BayesBinMix: an R Package for Model Based Clustering of Multivariate Binary Data

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Abstract: The BayesBinMix package offers a Bayesian framework for clustering binary data with or without missing values by fitting mixtures of multivariate Bernoulli distributions with an unknown number of components. It allows the joint estimation of the number of clusters and model parameters using Markov chain Monte Carlo sampling. Heated chains are run in parallel and accelerate the convergence to the target posterior distribution. Identifiability issues are addressed by implementing label switching algorithms. The package is demonstrated and benchmarked against the Expectation-Maximization algorithm using a simulation study as well as a real dataset.

Keywords and phrases: CRAN package, mixture models, clustering binary data, trans-dimensional MCMC, Metropolis-coupled MCMC.

1. Introduction

Clustering data is a fundamental task in a wide range of applications and finite mixture models are widely used for this purpose [27, 26, 10]. In this paper our attention is focused on binary datasets. A variety of studies aims at identifying patterns in binary data including, but not limited to, voting data [18], text classification [20], handwritten digit recognition [2], medical research [41], animal classification Li [23] and genetics [1].

Finite mixture models can be estimated under a frequentist approach using the Expectation-Maximization (EM) algorithm [9]. However, the likelihood surface of a mixture model can exhibit many local maxima and it is well known that the EM algorithm fails to converge to the main mode if it is initialized from a point close to a minor mode. Moreover, under a frequentist approach, the selection of the number of clusters is not straightforward: a mixture model for each possible value of number of clusters should be fitted and then the number of clusters is selected according to penalized likelihood criteria such as the Bayesian information criterion [38] or the Integrated complete likelihood criterion [6].

On the other hand, the Bayesian framework allows to put a prior distribution on both the number of clusters as well as the model parameters and then (approximately) sample from the joint posterior distribution using Markov chain Monte Carlo (MCMC) algorithms [36, 39, 28]. However this does not mean that the Bayesian approach is not problematic: At first, vanilla MCMC algorithms can become trapped to a minor mode and in such a case a very large number of iterations is demanded in order to fully explore the posterior surface. Second, identifiability issues arise due to the label switching phenomenon [35] which complicate the inference procedure.

The BayesBinMix package explicitly takes care of the previously mentioned problems for the problem of clustering multivariate binary data:

1. Allows missing values in the observed data
2. Performs MCMC sampling for estimating the posterior distribution of the number of clusters and model parameters
3. Produces a rapidly mixing MCMC sample by running parallel heated chains which can switch states
4. Post-processes the generated MCMC sample and produces meaningful posterior mean estimates using state of the art algorithms to deal with label switching.

The rest of the paper is organised as follows. The mixture model is presented in Section 2. Its prior assumptions and the corresponding hierarchical model is introduced in Section 3.

*https://CRAN.R-project.org/package=BayesBinMix
The basic MCMC scheme is detailed in Section 4.1. Section 4.2 deals with post-processing the generated MCMC sample in order to overcome identifiability issues due to the label switching problem. Finally, the basic sampler is embedded in a Metropolis-coupled MCMC algorithm as described in Section 4.3.

2. Model

Let \( x = (x_1, \ldots, x_n) \) denote a random sample of multivariate binary data, where \( x_i = (x_{i1}, \ldots, x_{id}) ; d > 1 \), for \( i = 1, \ldots, n \). Assume that the observed data has been generated from a mixture of independent Bernoulli distributions, that is,

\[
x_i \sim \sum_{k=1}^{K} p_k \prod_{j=1}^{d} f(x_{ij}; \theta_{kj}) = \sum_{k=1}^{K} p_k \prod_{j=1}^{d} \theta_{kj}^{x_{ij}} (1 - \theta_{kj})^{1-x_{ij}} \mathbb{I}_{[0,1]}(x_{ij}), \tag{2.1}
\]

independently for \( i = 1, \ldots, n \), where \( \theta_{kj} \in \Theta = (0,1) \) denotes the probability of success for the \( k \)-th cluster and \( j \)-th response for \( k = 1, \ldots, K; j = 1, \ldots, d \), \( p = (p_1, \ldots, p_K) \in \mathcal{P}_{K-1} = \{ p_k ; k = 1, \ldots, K - 1 : 0 \leq p_k \leq 1 ; p_K = 1 - \sum_{k=1}^{K-1} p_k \} \) corresponds to the vector of mixture weights and \( \mathbb{I}_A(\cdot) \) denotes the indicator function of a (measurable) subset \( A \).

It is straightforward to prove that the variance-covariance matrix of a mixture of independent Bernoulli distributions is not diagonal (see e.g. [7]), which is the case for a collection of independent Bernoulli distributions. Therefore, the mixture model exhibits richer covariance structure thus it can prove useful to discover correlations in heterogeneous multivariate binary data.

The observed likelihood of the model is written as

\[
L_K(p, \theta ; x) = \prod_{i=1}^{n} \sum_{k=1}^{K} p_k \prod_{j=1}^{d} \theta_{kj}^{x_{ij}} (1 - \theta_{kj})^{1-x_{ij}}, \quad (p, \theta) \in \mathcal{P}_{K-1} \times \Theta^{Kd} \tag{2.2}
\]

where \( x \in \mathcal{X}^n = \{0,1\}^{nd} \). For any fixed value of \( K \), Equation (2.2) can be further decomposed by considering that observation \( i \) has been generated from the \( z_i \)-th mixture component, that is,

\[
x_i | z_i = k \sim \prod_{j=1}^{d} f(x_{ij}; \theta_{kj}), \quad \text{independent for } i = 1, \ldots, n. \tag{2.3}
\]

Note that the allocation variables \( z_i \in \mathcal{Z}_K = \{1, \ldots, K\}; i = 1, \ldots, n \) are unobserved, so they are treated as missing data. Assume that

\[
P(z_i = k | p, K) = \frac{p_k}{\sum_k p_k}, \quad k = 1, \ldots, K \tag{2.4}
\]

and furthermore that \( (x_i, z_i) \) are independent for \( i = 1, \ldots, n \). Data augmentation [42] considers jointly the complete data \( \{ (x_i, z_i) ; i = 1, \ldots, n \} \) and it is a standard technique exploited both by the Expectation-Maximization algorithm [9] as well as the Gibbs sampler [11]. The complete likelihood is defined as

\[
L_K^c(p, \theta ; x, z) = \prod_{i=1}^{n} p_{z_i} \prod_{j=1}^{d} \theta_{z_{ij}}^{x_{ij}} (1 - \theta_{z_{ij}})^{1-x_{ij}} = \prod_{k=1}^{K} p_k \prod_{i=1}^{n} \mathbb{I}_{[0,1]}(z_i = k) \prod_{j=1}^{d} \theta_{kj}^{x_{ij}} (1 - \theta_{kj})^{n_k-x_{ij}}, \quad (p, \theta) \in \mathcal{P}_{K-1} \times \Theta^{Kd} \tag{2.5}
\]

where \( n_k = \sum_{i=1}^{n} \mathbb{I}(z_i = k) \) and \( s_{kj} = \sum_{i=1}^{n} \mathbb{I}(z_i = k) x_{ij} \), \( k = 1, \ldots, K; j = 1, \ldots, d \), for a given \( (x, z) \in \mathcal{X}^n \times \mathcal{Z}^n \).
3. Prior assumptions

Note that the quantities $p, \theta, z$ are defined conditionally on $K$. For convenience we will assume that $K \in K = \{1, \ldots, K_{\text{max}}\}$, where $K_{\text{max}}$ denotes an upper bound on the number of clusters. Hence, under a model-based clustering point of view, the vector $(K, p, \theta, z) \in A := K \times \mathcal{P}_{K-1} \times \Theta^D \times \mathcal{Z}_K$ summarizes all unknown parameters that we wish to infer.

The following prior assumptions are imposed

$$K \sim \text{Discrete}\{1, \ldots, K_{\text{max}}\} \quad (3.1)$$

$$p|K \sim \text{Dirichlet}(\gamma_1, \ldots, \gamma_K) \quad (3.2)$$

$$\theta_{kj}|K \sim \text{Beta}(\alpha, \beta) \quad (3.3)$$

independent for $k = 1, \ldots, K; j = 1, \ldots, d$. The discrete distribution in Equation (3.1) can be either a Uniform or a Poisson distribution with mean $\lambda = 1$ truncated on the set $\{1, \ldots, K_{\text{max}}\}$. Equations (3.2) and (3.3) correspond to typical prior distributions for the mixture weights and success probabilities, that furthermore enjoy conjugacy properties. Typically, we set $\gamma_1 = \ldots = \gamma_K = \gamma > 0$ so that the prior assumptions do not impose any particular information that separates the mixture components between them, which is also a recommended practice in mixture modelling.

According to Equations (2.4), (2.5), (3.1), (3.2) and (3.3), the joint probability density function of the introduced model is

$$f(x, K, z, p, \theta|K_{\text{max}}, \alpha, \beta, \gamma) \propto \Gamma \left( \sum_{k=1}^{K} \gamma_k \right) \prod_{k=1}^{K} \Gamma(\gamma_k) \left\{ \Gamma(\alpha + \beta) \Gamma(\alpha) \Gamma(\beta) \right\}^K f(K|K_{\text{max}})$$

$$\times \prod_{k=1}^{K} \left\{ p_k^{n_k+\gamma_k-1} \prod_{j=1}^{d} \theta_{kj}^{s_j+\gamma_k-1}(1-\theta_{kj})^{\delta+s_j-\gamma_k-1} \right\} I_A(K, p, \theta, z). \quad (4.1)$$

From the last expression it is straightforward to derive the full conditional distributions of the component specific parameters and latent allocation variables as follows:

$$p|K, z \sim \text{Dirichlet}(\gamma_1 + n_1, \ldots, \gamma_K + n_K) \quad (4.2)$$
\[ \theta_{kj} | K, z, x \sim \text{Beta}(\alpha + s_{kj}, \beta + n_k - s_{kj}) \] (4.3)

\[ P(z_i = k | K, x, p, \theta) \propto p_k \prod_{j=1}^{d} \theta_{kj}^i (1 - \theta_{kj})^{1 - x_{ij}}, \quad k = 1, \ldots, K, \]

independent for \( i = 1, \ldots, n; k = 1, \ldots, K; j = 1, \ldots, d. \)

A general framework for updating the number of mixture components (\( K \)) is given by trans-dimensional MCMC approaches, such as the reversible jump MCMC [15, 36, 31] or the Birth-Death MCMC [39] methodologies. However, the conjugate prior assumptions used for the component specific parameters \((p, \theta)\) allow us to use simpler techniques by integrating those parameters out from the model and perform collapsed sampling [25] on the space of \((K, z)\). We use the allocation sampler [28] which introduced this sampling scheme in the context of mixtures of normal distributions.

Let \( A_0 = \Theta^{Kd} \times \mathcal{P}_{K-1} \) and \( A_1 = K \times \{1, \ldots, K\}^n \). Integrating out \((\theta, p)\) from (4.1) we obtain

\[ f(K, z | x, K_{\text{max}}, \alpha, \beta, \gamma) = \int_{A_0} f(z, \theta, p, K | x, K_{\text{max}}, \alpha, \beta, \gamma) d\theta dp \]

\[ \propto \frac{\Gamma(\sum_{k=1}^{K} \gamma_k)}{\prod_{k=1}^{K} \Gamma(\gamma_k)} \left\{ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \right\}^{Kd} f(K | K_{\text{max}}) \mathbb{I}_{A_1}(K, z) \]

\[ \times \int_{A_0} \frac{\Gamma(\sum_{k=1}^{K} \gamma_k)}{\prod_{k=1}^{K} \Gamma(\gamma_k)} \left\{ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \right\}^{Kd} f(K | K_{\text{max}}) \mathbb{I}_{A_1}(K, z) \]

\[ \times \int_{\mathcal{P}_{K-1}} \frac{\Gamma(\sum_{k=1}^{K} \gamma_k)}{\prod_{k=1}^{K} \Gamma(\gamma_k)} \left\{ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \right\}^{Kd} f(K | K_{\text{max}}) \mathbb{I}_{A_1}(K, z). \] (4.4)

Let now \( z_{[-i]} = \{z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_n\} \) and also define the following quantities, for \( i = 1, \ldots, n:\)

\[ n_k[i] = \sum_{h \neq i} \mathbb{I}(z_h = k), k = 1, \ldots, K \]

\[ s_{kj}[i] = \sum_{h \neq i} \mathbb{I}(z_h = k) x_{hj}, k = 1, \ldots, K, j = 1, \ldots, d \]

\[ A_1[i] = \{j = 1, \ldots, d : x_{ij} = 1\} \]

\[ A_0[i] = \{j = 1, \ldots, d : x_{ij} = 0\}. \]

From Equation (4.4), the (collapsed) conditional posterior distribution of \( z_i \) is

\[ P(z_i = k | z_{[-i]}, K, x) \propto \frac{n_k[i] + \gamma_k}{(\alpha + \beta + n_k[i])^d} \prod_{j \in A_1[i]} (\alpha + s_{kj}[i]) \prod_{j \in A_0[i]} (\beta + n_k - s_{kj}[i]), \] (4.5)

\( k = 1, \ldots, K; i = 1, \ldots, n. \)

It is well known that draws from the conditional distributions in Equation (4.5) exhibit strong serial correlation, slowing down the convergence of the MCMC sampler. The mixing can be improved by proposing simultaneous updates of blocks of \( z | K \), by incorporating proper Metropolis-Hastings moves on \( z | K \). Following [28], we also propose jumps to configurations that massively update the allocation vector as follows:
1. **Move 1**: select two mixture components and propose a random reallocation of the assigned observations.
2. **Move 2**: select two mixture components and propose to move all assigned observations from the 1st to the 2nd one.
3. **Move 3**: select two mixture components and propose a reallocation of the assigned observations according to the full conditional probabilities given the already processed ones.

Each move is accepted according to the corresponding Metropolis-Hastings acceptance probability, see Nobile and Fearnside [28] for details.

The final step of the allocation sampler is to update the number of clusters ($K$). According to Nobile and Fearnside [28], this is achieved by performing a Metropolis-Hastings type move, namely a pair of absorption/ejection moves which decrease/increase $K$, respectively. Assume that the current state of chain is $\{K, z\}$. The following pseudocode describes the Absorption/Ejection step:

1. Attempt ejection with probability $p'_K$, where $p_k^e = 1/2$, $K = 2, \ldots, K_{\text{max}} - 1$, $p_1^e = 1$ and $p_k^e = 0$. Otherwise, an absorption move is attempted.
2. Suppose that an ejection is attempted. The candidate state is $\{K', z'\}$ with $K' = K + 1$.
   (a) Propose reallocation of observations assigned to the ejecting component between itself and the ejected component according to the Beta($\tilde{\alpha}$, $\tilde{\beta}$) distribution.
   (b) Accept the candidate state with probability $\min\{1, R\}$ where
   \[
   R = R(\tilde{\alpha}) = \frac{f(K', z'|x) P(\{K', z'\} \rightarrow \{K, z\})}{f(K, z|x) P(\{K, z\} \rightarrow \{K', z'\})} \tag{4.6}
   \]
3. If an absorption is attempted:
   (a) all observations allocated to the absorbed component are reallocated to the absorbing component.
   (b) the candidate state is accepted with probability $\min\{1, 1/R(\tilde{\alpha})\}$.

The parameter $\tilde{\alpha}$ is chosen in a way that ensures that the probability of ejecting an empty component is sufficiently large. For full details the reader is referred to Nobile and Fearnside [28].

The allocation sampler for mixtures of multivariate Bernoulli distributions is summarized in the following algorithm.

**Algorithm 1** (Allocation sampler for Bernoulli mixtures). *Given an initial state $\{K^{(0)}, z^{(0)}\} \in \mathcal{A}_1$ iterate the following steps for $t = 1, 2, \ldots$*

1. For $i = 1, \ldots, n$
   (a) Compute $n_k^{(i)} = \sum_{h \neq i} I(z_h = k)$, $s_k^{(i)} = \sum_{h \neq i} I(z_h = k)x_{hij}$, $k = 1, \ldots, K^{(t)}$, $j = 1, \ldots, d$.
   (b) Update $z_j^{(t)} | z_{[\cdots i]}, \cdots$ according to Equation (4.5).
2. Propose Metropolis-Hastings moves $M_1$, $M_2$ and $M_3$ to update $z^{(t)}$.
3. Propose an Absorption/Ejection move to update $\{K^{(t)}, z^{(t)}\}$.

Note in step 1.(a):

$$z_h = \begin{cases} z_h^{(t)}, & h < i \\ z_h^{(t-1)}, & h > i. \end{cases}$$

Finally, we mention that after the last step of Algorithm 1 we can also simulate the component-specific parameters $\theta$ and $\psi$ from their full conditional posterior distributions given in (4.2) and (4.3), respectively. Although this is not demanded in case that the user is only interested in inferring $K, z, z|x$, it will produce an (approximate) MCMC sample from the full posterior distribution of $K, \psi, \theta, z|x$. If the observed data contains missing entries an extra step is implemented in order to simulate the corresponding values. For this purpose we use the full conditional distribution derived from Equation (2.3), taking only into account the subset of $\{1, \ldots, d\}$ that contains missing values for a given $i = 1, \ldots, n$. 
4.2. Label switching issue and identifiability

Label switching [35] is a well known identifiability problem occurring in MCMC outputs of mixture models, arising from the symmetry of the likelihood with respect to permutations of components’ labels. A set of sufficient conditions under a general framework of missing data models that lead to label switching and its consequences is given in Papastamoulis and Iliopoulos [33]. In brief, if the prior distribution exhibits the same invariance property, which is usually the case, the posterior distribution corresponding to a model with $K$ components will have a multiple of $K!$ symmetric modes. Hence, the standard practice of estimating the posterior means and other parametric functions by ergodic averages becomes meaningless due to the fact that the labels across the MCMC run will be switching across the symmetric modes.

Many algorithms are available for the solution of this problem and they are mostly based on post-processing the MCMC sample by switching all simulated values back to one among the $K!$ symmetric areas of the posterior. From a modelling point of view, the main challenge is to make the permuted sample reflect the topology of the posterior surface by retaining exactly one copy of the genuine modes. From a computational point of view, the main issue is to apply efficient algorithms that can find fast the optimal permutation among the $K!$ ones, per MCMC iteration. For this purpose we have considered the ECR algorithm [32, 29, 37] as well as the KL algorithm [40]. Both of these algorithms are quite efficient and in most cases exhibit almost identical results, but ECR is significantly faster and computationally lightweight compared to KL. The implementation was performed in the R package label.switching [30].

Note here that in the case that $d = 1$, Equation (2.1) collapses to a single Bernoulli distribution. However, this is not true in general when $d > 1$. Hence, there are two types of identifiability issues in mixture models: the first one is related to the fact that the model is identifiable only up to a permutation of the parameters (label switching). The second one is generic non-identifiability which relates to the fact that for a mixture of discrete distributions (such as the multivariate Bernoulli) totally different parameter values can correspond to the same distribution. We are not dealing with this second source of identifiability problems since it has been demonstrated that it is not of great practical importance [8].

4.3. Metropolis-coupled MCMC sampler

Vanilla algorithms may behave poorly in terms of mixing when dealing with MCMC sampling from high-dimensional posterior distributions. The existence of minor modes is a common source of mixing problems. On the other hand, mixture models exhibit multiple symmetric modes, due to the presence of the label switching phenomenon. A typical behaviour in such cases is that the sampler may demand a very large number of iterations to escape from the vicinity of a single mode, thus the sufficient exploration of the whole posterior surface may become unappealing within a practical computing time. There are various strategies for improving MCMC sampling, see e.g. chapter 6 in [14]. In this study, the Metropolis-coupled MCMC (MC$^3$) [12, 13, 3] strategy is adopted.

An MC$^3$ sampler runs $m$ chains with different posterior distributions $f_i(\xi); i = 1, \ldots, m$. The target posterior distribution corresponds to $i = 1$, that is, $f_1(\xi) = f(\xi)$, while the rest of them are chosen in a way that the mixing is improved. This is typically achieved by considering “heated” versions of the original target, that is, $f_i(\xi) = f(\xi)^{h_i}$ where $h_1 = 1$ and $0 < h_i < 1$ for $i = 2, \ldots, m$ represents the heat value of the chain. Note that when raising the posterior distribution to a power $0 < h_i < 1$ makes the modified posterior surface flatter, thus, easier to explore compared to $f(\xi)$. Only the chain that corresponds to the target posterior distribution is used for the posterior inference, however, after each iteration a proposal attempts to swap the states of two randomly chosen chains. This improves the mixing of the chain since it is possible that an accepted swap between the cold and a heated chain will make the former move to another mode.

Let $\xi^{(t)}_i$ denote the state of chain $i$ at iteration $t$ and that a swap between chains $i$ and $j$ is proposed. Note that in our setup $\xi = (K, z)$ and $f$ is given in (4.4) (up to a normalizing
| Argument      | Description                                                                 |
|---------------|------------------------------------------------------------------------------|
| Kmax          | Maximum number of clusters (integer, at least equal to two).                 |
| nChains       | Number of parallel (heated) chains. It should be equal to the number of available threads. |
| heats         | nChains-dimensional vector specifying the temperature of each chain: the 1st entry should always be equal to 1 and the rest of them lie on the set: (0, 1]. |
| binaryData    | The observed binary data (array). Missing values are allowed as long as the corresponding entries are denoted as NA. |
| outPrefix     | The name of the produced output folder. An error is thrown if the directory exists. |
| ClusterPrior  | Character string specifying the prior distribution of the number of clusters. Available options: 'poisson' or 'uniform'. It defaults to the (truncated) Poisson distribution. |
| m             | The number of MCMC cycles. At the end of each cycle a swap between a pair of heated chains is attempted. Each cycle consists of 10 iterations. |
| alpha         | First shape parameter of the Beta prior distribution (strictly positive). Defaults to 1. |
| beta          | Second shape parameter of the Beta prior distribution (strictly positive). Defaults to 1. |
| gamma         | Kmax-dimensional vector (positive) corresponding to the parameters of the Dirichlet prior of the mixture weights. Default value: rep(1, Kmax). |
| z.true        | An optional vector of cluster assignments considered as the ground-truth clustering of the observations. It is only used to obtain a final permutation of the labels (after the label switching algorithms) in order to maximise the similarity between the resulting estimates and the real cluster assignments. Useful for simulations. |
| ejectionAlpha | Probability of ejecting an empty component. Defaults to 0.2. |
| burn          | Optional integer denoting the number of MCMC cycles that will be discarded as burn-in period. |

In order to take full advantage of computing power in modern-day computers, our MC³ sampler utilizes parallel computing in multiple cores. This is achieved by running each chain in parallel using the R packages `foreach` [4] and `doParallel` [5]. Every 10-th iteration a swap is proposed between a pair of chains.

**5. Using package BayesBinMix**

The main function of the BayesBinMix package is `coupledMetropolis`, with its arguments shown in Table 1. This function takes as input a binary data array (possibly containing missing values) and runs the allocation sampler for a series of heated chains which run in parallel while swaps between pairs of chains are proposed. In the case that the most probable number of mixture components is larger than 1, the label switching algorithms are applied.

The generated output can be quite large, hence everything is written to a set of files in the folder specified by `outPrefix`. The most important output files are listed below.

- ‘K.allChains.txt’ $m \times n$Chains matrix containing the simulated values of the number of clusters per chain.
- ‘K.txt’ the simulated values of the number of clusters (K) of the cold chain (posterior distribution) discarding the values specified by `burn`.
- ‘rawMCMC.mapK.KVALUE.txt’ the raw MCMC output which corresponds to the most probable model (not identifiable).
- ‘reorderedMCMC-ECR-ITERATIVE1.mapK.KVALUE.txt’ the reordered MCMC output which corresponds to the most probable model, reordered according to the ECR-ITERATIVE-1 algorithm.
- ‘reorderedMCMC-ECR.mapK.KVALUE.txt’ reordered MCMC output which corresponds to the most probable model, reordered according to the ECR algorithm.
- ‘reorderedMCMC-STEPHENS.mapK.KVALUE.txt’ reordered MCMC output which corresponds to the most probable model, reordered according to the STEPHENS algorithm.
‘reorderedSingleBestClusterings.mapK.KVALUE.txt’ the most probable allocation of each observation after reordering the MCMC sample which corresponds to the most probable number of clusters.

‘z-ECR-ITERATIVE1.mapK.KVALUE.txt’ reordered simulated latent allocations which corresponds to the most probable model, reordered according to the ECR-ITERATIVE-1 algorithm.

‘z-ECR.mapK.KVALUE.txt’ the reordered simulated latent allocations which corresponds to the most probable model, reordered according to the ECR algorithm.

‘z-KL.mapK.KVALUE.txt’ the reordered simulated latent allocations which corresponds to the most probable model, reordered according to the STEPHENS algorithm.

‘classificationProbabilities.mapK.KVALUE.csv’ the reordered classification probabilities per observation after reordering the most probable number of clusters with the ECR algorithm.

‘xEstimated.txt’ Observed data with missing values estimated by their posterior mean estimate. This file is produced only in the case that the observed data contains missing values.

As the function runs it prints some basic information on the screen such as the progress of the sampler as well as the acceptance rate of proposed swaps between chains.

6. Examples

In this section the usage of BayesBinMix package is described and various benchmarks are presented. At first we demonstrate a typical implementation on a single simulated dataset and inspect the simulated parameter values and estimates. Then we perform an extensive study on the number of estimated clusters and compare our findings to the FlexMix package \[21, 16, 17\]. An application to a real dataset is provided next.

6.1. Simulation study

At first, a single simulated dataset is used in order to give a brief overview of the implementation. We simulated \( n = 200 \) observations from the multivariate Bernoulli mixture model (2.1). The true number of clusters is set to \( K = 6 \) and the dimensionality of the multivariate distribution is equal to \( d = 100 \). The mixture weights are drawn from a Dirichlet \( D(1, 1, 1, 1, 1, 1) \) distributions resulting to \( (50, 46, 30, 36, 12, 26) \) generated observations from each cluster. For each cluster, true values for the probability of success were generated from a Uniform distribution, that is, \( \theta_{kj} \sim U(0, 1) \), independently for \( k = 1, \ldots, K; j = 1, \ldots, d \).

Furthermore, we introduce some missing values to the generated data: each row is allowed to contain missing values with probability 0.2: for such a row the total number of missing entries is drawn from the binomial distribution \( B(100, 0.3) \). Finally, the observed data is saved to the \( 200 \times 100 \) array \( x \) which contains a total of 1038 missing values corresponding to 34 rows.

We will run 4 parallel chains with the following temperatures: \((1, 0.8, 0.6, 0.4)\). Observe that the first chain should correspond to the actual posterior distribution, so its temperature equals to 1. Now apply the coupledMetropolis function as follows.

```r
> library('BayesBinMix')
> nChains <- 4
> heats <- seq(1,0.4,length = nChains)

# using the truncated Poisson prior distribution on the number of clusters
> coupledMetropolis(Kmax = 20, nChains = nChains, heats = heats, binaryData = x,
                  outPrefix = 'bbm-poisson', ClusterPrior = 'poisson', m = 1100,
                  z.true = z.true, burn = 100)

# using the uniform prior distribution on the number of clusters
> coupledMetropolis(Kmax = 20, nChains = nChains, heats = heats, binaryData = x,
                  outPrefix = 'bbm-uniform', ClusterPrior = 'poisson', m = 1100,
                  z.true = z.true, burn = 100)
```
Note that we have called the function twice using either the truncated Poisson or the Uniform prior on the set \{1, \ldots, 20\}. The total number of MCMC cycles corresponds to \(m = 1100\) and the first 100 cycles will be discarded as burn-in period. Recall that each cycle contains 10 usual MCMC iterations, so this is equivalent to keeping every 10th iteration of a chain with 11000 iterations. Since we are interested to compare against the true values used to generate the data, we also supply \(z\) which contains the true allocation of each observation. It is only used for making the inferred clusters agree to the labelling of the true values and it has no impact on the MCMC or label switching algorithms.

In order to check the behaviour of the algorithm to the space of the number of mixture components we can inspect the simulated values per chain. This information is contained to the file ‘K.allChains.txt’. Figures 2.(a) and 2.(b) illustrate the state of each chain according to the Poisson and Uniform prior distribution respectively. The actual posterior corresponds to the blue line. Note that as the temperature increases the posterior distribution of \(K\) has larger variability. In both cases, the most probable state corresponds to \(K = 6\) clusters, that is, the true value. In particular, the estimated posterior probability of six clusters equals to 0.97 (Poisson prior) and 0.75 (Uniform prior).

Next we inspect the MCMC output conditionally on the event that the number of clusters equals 6. By default, the package will apply the label switching algorithms corresponding to the selected number of clusters and will save the permuted MCMC output. At first, we can inspect the raw MCMC output, saved to the file ‘rawMCMC.mapK.6.txt’, by plotting e.g. the values of mixture weights. As shown in Figures 2.(c) and 2.(d), the raw MCMC values are not identifiable due to the presence of the label switching problem. Notice that the sample is mixing very well to the symmetric posterior surfaces, since in every iteration labels are changing. The corresponding reordered values (according to the ECR algorithm), saved in the file ‘reorderedMCMC-ECR.mapK.6.txt’, are shown in Figures 2.(e) and 2.(f) and it is obvious that the high posterior density areas are quite close to the true values of mixture weights (indicated by horizontal lines). Finally, Figures 2.(g) and 2.(h) display the posterior mean estimate (arising from the reordered MCMC sample) versus the true values of \(\theta_{kj}, k = 1, \ldots, 6; j = 1, \ldots, 100\).

Next we are dealing with model selection issues, that is, selecting the appropriate number of clusters. For this reason we compare BayesBinMix with the EM-algorithm implementation provided in FlexMix. Under a frequentist framework, the selection of the number of mixture components is feasible using penalized likelihood criteria, such as the BIC [38] or ICL [6], after fitting a mixture model for each possible value of \(K\). We used the ICL criterion since it has been shown to be more robust than BIC, see e.g. Papastamoulis, Martin-Magniette and Maugis-Rabusseau [34]. We considered that the true number of clusters ranges in the set \{1, 2, \ldots, 10\} and for each case we simulated 10 datasets using the same data generation procedure as previously but without introducing any missing values due to the fact that FlexMix does not handle missing data. The number of observations varies in the set \(n \in \{200, 300, 400, 500\}\). For each simulated data the general call is the following.

```r
> library('BayesBinMix')
> library('flexmix')
> nChains <- 8
> heats <- seq(1, 0.4, length = nChains)
> coupledMetropolis(Kmax = 20, nChains = nChains, heats = heats, binaryData = x,
                      outPrefix = 'sampler', ClusterPrior = 'poisson', m = 330, burn = 30)
# now run flexmix for binary data clustering
> ex <- initFlexmix(x ~ 1, k = 1:20, model = FLXMCmvbinary(),
                    control = list(minprior = 0), nrep = 10)
```

Note that for both algorithms the number of clusters varies in the set \(\{1, \ldots, 20\}\). Eight heated chains are considered for the MCMC scheme, while each run of the EM algorithm is initialised using \(nrep = 10\) different starting points in FlexMix. Here we used a total of only \(m = 330\) MCMC cycles in order to show that reliable estimates can be obtained using small number of iterations. Figure 3 displays the most probable number of mixture components estimated by BayesBinMix and the selected number of clusters using FlexMix, for each possible value of the true number of clusters used to simulate the data. Observe that when the number of clusters is less than 5 both methods are able to estimate the true number of mixture components. However, FlexMix tends to underestimate the number of clusters when \(K \geq 5\), while BayesBinMix is able to recover the true value in most cases.
FIG 2. Results for simulated dataset 1 using the Poisson (left) or Uniform (right) prior distribution on the number of clusters.
6.2. Real data

We consider the zoo database available at the UC Irvine Machine Learning Repository [24]. The database contains 101 animals, each of which has 15 boolean attributes and 1 discrete attribute (legs). The partition of animals into a total of 7 classes (mammal, bird, reptile, fish, amphibian, insect and invertebrate) can be considered as the ground-truth clustering of the data, provided in the vector \( z \text{.ground\_truth} \). Following Li [23], the discrete variable legs is transformed into six binary features, which correspond to 0, 2, 4, 5, 6 and 8 legs, respectively. Also we eliminate one of the two entries corresponding to frog. In total we consider an 100 \( \times \) 21 binary array \( x \) as the input data.

Recall that the Bernoulli mixture in Equation (2.1) assumes that each cluster consists of a product of independent Bernoulli distributions. Here this assumption is not valid due to the fact that the six new binary variables arising from legs are not independent: they should sum at 1. Nevertheless, it is interesting to see how our method performs in cases that the data is not generated by the assumed model.

We test our method considering both prior assumptions on the number of clusters, as well as different hyper-parameters on the prior distribution of \( \theta_{kj} \) in Equation (3.3): we consider \( \alpha = \beta = 1 \) (default values) as well as \( \alpha = \beta = 0.5 \). Note that the second choice corresponds to the Jeffreys prior [19] for a Bernoulli trial. Figure 4 displays the estimated posterior distribution of the number of clusters \( K \) when \( K \in \{1, \ldots, 20\} \). This is done with the following commands.

```r
# read data
> xOriginal <- read.table("zoo.data", sep="",)
> x <- xOriginal[, -c(1, 14, 18)]
> x <- x[-27, ] # delete 2nd frog
```
# now transform v14 into six binary variables
> v14 <- xOriginal[-27, 14]
> newV14 <- array(data = 0, dim = c(100, 6))
> for(i in 1:100){
+   if( v14[i] == 0 ){ newV14[i,1] = 1 }
+   if( v14[i] == 2 ){ newV14[i,2] = 1 }
+   if( v14[i] == 4 ){ newV14[i,3] = 1 }
+   if( v14[i] == 5 ){ newV14[i,4] = 1 }
+   if( v14[i] == 6 ){ newV14[i,5] = 1 }
+   if( v14[i] == 8 ){ newV14[i,6] = 1 }
+ }
> x <- as.matrix(cbind(x, newV14))

# apply BayesBinMix using 8 heated chains
> library('BayesBinMix')
> nChains <- 8
> heats <- seq(1, nChains)
> coupledMetropolis(Kmax = 2, nChains = nChains, heats = heats, binaryData = x,
+   outPrefix = 'poisson-uniform', ClusterPrior = 'poisson',
+   m = 4400, burn = 400, z.true = z.ground_truth)

# K ~ U{1,...,20}, theta_{kj} ~ Beta(0.5, 0.5)
> coupledMetropolis(Kmax = 2, nChains = nChains, heats = heats, binaryData = x,
+   outPrefix = 'poisson-jeffreys', ClusterPrior = 'poisson',
+   m = 4400, burn = 400, z.true = z.ground_truth)

# K ~ U{1,...,20}, theta_{kj} ~ Beta(0.5, 0.5)
> coupledMetropolis(Kmax = 2, nChains = nChains, heats = heats, binaryData = x,
+   outPrefix = 'uniform-jeffreys', ClusterPrior = 'uniform',
+   m = 4400, burn = 400, z.true = z.ground_truth)

Next, we compare the estimated clusters (for the most probable value of $K$) with the classification of the data into 7 classes (given in the vector $z.ground\_truth$). For this reason we provide the rand index (adjusted or not) based on the confusion matrix between the
estimated and ground-truth clusters, using the package \texttt{flexclust} [22].

```r
> library('flexclust')
> z <- array(data = NA, dim = c(100, 4))
> z[, 1] <- read.table('poisson-uniform/reorderedSingleBestClusterings.mapK.4.txt')$ECR
> z[, 2] <- read.table('uniform-uniform/reorderedSingleBestClusterings.mapK.4.txt')$ECR
> z[, 3] <- read.table('poisson-jeffreys/reorderedSingleBestClusterings.mapK.6.txt')$ECR
> z[, 4] <- read.table('uniform-jeffreys/reorderedSingleBestClusterings.mapK.7.txt')$ECR
> rand.index <- array(data = NA, dim = c(4, 3))
> rownames(rand.index) <- c('poisson-uniform', 'uniform-uniform',  
  'poisson-jeffreys', 'uniform-jeffreys')
> colnames(rand.index) <- c('K_map', 'rand_index', 'adjusted_rand_index')
> rand.index[, 1] <- c(4, 4, 6, 7)
> for(i in 1:4){
+   rand.index[i, 2] <- randIndex(table(z[, i], z.ground_truth), correct = F)
+   rand.index[i, 3] <- randIndex(table(z[, i], z.ground_truth))
+ }
> rand.index

| K_map        | rand_index | adjusted_rand_index |
|--------------|------------|---------------------|
| poisson-uniform | 4 | 0.9230303 | 0.7959666 |
| uniform-uniform | 4 | 0.9234343 | 0.7969233 |
| poisson-jeffreys | 6 | 0.9505051 | 0.8621216 |
| uniform-jeffreys | 7 | 0.9490909 | 0.8525556 |
```

Note that both rand indices (raw and adjusted) are larger for \( z[, 3] \), that is, the six-component mixture model that corresponds to the Poisson prior on \( K \) and the Jeffreys prior on \( \theta_{kj} \). A detailed view on the estimated clusters for this particular model is shown in Figure 5. We conclude that the estimated groups are characterized by animals belonging to the same taxonomy with very small deviations from the true clusters. Interestingly, in the case that an animal is wrongly assigned to a cluster, notice that the estimated grouping might still make sense: e.g. the sea mammals dolphin, porpoise and seal are assigned to the fourth cluster which is mainly occupied by the group ‘fish’.

7. \textbf{Summary and remarks}

The \texttt{BayesBinMix} package for fitting mixtures of Bernoulli distributions with an unknown number of components has been presented. The pipeline consists of a fully Bayesian treatment for the clustering of multivariate binary data: it allows the joint estimation of the number of clusters and model parameters, deals with identifiability issues as well as it
produces a rapidly mixing chain. Using a simulation study we concluded that the method outperforms the EM algorithm in terms of estimating the number of clusters and at the same time produces accurate estimates of the underlying model parameters. In the real dataset we explored the flexibility provided by using different prior assumptions and concluded that the estimated clusters are strongly relevant to the natural grouping of the data.

For the prior distribution on the number of clusters our experience suggests that the truncated Poisson distribution performs better than the uniform (see also Nobile and Fearnside [28]). Regarding the prior distribution on the Bernoulli parameters we recommend to try both the uniform distribution (default choice) as well as the Jeffreys prior, especially when the sample size is small. An important parameter is the number of heated chains which run in parallel, as well as the temperature of each chain. We suggest to run at least \( n_{\text{chains}} = 4 \) heated chains. The heat parameter for each presented example achieved an acceptance ratio of proposed swaps between pairs of chains between 10% and 60%. The default choice for the temperature vector is \( \text{heats} = \text{seq}(1, 0.3, \text{length} = n_{\text{chains}}) \), however we advise to try different values in case that the swap acceptance ratio is too small (e.g. < 2%) or too large (e.g. > 90%). Finally, we recommend running the algorithm using at least \( m = 1100 \) and \( \text{burn} = 100 \) for total number of MCMC cycles and burn-in period, respectively. For these particular values of \( n_{\text{chains}} \) and \( m \), Figure 6 displays the wall clock time demanded by the coupledMetropolis function.

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