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Rmixmod: The R Package of the Model-Based Unsupervised, Supervised and Semi-Supervised Classification Mixmod Library

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Abstract

Mixmod is a well-established software package for fitting a mixture model of multivariate Gaussian or multinomial probability distribution functions to a given data set with either a clustering, a density estimation or a discriminant analysis purpose. The **Rmixmod** S4 package provides a bridge between the C++ core library of **Mixmod** (**mixmodLib**) and the R statistical computing environment. In this article, we give an overview of the model-based clustering and classification methods, and we show how the R package **Rmixmod** can be used for clustering and discriminant analysis.

Keywords: model-based clustering, discriminant analysis, mixture models, visualization, R, **Rmixmod**.

1. Introduction

Clustering and discriminant analysis (or classification) methods are among the most important techniques in multivariate statistical learning. The goal of cluster analysis is to partition the observations into groups ("clusters") so that the pairwise dissimilarities between observations assigned to the same cluster tend to be smaller than observations in different clusters. The goal of classification is to design a decision function from a learning data set to assign new data to groups *a priori* known. *Mixture modeling* supposes that the data are an *i.i.d.* sample from some population described by a probability density function. This density function is characterized by a parameterized finite mixture of component density functions, each

component modeling one of the clusters. This model is fit to the data by maximum likelihood (Mclachlan and Peel 2000).

The **Mixmod** package (Mixmod Team 2008) is primarily devoted to clustering using mixture modeling and, to a lesser extent, to discriminant analysis (supervised and semi-supervised situations). Many options are available to specify the models and the strategy to be run. **Mixmod** is dealing with 28 multivariate Gaussian mixture models for quantitative data and 10 multivariate multinomial mixture models for qualitative data. Estimation of the mixture parameters is performed via the EM, the Stochastic EM or the Classification EM algorithms. These three algorithms can be chained and initialized in several different ways leading to original strategies (see Section 2.3). The model selection criteria BIC, ICL, NEC and cross-validation are proposed according to the modeling purpose (see Section 2.4 for a brief review).

Mixmod, developped since 2001, is a package written in C++. Its core library (**mixmodLib**) can be interfaced with any other softwares or libraries, or can be used in command line. It has been already interfaced with Scilab and Matlab (Biernacki *et al.* 2006). It was lacking an interface with R (R Development Core Team 2012). The **Rmixmod** package provides a bridge between the C++ core library of **Mixmod** and the R statistical computing environment. Both cluster analysis and discriminant analysis can be now performed using **Rmixmod**. User-friendly outputs and graphs allow for a relevant and nice visualisation of the results.

There exists a wide variety of packages in R dedicated to the estimation of mixture model. Among them let us cite **bgmm** (Biecek *et al.* 2012), **flexmix** (Leisch 2004; Grün and Leisch 2007, 2008), **mclust** (Fraley and Raftery 2007a,b), **mixtools** (Benaglia *et al.* 2009) but none of them offer the large set of possibilities of the newcomer **Rmixmod**.

This paper reviews in Section 2 the Gaussian and multinomial mixture models and the **Mixmod** library. An overview of the **Rmixmod** package is then given in Section 3 through a description of the main function and of other related companion functions. The practical use of this new package is illustrated in Section 4 on toy datasets for model-based clustering in a quantitative and qualitative setting (Section 4.1) and for discriminant analysis (Section 4.2). The last section (Section 5) evokes future works of the **Mixmod** project. The package is available from the Comprehensive R Archive Network at `http://cran.r-project.org/package=Rmixmod`.

2. Overview of the Mixmod library functionalities

2.1. Model-based classifications focus

"X-supervised" classifications

Roughly speaking, the **Mixmod** library is devoted to three kinds of different classification tasks. Its main task is unsupervised classification but supervised and semi-supervised classifications can benefit from its meaningful models, its efficient algorithms and its model selection criteria.

Unsupervised classification Unsupervised classification, called also cluster analysis, is concerned with discovering a group structure in a n by d data matrix $\mathbf{x} = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$ where

$\mathbf{x}_i$ is an individual in $\mathbb{X}_1 \times \ldots \times \mathbb{X}_d$. The space $\mathbb{X}_j$ $(j = 1, \ldots, d)$ depends on the type of data at hand: It is $\mathbb{R}$ for continuous data and it is $\{1, \ldots, m_j\}$ for categorical data with m_j levels. The result provided by clustering is typically a partition $\mathbf{z} = \{\mathbf{z}_1, ..., \mathbf{z}_n\}$ of $\mathbf{x}$ into K groups, $\mathbf{z}_i$'s being indicator vectors or *labels* with $\mathbf{z}_i = (z_{i1}, \ldots, z_{iK})$, $z_{ik} = 1$ or 0, according to the fact that $\mathbf{x}_i$ belongs to the kth group or not.

Supervised classification In discriminant analysis, data are composed by n observations $\mathbf{x} = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$ $(\mathbf{x}_i \in \mathbb{X}_1 \times \ldots \times \mathbb{X}_d)$ and a partition of $\mathbf{x}$ into K groups defined with the labels $\mathbf{z}$. The aim is to estimate the group $\mathbf{z}_{n+1}$ of any new individual $\mathbf{x}_{n+1}$ of $\mathbb{X}_1 \times \ldots \times \mathbb{X}_d$ with unknown label. Discriminant analysis in **Mixmod** is divided into two steps. The first step consists of a classification rule from the training data set $(\mathbf{x}, \mathbf{z})$. The second step consists of assigning the other observations to one of the groups.

Semi-supervised classification Usually all the labels $\mathbf{z}_i$ are completely unknown (unsupervised classification) or completely known (supervised classification). Nevertheless, partial labeling of data is possible, and it leads to the so-called semi-supervised classification. The **Mixmod** library handles situations where the data set $\mathbf{x}$ is divided into two subsets $\mathbf{x} = (\mathbf{x}^\ell, \mathbf{x}^u)$ where $\mathbf{x}^\ell = \{\mathbf{x}_1, ..., \mathbf{x}_g\}$ $(1 \leq g \leq n)$ are units with known labels $\mathbf{z}^\ell = \{\mathbf{z}_1, ..., \mathbf{z}_g\}$, and $\mathbf{x}^u = \{\mathbf{x}_{g+1}, ..., \mathbf{x}_n\}$ units with unknown labels $\mathbf{z}^u = \{\mathbf{z}_{g+1}, ..., \mathbf{z}_n\}$.

Usually, semi-supervised classification is concerned by the supervised classification purpose and it aims to estimate the group $\mathbf{z}_{n+1}$ of any new individual $\mathbf{x}_{n+1}$ of $\mathbb{X}_1 \times \ldots \times \mathbb{X}_d$ with unknown label by taking profit of the unlabeled data of the learning set.

Model-based classifications

The model-based point of view allows to consider all previous classification tasks in a unified manner.

Mixture models Let $\mathbf{x} = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$ be n independent vectors in $\mathbb{X}_1 \times \ldots \times \mathbb{X}_d$, where each $\mathbb{X}_j$ denotes some measurable space, and such that each $\mathbf{x}_i$ arises from a mixture probability distribution with density

$$f(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{k=1}^{K} p_k h(\mathbf{x}_i|\boldsymbol{\alpha}_k) \tag{1}$$

where the p_k's are the mixing proportions $(0 < p_k < 1$ for all $k = 1, ..., K$ and $p_1 + ... + p_K = 1)$, $h(\cdot|\boldsymbol{\alpha}_k)$ denotes a d-dimensional distribution parameterized by $\boldsymbol{\alpha}_k$. As we will see below, h is for instance the density of a Gaussian distribution with mean $\boldsymbol{\mu}_k$ and variance matrix Σ_k and, thus, $\boldsymbol{\alpha}_k = (\boldsymbol{\mu}_k, \Sigma_k)$. The whole vector parameter (to be estimated) of f is denoted by $\boldsymbol{\theta} = (p_1, \ldots, p_K, \boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_K)$.

Label estimation From a generative point of view, drawing the sample $\mathbf{x}$ from the mixture distribution f requires previously to draw a sample of labels $\mathbf{z} = \{\mathbf{z}_1, ..., \mathbf{z}_n\}$, with $\mathbf{z}_i = (z_{i1}, \ldots, z_{iK})$, $z_{ik} = 1$ or 0, according to the fact that $\mathbf{x}_i$ is arising from the kth mixture component or not. Depending of the fact that the sample $\mathbf{z}$ is completely unknown, completely known or only partially known, we retrieve respectively an unsupervised, a supervised or a semi-supervised classification problem. Mixture models are particularly well-suited for

modeling these different standard situations since an estimate of any label $\mathbf{z}_i$ ($i = 1, \ldots, n$ for unsupervised classification, $i = n + 1$ for supervised or semi-supervised classification) can be easily obtained by the following so-called *Maximum A posteriori* (MAP) rule

$$\hat{\mathbf{z}}(\boldsymbol{\theta}) = \text{MAP}(\mathbf{t}(\boldsymbol{\theta})) \quad \Leftrightarrow \quad \hat{z}_{ik}(\boldsymbol{\theta}) = \begin{cases} 1 & \text{if } k = \arg\max_{k' \in \{1,\ldots,K\}} t_{ik'}(\boldsymbol{\theta}) \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

where $\mathbf{t}(\boldsymbol{\theta}) = \{t_{ik}(\boldsymbol{\theta})\}$, $t_{ik}(\boldsymbol{\theta})$ denoting the following conditional probability that the observation $\mathbf{x}_i$ arises from the group $\mathbf{z}_i$:

$$t_{ik}(\boldsymbol{\theta}) = \frac{p_k h(\mathbf{x}_i|\boldsymbol{\alpha}_k)}{f(\mathbf{x}_i|\boldsymbol{\theta})}. \tag{3}$$

2.2. Parsimonious and meaningful models

The **Mixmod** library proposes many parsimonious and meaningful models, depending on the type of variables to be considered. Such models provide simple interpretation of groups.

Continuous variables: Fourteen Gaussian models

In the Gaussian mixture model, each $\mathbf{x}_i$ is assumed to arise independently from a mixture of d-dimensional Gaussian density with mean $\boldsymbol{\mu}_k$ and variance matrix Σ_k. In this case we have in Equation (1), with $\boldsymbol{\alpha}_k = (\boldsymbol{\mu}_k, \Sigma_k)$,

$$h(\mathbf{x}_i|\boldsymbol{\alpha}_k) = (2\pi)^{-d/2}|\Sigma_k|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \Sigma_k^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_k)\right\}. \tag{4}$$

Thus, clusters associated to the mixture components are ellipsoidal, centered at the means $\boldsymbol{\mu}_k$ and the variance matrices Σ_k determine their geometric characteristics.

Following Banfield and Raftery (1993) and Celeux and Govaert (1995), we consider a parameterization of the variance matrices of the mixture components consisting of expressing the variance matrix Σ_k in terms of its eigenvalue decomposition

$$\Sigma_k = \lambda_k D_k A_k D_k^\top \tag{5}$$

where $\lambda_k = |\Sigma_k|^{1/d}$, D_k is the matrix of eigenvectors of Σ_k and A_k is a diagonal matrix, such that $|A_k| = 1$, with the normalized eigenvalues of Σ_k on the diagonal in a decreasing order. The parameter λ_k determines the *volume* of the kth cluster, D_k its *orientation* and A_k its *shape*. By allowing some but not all of these quantities to vary between clusters, we obtain parsimonious and easily interpreted models which are appropriate to describe various group situations (see Table 1). More explanations about notation used in this table are given below.

The general family First, we can allow the volumes, the shapes and the orientations of clusters to vary or to be equal between clusters. Variations on assumptions on the parameters λ_k, D_k and A_k ($1 \leq k \leq K$) lead to eight general models of interest. For instance, we can assume different volumes and keep the shapes and orientations equal by requiring that $A_k = A$ (A unknown) and $D_k = D$ (D unknown) for $k = 1, \ldots, K$. We note this model $[\lambda_k DAD^\top]$ (or, shortly, $[\lambda_k C]$ where $C = DAD^\top$). With this convention, writing $[\lambda D_k A D_k^\top]$ means that we consider the mixture model with equal volumes, equal shapes and different orientations.

model	number of parameters	M step	**Rmixmod** model name
$[\lambda DAD^\top]$	$\alpha+\beta$	CF	`"Gaussian_*_L_C"`
$[\lambda_k DAD^\top]$	$\alpha+\beta+K-1$	IP	`"Gaussian_*_Lk_C"`
$[\lambda DA_k D^\top]$	$\alpha+\beta+(K-1)(d-1)$	IP	`"Gaussian_*_L_D_Ak_D"`
$[\lambda_k DA_k D^\top]$	$\alpha+\beta+(K-1)d$	IP	`"Gaussian_*_Lk_D_Ak_D"`
$[\lambda D_k AD_k^\top]$	$\alpha+K\beta-(K-1)d$	CF	`"Gaussian_*_L_Dk_A_Dk"`
$[\lambda_k D_k AD_k^\top]$	$\alpha+K\beta-(K-1)(d-1)$	IP	`"Gaussian_*_Lk_Dk_A_Dk"`
$[\lambda D_k A_k D_k^\top]$	$\alpha+K\beta-(K-1)$	CF	`"Gaussian_*_L_Ck"`
$[\lambda_k D_k A_k D_k^\top]$	$\alpha+K\beta$	CF	`"Gaussian_*_Lk_Ck"`
$[\lambda B]$	$\alpha+d$	CF	`"Gaussian_*_L_B"`
$[\lambda_k B]$	$\alpha+d+K-1$	IP	`"Gaussian_*_Lk_B"`
$[\lambda B_k]$	$\alpha+Kd-K+1$	CF	`"Gaussian_*_L_Bk"`
$[\lambda_k B_k]$	$\alpha+Kd$	CF	`"Gaussian_*_Lk_Bk"`
$[\lambda I]$	$\alpha+1$	CF	`"Gaussian_*_L_I"`
$[\lambda_k I]$	$\alpha+K$	CF	`"Gaussian_*_Lk_I"`

Table 1: Some characteristics of the 14 models. We have $\alpha = Kd+K-1$, * = pk in the case of free proportions and $\alpha = Kd$, * = p in the case of equal proportions, and $\beta = \frac{d(d+1)}{2}$; CF means that the M step is closed form, IP means that the M step needs an iterative procedure.

The diagonal family Another family of interest consists of assuming that the variance matrices Σ_k are diagonal. In the parameterization (5), it means that the orientation matrices D_k are permutation matrices. We write $\Sigma_k = \lambda_k B_k$ where B_k is a diagonal matrix with $|B_k| = 1$. This particular parameterization gives rise to four models: $[\lambda B]$, $[\lambda_k B]$, $[\lambda B_k]$ and $[\lambda_k B_k]$.

The spherical family The last family of models consists of assuming spherical shapes, namely $A_k = I$, I denoting the identity matrix. In such a case, two parsimonious models are in competition: $[\lambda I]$ and $[\lambda_k I]$.

Remark The **Mixmod** library provides also some Gaussian models devoted to high dimensional data. We do not describe them here since they are not yet available in the **Rmixmod** package but the reader can refer to the **Mixmod** website[1] for further informations.

Categorical variables: Five multinomial models

We consider now that the data are n objects described by d categorical variables, with respective number of levels $m_1, \ldots, m_d$. The data can be represented by n binary vectors $\mathbf{x}_i = (x_i^{jh}; j = 1, \ldots, d; h = 1, \ldots, m_j)$ $(i = 1, \ldots, n)$ where $x_i^{jh} = 1$ if the object i belongs to the level h of the variable j and 0 otherwise. Denoting $m = \sum_{j=1}^{d} m_j$ the total number of levels, the data matrix $\mathbf{x} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ has n rows and m columns. Binary data can be seen as a particular case of categorical data with d dichotomous variables, *i.e.,* $m_j = 2$ for any $j = 1, \ldots, d$.

The latent class model assumes that the d categorical variables are independent given the latent variable: Each $\mathbf{x}_i$ arises independently from a mixture of multivariate multinomial

[1] `http://www.mixmod.org/`

distributions (Everitt 1984). In this case we have in Equation (1)

$$h(\mathbf{x}_i|\boldsymbol{\alpha}_k) = \prod_{j=1}^{d}\prod_{h=1}^{m_j}(\alpha_k^{jh})^{x_i^{jh}} \tag{6}$$

with $\boldsymbol{\alpha}_k = (\alpha_k^{jh}; j = 1,\ldots,d; h = 1,\ldots,m_j)$. In (6), we recognize the product of d conditionally independent multinomial distributions of parameters $\boldsymbol{\alpha}_k^j = (\alpha_k^{j1},\ldots,\alpha_k^{jm_j})$. This model may present problems of identifiability (see for instance Goodman 1974) but most situations of interest are identifiable (Allman *et al.* 2009).

In order to propose more parsimonious models, we present the following extension of the parameterization of Bernoulli distributions used by Celeux and Govaert (1991a) for clustering and also by Aitchison and Aitken (1976) for kernel discriminant analysis. The basic idea is to impose the vector $\boldsymbol{\alpha}_k^j$ to have a unique modal value for one of its components, the other components sharing uniformly the remaining mass probability. Thus, $\boldsymbol{\alpha}_k^j$ takes the form $(\beta_k^j,\ldots,\beta_k^j,\gamma_k^j,\beta_k^j,\ldots,\beta_k^j)$ with $\gamma_k^j > \beta_k^j$. Since $\sum_{h=1}^{m_j}\alpha_k^{jh} = 1$, we have $(m_j-1)\beta_k^j + \gamma_k^j = 1$ and, consequently, $\beta_k^j = (1-\gamma_k^j)/(m_j-1)$. The constraint $\gamma_k^j > \beta_k^j$ becomes finally $\gamma_k^j > 1/m_j$. Equivalently and meaningfully, the vector $\boldsymbol{\alpha}_k^j$ can be reparameterized by a center $\mathbf{a}_k^j$ and a dispersion ε_k^j around this center with the following decomposition:

- **Center:** $\mathbf{a}_k^j = (a_k^{j1},\ldots,a_k^{jm_j})$ where $a_k^{jh} = 1$ if h is to the rank of γ_k^j (in the following, this rank will be noted $h(k,j)$), 0 otherwise;
- **Dispersion:** $\varepsilon_k^j = 1-\gamma_k^j$ the probability that the data $\mathbf{x}_i$, arising from the kth component, are such that $x_i^{jh(k,j)} \neq 1$.

Thus, it allows us to give an interpretation similar to the center and the variance matrix used for continuous data in the Gaussian mixture context. Since, the relationship between the initial parameterization and the new one is given by:

$$\alpha_k^{jh} = \begin{cases} 1-\varepsilon_k^j & \text{if } h = h(k,j) \\ \varepsilon_k^j/(m_j-1) & \text{otherwise,} \end{cases} \tag{7}$$

Equation (6) can be rewritten with $\mathbf{a}_k = (\mathbf{a}_k^j; j = 1,\ldots,d)$ and $\boldsymbol{\varepsilon}_k = (\varepsilon_k^j; j = 1,\ldots,d)$

$$h(\mathbf{x}_i|\boldsymbol{\alpha}_k) = \tilde{h}(\mathbf{x}_i|\mathbf{a}_k,\varepsilon_k) = \prod_{j=1}^{d}\prod_{h=1}^{m_j}\left((1-\varepsilon_k^j)^{a_k^{jh}}(\varepsilon_k^j/(m_j-1))^{1-a_k^{jh}}\right)^{x_i^{jh}}. \tag{8}$$

In the following, this model will be noted $[\varepsilon_k^j]$. In this context, three other models can be defined. We note $[\varepsilon_k]$ the model where ε_k^j is independent of the variable j, $[\varepsilon^j]$ the model where ε_k^j is independent of the component k and, finally, $[\varepsilon]$ the model where ε_k^j is independent of both the variable j and the component k. In order to maintain some unity in the notation, we will note also $[\varepsilon_k^{jh}]$ the most general model introduced at the previous section. The number of free parameters associated to each model is given in Table 2.

2.3. Efficient maximum "X-likelihood" estimation strategies

model	number of parameters	**Rmixmod** model name
$[\varepsilon]$	$\delta + 1$	`"Binary_*_E"`
$[\varepsilon^j]$	$\delta + d$	`"Binary_*_Ej"`
$[\varepsilon_k]$	$\delta + K$	`"Binary_*_Ek"`
$[\varepsilon_k^j]$	$\delta + Kd$	`"Binary_*_Ekj"`
$[\varepsilon_k^{jh}]$	$\delta + K\sum_{j=1}^{d}(m_j - 1)$	`"Binary_*_Ekjh"`

Table 2: Number of free parameters of the five multinomial models. We have $\delta = K - 1$, * = pk in the case of free proportions and $\delta = 0$, * = p in the case of equal proportions.

EM and EM-like algorithms focus

Estimation of the mixture parameter is performed either through maximization of the log-likelihood (ML) on $\boldsymbol{\theta}$

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{n} \ln f(\mathbf{x}_i|\boldsymbol{\theta}) \tag{9}$$

via the EM algorithm (*Expectation Maximization,* Dempster *et al.* 1997), the SEM algorithm (*Stochastic EM,* Celeux and Diebolt 1985) or through maximization of the completed log-likelihood on both $\boldsymbol{\theta}$ and $\mathbf{z}$

$$L_c(\boldsymbol{\theta}, \mathbf{z}) = \sum_{i=1}^{n}\sum_{k=1}^{K} z_{ik} \ln(p_k h(\mathbf{x}_i|\boldsymbol{\alpha}_k)), \tag{10}$$

via the CEM algorithm (*Clustering EM,* Celeux and Govaert 1992). We now describe these three algorithms at iteration q. The choice of the starting parameter $\boldsymbol{\theta}^{\{0\}}$ and of the stopping rules are both described later.

The EM algorithm It consists of repeating the following E and M steps:

- **E step:** Compute the conditional probabilities $\mathbf{t}(\boldsymbol{\theta}^{\{q\}})$ (see Equation 3).
- **M step:** Compute the parameter $\boldsymbol{\theta}^{\{q+1\}} = \text{argmax}_{\boldsymbol{\theta}}\, L_c(\boldsymbol{\theta}, \mathbf{t}(\boldsymbol{\theta}^{\{q\}}))$ (see Equation 10). Mixture proportions are given by $p_k^{\{q+1\}} = \sum_{i=1}^{n} t_{ik}(\boldsymbol{\theta}^{\{q\}})/n$. Detailed formula of other parameters $\boldsymbol{\alpha}^{\{q+1\}}$ depend on the model at hand and are given in the reference manual of **Mixmod** (Mixmod Team 2008).

The SEM algorithm It is a stochastic version of EM incorporating between the E and M steps a so-called S step restoring stochastically the unknown labels $\mathbf{z}$:

- **E step:** Like EM.
- **S step:** Draw labels $\mathbf{z}^{\{q\}}$ from $\mathbf{t}(\boldsymbol{\theta}^{\{q\}})$ with $\mathbf{z}_i^{\{q\}} \sim \text{multinomial}(t_{i1}(\boldsymbol{\theta}^{\{q\}}), \ldots, t_{iK}(\boldsymbol{\theta}^{\{q\}}))$.
- **M step:** Like EM but $\mathbf{t}(\boldsymbol{\theta}^{\{q\}})$ is replaced by $\mathbf{z}^{\{q\}}$.

It is important to notice that SEM does not converge pointwise. It generates a Markov chain whose stationary distribution is more or less concentrated around the ML estimate. A natural estimate from a SEM sequence $(\boldsymbol{\theta}^{\{q\}})_{q=1,\ldots,Q}$ of length Q is either the mean $\sum_{q=Q^-,\ldots,Q} \boldsymbol{\theta}^{\{q\}}/(Q-Q^-)$ (the first Q^- burning iterates are discarded) or the parameter value leading to the highest log-likelihood in the whole dequence.

The CEM algorithm It incorporates a classification step between the E and M steps of EM, restoring by a MAP the unknown labels $\mathbf{z}$:

- **E step:** Like EM.
- **C step:** Choose the most probable labels $\hat{\mathbf{z}}(\boldsymbol{\theta}^{\{q\}}) = \text{MAP}(\mathbf{t}(\boldsymbol{\theta}^{\{q\}}))$.
- **M step:** Like EM where $\mathbf{t}(\boldsymbol{\theta}^{\{q\}})$ is replaced by $\hat{\mathbf{z}}(\boldsymbol{\theta}^{\{q\}})$.

CEM leads to inconsistent estimates (Bryant and Williamson 1978; Mclachlan and Peel 2000, Section 2.21) but has faster convergence that EM since it converges with a finite number of iterations. It allows also to retrieve and generalize standard K-means like criteria both in the continuous case (Govaert 2009, Chap. 8) and in the categorical case (Celeux and Govaert 1991b).

Remark on the partial labelling case **Mixmod** allows partial labelling for all algorithms: It is straightforward since known labels $\mathbf{z}^l$ remain fixed in the E step for all of them. In that case the log-likelihood is expressed by

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{g} \ln f(\mathbf{x}_i|\boldsymbol{\theta}) + \sum_{i=g+1}^{n} \sum_{k=1}^{K} z_{ik} \ln(p_k h(\mathbf{x}_i|\boldsymbol{\alpha}_k)) \tag{11}$$

and the completed log-likelihood, noted now $L_c(\boldsymbol{\theta}, \mathbf{z}^u)$, is unchanged.

Remark on duplicated units In some cases, it arises that some units are duplicated. Typically, it happens when the number of possible values for the units is low in regard to the sample size. To avoid entering unnecessarily large lists of units, it is also possible to specify a weight w_i for each unit $\mathbf{y}_i$ $(i = 1, \ldots, r)$. The set $\mathbf{y}^w = \{(\mathbf{y}_1, w_1), \ldots, (\mathbf{y}_r, w_r)\}$ is strictly equivalent to the set with eventual replications $\mathbf{x} = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$, and we have the relation $n = w_1 + \ldots + w_r$.

Remark on spurious solutions In the Gaussian case, some solutions with (finite) high log-likelihood value can be uninteresting for the user since they correspond to ill-conditionned estimate covariance matrices for some mixture components. It corresponds to so-called *spurious situations* (Mclachlan and Peel 2000, Section 3.10 and 3.11). As far as we know such spurious solutions cannot be detected automatically and have to be discarded by hand.

Strategies for using EM and CEM

Both likelihood and completed likelihood functions usually suffer from multiple local maxima where EM and CEM algorithms can be trapped. Slow evolution of the objective function can be also encountered sometimes during a long period for some runs, in particular with EM.

Notice that SEM is not concerned by local maxima since it does not converge pointwise but slow evolution towards the stationary distribution cannot be excluded in some cases.

In order to avoid such drawbacks, **Mixmod** can act in three ways: Chained algorithms, starting strategies and stopping rules. More details can be found in the **Mixmod** reference manual (Mixmod Team 2008).

Chained algorithms strategies The three algorithms EM, CEM and SEM can be chained to obtain original fitting strategies (*e.g.,* CEM then EM with results of CEM) taking advantage of each of them in the estimation process.

Initialization strategies The available procedures of initialization are:

- `"random"`: Initialization from a random position is a standard way to initialize an algorithm. This random initial position is obtained by choosing at random centers in the data set. This simple strategy is repeated several times from different random positions and the position maximizing the likelihood or the completed lilkelihood is selected.
- `"smallEM"`: A predefined number of EM iterations is split into several short runs of EM launched from random positions. By a short run of EM, we mean that we do not wait for complete convergence but we stop it as soon as the log-likelihood growth is small in comparison to a predefined crude threshold (see details in Biernacki *et al.* 2003). Indeed, it appears that repeating runs of EM is generally profitable since using a single run of EM can often lead to suboptimal solutions.
- `"CEM"`: A given number of repetitions of a given number of iterations of the CEM algorithm are run. One advantage of initializing an algorithm with CEM lies in the fact that CEM converges generally in a small number of iterations. Thus, without consuming a large amount of CPU times, several runs of CEM are performed. Then EM (or CEM) is run with the best solution among all repetitions.
- `"SEMMax"`: A run of a given number of SEM iterations. The idea is that a SEM sequence is expected to enter rapidly in the neighborhood of the global maximum of the likelihood function.

Stopping rules strategies They are two ways to stop an algorithm:

- `"nbIterationInAlgo"`: All algorithms can be stopped after a pre-defined number of iterations.
- `"epsilonInAlgo"`: EM and CEM can be stopped when the relative change of the criterion at hand (L or L_c) is small.

2.4. Purpose dependent model selection

It is of high interest to automatically select a model or the number K of mixture components. However, choosing a sensible mixture model is highly dependent on the modeling purpose.

Before describing these criteria, it can be noted that if no information on K is available, it is recommended to vary it between 1 and the smallest integer larger than $n^{0.3}$ (Bozdogan 1993).

Density estimation

In a density estimation perspective, the BIC criterion must be preferred. It consists of choosing the model and/or K minimizing

$$\text{BIC} = -2L(\hat{\boldsymbol{\theta}}) + \nu \ln n \tag{12}$$

with $\hat{\boldsymbol{\theta}}$ the ML estimate and with ν the number of parameters to estimate. BIC is an asymptotic approximation of the integrated likelihood, valid under regularity conditions, and has been proposed by Schwarz (1978). Despite the fact that those regularity conditions are not fulfilled for mixtures, it has been proved that the criterion BIC is consistent if the likelihood remains bound (Keribin 2000) and has been proved to be efficient on a practical ground (see for instance Fraley and Raftery 1998).

Unsupervised classification

In the unsupervised setting, three criteria are available: BIC, ICL and NEC. But in a full cluster analysis perspective, ICL and NEC can provide more parsimonious answers.

The integrated likelihood does not take into account the ability of the mixture model to give evidence for a clustering structure of the data. An alternative is to consider the integrated completed likelihood. Asymptotic considerations lead to the ICL criterion to be minimized (Biernacki *et al.* 2000):

$$\begin{aligned} \text{ICL} &= -2L_c(\hat{\boldsymbol{\theta}}, \mathbf{t}(\hat{\boldsymbol{\theta}})) + \nu \ln n & (13)\\ &= \text{BIC} - 2\sum_{i=1}^{n}\sum_{k=1}^{K} t_{ik}(\hat{\boldsymbol{\theta}}) \ln t_{ik}(\hat{\boldsymbol{\theta}}) & (14) \end{aligned}$$

Notice that both expressions of ICL above allow to consider ICL either as L_c penalized by the model complexity or as BIC penalized by an entropy term measuring the mixture component overlap.

The NEC criterion measures the ability of a mixture model to provide well-separated clusters and is derived from a relation highlighting the differences between the maximum likelihood approach and the classification maximum likelihood approach to the mixture problem. It is defined by

$$\text{NEC}_K = \begin{cases} \frac{-\sum_{i=1}^{n}\sum_{k=1}^{K} t_{ik}(\hat{\boldsymbol{\theta}}_K) \ln t_{ik}(\hat{\boldsymbol{\theta}}_K)}{L(\hat{\boldsymbol{\theta}}_K) - L(\hat{\boldsymbol{\theta}}_1)} & \text{if } K > 1 \\ 1 & \text{otherwise} \end{cases} \tag{15}$$

with $\hat{\boldsymbol{\theta}}_K$ the ML estimate of $\boldsymbol{\theta}$ for K components. The index K is used to highlight that NEC is essentially devoted to choose the number of mixture components K, not the model parameterization (Celeux and Soromenho 1996; Biernacki *et al.* 1999). The chosen value of K corresponds to the lower value of NEC.

Supervised classification

In the supervised setting, note that only the model (not the number of mixture components) has to be selected. Two criteria are proposed in this situation: BIC and cross-validation. For

BIC, the completed log-likelihood (10), where $\mathbf{z}$ is fixed to its known value, has to be used. The cross-validation criterion (CV) is valid only in the discriminant analysis (supervised) context.The model leading to the highest CV criterion value is selected. Cross validation is a resampling method which can be summarized as follows: Consider random splits of the whole data set $(\mathbf{x}, \mathbf{z})$ into V independent datasets $(\mathbf{x}, \mathbf{z})^{(1)}, \ldots, (\mathbf{x}, \mathbf{z})^{(V)}$ of approximatively equal sizes $n_1, \ldots, n_V$. (If n/V is an integer h, we have $n_1 = \ldots = n_V = h$.) The CV criterion is then defined by

$$\mathrm{CV} = \frac{1}{n} \sum_{v=1}^{V} \sum_{i \in I_v} \delta(\hat{\mathbf{z}}_i(\hat{\boldsymbol{\theta}}^{(v)}), \mathbf{z}_i) \tag{16}$$

where I_v denotes the indexes i of data included in $(\mathbf{x}, \mathbf{z})^{(v)}$, δ corresponds to the 0-1 cost and $\hat{\mathbf{z}}_i(\hat{\boldsymbol{\theta}}^{(v)})$ denotes the group to which $\mathbf{x}_i$ is assigned when designing the assignment rule from the entire data set $(\mathbf{x}, \mathbf{z})$ without $(\mathbf{x}, \mathbf{z})^{(v)}$. When $V = n$ the cross validation is known as the *leave one out* procedure, and, in this case, fast estimation of the n discriminant rules is implemented in **Mixmod** in the Gaussian situation (Biernacki and Govaert 1999).

Semi-supervised classification

Two criteria are available in the semi-supervised context (supervised purpose): BIC and CV. For BIC, the partial labeling log-likelihood (11) has to be used. For CV, split at random in V blocks of approximately equal sizes the whole data set, including both the labeled and the unlabeled units, to obtain unbiased estimate of the error rate (Vandewalle *et al.* 2010). However, note that the CV criterion is quite expensive to be computed in the semi-supervised setting since it requires to run an EM algorithm V times to estimate $\hat{\boldsymbol{\theta}}^{(v)}$.

2.5. Mixmod library implementation and related packages

*The **Mixmod** library*

The **Mixmod** core library (**mixmodLib)** is the main product of the **Mixmod** software package. Developped since 2001, it has been downloaded from the **Mixmod** web site `http://www.mixmod.org` about 300 per year. Distributed under GNU GPL license, **mixmodLib** has been enhanced and improved for years (Biernacki *et al.* 2006). An important work has been done to improve performance of the **mixmodLib** which can today treat very large data sets quickly with accuracy and robustness. Currently, some arbitrarily large "hard" limits for the sample size and for the variable number are respectively fixed to 1 000 000 and 10 000. It is possible to change them but it requires to recompile the source code. The user must also be aware that to reach these limits in practice will essentially depend on its computing resources.

It contains about 80 C++ classes and can be used in command line or can be interfaced with any other software or library (in accordance with the terms of the GNU GPL license). Some of these C++ classes (top level classes) have been created to interface easily **mixmodLib**. Clustering can be performed with the top level XEMClusteringMain class (using XEMClusteringInput and XEMClusteringOutput classes) and Discriminant Analysis with the XEMLearnMain class (using XEMLearnInput and XEMLearnOutput classes) for the first step and the XEMPredictMain class (using XEMPredcitInput and XEMpredictOutput classes) for the second step (prediction).

The **Rmixmod** package uses also the **Rcpp** package (Eddelbuettel and François 2011) which provides C++ classes that greatly facilitate interfacing C or C++ code in R packages. Since the **Rcpp** package works only on R versions 2.15 and above, an up-to-date version of R is required for smooth installation of the package.

Existing related packages

To provide a suitable product for an increasingly large and various public, the **Mixmod** team has developped four products, available at `http://www.mixmod.org`:

- **mixmodLib** (developped since 2001), the core library which can be interfaced with any other sofware and can also be used in command line (for *expert* users);
- **mixmodForMatlab** package (developped since 2002), a collection of **Matlab** functions to call **mixmodLib** supplemented by some functions to visualise results;
- **mixmodGUI** (developped since 2009), a very user friendly software which provides all the clustering functionnalities of **mixmodLib** (we plan to make available soon also discriminant analysis functionnalities).

3. Overview of the Rmixmod functions

3.1. Main Rmixmod functions

Unsupervised classification and density estimation

Cluster analysis can be performed with the function `mixmodCluster()`. Illustration of use of this function is given in Section 4.1.

This function has two mandatory arguments: A data frame `x` and a list of number of groups. Default values for model and strategy will be used unless users specify a list of models with the `models` option (see Section 3.2) or a new strategy with the `strategy` option (see Section 3.3). By default only the BIC criterion is used to select models, but users can make a list of criteria by using the `criterion` option. In Table 3 the reader will find a summary of all the input parameters of the `mixmodCluster()` function with its default value if it is not a mandatory parameter.

The `mixmodCluster()` function returns an instance of the `MixmodCluster` class. Its two attributes will contain all outputs:

- `results`: A list of `MixmodResults` object containing all the results sorted in ascending order according to the given criterion.
- `bestResult`: A `MixmodResults` object containing the best model results.

Supervised and semi-supervised classification

Supervised and semi-supervised classification can be performed using the `mixmodLearn()` and the `mixmodPredict()` functions. Both functions are illustrated in Section 4.2.

Input Parameter	Description
`data`	Data frame containing quantitative or qualitative data. Rows correspond to observations and columns correspond to variables.
`nbCluster`	Numeric. List the number of clusters.
`dataType`	Character. Type of data is either `"quantitative"` or `"qualitative"`. Set as `NULL` by default, type will be guessed depending on variables type.
`models`	A `Model` object defining the list of models to run. For quantitative data, the model `"Gaussian_pk_Lk_C"` is called (see `mixmodGaussianModel()` Section 3.2 to specify other models). For qualitative data, the model `"Binary_pk_Ekjh"` is called (see `mixmodMultinomialModel()` Section 3.2 to specify other models)
`strategy`	A `Strategy` object containing the strategy to run. Call `mixmodStrategy()` Section 3.3 method by default.
`criterion`	List of characters defining the criterion to select the best model. The best model is the one with the lowest criterion value. Possible values: `"BIC"`, `"ICL"`, `"NEC"`, `c("BIC", "ICL", "NEC")`. Default is `"BIC"`.
`weight`	Numeric vector with n (number of individuals) rows. `weight` is optional. This option is to be used when weights are associated to the data.
`knownLabels`	Vector of size n. it will be used for semi-supervised classification when labels are known. Each cell corresponds to a cluster affectation.

Table 3: List of all the input parameters of the `mixmodCluster()` function.

`mixmodLearn()` function It has two mandatory arguments: A data matrix `x` and a vector containing the known labels `z`. As the `mixmodCluster()` function the three arguments `models`, `weight` and `criterion` are available. The default criterion is CV (Cross Validation). In Table 4 the reader will find a summary of all the input parameters of the `mixmodLearn()` function and default value if it is not a mandatory parameter.

The `mixmodLearn()` function returns an instance of the `MixmodLearn` class. Its two attributes will contain all outputs:

- `results`: A list of `MixmodResults` object containing all the results sorted in ascending order according to the given criterion (in descending order for the CV criterion).
- `bestResult`: A S4 `MixmodResults` object containing the best model results.

`mixmodPredict()` function It only needs two arguments: A data matrix of the remaining observations and a classification rule (see Table 5). It returns an instance of the `MixmodPredict` class which contains predicted partitions and probabilities.

Input Parameter	Description
`data`	Data frame containing quantitative or qualitative data. Rows correspond to observations and columns correspond to variables.
`knownLabels`	Vector of size number of observations. Each cell corresponds to a cluster affectation. So the maximum value is the number of clusters.
`dataType`	Character. Type of data is either `"quantitative"` or `"qualitative"`. Set as `NULL` by default, type will be guessed depending on variables type.
`models`	A `Model` object defining the list of models to run. For quantitative data, the model `"Gaussian_pk_Lk_C"` is called (see `mixmodGaussianModel()` Section 3.2, to specify other models). For qualitative data, the model `"Binary_pk_Ekjh"` is called (see `mixmodMultinomialModel()` Section 3.2, to specify other models).
`criterion`	List of characters defining the criterion to select the best model. Possible values: `"BIC"`, `"CV"` or `c("CV", "BIC")`. Default is `"CV"`.
`nbCVBlocks`	Integer which defines the number of blocks to perform the cross validation. This value will be ignored if the CV criterion is not chosen. Default value is 10.
`weight`	Numeric vector with n (number of individuals) rows. `weight` is optional. This option is to be used when weights are associated to the data.

Table 4: List of all the input parameters of the `mixmodLearn()` function.

3.2. Companion functions for model definition

Continuous variables: Gaussian models

All the Gaussian models summarized in Table 1 are available in **Rmixmod**. Users can get all the 28 models by calling `mixmodGaussianModel()`.

```
R> all <- mixmodGaussianModel()
R> all

****************************************
*** Mixmod Models:
* list =  Gaussian_pk_L_I Gaussian_pk_Lk_I Gaussian_pk_L_B Gaussian_pk_Lk_B
          Gaussian_pk_L_Bk Gaussian_pk_Lk_Bk Gaussian_pk_L_C Gaussian_pk_Lk_C
          Gaussian_pk_L_D_Ak_D Gaussian_pk_Lk_D_Ak_D Gaussian_pk_L_Dk_A_Dk
          Gaussian_pk_Lk_Dk_A_Dk Gaussian_pk_L_Ck Gaussian_pk_Lk_Ck
          Gaussian_p_L_I Gaussian_p_Lk_I Gaussian_p_L_B Gaussian_p_Lk_B
          Gaussian_p_L_Bk Gaussian_p_Lk_Bk Gaussian_p_L_C Gaussian_p_Lk_C
          Gaussian_p_L_D_Ak_D Gaussian_p_Lk_D_Ak_D Gaussian_p_L_Dk_A_Dk
```

Input Parameter	Description
`data`	Data frame containing quantitative or qualitative data. Rows correspond to observations and columns correspond to variables.
`classificationRule`	A `MixmodResults` object which contains the classification rule computed in the `mixmodLearn()` or `mixmodCluster()` step.

Table 5: List of the input parameters of the `mixmodPredict()` function.

```
          Gaussian_p_Lk_Dk_A_Dk Gaussian_p_L_Ck Gaussian_p_Lk_Ck
* This list includes models with free and equal proportions.
*************************************
```

This function has four parameters to specify some particular models in the family:

- `listModels` can be used when users want to use specific models;

  ```
  R> list.models <- mixmodGaussianModel(listModels = c("Gaussian_p_L_C",
  +   "Gaussian_p_L_Dk_A_Dk", "Gaussian_pk_Lk_B"))
  ```

- `free.proportions` and `equal.proportions` can be used to include or not models with free or equal proportions;

  ```
  R> only.free.proportions <- mixmodGaussianModel(equal.proportions = FALSE)
  ```

- `family` allows to include models from a specific family (`"general"`, `"diagonal"`, `"spherical"`, `"all"`).

  ```
  R> family.models <- mixmodGaussianModel(family = c("general", "spherical"),
  +   free.proportions = FALSE)
  ```

Categorical variables: Multinomial models

All the multinomial models summarized in Table 2 are available in **Rmixmod**. Users can get all the 10 models by calling `mixmodMultinomialModel()`.

```
R> all <- mixmodMultinomialModel()
R> all

*************************************
*** Mixmod Models :
* list =  Binary_pk_E Binary_pk_Ekj Binary_pk_Ekjh Binary_pkEj Binary_pk_Ek
          Binary_p_E Binary_p_Ekj Binary_p_Ekjh Binary_p_Ej Binary_p_Ek
* This list includes models with free and equal proportions.
*************************************
```

This function has five parameters. As `mixmodGaussianModel()` this function has the following parameters: `listModels`, `free.proportions` and `equal.proportions`.

```
R> only.free.proportions <- mixmodMultinomialModel(equal.proportions = FALSE)
R> list.models <- mixmodMultinomialModel(listModels = c("Binary_p_E",
+   "Binary_p_Ekjh", "Binary_pk_Ekj", "Binary_pk_Ej"))
```

But users can also use `variable.independency` and `component.independency` in order to include models which are independent of the variable j or independent of the component k.

```
R> var.independent <- mixmodMultinomialModel(variable.independency = TRUE)
R> var.comp.independent <- mixmodMultinomialModel(
+   variable.independency = TRUE, component.independency = TRUE)
```

3.3. Companion function for maximum likelihood estimation strategies

The strategies described in Section 2.3 can be tuned using the `mixmodStrategy()` function. The `mixmodStrategy()` function have no mandatory argument and the default arguments are the ones specified in the mixmod documentation (Mixmod Team 2008). In Table 6 the reader will find a summary of all the input parameters of the `mixmodStrategy()` function.

The `mixmodStrategy()` function returns an instance of the `MixmodStrategy` class. A default strategy can be defined in **Rmixmod** with the `mixmodStrategy()` function:

```
R> mixmodStrategy()

****************************************
*** MIXMOD Strategy:
* algorithm            =  EM
* number of tries      =  1
* number of iterations =  200
* epsilon              =  0.001
*** Initialization strategy:
* algorithm            =  smallEM
* number of tries      =  50
* number of iterations =  5
* epsilon              =  0.001
* seed                 =  NULL
****************************************
```

Here are other examples to show different ways to set a strategy:

```
R> strategy1 <- mixmodStrategy(algo = "CEM", initMethod = "random",
+   nbTry = 10, epsilonInInit = 0.000001)
R> strategy2 <- mixmodStrategy(algo = c("SEM", "EM"),
+   nbIterationInAlgo = c(200, 100), epsilonInAlgo = c(NA, 0.0001))
```

It is well-known that the number of local maxima of the log-likelihood function increases in conjunction with the number of parameters to be estimated. In such a situation, **Rmixmod** is able to avoid these traps by tuning its previous input parameters, in particular by increasing

Input Parameter	Description
`algo`	List of character string with the estimation algorithm. Possible values: `"EM"`, `"SEM"`, `"CEM"`, `c("EM", "SEM")`. Default value: `"EM"`.
`nbTry`	Integer defining the number of tries. `nbTry` must be a positive integer. Default value: 1.
`initMethod`	A character string with the method of initialization of the algorithm specified in the `algo` argument. Possible values: `"random"`, `"smallEM"`, `"CEM"`, `"SEMMax"`. Default value: `"smallEM"`.
`nbTryInInit`	Integer defining number of tries in `initMethod` algorithm. `nbTryInInit` must be a positive integer. Option available only if `initMethod` is `"smallEM"` or `"CEM"`. Default value: 50.
`nbIterationInInit`	Integer defining the number of `"EM"` or `"SEM"` iterations in `initMethod`. `nbIterationInInit` must be a positive integer. Only available if `initMethod` is `"smallEM"` or `"SEMMax"`. Default values: 5 if `initMethod` is `"smallEM"` and 100 if `initMethod` is `"SEMMax"`.
`nbIterationInAlgo`	List of integers defining the number of iterations if `nbIteration` is used as a stopping rule for the algorithm(s). Default value: 200.
`epsilonInInit`	Real defining the epsilon value in the initialization step. Only available if `initMethod` is `"smallEM"`. Default value: 0.001.
`epsilonInAlgo`	List of reals defining the epsilon value for the algorithm. Warning: `epsilonInAlgo` doesn't have any sense if `algo` is `"SEM"`, so it needs to be set as `NaN` in that case. Default value: 0.001.
`seed`	Random seed used in the random generator. Default value: NULL

Table 6: List of all the input parameters of the `mixmodStrategy()` function.

the value of `nbTry`. The need for this adjustement is easily detected by the fact that multiple re-runs of **Rmixmod** provide unstable results.

However, ability of **Rmixmod** to provide a good search over the log-likelihood function increases the frequency of spurious solutions in the Gaussian case (see a description in Section 2.3.1). Such solutions are then easily manually discarded.

In addition, for some specific reproducibility purposes, note that **Rmixmod** allows also to control exactly the random seed by providing the optional `seed` argument (see Table 6).

3.4. Other companion functions

Non-graphical functions

The `show`, the `print` and the `summary` methods have been redefined for the **Rmixmod** S4 classes `Strategy`, `Model`, `GaussianParameter`, `MultinomialParameter`, `MixmodResults`, `MixmodCluster`, `MixmodLearn` and `MixmodPredict`.

The **Rmixmod** package provides two other utility functions:

1. `nbFactorFromData()`: Allow to get the number of levels of each column of a data set;
2. `sortbyCriterion()`: After calling the `mixmodCluster()` or `mixmodLearn()` method, results will be sorted into ascending order according to the first given criterion (descending order for CV criterion). This method is able to reorder the list of results according to a given criterion. The input parameters are
   - `object`: A **Mixmod** object;
   - `criterion`: A string containing the criterion name.

Most of these functions will be illustrated in Section 4.

Graphical functions

The three methods `plot`, `hist` and `barplot` have been redefined for the **Rmixmod** S4 classes `MixmodResults`. `hist` and `barplot` are respectively specific for quantitative and qualitative data. All functions will be also illustrated in Section 4.

4. Rmixmod through examples

4.1. Unsupervised classification

Continuous variables: Geyser dataset

The outputs and graphs of clustering with **Rmixmod** are illustrated on the well-known `geyser` dataset (Azzalini and Bowman 1990). It is a data frame containing 272 observations from the Old Faithful Geyser in the Yellowstone National Park taken from the Modern Applied Statistics in S library (Venables and Ripley, 2002). Each observation consists of two measurements: The duration (in minutes) of the eruption and the waiting time (in minutes) to the next eruption. In this example we ignore the partition and we want to estimate the best Gaussian mixture model fitting the data set. The following code provides a way to do it by running a cluster analysis with a list of clusters (from 2 to 8 clusters), all the Gaussian models, the BIC, ICL and NEC model selection criteria, and `strategy2` defined in Section 3.3:

```
R> data("geyser")
R> xem.geyser <- mixmodCluster(data = geyser, nbCluster = 2:8,
+   criterion = c("BIC", "ICL", "NEC"), models = mixmodGaussianModel(),
+   strategy = strategy2)
```

The `xem.geyser` variable contains information both on input and ouput of the clustering:

```
R> xem.geyser

****************************************
*** INPUT:
****************************************
* nbCluster =  2 3 4 5 6 7 8
* criterion =  BIC ICL NEC
****************************************
*** MIXMOD Models:
* list =  Gaussian_pk_L_I Gaussian_pk_Lk_I Gaussian_pk_L_B Gaussian_pk_Lk_B
Gaussian_pk_L_BkGaussian_pk_Lk_Bk Gaussian_pk_L_C Gaussian_pk_Lk_C
Gaussian_pk_L_D_Ak_D Gaussian_pk_Lk_D_Ak_D Gaussian_pk_L_Dk_A_Dk
Gaussian_pk_Lk_Dk_A_Dk Gaussian_pk_L_Ck Gaussian_pk_Lk_Ck Gaussian_p_L_I
Gaussian_p_Lk_I Gaussian_p_L_B Gaussian_p_Lk_B Gaussian_p_L_Bk Gaussian_p_Lk_Bk
Gaussian_p_L_CGaussian_p_Lk_C Gaussian_p_L_D_Ak_D Gaussian_p_Lk_D_Ak_D
Gaussian_p_L_Dk_A_DkGaussian_p_Lk_Dk_A_Dk Gaussian_p_L_Ck Gaussian_p_Lk_Ck
* This list includes models with free and equal proportions.
****************************************
* data (limited to a 10x10 matrix) =
      Duration Waiting.Time
 [1,] 3.6      79
 [2,] 1.8      54
 [3,] 3.333    74
 [4,] 2.283    62
 [5,] 4.533    85
 [6,] 2.883    55
 [7,] 4.7      88
 [8,] 3.6      85
 [9,] 1.95     51
[10,] 4.35     85
* ... ...
****************************************
*** MIXMOD Strategy:
* algorithm            =  SEM EM
* number of tries      =  1
* number of iterations =  200 100
* epsilon              =  NaN 1e-04
*** Initialization strategy:
* algorithm            =  smallEM
* number of tries      =  50
* number of iterations =  5
* epsilon              =  0.001
* seed                 =  NULL
****************************************
```

```
****************************************
*** BEST MODEL OUTPUT:
*** According to the BIC criterion
****************************************
* nbCluster   =  3
* model name  =  Gaussian_p_L_C
* criterion   =  BIC(2312.5998) ICL(2434.3210) NEC(0.3831)
* likelihood  =  -1131.0738
****************************************
*** Cluster 1
* proportion =  0.3333
* means      =  2.0390 54.5078
* variances  = |     0.0795     0.5333 |
               |     0.5333    34.2083 |
*** Cluster 2
* proportion =  0.3333
* means      =  4.5545 81.0516
* variances  = |     0.0795     0.5333 |
               |     0.5333    34.2083 |
*** Cluster 3
* proportion =  0.3333
* means      =  3.9750 78.7151
* variances  = |     0.0795     0.5333 |
               |     0.5333    34.2083 |
****************************************
```

A summary of the previous information can also be obtained:

```
R > summary(xem.geyser)

************************************************************
* Number of samples    =  272
* Problem dimension    =  2
************************************************************
*       Number of cluster =  3
*              Model Type =  Gaussian_p_L_C
*               Criterion =  BIC(2312.5998) ICL(2434.3210) NEC(0.3831)
*              Parameters =  list by cluster
*                  Cluster  1 :
                         Proportion =  0.3333
                              Means =  2.0390 54.5078
                          Variances = |     0.0795     0.5333 |
                                      |     0.5333    34.2083 |
*                  Cluster  2 :
                         Proportion =  0.3333
                              Means =  4.5545 81.0516
```

```
                          Variances = |     0.0795     0.5333 |
                                      |     0.5333    34.2083 |
*                   Cluster  3 :
                          Proportion =  0.3333
                               Means =  3.9750 78.7151
                          Variances = |     0.0795     0.5333 |
                                      |     0.5333    34.2083 |
*           Log-likelihood =  -1131.0738
*************************************************************
```

The `plot()` function has been redefined to get on the same graph:

- On diagonal: A 1D representation with densities and data;
- On lower triangular: A 2D representation with isodensities, data points and partition.

The output of `plot(xem.geyser)` is displayed in Figure 1.

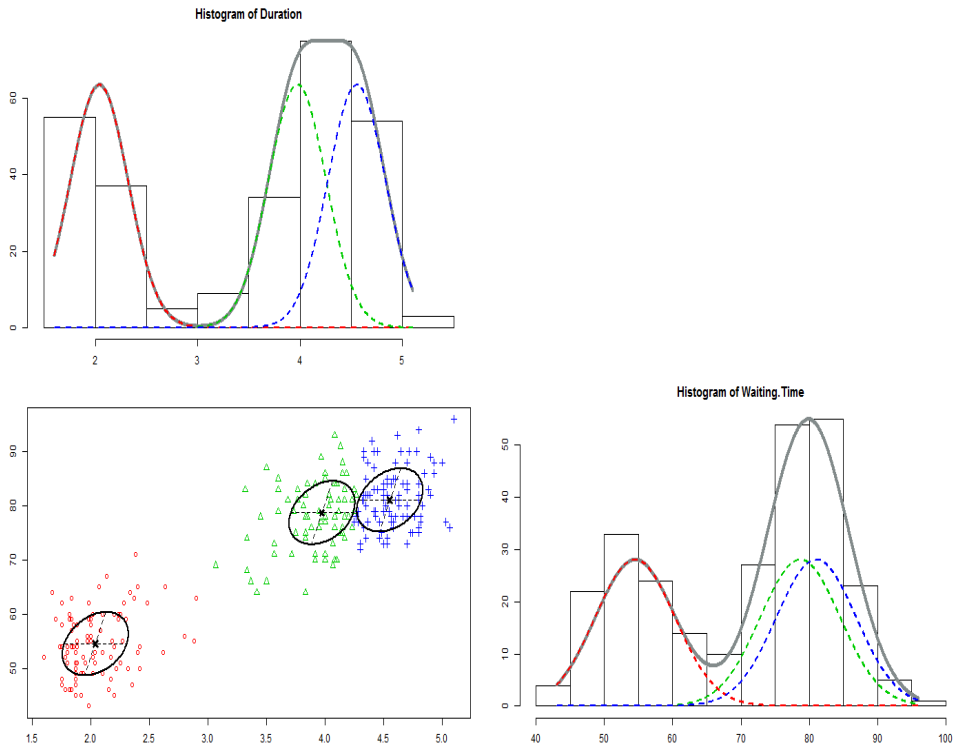


Figure 1: Output displayed by the `plot()` function for the geyser dataset.

By default, all models of the `xem.geyser@results` variable are sorted by the BIC criterion. Alternatively, it is easy to sort this list of models according to the ICL criterion value with the `sortByCriterion()` function. Then, by looking at the best result, we can see that ICL criterion selects two clusters (contrary to BIC which selects three clusters):

```
R> icl <- sortByCriterion(xem.geyser, "ICL")
R> icl["bestResult"]

* nbCluster   =  2
* model name  =  Gaussian_pk_Lk_D_Ak_D
* criterion   =  BIC(2320.2833) ICL(2321.3701) NEC(0.0034)
* likelihood  =  -1132.1126
**************************************
*** Cluster 1
* proportion =  0.3568
* means      =  2.0387 54.5040
* variances  = |     0.0783     0.6467 |
               |     0.6467    33.8916 |
*** Cluster 2
* proportion =  0.6432
* means      =  4.2915 79.9892
* variances  = |     0.1588     0.6810 |
               |     0.6810    35.7675 |
**************************************
```

A list with all results is also available, this list being sorted by criterion values:

```
R> xem.geyser["results"]
R> icl["results"]
```

Categorical variables: Birds of different subspecies

`birds` data set (Bretagnolle 2007) provides details on the morphology of birds (puffins). Each bird is described by five qualitative variables: One variable for the gender and four variables giving a morphological description of the birds. There are 69 puffins divided in two subclasses: *lherminieri* and *subalaris* (34 and 35 individuals respectively). Here we run a cluster analysis of birds with 2 clusters:

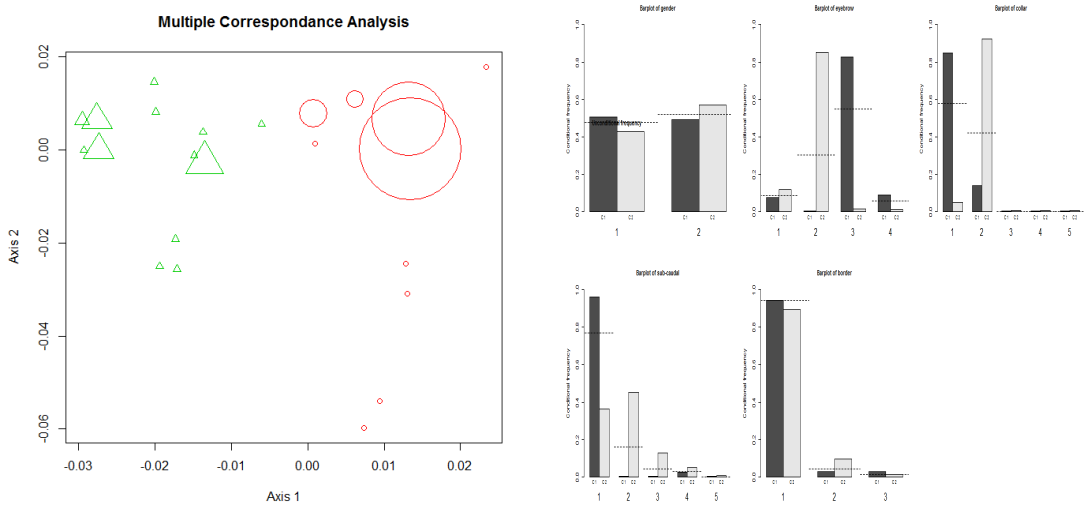
```
R> data("birds")
R> xem.birds <- mixmodCluster(birds, 2)
```

The `plot()` function has been redefined in the qualitative case: A multiple correspondance analysis is performed to get a 2-dimensional representation of the data set and a bigger symbol is used when observations are similar. The output of `plot(xem.birds)` is displayed in Figure 2(a).

The `barplot()` function has also been redefined. For each qualitative variable, we have:

- A barplot with the frequencies of the modalities;
- For each cluster a barplot with the probabilities for each modality to be in that cluster.

The output of `barplot(xem.birds)` is displayed in Figure 2(b).



(a) (b)

Figure 2: Output displayed (a) by the `plot()` function and (b) by the `barplot()` function for the birds dataset.

4.2. Supervised classification

The following example concerns quantitative data. But, obviously, discriminant analysis also works with qualitative datasets in **Rmixmod**.

The outputs and graphs of discriminant analysis with **Rmixmod** are illustrated through prediction of the company's ability to cover its financial obligations (Du Jardin and Séverin 2010; Lourme and Biernacki 2011). It is an important question that requires a strong knowledge of the mechanism leading to bankruptcy. The original first sample (year 2002) is made up of 216 healthy firms and 212 bankruptcy firms. The second sample (year 2003) is made up of 241 healthy firms and 220 bankruptcy firms. Four financial ratios expected to provide some meaningful information about the company's health are considered: EBITDA/Total Assets, Value Added/Total Sales, Quick Ratio, Accounts Payable/Total Sales.

First step: Learning

After spliting data into years 2002 and 2003, we learn the discriminant rule on year 2002 then we have a look at the best result:

```
R> data("finance")
R> ratios2002 <- finance[finance["Year"] == 2002, 3:6]
R> health2002 <- finance[finance["Year"] == 2002, 2]
R> ratios2003 <- finance[finance["Year"] == 2003, 3:6]
R> health2003 <- finance[finance["Year"] == 2003, 2]
R> learn <- mixmodLearn(ratios2002, health2002)
R> learn["bestResult"]

* nbCluster   =  2
```

```
* model name  =  Gaussian_pk_Lk_C
* criterion   =  CV(0.8201)
* likelihood  =  444.9579
**************************************
*** Cluster 1
* proportion =  0.4953
* means      =  -0.0386 0.2069 0.6089 0.1774
* variances  = |     0.0226     0.0064     0.0186    -0.0023 |
               |     0.0064     0.0166     0.0076    -0.0006 |
               |     0.0186     0.0076     0.2728    -0.0095 |
               |    -0.0023    -0.0006    -0.0095     0.0079 |
*** Cluster 2
* proportion =  0.5047
* means      =  0.1662 0.2749 1.0661 0.1079
* variances  = |     0.0172     0.0049     0.0142    -0.0017 |
               |     0.0049     0.0126     0.0058    -0.0005 |
               |     0.0142     0.0058     0.2076    -0.0073 |
               |    -0.0017    -0.0005    -0.0073     0.0060 |
**************************************
* Classification with CV:
           | Cluster 1 | Cluster 2 |
---------- ----------- -----------
 Cluster 1 |       167 |        32 |
 Cluster 2 |        45 |       184 |
---------- ----------- -----------
* Error rate with CV =  17.99 %

* Classification with MAP:
           | Cluster 1 | Cluster 2 |
---------- ----------- -----------
 Cluster 1 |       212 |         0 |
 Cluster 2 |         0 |       216 |
---------- ----------- -----------
* Error rate with MAP =  0.00 %
**************************************
```

We call now the `plot()` function to a get a visualisation of the best result. The output of `plot(learn)` is displayed in Figure 3. It is also allowed to specify a subset of variables to be combined on the figure; For instance the command line `plot(learn,c(1,3))` would display only variables 1 and 3. Equivalently, names of variables 1 and 3 could be used: `plot(learn,c("EBITDA.Total.Assets","Quick.Ratio"))`. This functionality could be particularly useful when many variables are available.

Second step: Prediction

We perform predictions on year 2003, then we get a summary (note that `[...]` indicates that output has been truncated) and finally we compare predictions of health 2003 with the

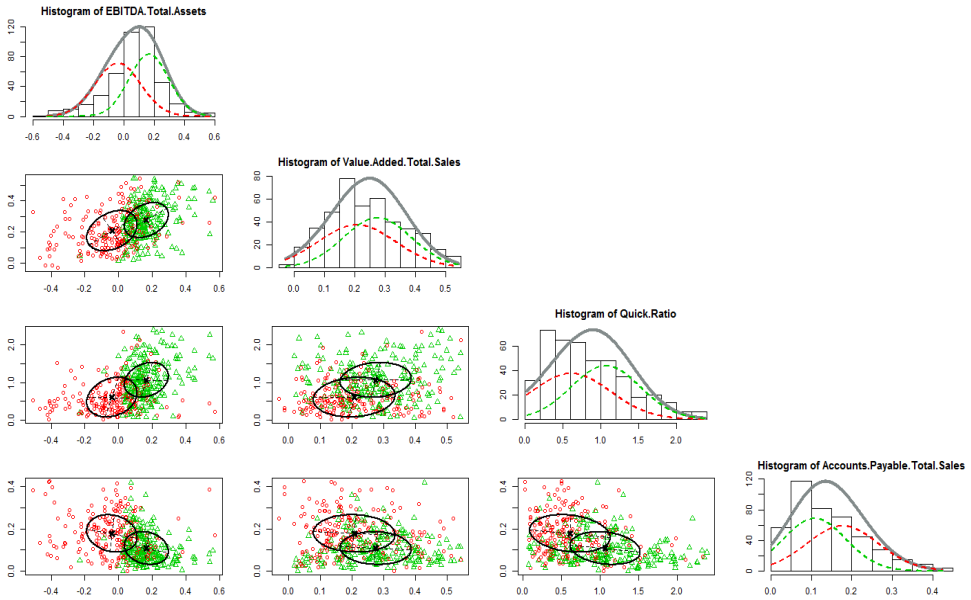


Figure 3: Output displayed by the `plot()` function for the finance dataset.

true health 2003 (75.7% of good classification):

```
R> prediction <- mixmodPredict(data = ratios2003,
+   classificationRule = learn["bestResult"])
R> summary(prediction)

**************************************************************
* partition     =  2 1 1 1 [...] 1 2
* probabilities = |   0.4966   0.5034 |
                  |   0.8125   0.1875 |
                  |   0.8851   0.1149 |
                  |   0.8329   0.1671 |
                              [...]
                  |   0.5626   0.4374 |
                  |   0.0308   0.9692 |
**************************************************************

R> mean(as.integer(health2003) == prediction["partition"])

[1] 0.7570499
```

5. Further works

The **Rmixmod** package interfaces almost every functionality of the **Mixmod** library. Some particular initializations strategies and models to deal with high-dimensional data have not

been implemented in the package. But initialization strategies of most interest are available in **Rmixmod** and the package **HDclassif** (Bergé *et al.* 2012) has been recently released to the clustering and the discriminant analysis of high-dimensional data.

We have proposed some tools to visualize outcomes but data visualization in **Rmixmod** can be enhanced. In addition, supervised and semi-supervised classification currently implemented could be greatly improved by including a variable selection procedure for instance (see Maugis *et al.* 2011). Moreover, we encourage users to contribute by suggesting new graphics or other utility functions.

The **Mixmod** project is currently implementing some other recent advances in model-based clustering in order to provide associated efficient `R` packages. It concerns for instance co-clustering (partioning simultaneaously rows and colums of a dataset) and clustering of mixed data (dealing with quantitative and qualitative data in the same exercise). The next versions of **Rmixmod** will include these latter functionalities.

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