = "REBMVNORM", Dataset = a.Dataset(mvnorm.simulated),
+   Preprocessing = "histogram", cmax = 20, K = K, Criterion = "BIC",
+   EMcontrol = EM)
R> summary(mvnormest.em)
```

```
      Dataset Preprocessing Criterion c v/k   IC logL   M
1 mvnormdataset    histogram      BIC 5   11 2125 -982 29
Maximum logL = -982 at pos = 1.
```

#### 4.3.8 Clustering with exhaustive REBMIX&ECM strategy and ICL criterion

```
R> CEM <- new("EM.Control", strategy = "exhaustive", variant = "ECM",
+   acceleration = "fixed", acceleration.multiplier = 1, tolerance = 1e-04,
+   maximum.iterations = 1000, K = 0)
R> mvnormest.cem <- REBMIX(model = "REBMVNORM", Dataset = a.Dataset(mvnorm.simulated),
+   Preprocessing = "histogram", cmax = 10, Criterion = "ICL",
+   EMcontrol = CEM)
R> mvnorm.clu <- RCLRMIX(model = "RCLRMVNORM", x = mvnormest.cem)
```

#### 4.3.9 Acceleration of the EM algorithm

Standard EM algorithm with fixed acceleration.multiplier of  $a_{EM} = 1.0$ :

```
R> EM.normal <- new("EM.Control", strategy = "exhaustive", variant = "EM",
+   acceleration = "fixed", acceleration.multiplier = 1, tolerance = 1e-04,
+   maximum.iterations = 1000, K = 0)
R> mvnormestest.em.normal <- REBMIX(model = "REBMVNORM", Dataset = a.Dataset(mvnorm.simulated),
+   Preprocessing = "histogram", cmax = 15, Criterion = "BIC",
+   EMcontrol = EM.normal)
R> cat("Total number of EM algorithm iterations: ", a.summary.EM(mvnormestest.em.normal,
+   pos = 1, col.name = "total.iterations.nbr"), ". Value of BIC: ",
+   a.summary(mvnormestest.em.normal, pos = 1, col.name = "IC"))
```

Total number of EM algorithm iterations: 461 . Value of BIC: 2125

Standard EM algorithm with fixed acceleration.multiplier of  $a_{EM} = 1.5$ :

```
R> EM.fixed1.5 <- new("EM.Control", strategy = "exhaustive", variant = "EM",
+   acceleration = "fixed", acceleration.multiplier = 1.5, tolerance = 1e-04,
+   maximum.iterations = 1000, K = 0)
R> mvnormest.em.fixed1.5 <- REBMIX(model = "REBMVNORM", Dataset = a.Dataset(mvnorm.simulated),
+   Preprocessing = "histogram", cmax = 15, Criterion = "BIC",
+   EMcontrol = EM.fixed1.5)
R> cat("Total number of EM algorithm iterations: ", a.summary.EM(mvnormest.em.fixed1.5,
+   pos = 1, col.name = "total.iterations.nbr"), ". Value of BIC: ",
+   a.summary(mvnormest.em.fixed1.5, pos = 1, col.name = "IC"))
```

Total number of EM algorithm iterations: 373 . Value of BIC: 2125

Standard EM algorithm with line search for optimal increment  $a_{EM}$  in each iteration:

```
R> EM.line <- new("EM.Control", strategy = "exhaustive", variant = "EM",
+   acceleration = "line", acceleration.multiplier = 1, tolerance = 1e-04,
+   maximum.iterations = 1000, K = 0)
R> mvnormest.em.line <- REBMIX(model = "REBMVNORM", Dataset = a.Dataset(mvnorm.simulated),
```

```

+     Preprocessing = "histogram", cmax = 15, Criterion = "BIC",
+     EMcontrol = EM.line)
R> cat("Total number of EM algorithm iterations: ", a.summary.EM(mvnormest.em.line,
+     pos = 1, col.name = "total.iterations.nbr"), ". Value of BIC: ",
+     a.summary(mvnormest.em.line, pos = 1, col.name = "IC"))

```

Total number of EM algorithm iterations: 374 . Value of BIC: 2125

Standard EM algorithm with golden search for optimal increment  $a_{EM}$  in each iteration:

```

R> EM.golden <- new("EM.Control", strategy = "exhaustive", variant = "EM",
+     acceleration = "golden", acceleration.multiplier = 1, tolerance = 1e-04,
+     maximum.iterations = 1000, K = 0)
R> mvnormest.em.golden <- REBMIX(model = "REBMVNORM", Dataset = a.Dataset(mvnorm.simulated),
+     Preprocessing = "histogram", cmax = 15, Criterion = "BIC",
+     EMcontrol = EM.golden)
R> cat("Total number of EM algorithm iterations: ", a.summary.EM(mvnormest.em.golden,
+     pos = 1, col.name = "total.iterations.nbr"), ". Value of BIC: ",
+     a.summary(mvnormest.em.golden, pos = 1, col.name = "IC"))

```

Total number of EM algorithm iterations: 363 . Value of BIC: 2125

#### 4.4 Multivariate sensorlessdrive dataset

These data are a result of the sensorless drive diagnosis procedure. The features are extracted from electric current drive signals (Bator et al., 2012). The main objective is the sensorless fault detection and classification.

```

R> data(sensorlessdrive)
R> set.seed(5)
R> Drive <- split(p = 0.75, Dataset = sensorlessdrive, class = 4)

```

##### 4.4.1 Finite mixture estimation

```

R> driveest <- REBMIX(model = "REBMVNORM", Dataset = a.train(Drive),
+     Preprocessing = "histogram", cmax = 15, Criterion = "BIC")

```

##### 4.4.2 Classification

```

R> drivecla <- RCLSMIX(model = "RCLSMVNORM", x = list(driveest),
+     Dataset = a.test(Drive), Zt = a.Zt(Drive))

```

##### 4.4.3 Show and summary methods

```
R> drivecla
```

An object of class "RCLSMVNORM"  
Slot "CM":

	1	2	3	4	5	6	7	8	9	10	11
1	1017	0	0	0	0	234	0	0	79	0	0
2	0	1201	0	0	1	0	0	0	15	113	0
3	0	0	1231	18	79	1	0	0	1	0	0
4	0	0	7	1283	38	0	0	2	0	0	0
5	0	0	96	26	1036	0	0	172	0	0	0
6	136	0	4	0	0	988	0	0	202	0	0

7	0	1	0	0	0	0	1329	0	0	0	0
8	0	0	24	29	324	0	0	952	0	1	0
9	159	6	0	1	0	467	0	0	696	1	0
10	0	164	0	0	0	0	0	0	6	1160	0
11	0	0	0	0	0	0	0	0	0	0	1330

Slot "Error":

[1] 0.165

Slot "Precision":

[1] 0.765 0.903 0.926 0.965 0.779 0.743 0.999 0.716 0.523 0.872 1.000

Slot "Sensitivity":

[1] 0.775 0.875 0.904 0.945 0.701 0.585 1.000 0.845 0.697 0.910 1.000

Slot "Specificity":

[1] 0.999 1.003 1.002 1.002 1.011 1.028 1.000 0.985 0.976 0.996 1.000

Slot "Chunks":

[1] 1

R> summary(drivecla)

	Test	Predictive	Frequency
1	1	1	1017
2	2	1	0
3	3	1	0
4	4	1	0
5	5	1	0
6	6	1	136
7	7	1	0
8	8	1	0
9	9	1	159
10	10	1	0
11	11	1	0
12	1	2	0
13	2	2	1201
14	3	2	0
15	4	2	0
16	5	2	0
17	6	2	0
18	7	2	1
19	8	2	0
20	9	2	6
21	10	2	164
22	11	2	0
23	1	3	0
24	2	3	0
25	3	3	1231
26	4	3	7
27	5	3	96
28	6	3	4
29	7	3	0
30	8	3	24
31	9	3	0
32	10	3	0
33	11	3	0
34	1	4	0
35	2	4	0

36	3	4	18
37	4	4	1283
38	5	4	26
39	6	4	0
40	7	4	0
41	8	4	29
42	9	4	1
43	10	4	0
44	11	4	0
45	1	5	0
46	2	5	1
47	3	5	79
48	4	5	38
49	5	5	1036
50	6	5	0
51	7	5	0
52	8	5	324
53	9	5	0
54	10	5	0
55	11	5	0
56	1	6	234
57	2	6	0
58	3	6	1
59	4	6	0
60	5	6	0
61	6	6	988
62	7	6	0
63	8	6	0
64	9	6	467
65	10	6	0
66	11	6	0
67	1	7	0
68	2	7	0
69	3	7	0
70	4	7	0
71	5	7	0
72	6	7	0
73	7	7	1329
74	8	7	0
75	9	7	0
76	10	7	0
77	11	7	0
78	1	8	0
79	2	8	0
80	3	8	0
81	4	8	2
82	5	8	172
83	6	8	0
84	7	8	0
85	8	8	952
86	9	8	0
87	10	8	0
88	11	8	0

89	1	9	79
90	2	9	15
91	3	9	1
92	4	9	0
93	5	9	0
94	6	9	202
95	7	9	0
96	8	9	0
97	9	9	696
98	10	9	6
99	11	9	0
100	1	10	0
101	2	10	113
102	3	10	0
103	4	10	0
104	5	10	0
105	6	10	0
106	7	10	0
107	8	10	1
108	9	10	1
109	10	10	1160
110	11	10	0
111	1	11	0
112	2	11	0
113	3	11	0
114	4	11	0
115	5	11	0
116	6	11	0
117	7	11	0
118	8	11	0
119	9	11	0
120	10	11	0
121	11	11	1330

Error = 0.165.

#### 4.4.4 Plot method

#### 4.4.5 Estimation of using the histogram based EM algorithm

When dealing with large datasets it is useful to shrink datasets to reduce the computational overload of the EM algorithm. The histogram based EM algorithm can be used for this purpose. The dataset is discretized and the EM is computed with the binned data. Integer parameter K from the `EM.Control` object is used to set the shrinkage level. A smaller value means less containers while a larger value implicates more containers.

```
R> EM <- new("EM.Control", strategy = "exhaustive", variant = "EM",
+   acceleration = "fixed", acceleration.multiplier = 1, tolerance = 1e-04,
+   maximum.iterations = 1000, K = 300)
R> driveest <- REBMIX(model = "REBMVNORM", Dataset = a.train(Drive),
+   Preprocessing = "histogram", cmax = 15, Criterion = "BIC",
+   EMcontrol = EM)
R> drivecla <- RCLSMIX(model = "RCLSMVNORM", x = list(driveest),
+   Dataset = a.test(Drive), Zt = a.Zt(Drive))
R> summary(drivecla)
```

	Test	Predictive	Frequency
1	1	1	1017
2	2	1	0
3	3	1	0
4	4	1	0
5	5	1	0
6	6	1	136
7	7	1	0
8	8	1	0
9	9	1	159
10	10	1	0
11	11	1	0
12	1	2	0
13	2	2	1201
14	3	2	0
15	4	2	0
16	5	2	0
17	6	2	0
18	7	2	1
19	8	2	0
20	9	2	6
21	10	2	164
22	11	2	0
23	1	3	0
24	2	3	0
25	3	3	1231
26	4	3	7
27	5	3	96
28	6	3	4
29	7	3	0
30	8	3	24
31	9	3	0
32	10	3	0
33	11	3	0
34	1	4	0
35	2	4	0
36	3	4	18
37	4	4	1283
38	5	4	26
39	6	4	0
40	7	4	0
41	8	4	29
42	9	4	1
43	10	4	0
44	11	4	0
45	1	5	0
46	2	5	1
47	3	5	79
48	4	5	38
49	5	5	1036
50	6	5	0
51	7	5	0
52	8	5	324

53	9	5	0
54	10	5	0
55	11	5	0
56	1	6	234
57	2	6	0
58	3	6	1
59	4	6	0
60	5	6	0
61	6	6	988
62	7	6	0
63	8	6	0
64	9	6	467
65	10	6	0
66	11	6	0
67	1	7	0
68	2	7	0
69	3	7	0
70	4	7	0
71	5	7	0
72	6	7	0
73	7	7	1329
74	8	7	0
75	9	7	0
76	10	7	0
77	11	7	0
78	1	8	0
79	2	8	0
80	3	8	0
81	4	8	2
82	5	8	172
83	6	8	0
84	7	8	0
85	8	8	952
86	9	8	0
87	10	8	0
88	11	8	0
89	1	9	79
90	2	9	15
91	3	9	1
92	4	9	0
93	5	9	0
94	6	9	202
95	7	9	0
96	8	9	0
97	9	9	696
98	10	9	6
99	11	9	0
100	1	10	0
101	2	10	113
102	3	10	0
103	4	10	0
104	5	10	0
105	6	10	0

```

106    7      10      0
107    8      10      1
108    9      10      1
109   10      10    1160
110   11      10      0
111    1      11      0
112    2      11      0
113    3      11      0
114    4      11      0
115    5      11      0
116    6      11      0
117    7      11      0
118    8      11      0
119    9      11      0
120   10      11      0
121   11      11    1330

```

Error = 0.165.

## 4.5 Multivariate adult dataset

The `adult` dataset containing 48842 instances with 16 continuous, binary and discrete variables was extracted from the census bureau database Asuncion and Newman (2007). Extraction was done by Barry Becker from the 1994 census bureau database. The `adult` dataset is loaded, complete cases are extracted and levels are replaced with numbers.

```

R> data(adult)
R> adult <- adult[complete.cases(adult), ]
R> adult <- as.data.frame(data.matrix(adult))

```

Numbers of unique values for variables are determined and displayed.

```

R> cmax <- unlist(lapply(apply(adult[, c(-1, -16)], 2, unique),
+   length))
R> cmax

```

	Age	Workclass	Fnlwgt	Education	Education.Num
	74	7	26741	16	16
Marital.Status	Occupation	Relationship	Race	Sex	
	7	14	6	5	2
Capital.Gain	Capital.Loss	Hours.Per.Week	Native.Country		
	121	97	96	41	

The dataset is split into train and test subsets for the two incomes and the `Type` and `Income` columns are removed.

```

R> Adult <- split(p = list(type = 1, train = 2, test = 1), Dataset = adult,
+   class = 16)

```

### 4.5.1 Finite mixture estimation

Number of components, component weights and component parameters are estimated assuming that the variables are independent for the set of chunks  $y_{1j}, y_{2j}, \dots, y_{14j}$ .

```

R> adulctest <- list()
R> for (i in 1:14) {
+   adulctest[[i]] <- REBMIX(Dataset = a.train(chunk(Adult, i)),

```

```
+      Preprocessing = "histogram", cmax = min(120, cmax[i]),
+      Criterion = "BIC", pdf = "Dirac", K = 1)
+ }
```

#### 4.5.2 Classification

The class membership prediction is based upon the best first search algorithm.

```
R> adultcla <- BFSMIX(x = adulttest, Dataset = a.test(Adult), Zt = a.Zt(Adult))
```

#### 4.5.3 Show and summary methods

```
R> adultcla
```

An object of class "RCLSMIX"

Slot "CM":

	1	2
1	10649	711
2	1397	2303

Slot "Error":

```
[1] 0.14
```

Slot "Precision":

```
[1] 0.937 0.622
```

Slot "Sensitivity":

```
[1] 0.884 0.764
```

Slot "Specificity":

```
[1] 1.228 0.943
```

Slot "Chunks":

```
[1] 11 12 4 8 1
```

```
R> summary(adultcla)
```

	Test	Predictive	Frequency
1	1	1	10649
2	2	1	1397
3	1	2	711
4	2	2	2303

Error = 0.14.

#### 4.5.4 Plot method

## 5 Summary

The users of the `rebmix` package are kindly encouraged to inform the authors about bugs and wishes.

## References

- A. Asuncion and D. J. Newman. Uci machine learning repository, 2007. URL <http://archive.ics.uci.edu/ml>.
- M. Bator, A. Dicks, U. Mönks, and V. Lohweg. Feature extraction and reduction applied to sensorless drive diagnosis. 12 2012. doi: 10.13140/2.1.2421.5689.

- G. Celeux and G. Govaert. A classification em algorithm for clustering and two stochastic versions. *Computational Statistics & Data Analysis*, 14(3):315–332, 1992. doi: 10.1016/0167-9473(92)90042-E.
- A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the em algorithm. *Journal of the Royal Statistical Society B*, 39(1):1–38, 1977. URL <https://www.jstor.org/stable/2984875>.
- K. H. Knuth. Optimal data-based binning for histograms and histogram-based probability density models. *Digital Signal Processing*, 95:102581, 2019. doi: 10.1016/j.dsp.2019.102581.
- J. Ma, J. Liu, and Z. Ren. Parameter estimation of poisson mixture with automated model selection through byy harmony learning. *Pattern Recognition*, 42(11):2659–2670, 2009. doi: 10.1016/j.patcog.2009.03.029.
- M. Nagode. Finite mixture modeling via rebmix. *Journal of Algorithms and Optimization*, 3(2):14–28, 2015. URL <https://repozitorij.uni-lj.si/Dokument.php?id=127674&lang=eng>.
- M. Nagode. Multivariate normal mixture modeling, clustering and classification with the rebmix package. *ArXiv e-prints*, Jan. 2018.
- M. Nagode and M. Fajdiga. The rebmix algorithm for the univariate finite mixture estimation. *Communications in Statistics - Theory and Methods*, 40(5):876–892, 2011a. doi: 10.1080/03610920903480890.
- M. Nagode and M. Fajdiga. The rebmix algorithm for the multivariate finite mixture estimation. *Communications in Statistics - Theory and Methods*, 40(11):2022–2034, 2011b. doi: 10.1080/03610921003725788.
- B. Panić, J. Klemenc, and M. Nagode. Improved initialization of the em algorithm for mixture model parameter estimation. *Mathematics*, 8(3):373, 2020a. doi: 10.3390/math8030373. URL <https://www.mdpi.com/2227-7390/8/3/373/htm>.
- B. Panić, J. Klemenc, and M. Nagode. Optimizing the estimation of a histogram-bin width-application to the multivariate mixture-model estimation. *Mathematics*, 8(7):1090, 2020b. doi: 10.3390/math8071090. URL <https://www.mdpi.com/2227-7390/8/7/1090>.
- B. Panić, J. Klemenc, and M. Nagode. Gaussian mixture model based classification revisited: Application to the bearing fault classification. *Journal of Mechanical Engineering*, 66(4):215–226, 2020c. doi: 10.5545/sv-jme.2020.6563. URL <https://www.sv-jme.eu/article/gaussian-mixture-model-based-classification-revisited-application-to-the-bearing-fault-classification>.
- P. F. Velleman. Interactive computing for exploratory data analysis i: Display algorithms. In *Proceedings of the Statistical Computing Section*, Washington, D.C., 1976. American Statistical Association.
- M. Wiper, D. R. Insua, and F. Ruggeri. Mixtures of gamma distributions with applications. *Journal of Computational and Graphical Statistics*, 10(3):440–454, 2001. URL <http://www.jstor.org/stable/1391098>.

Marko Nagode  
 University of Ljubljana  
 Faculty of Mechanical Engineering  
 Aškerčeva 6  
 1000 Ljubljana  
 Slovenia  
 Marko.Nagode@fs.uni-lj.si.

```
R> plot(poissonest, pos = 1, what = c("pdf", "marginal pdf", "IC",
+   "D", "logL"), nrow = 2, ncol = 3, npts = 1000)
```

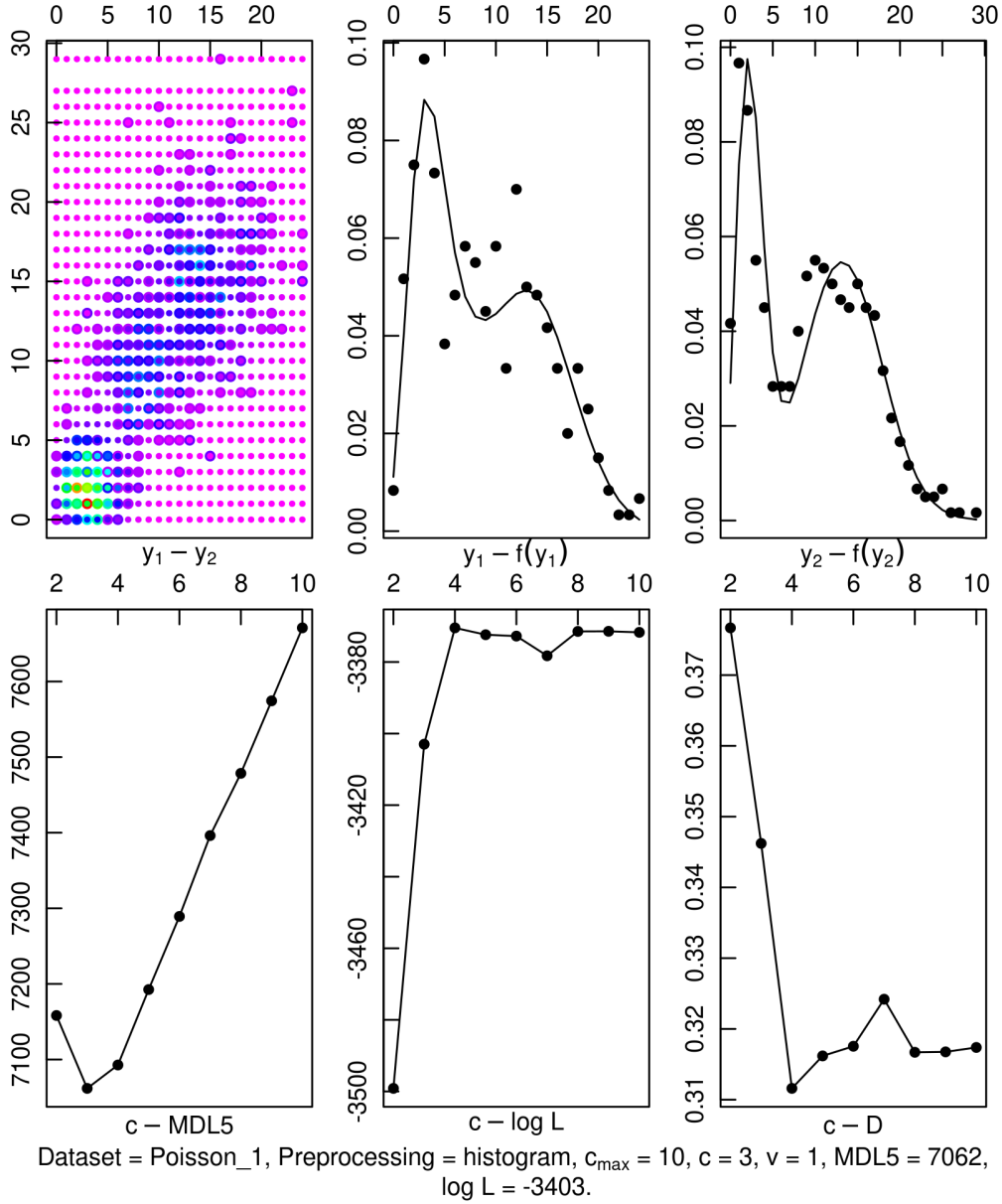


Figure 2: Poisson dataset. Empirical densities (coloured large circles), predictive multivariate Poisson-Poisson mixture density (coloured small circles), empirical densities (circles), predictive univariate marginal Poisson mixture densities and progress charts (solid line).

```
R> poissonclu <- RCLRMIX(x = poissonest, pos = 1, Zt = a.Zt(poisson))
R> plot(poissonclu)
```

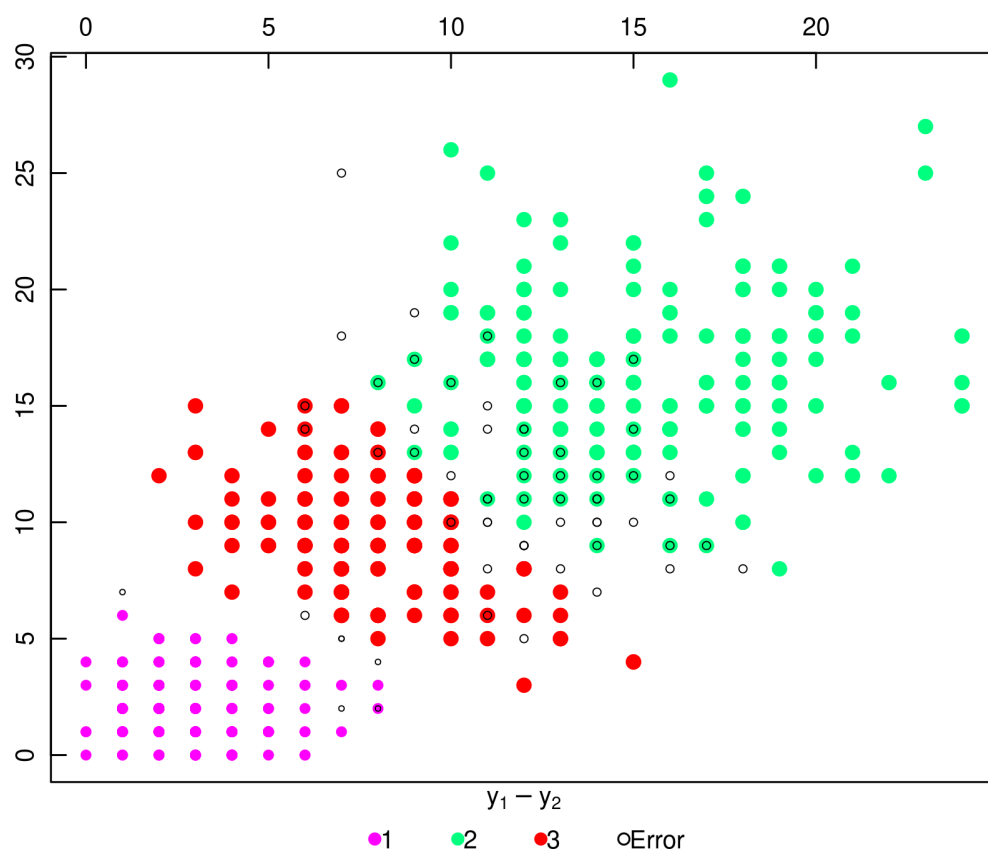


Figure 3: Poisson dataset. Predictive cluster membership (coloured circles), error (black circles).

```
R> plot(mvnormest)
```

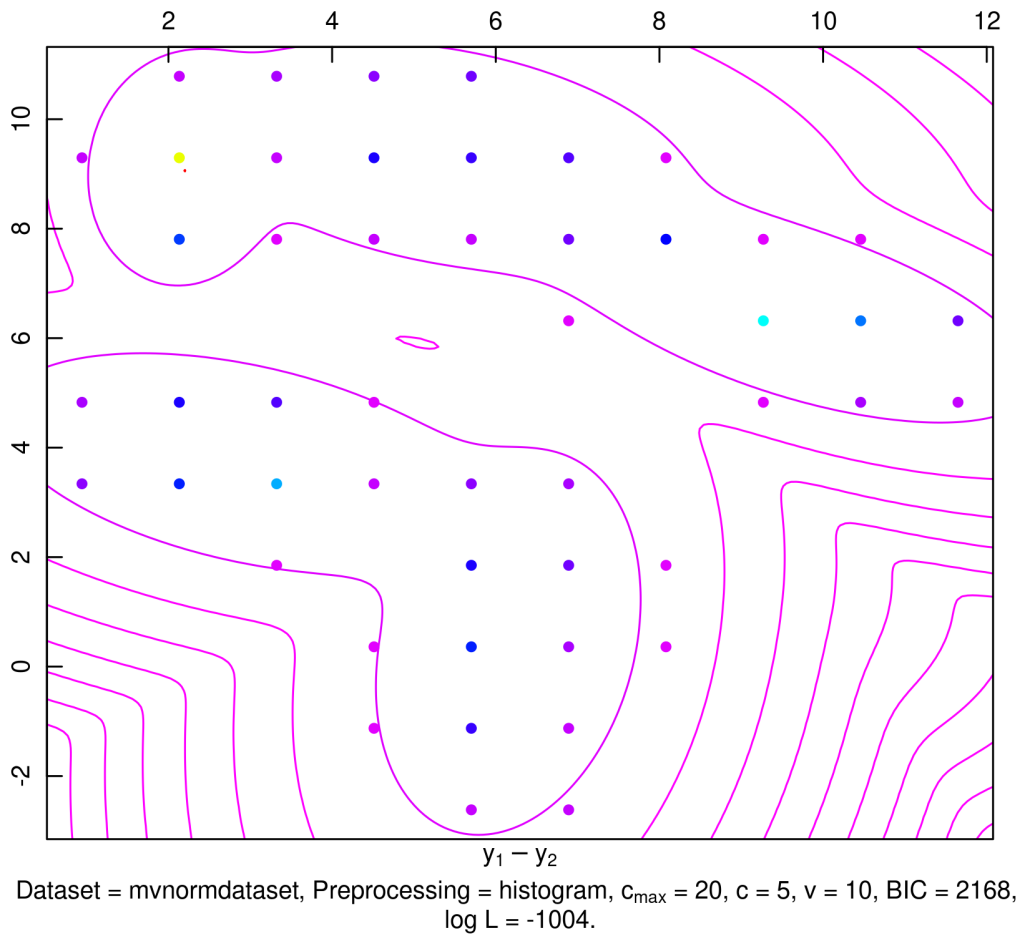


Figure 4: Dataset `mvnorm`. Empirical densities (coloured circles), predictive multivariate normal mixture density (coloured lines).

```
R> mvnormclu <- RCLRMIX(model = "RCLRMVNORM", x = mvnormest)
R> plot(mvnormclu)
```

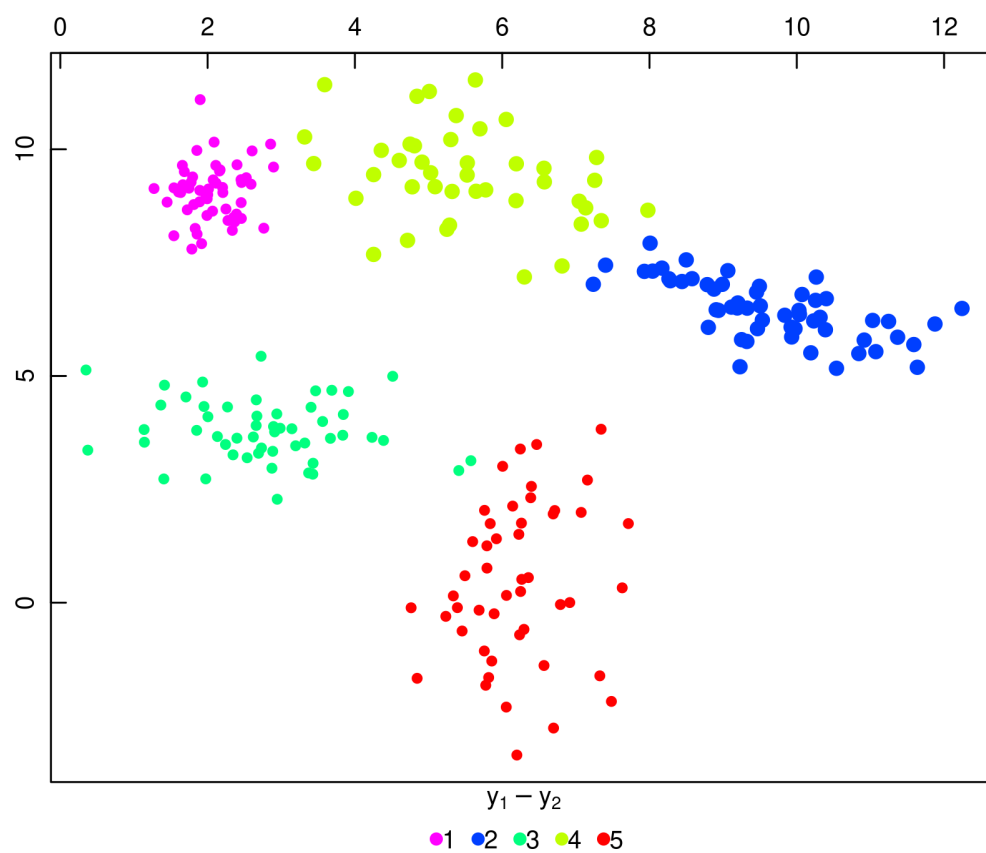


Figure 5: Dataset `mvnorm`. Predictive cluster membership (coloured circles).

```
R> plot(mvnorm.clu)
```

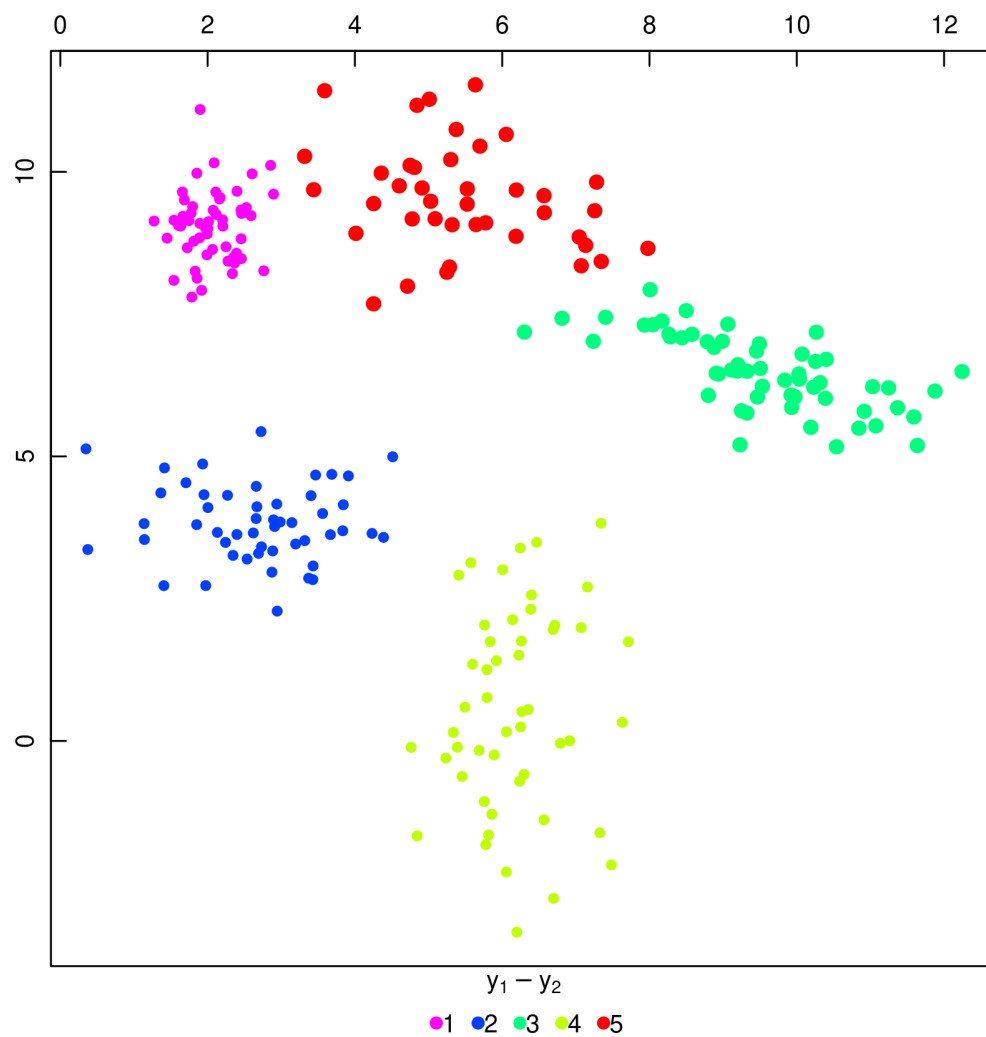


Figure 6: Dataset `mvnorm`. Predictive cluster membership (coloured circles) for exhaustive REB-MIX&ECM strategy and ICL criterion.

```
R> plot(drivecla, nrow = 3, ncol = 2)
```

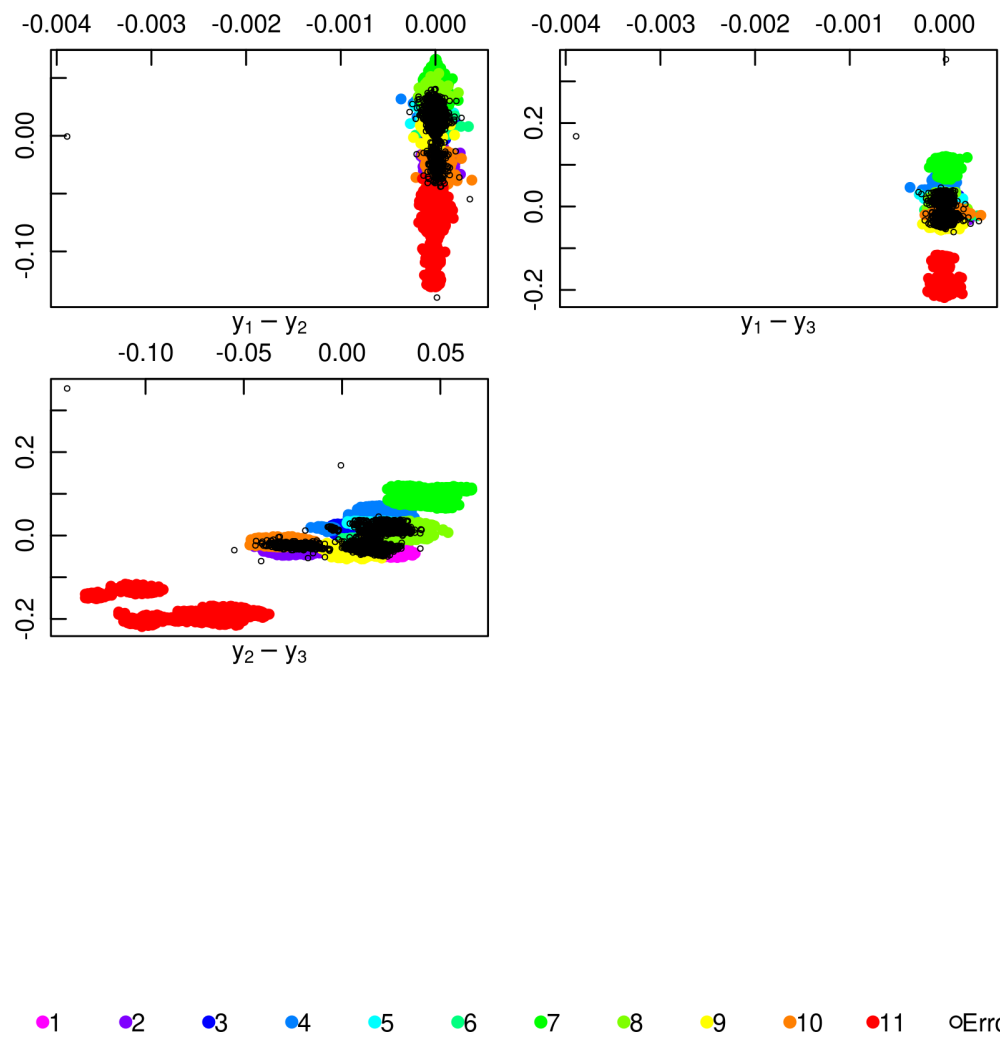


Figure 7: Dataset `iris`. Predictive class membership (coloured circles), error (black circles).

```
R> plot(adultcla, nrow = 5, ncol = 2)
```

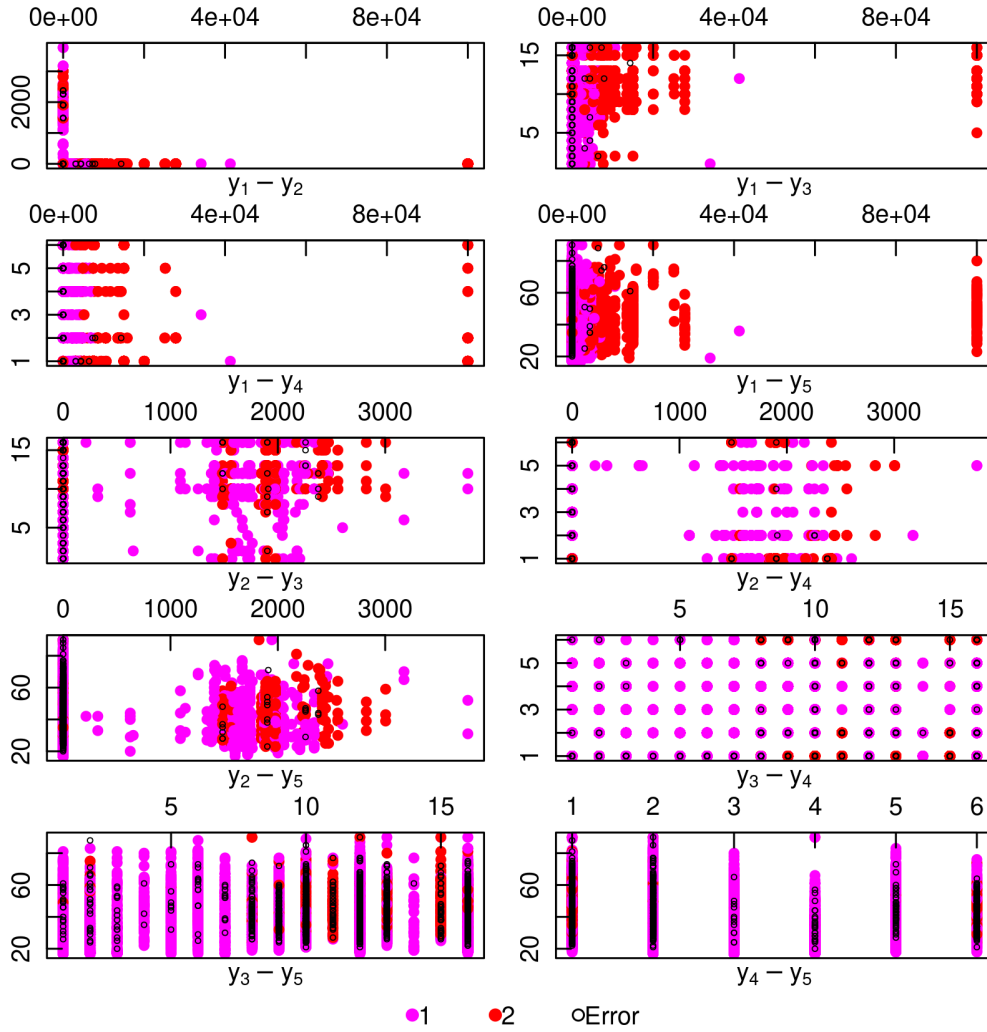


Figure 8: Dataset `adult`. Predictive class membership (coloured circles), error (black circles).