

rebmix: Finite Mixture Modeling, Clustering & Classification

Marko Nagode

January 24, 2017

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 or Dirac parametric families.

1 Introduction

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

2 What's new in version 2.9.0

This version 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)
```

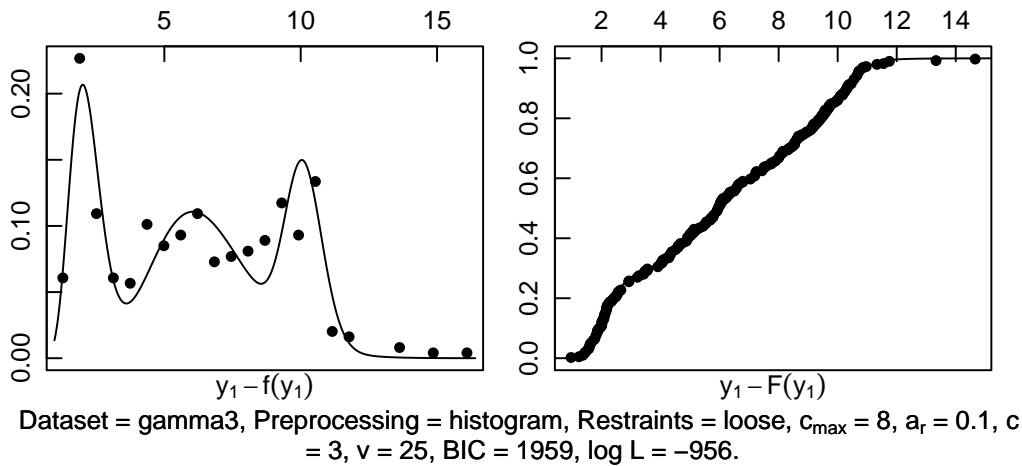


Figure 1: Gamma 3 dataset. Empirical density (circles) and predictive gamma mixture density in black solid line.

3.1.4 Summary and coef methods

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

```
Dataset Preprocessing Criterion c v/k IC logL M
1 gamma2 histogram BIC 2 22 -1336 683 5
Maximum logL = 683 at pos = 1.
```

```
R> coef(gamma1est, pos = 2)
```

```

      comp1 comp2 comp3 comp4
w 0.251 0.249 0.251 0.249
      1
theta1.1 0.0127
theta1.2 0.0111
theta1.3 0.0087
theta1.4 0.0114
      1
theta2.1 159
theta2.2 357
theta2.3 918
theta2.4 520

```

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] 4 3 3 4 3 3 3 3 3 4
Slot "c.se":
 [1] 0.483
Slot "c.cv":
 [1] 0.146
Slot "c.mode":
 [1] 3
Slot "c.prob":
 [1] 0.7

```

```

R> summary(gamma3boot)

```

```

      comp1 comp2 comp3
w.cv 0.0645 0.144 0.145
      1
theta1.1.cv 0.409
theta1.2.cv 0.828
theta1.3.cv 0.436
      1
theta2.1.cv 1.893
theta2.2.cv 0.673
theta2.3.cv 1.005
Mode probability = 0.7 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

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

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_{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

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

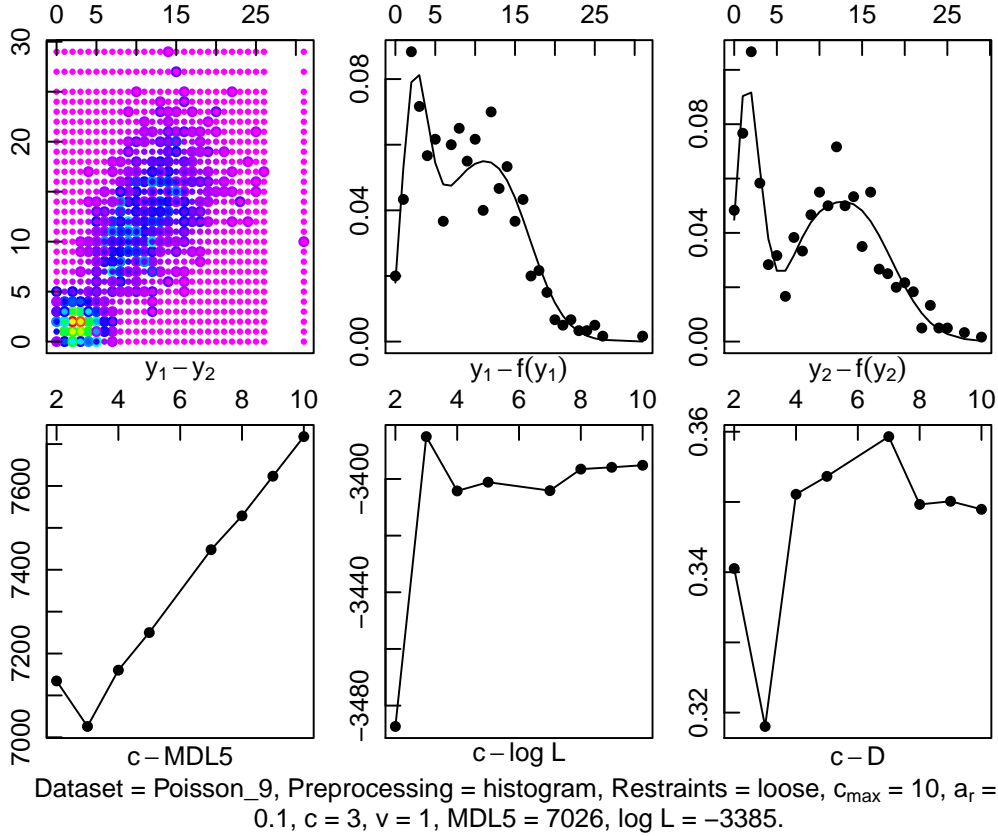


Figure 2: Poisson dataset. Empirical densities (coloured large circles), predictive multivariate Poisson-Poisson mixture density (coloured small circles), empirical densities (circles), predictive univariate marginal Poisson mixture densities and progress charts (solid line).

3.2.4 Clustering

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

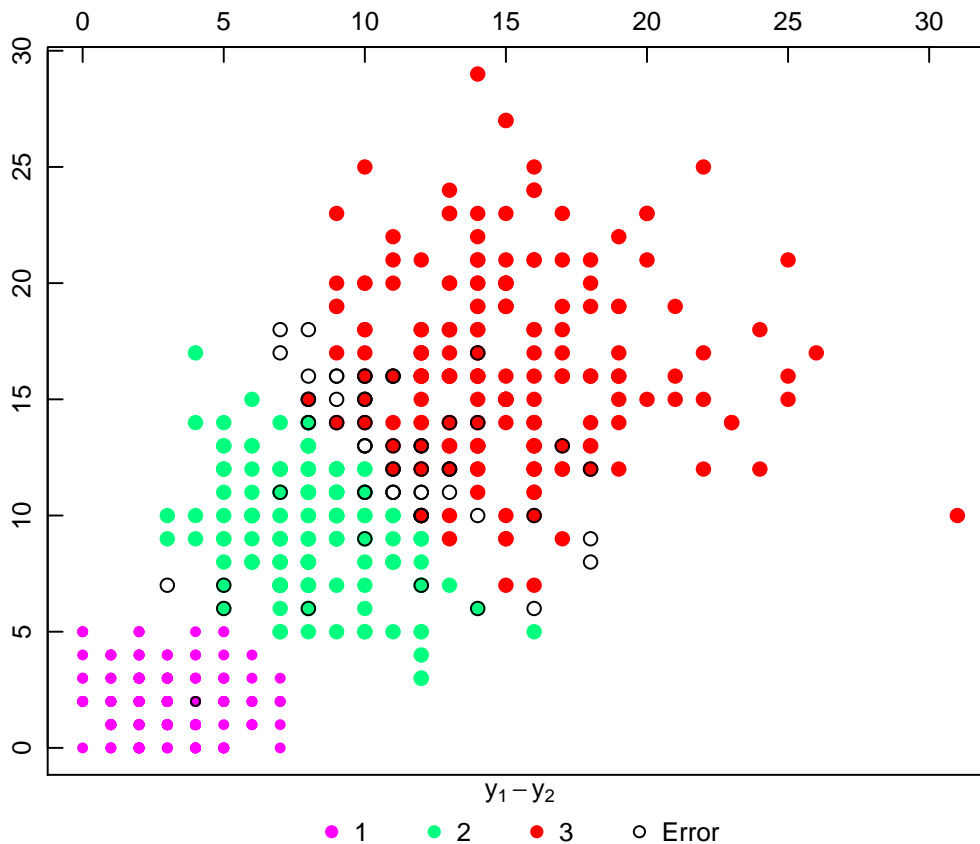


Figure 3: Poisson dataset. Predictive cluster membership (coloured circles), error (black circles).

3.2.5 Summary and coef methods

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

	Dataset	Preprocessing	Criterion	c	v/k	IC	logL	M
1	Poisson_1	histogram	MDL5	2	1	7151	-3496	5
2	Poisson_2	histogram	MDL5	2	1	7222	-3531	5
3	Poisson_3	histogram	MDL5	5	1	7242	-3397	14
4	Poisson_4	histogram	MDL5	3	1	7027	-3386	8
5	Poisson_5	histogram	MDL5	3	1	7132	-3438	8
6	Poisson_6	histogram	MDL5	3	1	7130	-3437	8
7	Poisson_7	histogram	MDL5	3	1	7181	-3462	8
8	Poisson_8	histogram	MDL5	3	1	7072	-3408	8
9	Poisson_9	histogram	MDL5	3	1	7026	-3385	8
10	Poisson_10	histogram	MDL5	2	1	7098	-3469	5

Maximum logL = -3385 at pos = 9.

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

```
comp1 comp2 comp3
w 0.335 0.25 0.415
    1    2
```

```

theta1.1  2.93  2.01
theta1.2  8.25  9.31
theta1.3 13.98 15.46
      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.

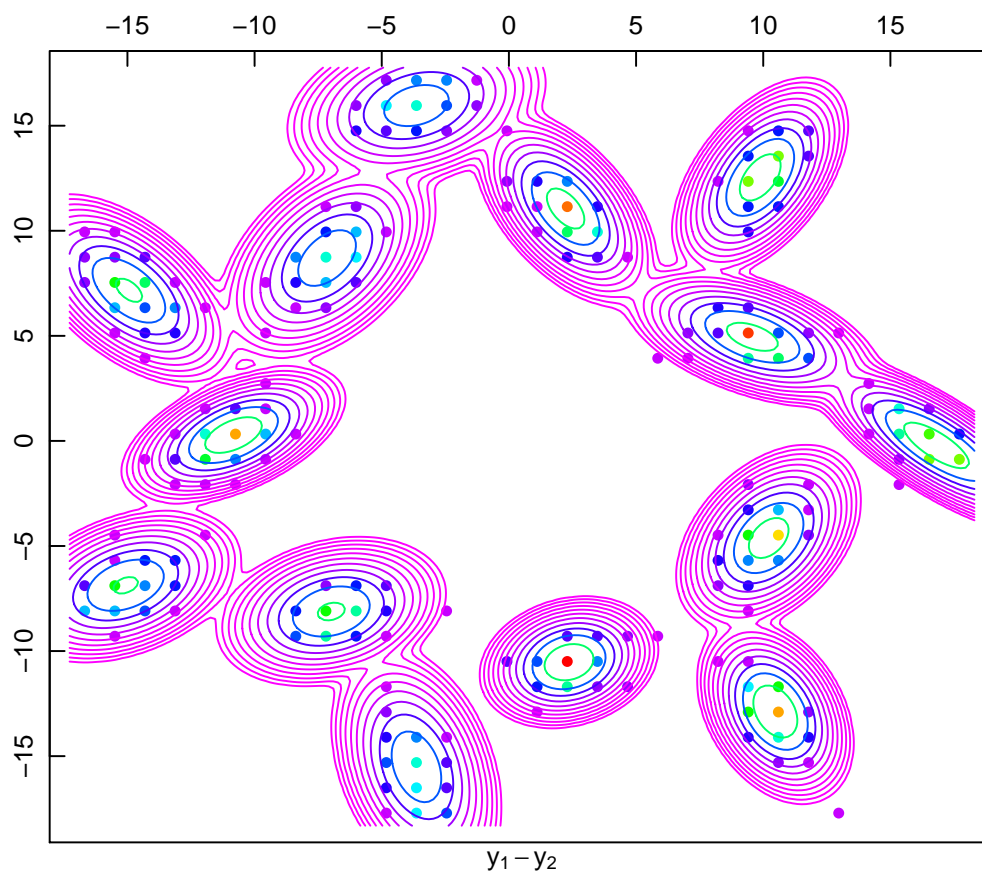
```
R> data("wreath", package = "mclust")
```

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

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



Dataset = dataset1, Preprocessing = histogram, Restraints = loose, $c_{\max} = 20$, $a_r = 0.1$, $c = 14$, $v = 30$, BIC = 11476, log L = -5451.

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

3.3.3 Clustering

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

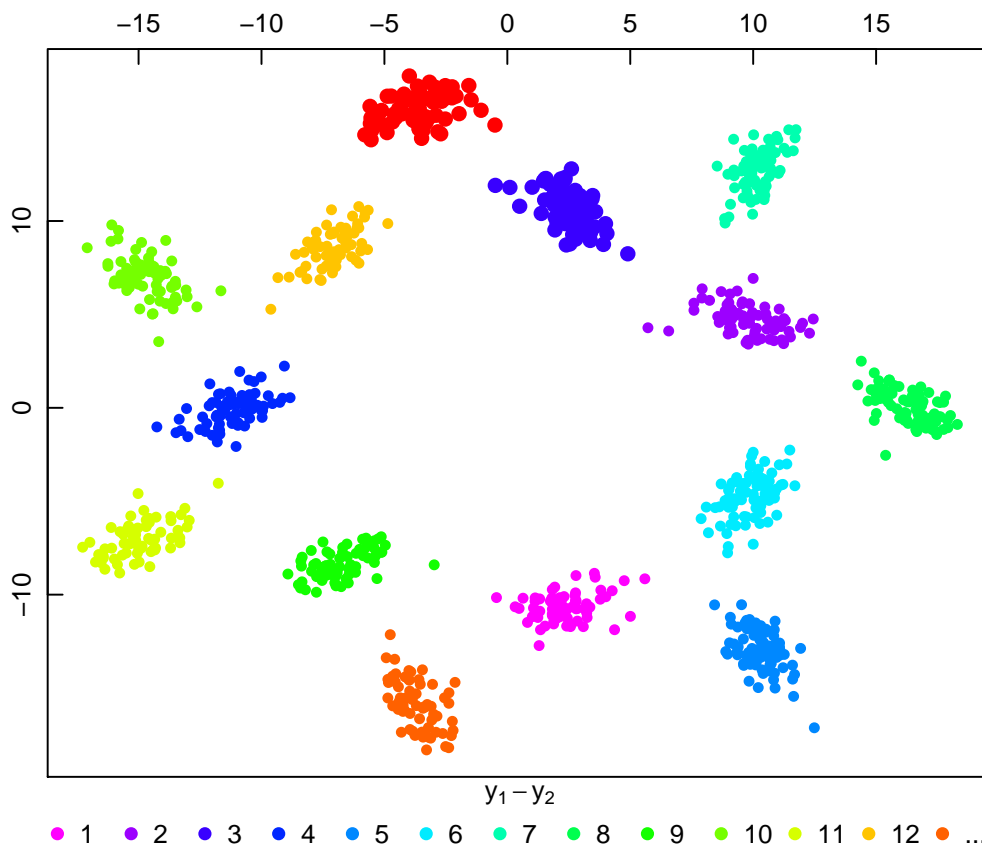


Figure 5: Dataset `wreath`. Predictive cluster membership (coloured circles).

3.3.4 Summary and coef methods

```
R> summary(wreathest)
```

```
Dataset Preprocessing Criterion c v/k IC logL M
1 dataset1 histogram BIC 14 30 11476 -5451 83
Maximum logL = -5451 at pos = 1.
```

```
R> coef(wreathest)
```

```
comp1 comp2 comp3 comp4 comp5 comp6 comp7 comp8 comp9 comp10 comp11
w 0.0684 0.0734 0.0715 0.0744 0.0824 0.0774 0.0774 0.0804 0.0673 0.0703 0.0663
comp12 comp13 comp14
w 0.0633 0.0664 0.0612

      1      2
theta1.1 2.36 -10.529
theta1.2 9.57 4.952
theta1.3 2.23 11.058
theta1.4 -10.83 0.279
theta1.5 10.48 -12.879
theta1.6 10.21 -4.620
theta1.7 9.88 12.540
```

```

theta1.8    16.81  -0.212
theta1.9    -6.98  -8.115
theta1.10   -14.94   7.168
theta1.11   -15.07  -6.869
theta1.12    -7.15   8.702
theta1.13    -3.64 -15.509
theta1.14    -3.64  15.958

          1-1    1-2    2-1    2-2
theta2.1    0.862  0.144  0.144  0.691
theta2.2    1.846 -0.615 -0.615  0.810
theta2.3    0.934 -0.664 -0.664  1.574
theta2.4    1.376  0.541  0.541  0.798
theta2.5    0.661 -0.327 -0.327  1.357
theta2.6    0.954  0.471  0.471  1.425
theta2.7    0.858  0.615  0.615  1.622
theta2.8    1.784 -1.167 -1.167  1.283
theta2.9    1.521  0.289  0.289  0.943
theta2.10   1.349 -0.806 -0.806  1.562
theta2.11   1.537  0.441  0.441  1.013
theta2.12   1.423  0.764  0.764  1.939
theta2.13   0.861 -0.499 -0.499  2.566
theta2.14   2.041  0.437  0.437  1.207

```

3.3.5 Summary method

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

Number of clusters	1	2	3	4	5
From cluster	9	7	11	3	4
To cluster	1	1	1	1	3
Entropy	1.11e-14	5.24e-04	1.55e-03	8.40e-03	1.82e-02
Entropy decrease	0.000524	0.001026	0.006848	0.009838	0.025222
Number of clusters	6	7	8	9	10
From cluster	10	2	5	12	13
To cluster	3	1	1	10	9
Entropy	4.35e-02	6.93e-02	9.56e-02	1.23e-01	1.88e-01
Entropy decrease	0.025846	0.026283	0.027789	0.064156	0.094180
Number of clusters	11	12	13		
From cluster	6	8	14		
To cluster	5	2	3		
Entropy	2.82e-01	3.83e-01	7.05e-01		
Entropy decrease	0.101439	0.321624	0.664999		

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)
```

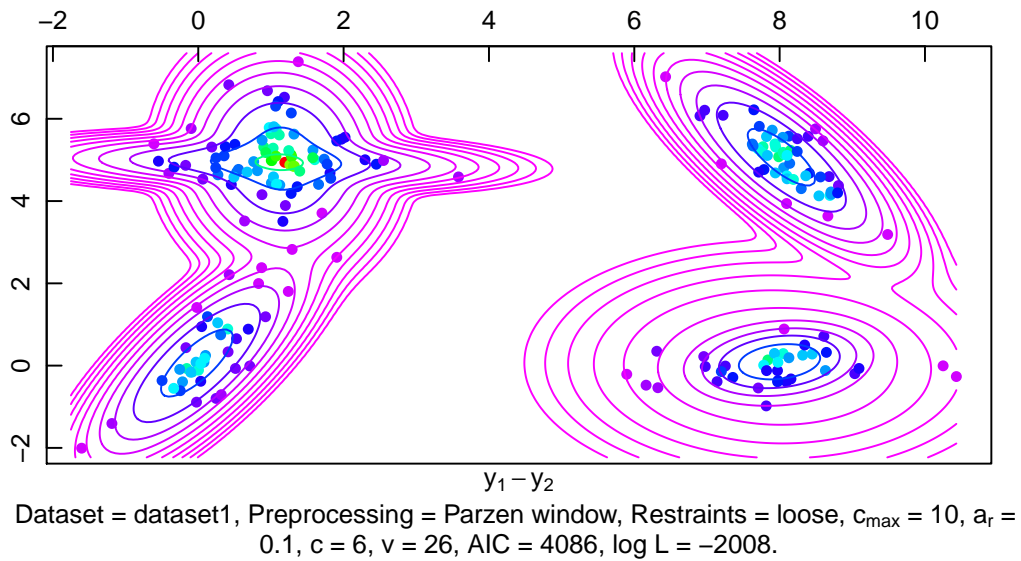


Figure 6: Dataset ex4.1. Empirical densities (coloured circles), predictive multivariate normal mixture density (coloured lines).

3.4.3 Clustering

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

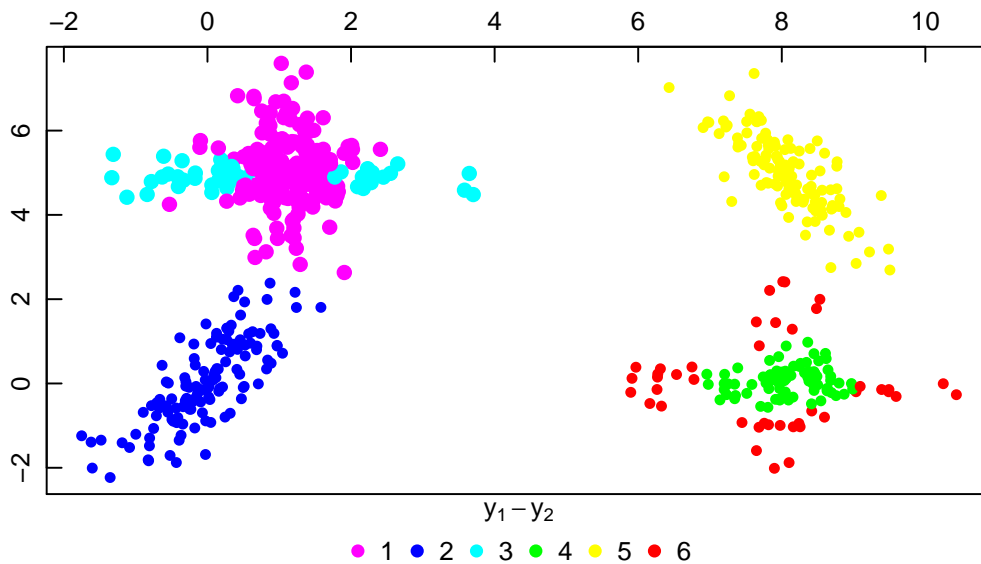


Figure 7: Dataset ex4.1. Predictive cluster membership (coloured circles).

3.4.4 Summary method

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

Dataset	Preprocessing	Criterion	c	v/k	IC	logL	M
---------	---------------	-----------	---	-----	----	------	---

```
1 dataset1 Parzen window      AIC 6  26 4086 -2008 35
Maximum logL = -2008 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 12  1
3  0  2 11
```

Slot "Error":

```
[1] 0.0769
```

Slot "Precision":

```
[1] 1.000 0.923 0.846
```

Slot "Sensitivity":

```
[1] 1.000 0.857 0.917
```

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	12
6	3	2	2
7	1	3	0
8	2	3	1
9	3	3	11

Error = 0.0769.

3.5.4 Plot method

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

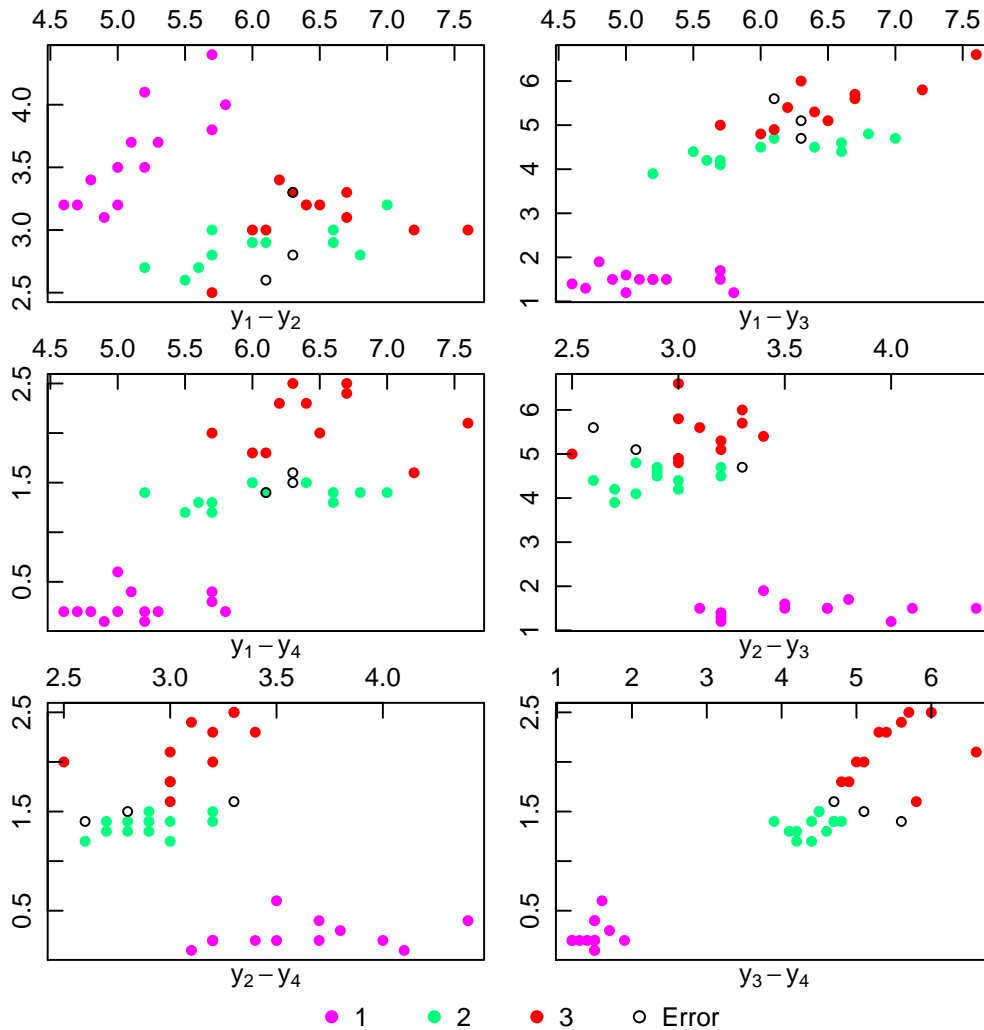


Figure 8: Dataset *iris*. Predictive class membership (coloured circles), error (black circles).

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
```

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 $y_{1j}, y_{2j}, \dots, y_{14j}$.

```
R> adultest <- list()
R> for (i in 1:14) {
+   adultest[[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

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

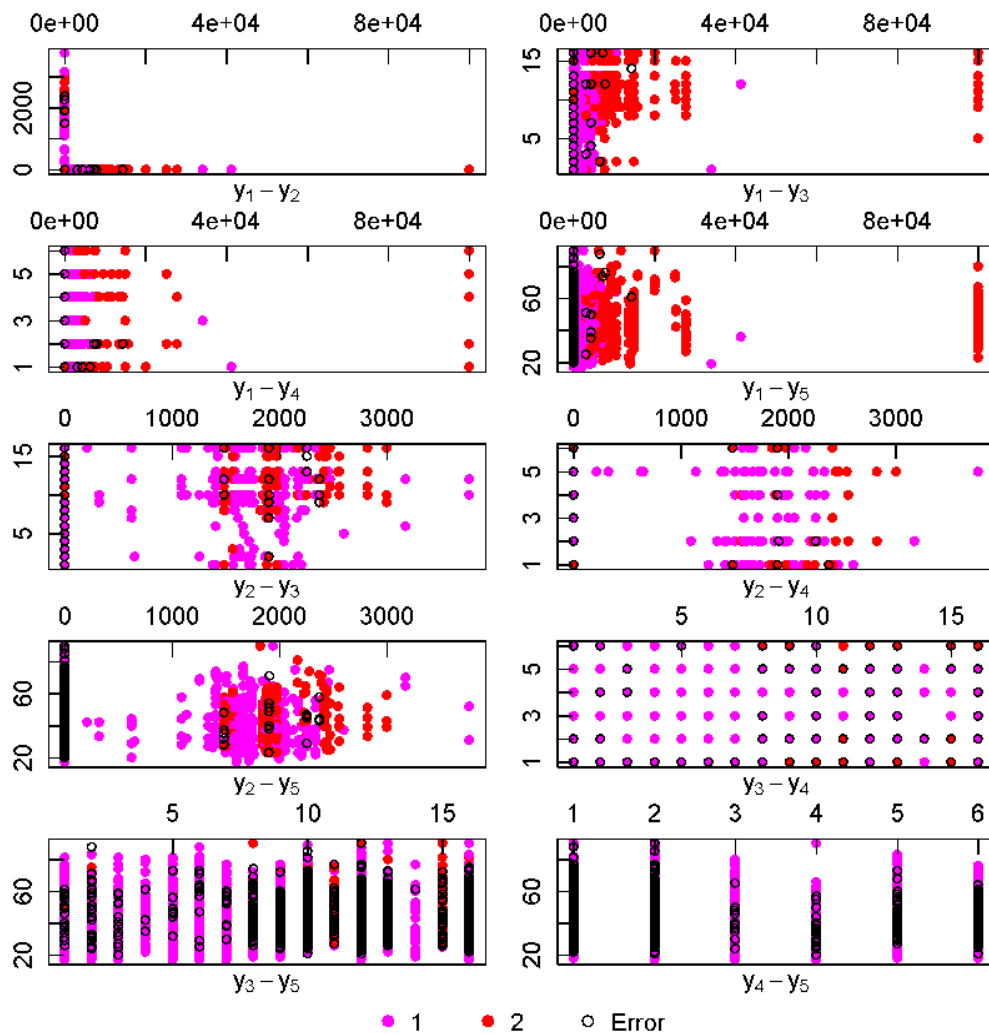


Figure 9: Dataset `adult`. Predictive class membership (coloured circles), error (black circles).

4 Summary

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

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.
- J. Ma, J. Liu, and Z. Ren. Parameter estimation of poisson mixture with automated model selection through by 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. doi: 10.5963/JAO0302001.
- 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.
- 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.