Journal of Statistical Software

November 2012, Volume 51, Issue 12. *http://www.jstatsoft.org/*

MixSim: An R Package for Simulating Data to Study Performance of Clustering Algorithms

Volodymyr Melnykov
The University of Alabama

Wei-Chen Chen
Oak Ridge
National Laboratory

Ranjan Maitra
Iowa State University

Abstract

The R package **MixSim** is a new tool that allows simulating mixtures of Gaussian distributions with different levels of overlap between mixture components. Pairwise overlap, defined as a sum of two misclassification probabilities, measures the degree of interaction between components and can be readily employed to control the clustering complexity of datasets simulated from mixtures. These datasets can then be used for systematic performance investigation of clustering and finite mixture modeling algorithms. Among other capabilities of **MixSim**, there are computing the exact overlap for Gaussian mixtures, simulating Gaussian and non-Gaussian data, simulating outliers and noise variables, calculating various measures of agreement between two partitionings, and constructing parallel distribution plots for the graphical display of finite mixture models. All features of the package are illustrated in great detail. The utility of the package is highlighted through a small comparison study of several popular clustering algorithms.

Keywords: Gaussian mixture model, data simulation, pairwise overlap, parallel distribution plot, R.

1. Introduction

The main goal of clustering is to form groups of similar observations while also separating dissimilar ones. Many clustering algorithms have been developed, such as the iterative k-means (Forgy 1965; MacQueen 1967) and k-medoids (Kaufman and Rousseuw 1990) algorithms, hierarchical (both agglomerative and divisive) algorithms with different merging/splitting criteria called linkages – e.g., Ward's (Ward 1963), single (Sneath 1957), complete (Sorensen 1948) and other – and the probabilistic model-based clustering algorithms, where the observations are assumed to be sampled from an underlying finite mixture model (Melnykov and Maitra 2010). For a comprehensive review of clustering methods, see Xu and Wunsch (2009).

Clustering is a difficult problem with, consequently, many suggested methodologies, but no uniformly best performer in all situations. Thus, it is of interest to understand the scenarios in which different clustering algorithms perform better, worse, or indifferently. This requires an objective measure that would allow the clustering complexity of a simulated dataset to be controlled and different procedures to be calibrated with regard to this complexity. Performance of clustering algorithms depends on many factors such as cluster representation, orientation, elongation, multimodality, overlap, presence of noise, and others. The majority of procedures aiming to control clustering complexity focus on finding a good measure for the level of separation or overlap among clusters.

There have been many attempts made to define clustering complexity and to evaluate clustering algorithms in different settings. We refer our reader to Steinley and Henson (2005) and Maitra and Melnykov (2010) for a comprehensive review, while focusing our discussion here on a few most recent ones. Dasgupta (1999)'s c-separation for two p-dimensional Gaussian densities with mean vectors $\boldsymbol{\mu}_i$ and covariance matrices $\boldsymbol{\Sigma}_i$ for $i = 1, 2$ is defined as $c \leq ||\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2||/\sqrt{p \max\{\lambda_{(p)}(\boldsymbol{\Sigma}_1), \lambda_{(p)}(\boldsymbol{\Sigma}_2)\}}$, where $\lambda_{(p)}$ represents the largest eigenvalue in the corresponding covariance matrix $\boldsymbol{\Sigma}_i$. c-separation is widely used by researchers but cannot serve as an adequate measure of the interaction between distributions as it does not take into consideration the structure of both covariance matrices relying in its inference just on the largest eigenvalue and the norm of two mean vectors. Another approach to generating clustered data was proposed by Steinley and Henson (2005). The algorithm is implemented in the MATLAB function **OCLUS** and conveniently generates clusters of different shapes from various distributions. However, there are some limitations of this approach as well: clusters are marginally independent by construction and the number of overlapping clusters is restricted. A novel separation index was proposed by Qiu and Joe (2006b) and implemented in their package **clusterGeneration** (Qiu and Joe 2006a) for R (R Development Core Team 2012). In a univariate setting, the developed index is calculated as $(q_{l,2} - q_{u,1})/(q_{u,2} - q_{l,1})$, where $q_{l,1}$ and $q_{u,1}$ are the lower and upper quantiles of the first cluster and $q_{l,2}$ and $q_{u,2}$ are the corresponding quantiles of the second cluster. The probability associated with the quantiles is an additional parameter commonly chosen to be equal to 0.05. When two clusters are distant, this index takes values close to 1. It can take negative values but no less than -1 for clusters that are poorly separated. The advantage of this index is its simplicity and applicability for clusters of any shapes. At the same time, while being exact in the univariate framework, this index cannot be readily generalized to the case of two and more dimensions. The authors propose finding the best projection onto a one-dimensional space that maximizes the separation of clusters first. Then, their index can be employed as in the univariate case. Unfortunately, the substantial amount of information can be lost while projecting multidimensional clusters; hence, conclusions can be partial or incorrect. Very recently, Maitra and Melnykov (2010) have provided the only known exact measure capable of measuring interaction between two clusters in terms of the pairwise overlap ω, which is defined for Gaussian mixtures as the sum of two misclassification probabilities and can be calculated in a univariate as well as multivariate framework. More details about this measure can be found in Section 2. Maitra and Melnykov (2010) also developed algorithms which can be used to simulate data from a finite mixture model with specified clustering complexity. Further, they developed the open-source **CARP** package (Melnykov and Maitra 2011) to evaluate clustering algorithms from a command-line interface.

This paper details the use and applicability of **MixSim**, an R package with kernel written in C. The package is available from the Comprehensive R Archive Network at http://CRAN.R-project.org/package=MixSim and allows for the simulation of mixtures with the pre-specified level of average or/and maximum pairwise overlap. Thus, the package can be employed by the user for convenient and systematic comparisons of existing and newly developed clustering procedures. We discuss the use of this package in Section 3, following up with a small utility demonstrator in Section 4. The paper concludes with a discussion in Section 5.

2. Methodological and algorithmic details

This section briefly defines the basics of the overlap measure for the reader and discusses two mixture simulating schemes adopted by **MixSim**. It also summarizes several indices frequently used for comparing two partitionings.

2.1. Pairwise overlap

As mentioned in Section 1, the notion of pairwise overlap was recently introduced by Maitra and Melnykov (2010). We refer the reader to their paper for the detailed analysis of the measure and its properties. Here, we briefly explain mechanics behind the measure.

Let $\boldsymbol{X}$ be distributed according to the finite mixture model $g(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k \phi(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, where $\phi(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ is a multivariate Gaussian density of the kth component with mean vector $\boldsymbol{\mu}_k$ and covariance matrix $\boldsymbol{\Sigma}_k$. Then, the overlap between ith and jth components is defined as $\omega_{ij} = \omega_{i|j} + \omega_{j|i}$, where $\omega_{j|i}$ is the misclassification probability that the random variable $\boldsymbol{X}$ originated from the ith component but was mistakenly assigned to the jth component; $\omega_{i|j}$ is defined similarly. Thus, $\omega_{j|i}$ is given by

$$\omega_{j|i} = \Pr\left[\pi_i \phi(\boldsymbol{X}; \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) < \pi_j \phi(\boldsymbol{X}; \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j) \mid \boldsymbol{X} \sim N_p(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)\right].$$

Overlap has nice closed form expressions in some special cases. For example, when $\pi_i = \pi_j$ as well as $\boldsymbol{\Sigma}_i = \boldsymbol{\Sigma}_j \equiv \boldsymbol{\Sigma}$, we obtain

$$\omega_{ij} = 2\Phi\left(-\frac{1}{2}\sqrt{(\boldsymbol{\mu}_j - \boldsymbol{\mu}_i)'\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_j - \boldsymbol{\mu}_i)}\right),$$

where Φ is the standard normal cumulative density function. For spherical clusters, the above reduces to $\omega_{ij} = 2\Phi\left(-\frac{1}{2\sigma}\left\|\mu_i - \mu_j\right\|\right)$. In general, misclassification probabilities are given by

$$\omega_{j|i} = \Pr{}_{N_p(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)}\left[\sum_{\substack{l=1\\ l:\lambda_l \neq 1}}^{p} (\lambda_l - 1)U_l + 2\sum_{\substack{l=1\\ l:\lambda_l = 1}}^{p} \delta_l W_l \leq \sum_{\substack{l=1\\ l:\lambda_l \neq 1}}^{p} \frac{\lambda_l \delta_l^2}{\lambda_l - 1} - \sum_{\substack{l=1\\ l:\lambda_l = 1}}^{p} \delta_l^2 + \log\frac{\pi_j^2 \mid \boldsymbol{\Sigma}_i \mid}{\pi_i^2 \mid \boldsymbol{\Sigma}_j \mid}\right],$$

where $\lambda_1, \lambda_2, \ldots, \lambda_p$ are eigenvalues of the matrix $\boldsymbol{\Sigma}_i^{\frac{1}{2}}\boldsymbol{\Sigma}_j^{-1}\boldsymbol{\Sigma}_i^{\frac{1}{2}}$ and $\boldsymbol{\gamma}_1, \boldsymbol{\gamma}_2, \ldots, \boldsymbol{\gamma}_p$ are the corresponding eigenvectors, U_l's are independent noncentral χ^2 random variables with one degree of freedom and noncentrality parameter given by $\lambda_l^2\delta_l^2/(\lambda_l - 1)^2$ with $\delta_l = \gamma_l'\boldsymbol{\Sigma}_i^{-\frac{1}{2}}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)$, independent of W_l's, which are independent $N(0,1)$ random variables. This provides an efficient way of calculating $\omega_{i|j}$ and $\omega_{j|i}$ due to the algorithm AS155 (Davies 1980) that computes probabilities for linear combinations of noncentral χ^2 random variables.

Note that if the covariance matrices are multiplied by some positive constant c, it causes inflation ($c > 1$) or deflation ($c < 1$) of the components. Thus, we can manipulate the value of c in order to reach the pre-specified level of overlap $\omega_{ij}(c)$ between the components. According to Maitra and Melnykov (2010), the function $\omega_{ij}(c)$ does not have to be monotone increasing; however, $\omega_{ij}(c)$ enjoys monotonicity in the overwhelming number of simulated mixtures. In those rare cases when monotonicity is violated, the simplest solution is to drop the current mixture and simulate a new one.

If $c \to \infty$ and clusters are heterogeneous, the above expression reduces to

$$\omega_{j|i}^{\infty} = \Pr_{N_p(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)} \left[\sum_{\substack{l=1 \\ l:\lambda_l \neq 1}}^{p} (\lambda_l - 1) U_l \leq \log \frac{\pi_j^2 \mid \boldsymbol{\Sigma}_i \mid}{\pi_i^2 \mid \boldsymbol{\Sigma}_j \mid} \right],$$

where U_l's are independent central χ^2 random variables with one degree of freedom.

Maitra and Melnykov (2010) do not discuss the case of homogenenous clusters but it can be also addressed as follows. If all clusters are homogeneous, the expression for $\omega_{j|i}$ reduces to

$$\omega_{j|i} = \Phi \left(-\frac{1}{2} \sqrt{\sum_{l=1}^{p} \delta_l^2} + \frac{\log \pi_j / \pi_i}{\sqrt{\sum_{l=1}^{p} \delta_l^2}} \right).$$

When $c \to \infty$, $\delta_l^2 \to 0$ for $l = 1, 2, \ldots, p$. This yields $\omega_{j|i}^{\infty} = 0$ for $\pi_j < \pi_i$, $\omega_{j|i}^{\infty} = \frac{1}{2}$ for $\pi_j = \pi_i$, and $\omega_{j|i}^{\infty} = 1$ for $\pi_j > \pi_i$. This indicates that the value of asymptotic overlap for homogeneous clusters is $\omega_{ij}^{\infty} = \omega_{j|i}^{\infty} + \omega_{i|j}^{\infty} = 1$ for any mixing proportions π_i and π_j.

2.2. Mixture model and data generation

Having detailed the pairwise overlap and its implementation in Section 2.1, the overlap can now be employed to control the degree of interaction among mixture components. Before we proceed to the next section describing algorithms for generating mixtures with a pre-specified overlap characteristic, we discuss how mixture model parameters are simulated.

Mean vectors of Gaussian mixture components $\boldsymbol{\mu}_k$ are obtained as K independent realizations from a uniform p-variate hypercube with bounds specified by the user. Covariance matrices $\boldsymbol{\Sigma}_k$ are taken as draws from the Wishart distribution with parameter p and $p + 1$ degrees of freedom. The low number of degrees of freedom provides us with random covariance matrices of different orientation and elongation. Finally, mixing proportions π_k are generated on the $[0, 1]$ interval subject to the restriction $\sum_{k=1}^{K} \pi_k = 1$ with the lower bound pre-specified by the user. To simulate a dataset from a generated mixture, first, cluster sizes are obtained as a draw from a multinomial distribution based on mixing proportions. Then, the corresponding number of realizations are obtained from each multivariate normal component.

2.3. Algorithms

Maitra and Melnykov (2010) provided two algorithms that simulate Gaussian mixtures according to pre-specified values of average ($\bar{\omega}$) or/and maximum ($\check{\omega}$) overlap. The algorithms are briefly summarized below.

Generate mixture model controlling the average or maximum overlap

The first algorithm generates a mixture model with respect to the level of average or maximum overlap. The algorithm consists of the following three steps.

1. *Generating initial parameters.* Generate K mixing proportions, mean vectors and covariance matrices as discussed in Section 2.2. Compute limiting average ($\bar{\omega}^{\infty}$) (maximum ($\check{\omega}^{\infty}$)) overlap. If $\bar{\omega} > \bar{\omega}^{\infty}$ ($\check{\omega} > \check{\omega}^{\infty}$), discard the realization and start Step 1 again.

2. *Calculating pairwise overlaps.* Compute all pairwise overlaps. Calculate the current estimate of $\hat{\bar{\omega}}$ ($\hat{\check{\omega}}$). If the difference between $\hat{\bar{\omega}}$ and $\bar{\omega}$ ($\hat{\check{\omega}}$ and $\check{\omega}$) is negligible, stop the algorithm and provide the current parameters.

3. *Scaling clusters.* Use root-finding techniques to find a covariance matrix multiplier c such that the difference between $\hat{\bar{\omega}}(c)$ and $\bar{\omega}$ ($\hat{\check{\omega}}(c)$ and $\check{\omega}$) is negligible.

For finding roots, **MixSim** obtains bounds of an interval that contains the root by considering positive or negative powers of 2, and then applies the approach of Forsythe, Malcolm, and Moler (1980) to find the root.

Generate mixture model controlling the average and maximum overlap

The second algorithm deals with both characteristics $\bar{\omega}$ and $\check{\omega}$ simultaneously. It can be preferred over the first algorithm to better control the overlap between simulated components.

1. *Scaling clusters to reach $\check{\omega}$.* Use the first algorithm to obtain the set of parameters that satisfies $\check{\omega}$ and fix two components that produced the highest overlap; their covariance matrices will not be involved in inflation/deflation process.

2. *Finding $c_{\vee}$.* Find the largest value of c (say $c_{\vee}$) such that none of pairwise overlaps $\omega_{ij}(c_{\vee})$ exceeds $\check{\omega}$. If $\hat{\bar{\omega}}(c_{\vee}) < \bar{\omega}$, discard the realization and return to Step 1.

3. *Limited scaling.* While keeping the two fixed components unchanged, apply Step 3 of the first algorithm to the rest of components to reach the desired $\bar{\omega}$. If the obtained parameters satisfy $\bar{\omega}$ and $\check{\omega}$, report them. Otherwise, start with Step 1 again.

It can be noticed that not every combination of $\check{\omega}$ and $\bar{\omega}$ can be obtained. Immediate restrictions are $\bar{\omega} \leq \check{\omega}$ and $\check{\omega} \leq \bar{\omega}K(K-1)/2$, where K is the number of mixture components. Also, some combinations of $\check{\omega}$ and $\bar{\omega}$ can be more difficult to reach than the others. In this case, a higher number of mixture resimulations may be needed to find a targeted mixture.

2.4. Classification indices

One application of **MixSim** is the systematic investigation of the properties of clustering algorithms. In order to assess the level of similarity between partitioning vectors, some measure has to be used. There are multiple indices that have been developed for this purpose – see Meilă (2006) for a detailed review. Here, we summarize those indices that are implemented in **MixSim**. Meilă (2006) brackets all indices into one of three groups. The first group of indices compares clusterings counting the pairs of points that are assigned to the same or different clusters under both partitionings. The Rand (1971) index falls into this category and is defined as

$$R(\boldsymbol{c}_1, \boldsymbol{c}_2) = \frac{N_{11} + N_{00}}{\binom{n}{2}},$$

where $\boldsymbol{c}_1$ and $\boldsymbol{c}_2$ are the first and second partitioning vectors respectively, N_{11} is the number of pairs of points in the same cluster under $\boldsymbol{c}_1$ and $\boldsymbol{c}_2$, and N_{00} is the number of pairs in different clusters under $\boldsymbol{c}_1$ and $\boldsymbol{c}_2$; n represents the number of points in partitioning vectors. The more commonly used modification of $R(\boldsymbol{c}_1, \boldsymbol{c}_2)$ involves adjustment with its $E(R(\boldsymbol{c}_1, \boldsymbol{c}_2))$, providing the adjusted Rand index (Hubert and Arabie 1985):

$$AR(\boldsymbol{c}_1, \boldsymbol{c}_2) = \frac{R(\boldsymbol{c}_1, \boldsymbol{c}_2) - E(R(\boldsymbol{c}_1, \boldsymbol{c}_2))}{1 - E(R(\boldsymbol{c}_1, \boldsymbol{c}_2))}.$$

Another, albeit less popular, adjustment of the Rand index was proposed by Mirkin (1996):

$$M(\boldsymbol{c}_1, \boldsymbol{c}_2) = n(n-1)(1 - R(\boldsymbol{c}_1, \boldsymbol{c}_2)).$$

An interesting index proposed by Fowlkes and Mallows (1983) combines two asymmetric criteria of Wallace (1983), $W_1(\boldsymbol{c}_1, \boldsymbol{c}_2)$ and $W_2(\boldsymbol{c}_1, \boldsymbol{c}_2)$:

$$F(\boldsymbol{c}_1, \boldsymbol{c}_2) = \sqrt{W_1(\boldsymbol{c}_1, \boldsymbol{c}_2) W_2(\boldsymbol{c}_1, \boldsymbol{c}_2)},$$

where

$$W_i(\boldsymbol{c}_1, \boldsymbol{c}_2) = \frac{2N_{11}}{\sum_{k=1}^{K^{(i)}} n_k^{(i)}(n_k^{(i)} - 1)}$$

for $i = 1, 2$ with $n_k^{(i)}$ representing the size of the kth cluster according to the partitioning $\boldsymbol{c}_i$ and $K^{(i)}$ representing the number of clusters in $\boldsymbol{c}_i$. Indices R, AR, and F have upper bounds equal to 1 which can be achieved only in the case of the same partitioning, i.e., $\boldsymbol{c}_1 = \boldsymbol{c}_2$. On the contrary, the Mirkin index reaches 0 for identical partitioning vectors; otherwise, it takes positive integer values. These four indices are implemented in **MixSim**'s function `RandIndex()`.

A second group of indices compares partitionings by set matching. The most well-known index here is the proportion of observations that agree on classification for both partitioning vectors. It may be noted that label-switching plays an important role here as the result is label-dependent. **MixSim**'s function `ClassProp()` calculates this proportion considering all possible permutations of labels and choosing the permutation yielding the highest proportion of agreement between two partitionings. Of course, this approach becomes restrictive for a high number of classes. In this case, heuristic approaches for matching classes, such as provided by the function `matchClasses()` from the package **e1071** (Meyer, Dimitriadou, Hornik, Weingessel, and Leisch 2012), can be applied.

The last category of indices is based on the analysis of the variation of information in two partitioning vectors. Meilă (2006) developed an index defined as

$$VI(\boldsymbol{c}_1, \boldsymbol{c}_2) = H(\boldsymbol{c}_1) + H(\boldsymbol{c}_2) - 2I(\boldsymbol{c}_1, \boldsymbol{c}_2),$$

where $H(\boldsymbol{c}_i)$ is the entropy associated with $\boldsymbol{c}_i$ defined as

$$H(\boldsymbol{c}_i) = -\sum_{k=1}^{K^{(i)}} \frac{n_k^{(i)}}{n} \log \frac{n_k^{(i)}}{n}$$

for $i = 1, 2$. $I(\boldsymbol{c}_1, \boldsymbol{c}_2)$ represents the mutual information between two partitionings and is defined as

$$I(\boldsymbol{c}_1, \boldsymbol{c}_2) = \sum_{k=1}^{K^{(1)}} \sum_{r=1}^{K^{(2)}} \frac{n_{kr}}{n} \log \frac{n_{kr} n}{n_k^{(1)} n_r^{(2)}},$$

where n_{kr} is the number of observations being assigned simultaneously to the kth and rth clusters under partitionings $\boldsymbol{c}_1$ and $\boldsymbol{c}_2$ respectively. When $\boldsymbol{c}_1 = \boldsymbol{c}_2$, $VI(\boldsymbol{c}_1, \boldsymbol{c}_2) = 0$. The upper bound for VI is equal to $\log n$. The **MixSim** function responsible for calculating VI is called `VarInf()`. It is worth pointing out that all the indices listed above and implemented in **MixSim** are symmetric, which means that for any index, $Index(\boldsymbol{c}_1, \boldsymbol{c}_2) = Index(\boldsymbol{c}_2, \boldsymbol{c}_1)$.

3. Package description and illustrative examples

In this section we provide a detailed description of **MixSim**'s capabilities, along with illustrations. First, we briefly summarize **MixSim**'s functionality which includes the following features:

- simulating Gaussian mixture models with homogeneous or heterogeneous, spherical or ellipsoidal covariance matrices according to the pre-specified level of average or/and maximum overlap;
- simulating datasets from Gaussian mixtures;
- calculating pairwise overlap for Gaussian mixture components;
- simulating outliers, noise and inverse Box-Cox transformed variables;
- constructing parallel distribution plots to display multivariate Gaussian mixtures;
- calculating various indices for measuring the classification agreement between two examined partitionings.

The complete list of functions included in the package along with their brief descriptions can be found in Table 1. More details and illustrative examples for each function are provided in the following sections. Our illustrative examples can be run by the function `demo()` in all considered cases. For instance, the code of the first example in Section 3.1 can be reproduced using the command `demo("sec3.1_ex1", package = "MixSim")`. If there are several

Function	Description
`MixSim()`	Simulates a mixture with pre-specified level of $\bar{\omega}$ or/and $\check{\omega}$
`overlap()`	Calculates the exact overlap given the parameters of a mixture
`simdataset()`	Simulates datasets given the parameters of a mixture
`pdplot()`	Constructs a parallel distribution plot
`RandIndex()`	Calculates Rand, adjusted Rand, Fowlkes-Mallows, and Merkin indices
`ClassProp()`	Calculates the agreement proportion between two classification vectors
`VarInf()`	Calculates the variation of information for two classification vectors
`perms()`	Returns all permutations given the number of elements

Table 1: Summary of functions implemented in **MixSim**.

Section	Demo names
Section 3.1	`"sec3.1_ex1"`, `"sec3.1_ex2"`, `"sec3.1_ex3"`
Section 3.2	`"sec3.2_ex1"`

Section 3.3	`"sec3.3_ex1a"`, `"sec3.3_ex1b"`, `"sec3.3_ex2c"`, `"sec3.3_ex2d"`
	`"sec3.3_ex3a"`, `"sec3.3_ex3b"`, `"sec3.3_ex4c"`, `"sec3.3_ex4d"`

Section 3.4	`"sec3.4_ex1"`, `"sec3.4_ex2b"`, `"sec3.4_ex2c"`
Section 4	`"sec4_ex1"`

Table 2: Summary of demos included in **MixSim**.

plots produced in the example, the plot name is also included in the demo name, for example: `demo("sec3.3_ex1a", package = "MixSim")`. The names of all demo programs are provided in Table 2.

3.1. Simulating mixtures with the function `MixSim()`

`MixSim()` is the main function of the package and is responsible for finding a Gaussian mixture model satisfying the user-specified level of average or/and maximum overlap. The command has the following syntax:

```
MixSim(BarOmega = NULL, MaxOmega = NULL, K, p, sph = FALSE, hom = FALSE,
  ecc = 0.90, PiLow = 1.0, int = c(0.0, 1.0), resN = 100, eps = 1e-06,
  lim = 1e06)
```

The parameters of the function are listed in Table 3.

When both parameters `BarOmega` and `MaxOmega` are specified, the second algorithm from Section 2.3 is run. If only one of the above parameters is provided, the first algorithm from Section 2.3 is employed. The smallest allowed number of components `K` is 2; in this case, `BarOmega` $\equiv$ `MaxOmega`. `MixSim()` allows the simulation of mixtures with spherical or general covariance structure as well as with homogenenous or nonhomogeneous components. In order to better control the shape of produced components, the parameter `ecc` specifying the maximum eccentricity can be used. Maitra and Melnykov (2010) defined the multidimensional eccentricity by extending its definition for two-dimensional ellipses: $e = \sqrt{1 - \lambda_{\min}/\lambda_{\max}}$ with $\lambda_{\min}$ and $\lambda_{\max}$ being correspondingly the smallest and largest eigenvalues of the (covariance) matrix. If some simulated dispersion matrices have $e > e_{\max}$ specified by `ecc`, all eigenvalues will be scaled in order to have $e_{\mathrm{new}} = e_{\max}$. `PiLow` controls the minimum of the mixing proportions, with `PiLow = 1` indicating equality of all mixing proportions. Option `int` specifies a side of a hypercube on which mean vectors are generated. If `int` is not provided, the default interval is $(0, 1)$. The last three options `resN`, `eps`, and `lim` described in Table 3 specify technical parameters used in `MixSim()`. `resN` sets the maximum number of resimulations allowed when the desired overlap cannot be reached easily. This happens, for example, when asymptotic maximum or average overlap is lower than the corresponding value specified by the user. `eps` represents the error bound used in our root-finding procedure and Davies (1980)'s algorithm approximating the distribution of a linear combination of χ^2 random variables based on the numerical invertion of the characteristic function. Finally, `lim` specifies the maximum number of terms allowed in numerical integration involved in Davies (1980)'s procedure. We next illustrate three sample usages of `MixSim()`.

Arguments	Description
`BarOmega`	Average pairwise overlap $\bar{\omega}$
`MaxOmega`	Maximum pairwise overlap $\check{\omega}$
`K`	Number of mixture components
`p`	Number of dimensions
`sph`	Nonspherical (`FALSE`) or spherical (`TRUE`) mixture components
`hom`	Nonhomogeneous (`FALSE`) or homogenenous (`TRUE`) mixture components
`ecc`	Maximum eccentricity
`PiLow`	Smallest mixing proportion
`int`	Side of a hypercube for simulating mean vectors
`resN`	Maximum number of mixture resimulations
`eps`	Error bound
`lim`	Maximum number of integration terms according to Davies (1980)
Values	Description
`$Pi`	Vector of mixing proportions
`$Mu`	Mean vectors
`$S`	Covariance matrices
`$OmegaMap`	Map of misclassification probabilities
`$BarOmega`	Average pairwise overlap $\bar{\omega}$
`$MaxOmega`	Maximum pairwise overlap $\check{\omega}$
`$rcMax`	Index of the pair of clusters producing maximum overlap
`$fail`	Flag of successful completion

Table 3: Summary of available arguments and values returned by the function `MixSim()`.

Simulating a mixture with non-homogeneous mixture components, equal mixing proportions and pre-specified values of maximum and average pairwise overlap

Here, we illustrate the use of `MixSim()` in simulating a 5-dimensional mixture with 4 components, and average and maximum overlaps equal to 0.05 and 0.15 correspondingly. The following example (`"sec3.1_ex1"`) beginning with `set.seed(1234)` for reproducibility illustrates the use of the function. Since the parameter `PiLow` is not specified, the mixture model has equal mixing proportions. As options `sph` and `hom` are not provided, nonhomogeneous and general (ellipsoidal) covariance matrices are simulated.

```
R> set.seed(1234)
R> (ex.1 <- MixSim(BarOmega = 0.05, MaxOmega = 0.15, K = 4, p = 5))


K = 4, p = 5, BarOmega = 0.04999942, MaxOmega = 0.1499996, success = TRUE.

Pi:
[1] 0.25 0.25 0.25 0.25

Mu:
          p.1        p.2        p.3        p.4        p.5
K.1 0.8446347 0.02955681 0.59976935 0.26841977 0.12060890
K.2 0.1007055 0.74816114 0.01596063 0.04946115 0.74762379
```

```
K.3 0.3572377 0.75895820 0.37595634 0.79946271 0.02569277
K.4 0.5063586 0.82122865 0.54475658 0.26668445 0.34463732

S: ... too long and skipped. Use operator $ to access.
```

```
R> summary(ex.1)
```

```
OmegaMap:
             k.1          k.2         k.3        k.4
k.1 1.0000000000 0.0004152306 0.002332968 0.01901556
k.2 0.0009103698 1.0000000000 0.014849260 0.08575316
k.3 0.0031164483 0.0079691289 1.000000000 0.02517269
k.4 0.0355134505 0.0642464525 0.040701777 1.00000000

rcMax: 2 4
```

From the output, we can see that mixture components with numbers 2 and 4 provide the largest overlap (see vector `ex.1$rcMax`). The corresponding probabilities of mislcassification can be found in the matrix `ex.1$OmegaMap`: they are 0.0642 and 0.0858. The map of misclassification probabilities as well as the numbers of components producing the largest pairwise overlap can be conveniently accessed by function `summary()`. Both desired values, $\check{\omega}$ and $\bar{\omega}$, have been reached within the error bound as we can see from `ex.1$BarOmega` and `ex.1$MaxOmega` correspondingly.

Simulating a mixture with non-homogeneous spherical mixture components, unequal mixing proportions and pre-specified value of maximum pairwise overlap

The following example (`"sec3.1_ex2"`) simulates a bivariate mixture with three spherical components, mixing proportions no less than 0.1 and maximum pairwise overlap 0.1. Parameter `hom` is not provided, thus nonhomogeneous components are simulated.

```
R> set.seed(1234)
R> (ex.2 <- MixSim(MaxOmega = 0.1, K = 3, p = 2, sph = TRUE, PiLow = 0.1))
```

```
K = 3, p = 2, BarOmega = 0.03672386, MaxOmega = 0.09999973, success = TRUE.

Pi:
[1] 0.1048634 0.4386534 0.4564832

Mu:
          p.1       p.2
K.1 0.2325505 0.6660838
K.2 0.5142511 0.6935913
K.3 0.5449748 0.2827336

S: ... too long and skipped. Use operator $ to access.
```

```
R> summary(ex.2)
```

```
OmegaMap:
              k.1         k.2          k.3
k.1 1.000000e+00 0.075664063 4.520316e-05
k.2 2.433567e-02 1.000000000 6.629426e-03
k.3 9.497808e-06 0.003487719 1.000000e+00

rcMax: 1 2
```

As we can see from the above output, the desired maximum overlap has been reached. It is produced by the components 1 and 2 with misclassification probabilities 0.0243 and 0.0757 respectively.

Simulating a mixture with homogeneous spherical components, equal mixing proportions and pre-specified value of average pairwise overlap

The last illustration (`"sec3.1_ex3"`) of the function `MixSim()` deals with a 4-dimensional mixture with 2 components. The average overlap is specified at the level 0.05. To increase accuracy, we let `eps` be equal to 1e-10. Coordinates of mean vectors are simulated between 0 and 10. Since arguments `sph` and `hom` are specified as `TRUE`, clusters should be spherical and homogeneous.

```
R> set.seed(1234)
R> (ex.3 <- MixSim(BarOmega = 0.05, K = 2, p = 4, sph = TRUE, hom = TRUE,
+    int = c(0, 10), eps = 1e-10))

K = 2, p = 4, BarOmega = 0.05, MaxOmega = 0.05, success = TRUE.

Pi:
[1] 0.5 0.5

Mu:
         p.1      p.2        p.3      p.4
K.1 1.137034 6.222994 6.09274733 6.233794
K.2 8.609154 6.403106 0.09495756 2.325505

S: ... too long and skipped. Use operator $ to access.

R> summary(ex.3)

OmegaMap:
      k.1   k.2
k.1 1.000 0.025
k.2 0.025 1.000

rcMax: 1 2
```

As we can see from the obtained output, the average and maximum overlaps provided in `ex.3$BarOmega` and `ex.3$MaxOmega` respectively are equal to each other. It happens because

Arguments	Description
`Pi`	Vector of mixing proportions
`Mu`	Mean vectors
`S`	Covariance matrices
`eps`	Error bound
`lim`	Maximum number of integration terms according to Davies (1980)
Values	Description
`$OmegaMap`	Map of misclassification probabilities
`$BarOmega`	Average pairwise overlap $\bar{\omega}$
`$MaxOmega`	Maximum pairwise overlap $\check{\omega}$
`$rcMax`	Index of the pair of clusters producing maximum overlap

Table 4: Summary of available arguments and values returned by the function `overlap()`.

we have only two mixture components. Misclassification probabilities provided in the matrix `ex.3$OmegaMap` are both equal to 0.025 because the components are homogeneous and mixing proportions are equal to each other. From the output, we can also see the effect of the increased accuracy.

3.2. Calculating exact overlap with the function `overlap()`

In this section we discuss the capability of **MixSim** to calculate the exact overlap when given the parameters of a Gaussian mixture model. This feature is useful if it is desired to estimate the level of clustering complexity for an existing classification dataset. This is another important application of **MixSim**. There exist numerous classification datasets widely used for testing clustering algorithms. However, the knowledge about these datasets is usually very limited: the investigator typically knows only which clusters are problematic having no information about the level of interaction among the clusters. Function `overlap()` provides the user with the map of misclassification probabilities. The command has the following syntax:

```
overlap(Pi, Mu, S, eps = 1e-06, lim = 1e06)
```

The parameters accepted by `overlap` as well as values returned by the function are provided in Table 4. All five arguments – `Pi`, `Mu`, `S`, `eps`, and `lim` – have the same meaning as in the function `MixSim()` discussed in Section 3.1. The returned values are also discussed in the same section.

Finding exact overlap for the Iris dataset

Here, we analyze the celebrated *Iris* dataset of Anderson (1935) and Fisher (1936). The data consist of 150 4-dimensional points measuring the width and length of petals and sepals; there are 50 observations from each of three different species of Iris: *Setosa*, *Versicolor*, and *Virginica*. It is well-known that *Virginica* and *Versicolor* are difficult to separate while *Setosa* creates a very distinct cluster. The following code (`"sec3.2_ex1"`) estimates the parameters of a Gaussian mixture model with three components for *Iris*, provided the true classification vector. Then, the exact overlap is calculated using the function `overlap()`.

```
R> data("iris", package = "datasets")
R> p <- ncol(iris) - 1
```

```
R> id <- as.integer(iris[, 5])
R> K <- max(id)
R> Pi <- prop.table(tabulate(id))
R> Mu <- t(sapply(1:K, function(k){ colMeans(iris[id == k, -5]) }))
R> S <- sapply(1:K, function(k){ var(iris[id == k, -5]) })
R> dim(S) <- c(p, p, K)
R> overlap(Pi = Pi, Mu = Mu, S = S)

$OmegaMap
             [,1]         [,2]       [,3]
[1,] 1.000000e+00 7.201413e-08 0.00000000
[2,] 1.158418e-07 1.000000e+00 0.02302315
[3,] 0.000000e+00 2.629446e-02 1.00000000

$BarOmega
[1] 0.01643926

$MaxOmega
[1] 0.0493176

$rcMax
[1] 2 3
```

As we can see from the output, the substantial maximum overlap of 0.0493 is produced by the second and third components: *Virginica* and *Versicolor*. At the same time, these two clusters almost do not overlap with *Setosa*. This explains why the majority of clustering methods prefer two-cluster solutions combining *Virginica* and *Versicolor* together.

3.3. Simulating datasets with the function `simdataset()`

In this section, we discuss some capabilities of **MixSim** for simulating datasets, along with outliers, from a given (perhaps simulated) mixture model. The function responsible for data generation is called `simdataset()` and has the following form:

```
simdataset(n, Pi, Mu, S, n.noise = 0, n.out = 0, alpha = 0.001,
  max.out = 100000, int = NULL, lambda = NULL)
```

The arguments and returned values are listed in Table 5. Parameters `Pi`, `Mu`, and `S` have the same meaning as before. The size of a generated dataset is defined as `n + n.out`, where `n.out` specifies the number of outliers needed. If the parameter `n.out` is not specified, no outliers are produced by `simdataset`. Parameter `max.out` specifies the maximum number of outlier resimulations with the default value of 1e05. `alpha` specifies ellipsoidal contours beyond which outliers have to be simulated. The number of dimensions for the dataset is defined as `dim(Mu)[2] + n.noise`. By default, `n.noise = 0`. The interval `int` defines a side of a hypercube for outlier simulation. It is also used for simulating noise variables if `n.noise` is greater than 0. Both outliers and noise variables are simulated from a uniform hypercube. When `int` is not provided, the interval bounds are chosen to be equal to the smallest and

Arguments	Description
`n`	Sample size
`Pi`	Vector of mixing proportions
`Mu`	Mean vectors
`S`	Covariance matrices
`n.noise`	Number of noise variables
`n.out`	Number of outliers
`alpha`	Level for 1 - alpha contour for simulating outliers
`max.out`	Maximum number of trials to simulate outliers
`int`	Interval to simulate outliers or/and noise variables
`lambda`	Vector of coefficients for an inverse Box-Cox transformation
Values	**Description**
`$X`	Produced dataset
`$id`	Classification vector for the produced dataset

Table 5: Summary of available arguments and values returned by the function `simdataset()`.

largest coordinates in mean vectors correspondingly. The last parameter, `lambda`, specifies a vector of size `dim(Mu)[2] + n.noise` that performs an inverse Box-Cox transformation for every coordinate. By default, `simdataset()` generates datasets from Gaussian mixture models. If the user wants to produce data that are not normally distributed, the argument `lambda` can be helpful. The procedure uses the multivariate Box-Cox transformation given by $x^* = (x^\lambda - 1)/\lambda$, where x and x^* represent the original and transformed observations, respectively. x^* is approximately normally distributed for some value λ. We use an idea related to inverting the Box-Cox transformation to provide non-normally distributed data. The transformation we propose is given by $x = (\lambda x^* + 1)^{\frac{1}{\lambda}} - 1$. When $\lambda = 1$, the identity transformation is employed. Thus, the parameter `lambda` specifies desired transformations for each coordinate.

The following examples illustrate the capabilities of the function.

Simulating datasets from Gaussian mixtures

The following code illustrates how `simdataset()` can be used to simulate data from the mixture obtained by `MixSim`. Here, we obtain a two-dimensional mixture with 5 components, average overlap 0.05 and maximum overlap 0.20. Then, 500 observations are simulated from the mixture. Two samples obtained this way are provided in Figure 1a,b. The following commands (`"sec3.3_ex1a"`) construct the Figure 1a:

```
R> set.seed(1234)
R> Q <- MixSim(MaxOmega = 0.20, BarOmega = 0.05, K = 5, p = 2)
R> A <- simdataset(n = 500, Pi = Q$Pi, Mu = Q$Mu, S = Q$S)
R> colors <- c("red", "green", "blue", "brown", "magenta")
R> par(mar = c(0.1, 0.1, 0.1, 0.1))
R> plot(A$X, col = colors[A$id], pch = 19, cex = 0.8,
+    xlab = "", ylab = "", axes = FALSE)
R> box()
```

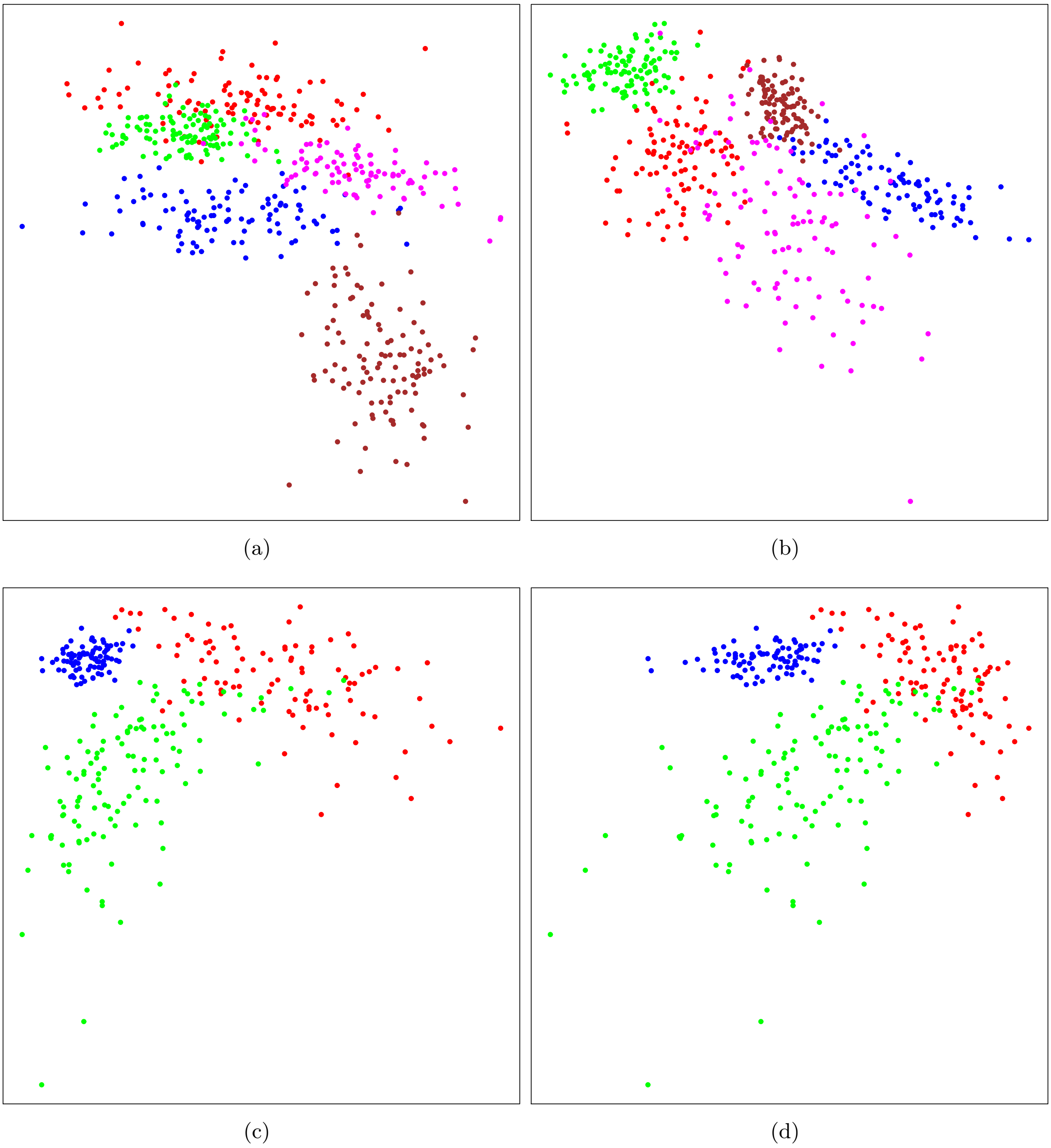


Figure 1: Simulated datasets obtained (a–b) from Gaussian mixture models and (c–d) by an inverse Box-Cox transformation.

The code for the Figure 1b is identical with the only difference in the seed value. The user needs to run `set.seed(1235)`.

Simulating datasets with inverse Box-Cox transformation

The following short example (`"sec3.3_ex1c"`) provides an illustration to an inverse Box-Cox transformation. First, we simulate a bivariate mixture with three components and maximum overlap 0.1; mean vectors are simulated from a hypercube with a side $(0, 1)$. Then, a dataset with 300 observations is simulated. The dataset is transformed using coefficients provided by option `lambda`. Two illustrative plots are included in Figure 1c,d. In both cases, we can see that obtained clusters do not follow patterns typical for normal distributions. The plots can be constructed running the following commands:

```
R> set.seed(1238)
R> Q <- MixSim(MaxOmega = 0.1, K = 3, p = 2, int = c(0.2, 1))
R> A <- simdataset(n = 300, Pi = Q$Pi, Mu = Q$Mu, S = Q$S,
+    lambda = c(0.1, 10))
R> colors <- c("red", "green", "blue")
R> par(mar = c(0.1, 0.1, 0.1, 0.1))
R> plot(A$X, col = colors[A$id], pch = 19, cex = 0.8,
+    xlab = "", ylab = "", axes = FALSE)
R> box()
```

To obtain the Figure 1d, use `lambda = c(10, 10)` instead of `lambda = c(0.1, 10)` used for the construction of the Figure 1c. This is the only change needed in the above code.

Simulating datasets with outliers

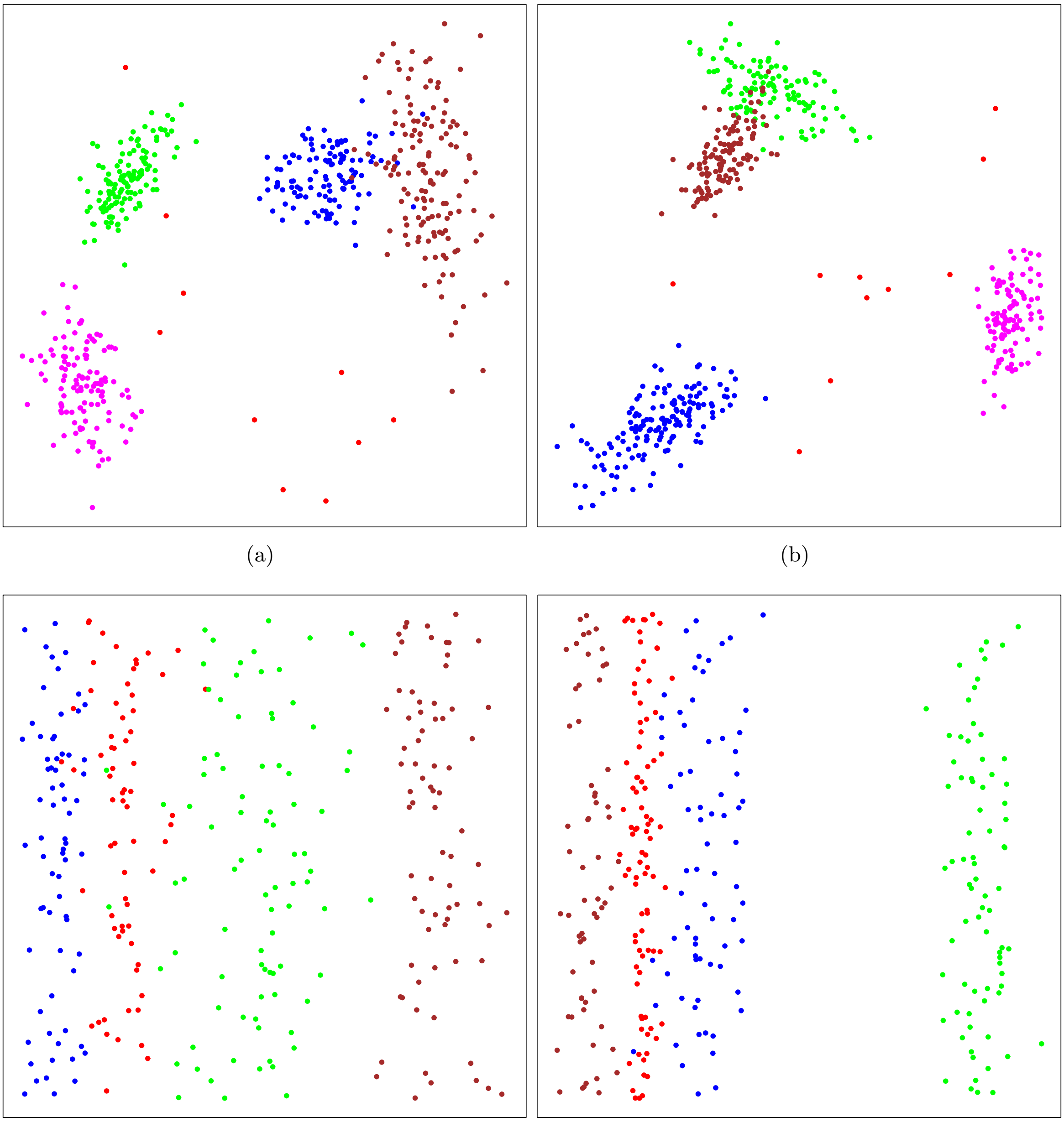
If it is desired to include outliers into a simulated dataset to increase clustering complexity or check the performance of clustering algorithms in the presence of scatter, the corresponding option `n.out` has to be specified. The following example demonstrates how `simdataset()` can be employed for simulating datasets with outlying observations. First, bivariate normal mixtures with 4 components and average overlap 0.01 are simulated similar to the previous examples. Then, the function `simdataset()` is employed to generate a dataset of 500 observations and introduce 10 outliers. Figure 2a,b demonstrates two datasets obtained this way. Red color points represent outlying observations. `id` is equal to 0 for such points. To obtain the plots, the user needs to run the following commands (`"sec3.3_ex3a"`).

```
R> set.seed(1234)
R> Q <- MixSim(BarOmega = 0.01, K = 4, p = 2)
R> A <- simdataset(n = 500, Pi = Q$Pi, Mu = Q$Mu, S = Q$S, n.out = 10)
R> colors <- c("red", "green", "blue", "brown", "magenta")
R> par(mar = c(0.1, 0.1, 0.1, 0.1))
R> plot(A$X, col = colors[A$id+1], pch = 19, cex = 0.8,
+    xlab = "", ylab = "", axes = FALSE)
R> box()
```

In order to obtain the Figure 2b, the seed 1237 has to be used: `set.seed(1237)`.

Simulating datasets with noise variables

To increase the complexity of clustering or test procedures reducing dimensionality, it can be needed to simulate datasets with noise variables. Here, we illustrate the use of `simdataset()` for simulating data from a one-dimensional mixture with 4 components and maximum overlap 0.1. One noise variable is added after that. As we can see from Figure 2c,d, it is obvious



(a)

(b)

(c)

(d)

Figure 2: Simulated datasets with (a–b) outlying observations and (c–d) noise variables.

that the second variable introduces substantial clustering complexity. The Figure 2c can be obtained by running the following code ("sec3.3_ex4c").

```
R> set.seed(1235)
R> Q <- MixSim(MaxOmega = 0.1, K = 4, p = 1)
R> A <- simdataset(n = 300, Pi = Q$Pi, Mu = Q$Mu, S = Q$S, n.noise = 1)
R> colors <- c("red", "green", "blue", "brown")
R> par(mar = c(0.1, 0.1, 0.1, 0.1))
```

```
R> plot(A$X, col = colors[A$id], pch = 19, cex = 0.8,
+       xlab = "", ylab = "", axes = FALSE)
R> box()
```

For the Figure 2d, the seed has to be changed to 1236.

3.4. Constructing a parallel distribution plot with the function `pdplot()`

The next function illustrated here is `pdplot()` – parallel distribution plot – described in detail by Maitra and Melnykov (2010). This plot is a convenient tool for visualizing multidimensional mixture models and components' interaction. The plot displays the principal components of a Gaussian mixture model. The first several components can serve as a good indicator of the major source of variability in a mixture. Table 6 lists the arguments acceptable in `pdplot()`. `Pi`, `Mu`, and `S` are the usual mixture parameters. `file` is the name of the pdf-file the plot has to be written to. Parameters `Nx` and `Ny` provide the numbers of horizontal and vertical smoothing intervals respectively. `MaxInt` sets the level of maximum color intensity while `marg` specifies plot margins. The function call has the following form:

```
pdplot(Pi, Mu, S, file = NULL, Nx = 5, Ny = 5, MaxInt = 1,
  marg = c(2, 1, 1, 1))
```

We illustrate the use of the function with several examples.

Parallel distribution plot for the Iris dataset

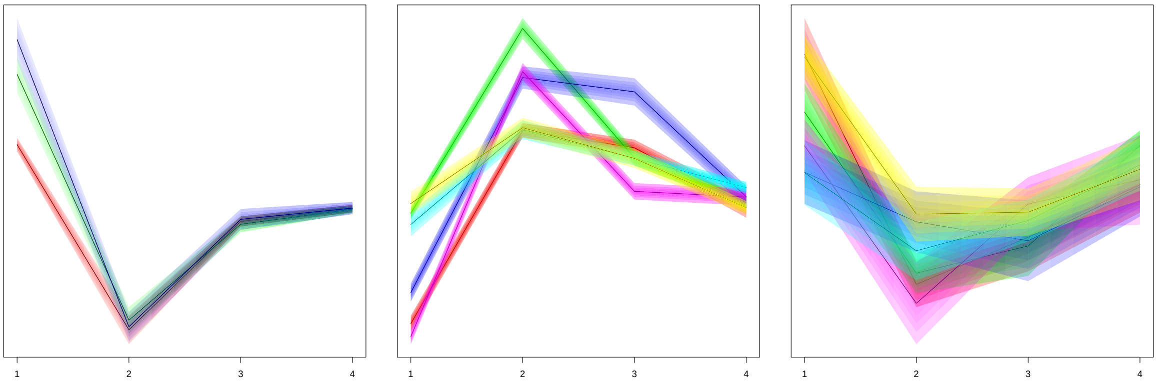
For the *Iris* dataset, we first estimate mixture parameters using the true classification vector. Then, we employ `pdplot()` function to construct a parallel distribution plot and save it into the file "Iris.pdf". The obtained plot is presented in Figure 3a. It can be clearly seen that the blue and green components have substantial overlap being close to each other in every principal component while the red one is well separated. It agrees well with our findings in Section 3.2. To construct the plot, the user has to estimate the mixture parameters using the code from the example in Section 3.2 first, and then to run the following command:

```
R> pdplot(Pi = Pi, Mu = Mu, S = S)
```

Parallel distribution plot for simulated mixtures

Arguments	Description
`Pi`	Vector of mixing proportions
`Mu`	Mean vectors
`S`	Covariance matrices
`file`	Name of the output pdf-file
`Nx`	Number of horizontal smoothing regions
`Ny`	Number of vertical smoothing regions
`MaxInt`	Maximum color intensity
`marg`	Plot margins

Table 6: Summary of available arguments in the function `pdplot()`.



(a) (b) (c)

Figure 3: Parallel distribution plots for (a) *Iris* dataset, (b) 6-component mixture with well-separated clusters ($\bar{\omega} = 0.001$), and (c) 6-component mixture with substantial overlap ($\bar{\omega} = 0.05$).

This example illustrates the difference between parallel distribution plots for well and poorly separated mixtures. We simulate two 4-dimensional mixtures with 6 components and average overlap 0.001 and 0.05 correspondingly. Figure 3b,c provides their parallel distribution plots. As can be seen, there is substantial difference between patterns in pictures. In the plot b, between-cluster variability dominates over within-cluster variability. This is an indication of well-separated clusters. The plot c suggests that in-cluster variability dominates over between-cluster variability implying larger overlap. The two plots can be easily reproduced with the following code (`"sec3.4_ex1b"` and `"sec3.4_ex1c"`).

```
R> set.seed(1234)
R> Q <- MixSim(BarOmega = 0.001, K = 6, p = 4)
R> pdplot(Pi = Q$Pi, Mu = Q$Mu, S = Q$S)
R> set.seed(1232)
R> Q <- MixSim(BarOmega = 0.05, K = 6, p = 4)
R> pdplot(Pi = Q$Pi, Mu = Q$Mu, S = Q$S)
```

3.5. Calculating indices with functions `RandIndex()`, `ClassProp()`, `VarInf()`

MixSim implements all indices described in Section 2.4. Three functions responsible for them are `RandIndex()`, `ClassProp()`, and `VarInf()`. Table 7 provides their brief description. The first function returns values of four indices based on counting the pairs of points in clusterings, `ClassProp()` calculates the agreement proportion for two classifications, while the latter one, `VarInf()`, computes the variation in information for two clusterings. The functions have the following syntax:

```
RandIndex(id1, id2)
ClassProp(id1, id2)
VarInf(id1, id2)
```

The following examples are illustrations of the use of all the three functions.

Function	Values	Description
`RandIndex()`	`$R`	Rand index
	`$AR`	Adjusted Rand index
	`$F`	Fowlkes and Mallows index
	`$M`	Mirkin index
`ClassProp()`		Agreement proportion in classification vectors
`VarInf()`		Variation in information of classification vectors

Table 7: Summary of values returned by functions `RandIndex()`, `ClassProp()`, and `VarInf()`. All three functions take two arguments `id1` and `id2` with the first and second classification vector, respectively.

```
R> id1 <- c(1, 1, 1, 1, 2, 2, 2, 3, 3, 3)
R> id2 <- c(1, 1, 1, 2, 2, 2, 3, 2, 3, 3)
R> RandIndex(id1, id2)

$R
[1] 0.6888889

$AR
[1] 0.2045455

$F
[1] 0.4166667

$M
[1] 28

R> ClassProp(id1, id2)

[1] 0.7

R> VarInf(id1, id2)

[1] 1.213685
```

3.6. Other auxiliary capabilities

The last function discussed in this section is `perms()`, which returns all possible permutations given the number of elements in a vector. Although this function is not directly related to other capabilities of **MixSim**, it is needed in the construction of `ClassProp()` since it is a faster implementation of the capability also provided by `permn()` available from package **combinat** (Chasalow 2012). The function has the following syntax:

```
perms(n)
```

A small example below illustrates the use of the function.

```
R> perms(3)

     [,1] [,2] [,3]
[1,]    1    2    3
[2,]    1    3    2
[3,]    2    1    3
[4,]    2    3    1
[5,]    3    1    2
[6,]    3    2    1
```

4. Illustrative use of the package

This section provides a brief illustration of the utility of **MixSim**. Here, we investigate and compare performances of four clustering methods realized in R. The first method is model-based clustering by means of the EM algorithm, the second and third ones are k-means and partitioning around medoids algorithms respectively, while the last method is hierarchical clustering with Ward's linkage. The algorithms are tested on datasets simulated from 4-dimensional mixtures with 6 heterogeneous non-spherical components and equal mixing proportions. The value of average overlap $\bar{\omega}$ varies from extreme (0.4) to very low (0.001). For each overlap, 100 mixtures are simulated with `MixSim()`, then a dataset of size 200 is generated from each mixture using function `simdataset()`. It is worth mentioning that we obtain exactly one dataset from each simulated mixture. Indeed, one can simulate more than one set from a mixture and even multiple datasets from the only mixture model. In this experiment, however, we are interested in examining as widely varying datasets as possible, subject to the only condition that simulated mixture models satisfy the pre-specified degree of average overlap. Variation in data patterns is substantially higher when we use different mixtures. Hence, we simulated just one set from each mixture, although in some other problems, a different strategy can be preferred.

The performance of methods is evaluated based on the adjusted Rand index, proportion of correct classifications, and variation in information for two partitionings. We use the original true and estimated classifications obtained from each clustering method to calculate the value of each index. Functions `RandIndex()`, `ClassProp()`, and `VarInf()` were employed. We calculate sample mean μ and standard deviation s for each characteristic over 100 simulated datasets for every level of $\bar{\omega}$. The results are provided in Table 8. Function `Mclust()` from the package **mclust** (Fraley and Raftery 2006) was employed for the EM algorithm. Functions `kmeans()` and `hclust()` were used for k-means and hierarchal clustering algorithms. The partitioning around medoids algorithm was employed by means of the function `PAM()` from the package **cluster** (Mächler, Rousseeuw, Struyf, Hubert, and Hornik 2012). The experiment can be reproduced by running the demo `"sec4_ex1"` or by using the code provided in the supplementary materials.

The obtained results are summarized in Table 8. As we can see, there is no uniform winner among the considered four clustering methods. The results suggest that k-means algorithm should be preferred over the rest of the field for substantial and moderate overlaps. The model-based clustering, however, is the clear winner for well-separated clusters ($\bar{\omega} \leq 0.01$). Hierarchical clustering with Ward's linkage slightly outperforms k-means for well-separated

		$\bar{\omega}$	0.400	0.300	0.250	0.200	0.150	0.100	0.050	0.010	0.005	0.001
Model-based	AR	μ	0.057	0.106	0.143	0.200	0.272	0.409	0.608	0.900	0.938	0.986
		s	0.024	0.043	0.054	0.061	0.064	0.086	0.081	0.055	0.044	0.021
	P	μ	0.321	0.761	1.185	0.454	0.520	0.621	0.768	0.951	0.970	0.993
		s	0.032	3.863	5.506	0.054	0.055	0.078	0.065	0.038	0.032	0.017
	VI	μ	2.972	2.737	2.579	2.382	2.086	1.640	1.064	0.278	0.181	0.044
		s	0.125	0.178	0.200	0.193	0.200	0.247	0.186	0.118	0.099	0.049
k-means	AR	μ	0.082	0.141	0.188	0.240	0.309	0.423	0.611	0.865	0.919	0.974
		s	0.026	0.033	0.042	0.047	0.045	0.070	0.066	0.059	0.043	0.038
	P	μ	0.349	0.406	0.443	0.493	0.552	0.634	0.772	0.929	0.959	0.986
		s	0.035	0.042	0.048	0.048	0.048	0.071	0.060	0.052	0.037	0.034
	VI	μ	2.938	2.681	2.480	2.280	2.002	1.635	1.077	0.362	0.232	0.077
		s	0.117	0.129	0.155	0.157	0.133	0.196	0.161	0.119	0.091	0.074
PAM	AR	μ	0.075	0.128	0.179	0.229	0.295	0.412	0.593	0.864	0.918	0.974
		s	0.023	0.031	0.043	0.052	0.051	0.069	0.074	0.051	0.039	0.020
	P	μ	0.340	0.390	0.436	0.483	0.540	0.623	0.758	0.933	0.962	0.989
		s	0.034	0.038	0.048	0.052	0.057	0.069	0.068	0.038	0.025	0.009
	VI	μ	2.995	2.740	2.533	2.322	2.065	1.679	1.126	0.373	0.245	0.085
		s	0.114	0.121	0.153	0.177	0.157	0.194	0.184	0.112	0.100	0.059
Ward	AR	μ	0.070	0.125	0.168	0.219	0.286	0.403	0.586	0.866	0.922	0.980
		s	0.025	0.035	0.042	0.051	0.053	0.070	0.070	0.062	0.045	0.022
	P	μ	0.335	0.389	0.425	0.476	0.533	0.619	0.753	0.935	0.963	0.991
		s	0.033	0.038	0.047	0.047	0.052	0.064	0.065	0.037	0.028	0.011
	VI	μ	2.971	2.716	2.536	2.330	2.060	1.665	1.108	0.360	0.222	0.064
		s	0.128	0.139	0.154	0.177	0.168	0.190	0.166	0.142	0.102	0.061

Table 8: Performance of the model-based, k-means, partitioning around medoids, and hierarchical clustering with Ward's linkage algorithms in clustering 4-dimensional datasets of size 200 with 6 groups. μ and s represent the sample mean and standard deviation for the adjusted Rand index (AR), proportion of correct classifications (P), and variation in information (VI) obtained over 100 replications.

clusters but loses to it in the cases of substantial and moderate overlap. Overall, k-means performs slightly better than the partitioning around medoids algorithm. All three indices considered agree on the suggested conclusions. Of course, this is a small example demonstrating the potential of **MixSim**, but it illustrates the utility of the package well.

5. Summary

This paper describes the R package **MixSim** which provides a convenient and friendly tool for simulating Gaussian mixture models and datasets according to the pre-specified level of clustering complexity expressed in terms of the average and maximum pairwise overlap among mixture components. **MixSim**'s functions are described and carefully illustrated on multiple examples. A small study illustrating the utility of the package is provided. The package is meant to be of interest to a broad audience working in the area of machine learning, clustering and classification.

Acknowledgments

The authors acknowledge partial support by the National Science Foundation CAREER Grant # DMS-0437555. We also thank the associate editor and reviewers whose comments and suggestions substantially improved the paper.

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Affiliation:

Volodymyr Melnykov
Department of Information Systems, Statistics, and Management Science
The University of Alabama
Tuscaloosa, AL 35487, United States of America
E-mail: vmelnykov@ua.edu
URL: http://cba.ua.edu/personnel/vmelnykov

Wei-Chen Chen
Computer Science and Mathematics Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831, United States of America
E-mail: wccsnow@gmail.com
URL: http://thirteen-01.stat.iastate.edu/snoweye

Ranjan Maitra
Department of Statistics and Statistical Laboratory
Iowa State University
Ames, IA 50011, United States of America
E-mail: maitra@iastate.edu
URL: http://maitra.public.iastate.edu

Journal of Statistical Software http://www.jstatsoft.org/
published by the American Statistical Association http://www.amstat.org/
Volume 51, Issue 12 *Submitted:* 2010-12-04
November 2012 *Accepted:* 2012-08-13