rebmix: Finite Mixture Modeling, Clustering & Classification

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Abstract

The **rebmix** package provides R functions for random univariate and multivariate finite mixture model generation, estimation, clustering 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). For theoretical backgrounds please upload also `http://doi.org/10.5963/JAO0302001`.

2 What's new in version `2.10.2`

Method `split` is improved and examples for its proper use are added. GCC 8.1 notes and warnings in C++ functions are eliminated in version 2.10.2, too. Cholesky decomposition is now used to calculate logarithm of determinant and inverse of variance-covariance matrices instead of LU decomposition. Special attention is put in resolving numerical problems related to high dimensional datasets. Version 2.10.1 is further debugged version 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

$$v_{\max} = \frac{1+d}{d} n^{\frac{d}{1+d}}. \tag{1}$$

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

$$A = \left. \frac{1 - a_{\mathrm{r}}}{a_{\mathrm{r}}(D_l w_l - D_{\min})} \right|_{I_2=1} \tag{2}$$

is calculated. Acceleration rate a_{r} at $I_2 = 1$ always equals the value stored in the input argument `ar`. Otherwise

$$a_{\mathrm{r}} = \left. \frac{1}{A(D_l w_l - D_{\min}) + 1} \right|_{I_2>1}. \tag{3}$$

The Newton-Raphson root finding in `C++` functions is improved in version 2.9.3, too. This affects only Weibull, gamma and von Mises parametric families. Circular von Mises parametric family is added and further debugging is done in version 2.9.2. Version 2.9.1 is further debugged version 2.8.4. The R code is extended and rewritten in S4 class system. The background C code is extended and rewritten as object-oriented `C++` code, too. The package can easier be extended to other parametric families. Multivariate normal mixtures with unrestricted variance-covariance matrices are added. Clustering is added and classification is improved.

3 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)
```

3.1 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

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

3.1.1 Finite mixture generation

```
R> n <- c(100, 100, 100, 100)
R> Theta <- list(pdf1 = "gamma", theta1.1 = c(1/100, 1/100, 1/100,
+      1/100), theta2.1 = c(200, 400, 600, 800))
R> gamma1 <- RNGMIX(Dataset.name = "gamma1", n = n, Theta = Theta)
R> n <- c(40, 360)
R> Theta <- list(pdf1 = "gamma", theta1.1 = c(1/27, 1/270), theta2.1 = c(9,
+      90))
R> gamma2 <- RNGMIX(Dataset.name = "gamma2", n = n, Theta = Theta)
R> n <- c(80, 240, 80)
R> Theta <- list(pdf1 = "gamma", theta1.1 = c(1/20, 1, 1/20), theta2.1 = c(40,
+      6, 200))
R> gamma3 <- RNGMIX(Dataset.name = "gamma3", rseed = -4, n = n,
+      Theta = Theta)
```

3.1.2 Finite mixture estimation

```
R> gamma1est <- REBMIX(Dataset = gamma1@Dataset, Preprocessing = "Parzen window",
+      cmax = 8, Criterion = c("AIC", "BIC"), pdf = "gamma")
R> gamma2est <- REBMIX(Dataset = gamma2@Dataset, Preprocessing = "histogram",
+      cmax = 8, Criterion = "BIC", pdf = "gamma")
R> gamma3est <- REBMIX(Dataset = gamma3@Dataset, Preprocessing = "histogram",
+      cmax = 8, Criterion = "BIC", pdf = "gamma", K = 23:27)
```

3.1.3 Plot method

```
R> plot(gamma3est, pos = 1, what = c("den", "dis"), ncol = 2, npts = 1000)
```

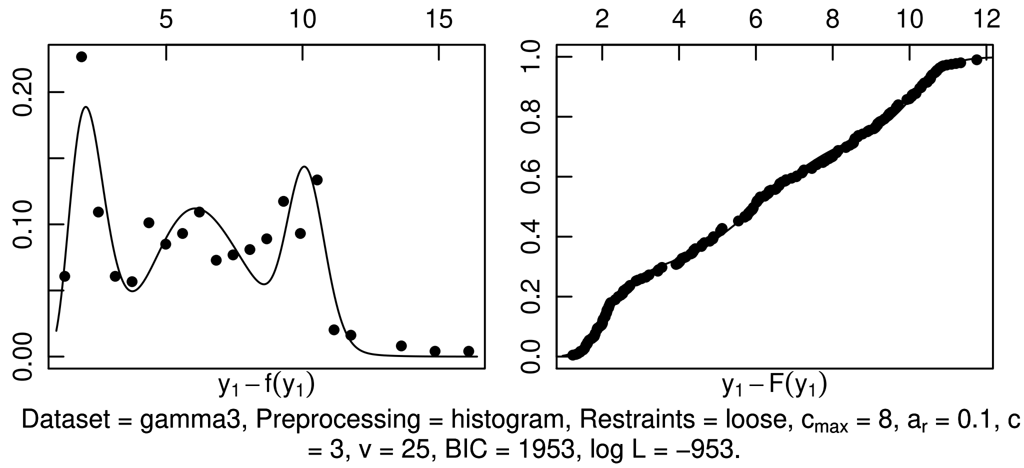


Figure 1: Gamma 3 dataset. Empirical density (circles) and predictive gamma mixture density in black solid line.

3.1.4 Summary and coef methods

```
R> summary(gamma2est)

  Dataset Preprocessing Criterion c v/k    IC logL M
1  gamma2     histogram       BIC 2  16 -1321  676 5
Maximum logL = 676 at pos = 1.

R> coef(gamma1est, pos = 2)

  comp1 comp2 comp3 comp4
w  0.25  0.25  0.25  0.25
                1
theta1.1 0.01027
theta1.2 0.00921
theta1.3 0.00870
theta1.4 0.01118
            1
theta2.1 195
theta2.2 437
theta2.3 918
theta2.4 535
```

3.1.5 Bootstrap methods

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

An object of class "REBMIX.boot"
Slot "c":
 [1] 3 3 3 3 3 3 3 3 3 3
Slot "c.se":
[1] 0
Slot "c.cv":
[1] 0
Slot "c.mode":
```

```
[1] 3
Slot "c.prob":
[1] 1
```

```
R> summary(gamma3boot)
```

```
     comp1 comp2 comp3
w.cv 0.122   0.2 0.175
                1
theta1.1.cv 0.457
theta1.2.cv 0.840
theta1.3.cv 0.508
                1
theta2.1.cv 2.149
theta2.2.cv 0.697
theta2.3.cv 1.083
Mode probability = 1 at c = 3 components.
```

3.2 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

$$
\begin{array}{ll}
\boldsymbol{\theta}_1 = (3, 2)^\top & n_1 = 200 \\
\boldsymbol{\theta}_2 = (9, 10)^\top & n_2 = 200 \\
\boldsymbol{\theta}_3 = (15, 16)^\top & n_3 = 200
\end{array}
$$

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_{seed} ranging from -1 to -10.

3.2.1 Finite mixture generation

```
R> n <- c(200, 200, 200)
R> Theta <- list(pdf1 = rep("Poisson", 2), theta1.1 = c(3, 2), theta2.1 = c(NA,
+      NA), pdf2 = rep("Poisson", 2), theta1.2 = c(9, 10), theta2.2 = c(NA,
+      NA), pdf3 = rep("Poisson", 2), theta1.3 = c(15, 16), theta2.3 = c(NA,
+      NA))
R> poisson <- RNGMIX(Dataset.name = paste("Poisson_", 1:10, sep = ""),
+      n = n, Theta = Theta)
```

3.2.2 Finite mixture estimation

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

3.2.3 Plot method

3.2.4 Clustering

```
R> plot(poissonest, pos = 9, what = c("dens", "marg", "IC", "D",
+       "logL"), nrow = 2, ncol = 3, npts = 1000)
```

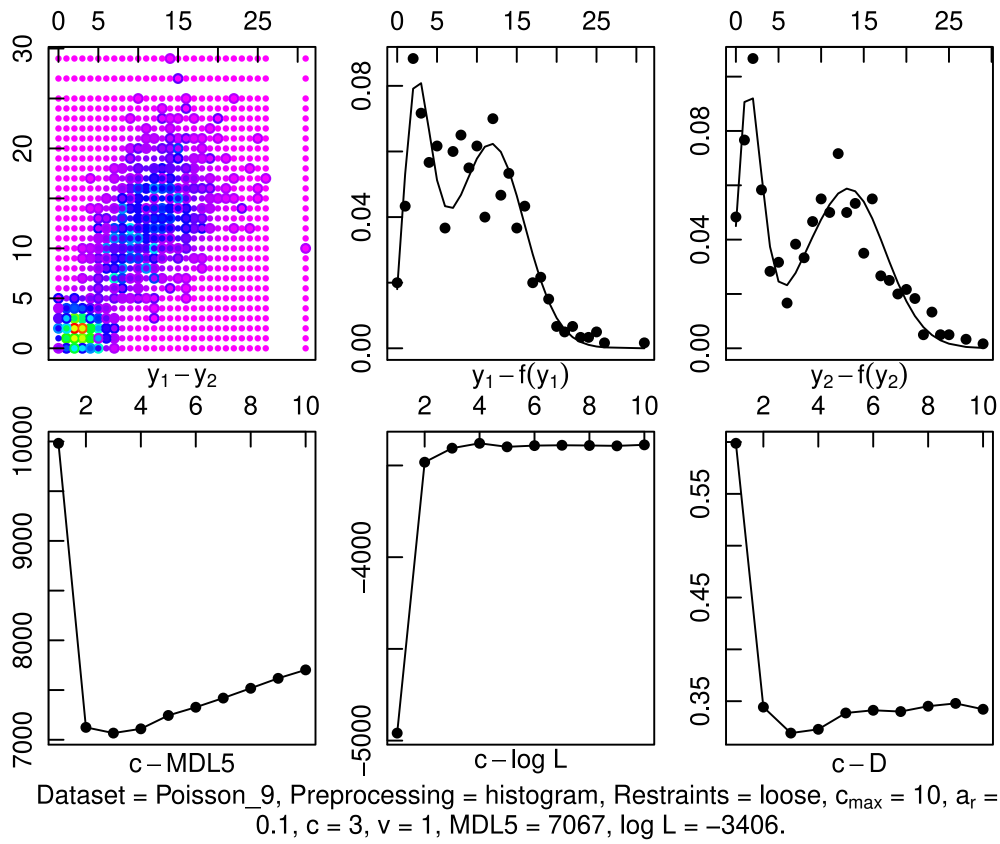


Figure 2: Poisson dataset. Empirical densities (coloured large circles), predictive multivariate Poisson-Poisson mixture density (coloured small circles), empirical densities (circles), predictive univariate marginal Poisson mixture densities and progress charts (solid line).

3.2.5 Summary and coef methods

```
R> summary(poissonest)

      Dataset Preprocessing Criterion c v/k   IC  logL M
1   Poisson_1     histogram      MDL5 3   1 6992 -3368 8
2   Poisson_2     histogram      MDL5 2   1 7180 -3510 5
3   Poisson_3     histogram      MDL5 3   1 7030 -3387 8
4   Poisson_4     histogram      MDL5 3   1 7005 -3375 8
5   Poisson_5     histogram      MDL5 3   1 6992 -3368 8
6   Poisson_6     histogram      MDL5 3   1 7044 -3394 8
7   Poisson_7     histogram      MDL5 2   1 7239 -3539 5
8   Poisson_8     histogram      MDL5 3   1 7036 -3390 8
9   Poisson_9     histogram      MDL5 3   1 7067 -3406 8
10 Poisson_10     histogram      MDL5 3   1 7008 -3376 8
Maximum logL = -3368 at pos = 5.
```

```
R> coef(poissonest, pos = 9)

  comp1 comp2 comp3
w 0.336 0.155 0.509
             1     2
theta1.1  2.93  2.01
```

```
R> poissonclu <- RCLRMIX(x = poissonest, pos = 9, Zt = poisson@Zt)
R> plot(poissonclu)
```

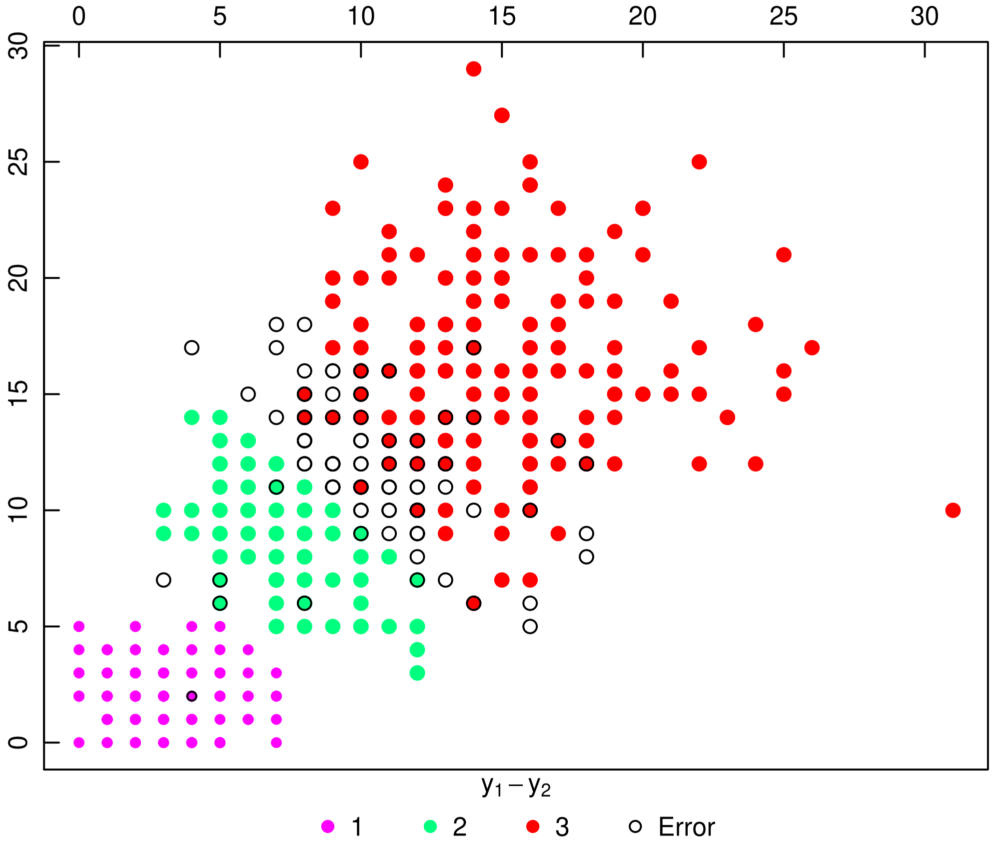


Figure 3: Poisson dataset. Predictive cluster membership (coloured circles), error (black circles).

```
theta1.2  7.75  8.68
theta1.3 13.05 14.42
         1 2
theta2.1 0 0
theta2.2 0 0
theta2.3 0 0
```

3.3 Multivariate normal `wreath` dataset

A `wreath` dataset (Fraley et al., 2005) consist of 1000 observations drawn from a 14-component normal mixture in which the covariances of the components have the same size and shape but differ in orientation.

```
R> data("wreath", package = "mclust")
```

3.3.1 Finite mixture estimation

```
R> wreathest <- REBMIX(model = "REBMVNORM", Dataset = list(as.data.frame(wreath)),
+      Preprocessing = "histogram", cmax = 20, Criterion = "BIC")
```

3.3.2 Plot method

3.3.3 Clustering

```
R> plot(wreathest)
```

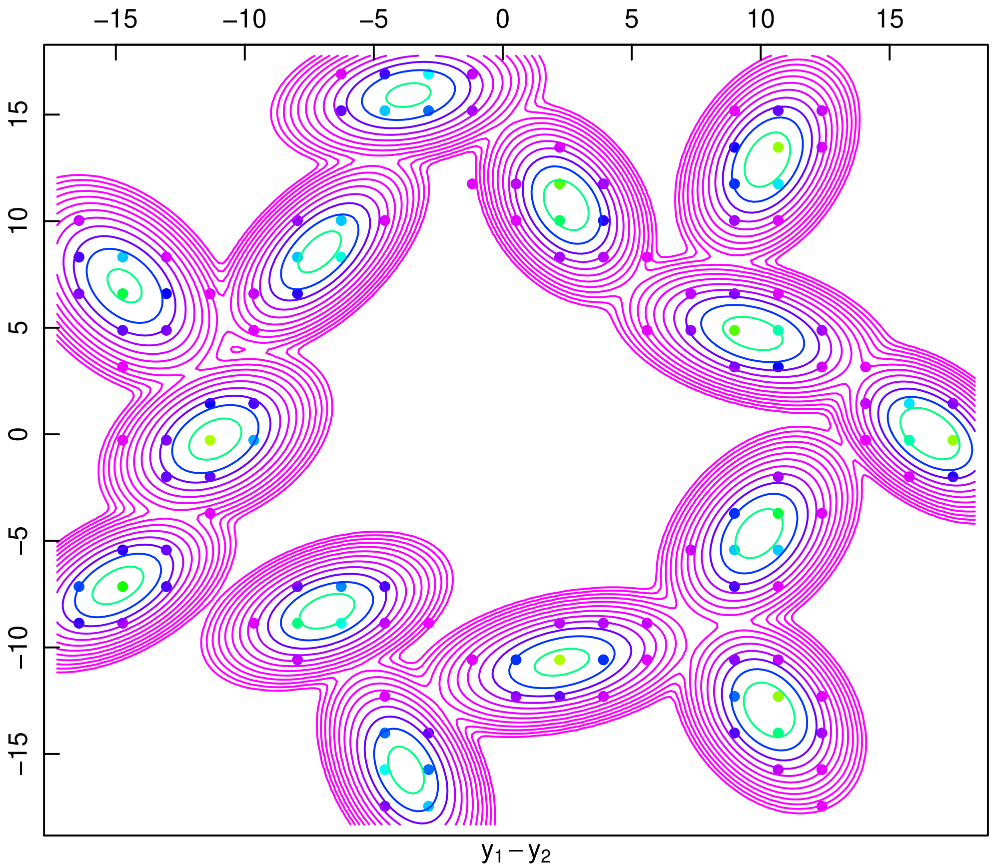


Figure 4: Dataset `wreath`. Empirical densities (coloured circles), predictive multivariate normal mixture density (coloured lines).

3.3.4 Summary and coef methods

```
R> summary(wreathest)

   Dataset Preprocessing Criterion  c v/k    IC  logL  M
1 dataset1     histogram       BIC 14  21 11174 -5300 83
Maximum logL = -5300 at pos = 1.
```

```
R> coef(wreathest)

   comp1  comp2  comp3  comp4  comp5  comp6  comp7  comp8  comp9 comp10 comp11
w 0.0699 0.0753 0.0772 0.0803 0.0823 0.0702 0.0752 0.0652 0.0771 0.0701 0.0673
  comp12 comp13 comp14
w 0.0631 0.0611 0.0657
               1        2
theta1.1    2.30 -10.6940
theta1.2  -11.14  -0.2258
theta1.3   10.26  12.8882
theta1.4   16.56   0.0341
theta1.5   10.33 -12.9260
theta1.6    2.46  10.7556
theta1.7    9.69   4.7299
theta1.8  -14.92  -7.0925
```

```
R> wreathclu <- RCLRMIX(model = "RCLRMVNORM", x = wreathest)
R> plot(wreathclu, s = 14)
```

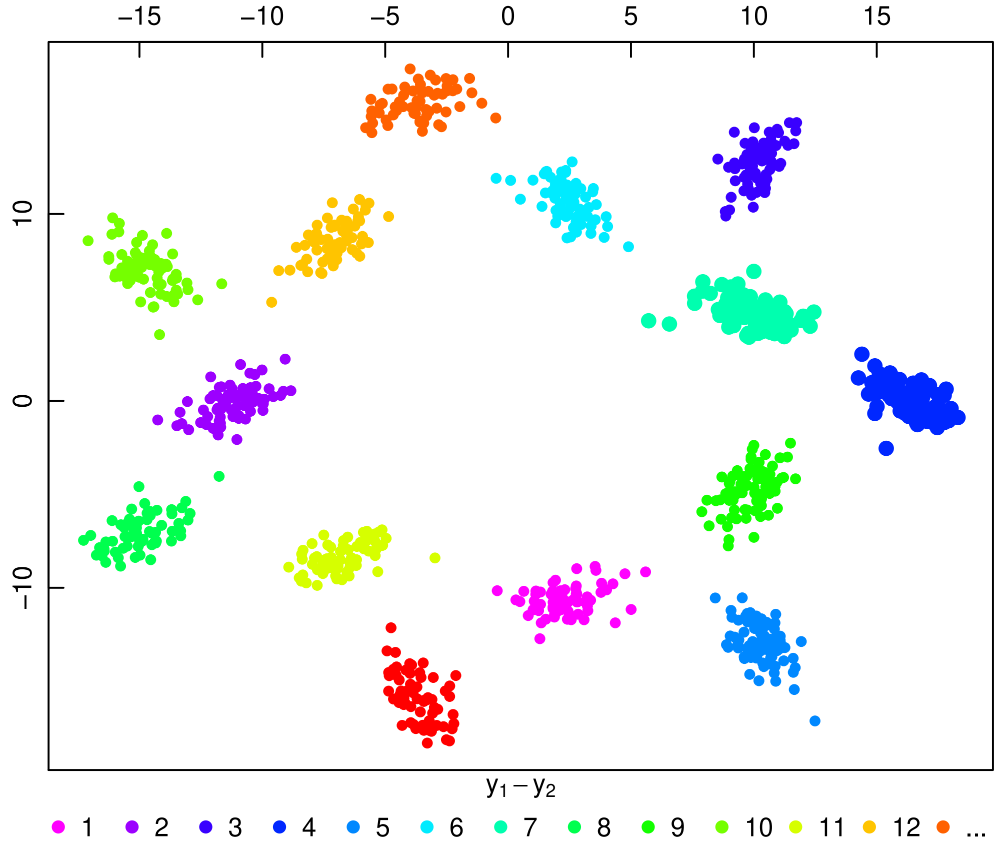


Figure 5: Dataset `wreath`. Predictive cluster membership (coloured circles).

```
theta1.9     9.94  -4.6601
theta1.10 -14.66   6.9672
theta1.11  -6.81  -8.3005
theta1.12  -7.09   8.5617
theta1.13  -3.65  15.9168
theta1.14  -3.75 -15.7497
             1-1    1-2    2-1   2-2
theta2.1   2.116  0.426  0.426 0.749
theta2.2   1.230  0.412  0.412 1.117
theta2.3   0.758  0.400  0.400 1.579
theta2.4   0.941 -0.443 -0.443 1.037
theta2.5   0.826 -0.343 -0.343 1.389
theta2.6   0.723 -0.328 -0.328 1.325
theta2.7   1.835 -0.437 -0.437 0.825
theta2.8   1.250  0.545  0.545 0.996
theta2.9   0.944  0.466  0.466 1.501
theta2.10 1.192 -0.569 -0.569 1.669
theta2.11 1.426  0.436  0.436 0.832
theta2.12 1.083  0.757  0.757 1.482
theta2.13 1.743  0.282  0.282 0.728
theta2.14 0.718 -0.445 -0.445 1.763
```

3.3.5 Summary method

```
R> summary(wreathclu)
```

```
Number of clusters  1         2         3         4         5
From cluster        3         2         13        5         4
To cluster          1         1         1         1         1
Entropy             2.03e-14  3.34e-03  8.28e-03  1.38e-02  2.28e-02
Entropy decrease    0.00334   0.00494   0.00552   0.00901   0.00751

Number of clusters  6         7         8         9         10
From cluster        9         14        10        11        12
To cluster          4         1         2         1         10
Entropy             3.03e-02  3.89e-02  5.83e-02  7.95e-02  1.20e-01
Entropy decrease    0.00858   0.01943   0.02119   0.04050   0.14527

Number of clusters  11        12        13
From cluster        6         8         7
To cluster          4         2         4
Entropy             2.65e-01  5.90e-01  1.10e+00
Entropy decrease    0.32504   0.51374   0.74344
```

3.4 Multivariate normal ex4.1 dataset

A ex4.1 dataset (Baudry et al., 2010; Fraley et al., 2016) consist of 600 two dimensional observations.

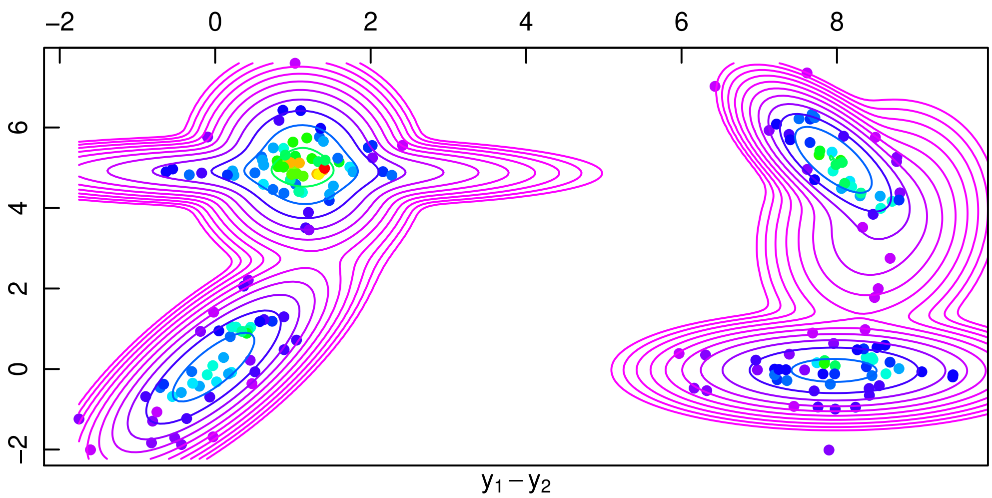
```
R> data("Baudry_etal_2010_JCGS_examples", package = "mclust")
```

3.4.1 Finite mixture estimation

```
R> ex4.1est <- REBMIX(model = "REBMVNORM", Dataset = list(as.data.frame(ex4.1)),
+      Preprocessing = "Parzen window", cmax = 10, Criterion = "AIC")
```

3.4.2 Plot method

```
R> plot(ex4.1est, pos = 1, what = c("dens"), nrow = 1, ncol = 1)
```



Dataset = dataset1, Preprocessing = Parzen window, Restraints = loose, c_{max} = 10, a_r = 0.1, c = 6, v = 28, AIC = 4084, log L = –2007.

Figure 6: Dataset ex4.1. Empirical densities (coloured circles), predictive multivariate normal mixture density (coloured lines).

3.4.3 Clustering

```
R> ex4.1clu <- RCLRMIX(model = "RCLRMVNORM", x = ex4.1est)
R> plot(ex4.1clu)
```

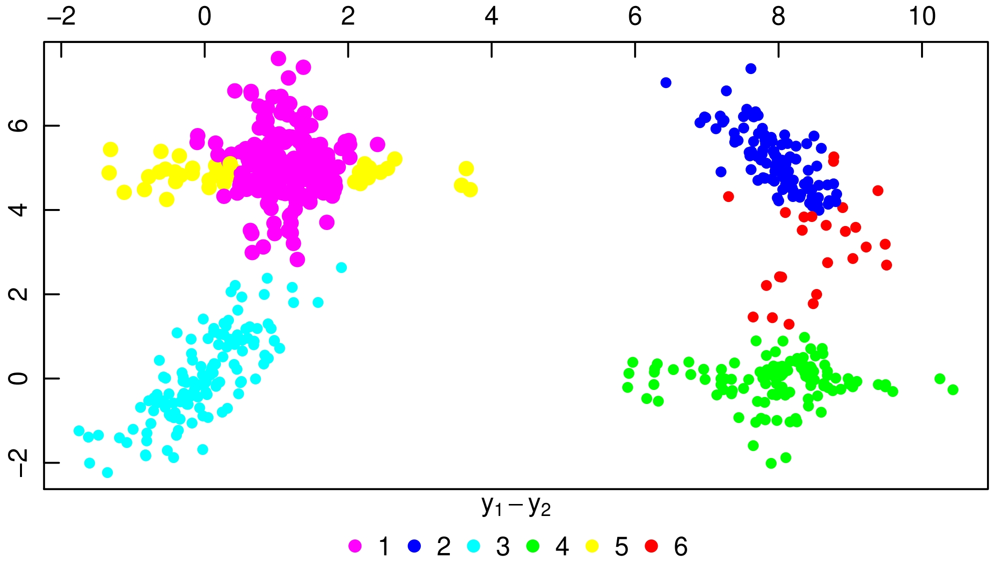


Figure 7: Dataset ex4.1. Predictive cluster membership (coloured circles).

3.4.4 Summary method

```
R> summary(ex4.1est)

   Dataset Preprocessing Criterion c v/k   IC  logL  M
1 dataset1 Parzen window       AIC 6  28 4084 -2007 35
Maximum logL = -2007 at pos = 1.
```

3.5 Multivariate iris dataset

The well known set of iris data as collected originally by Anderson (1936) and first analysed by Fisher (1936) is considered here. It is available at Asuncion and Newman (2007) consisting of the measurements of the length and width of both sepals and petals of 50 plants for each of the three types of iris species setosa, versicolor and virginica. The iris dataset is loaded, split into three subsets for the three classes and the `Class` column is removed.

```
R> data("iris")
R> levels(iris[["Class"]])

[1] "iris-setosa"     "iris-versicolor" "iris-virginica"

R> set.seed(5)
R> Iris <- split(p = 0.75, Dataset = iris, class = 5)
```

3.5.1 Finite mixture estimation

```
R> irisest <- REBMIX(model = "REBMVNORM", Dataset = Iris@train,
+       Preprocessing = "Parzen window", cmax = 10, Criterion = "ICL-BIC")
```

3.5.2 Classification

```
R> iriscla <- RCLSMIX(model = "RCLSMVNORM", x = list(irisest), Dataset = Iris@test,
+       Zt = Iris@Zt)
```

3.5.3 Show and summary methods

```
R> iriscla

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

     1  2  3
  1 13  0  0
  2  0 13  0
  3  0  1 12
Slot "Error":
[1] 0.0256
Slot "Precision":
[1] 1.000 1.000 0.923
Slot "Sensitivity":
[1] 1.000 0.929 1.000
Slot "Specificity":
[1] 1.000 1.040 0.963
Slot "Chunks":
[1] 1

R> summary(iriscla)

  Test Predictive Frequency
1    1          1        13
2    2          1         0
3    3          1         0
4    1          2         0
5    2          2        13
6    3          2         1
7    1          3         0
8    2          3         0
9    3          3        12
Error = 0.0256.
```

3.5.4 Plot method

3.6 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
```

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

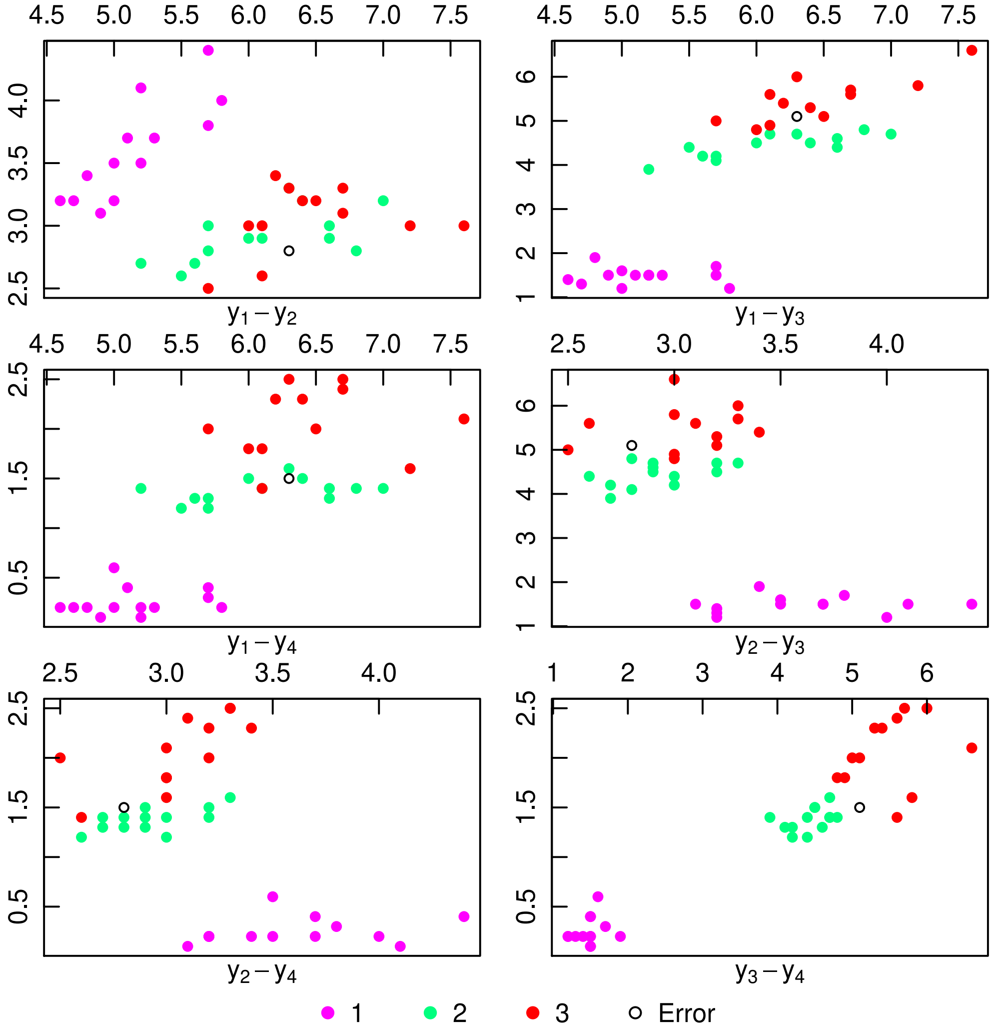


Figure 8: Dataset `iris`. Predictive class membership (coloured circles), error (black circles).

```
           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)
```

3.6.1 Finite mixture estimation

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

```
R> adulttest <- list()
R> for (i in 1:14) {
+       adulttest[[i]] <- REBMIX(Dataset = chunk(Adult, i)@train,
+           Preprocessing = "histogram", cmax = min(120, cmax[i]),
```

```
+           Criterion = "BIC", pdf = "Dirac", K = 1)
+  }
```

3.6.2 Classification

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

```
R> adultcla <- BFSMIX(x = adultest, Dataset = Adult@test, Zt = Adult@Zt)
```

3.6.3 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.
```

3.6.4 Plot method

4 Summary

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

5 Acknowledgement

The author thanks Branislav Panić for his contribution to the Velleman (1976) rule extension to multidimensions and for his other valuable suggestions on the package from version 2.9.0 on.

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

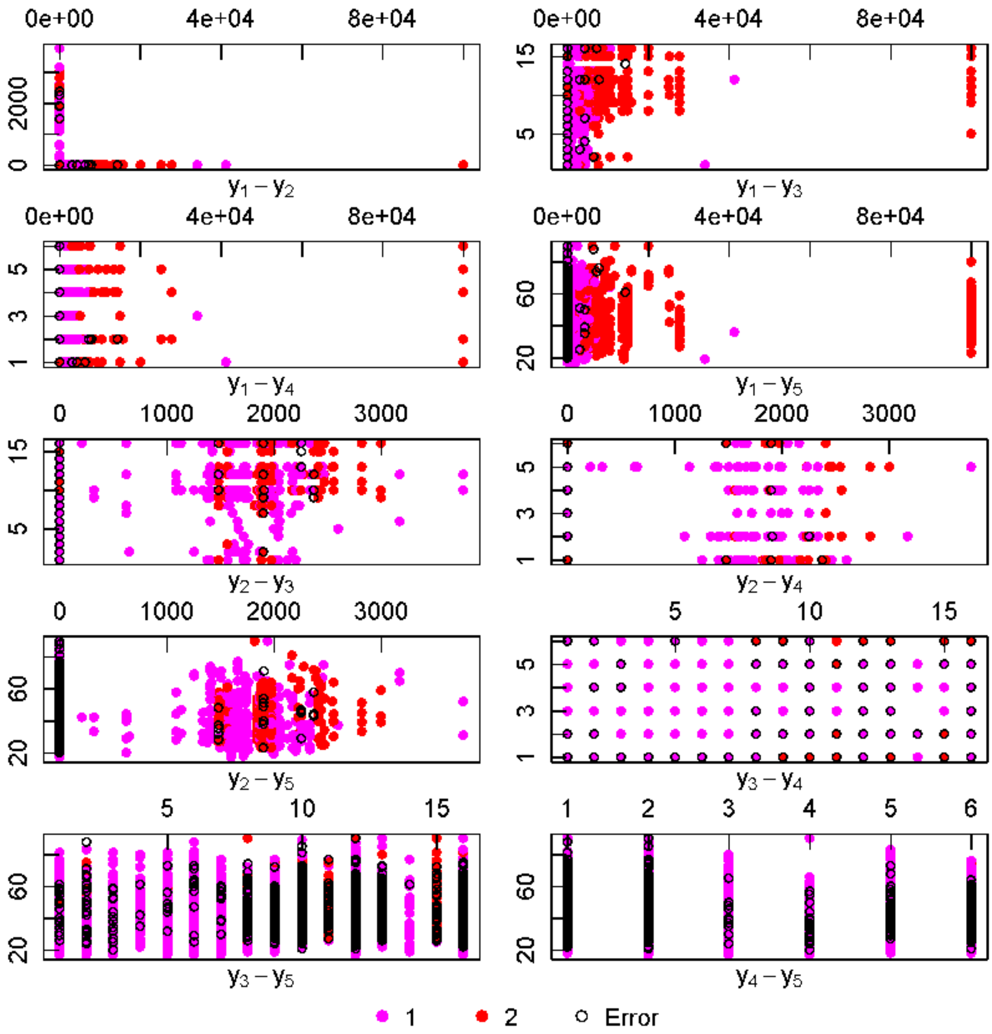


Figure 9: Dataset `adult`. Predictive class membership (coloured circles), error (black circles).

References

E. Anderson. The species problem in iris. *Annals of the Missouri Botanical Garden*, 23(3):457–509, 1936. doi: 10.2307/2394164.

A. Asuncion and D. J. Newman. Uci machine learning repository, 2007. URL `http://archive.ics.uci.edu/ml`.

J. P. Baudry, A. E. Raftery, G. Celeux, K. Lo, and R. Gottardo. Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332–353, 2010. doi: 10.1198/jcgs.2010.08111.

R. A. Fisher. The use of multiple measurements in taxonomic problems. *Annals of Eugenics*, 7(3):179–188, 1936. doi: 10.1111/j.1469-1809.1936.tb02137.x.

C. Fraley, A. Raftery, and R. Wehrens. Incremental model-based clustering for large datasets with small clusters. *Journal of Computational and Graphical Statistics*, 14(3):529–546, 2005. doi: 10.1198/106186005X59603.

C. Fraley, A. E. Raftery, L. Scrucca, T. B. Murphy, and M. Fop. *mclust: Normal Mixture Modelling for Model-Based Clustering, Classification, and Density Estimation*, 2016. URL `http://CRAN.R-project.org/package=mclust`. R package version 5.1.

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