Bayesian Mixture Labelling by Highest Posterior Density

Weixin Yao and Bruce G. Lindsay

Abstract

A fundamental problem for Bayesian mixture model analysis is label switching, which occurs due to the non-identifiability of the mixture components under symmetric priors. We propose two labelling methods to solve this problem. The first method, denoted by PM(ALG), is based on the posterior modes and an ascending algorithm generically denoted ALG. We use each Markov chain Monte Carlo (MCMC) sample as the starting point in an ascending algorithm, and label the sample based on the mode of the posterior to which it converges. Our natural assumption here is that the samples converged to the same mode should have the same labels. The PM(ALG) labelling method has some computational advantages over other popular labelling methods. Additionally, it automatically matches the "ideal" labels in the highest posterior density credible regions. The second method does labelling by maximizing the normal likelihood of the labelled Gibbs samples. Using a Monte Carlo simulation study and a real data set, we demonstrate the success of our new methods in dealing with the label switching problem.

KEYWORDS: Label switching; Bayesian approach; Morkov chain Monte Carlo; Mixture model; Posterior modes

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Weixin Yao is Assistant Professor, Department of Statistics, Kansas State University, Manhattan, KS 66506 (E-mail: wxyao@ksu.edu). Bruce G. Lindsay is Willaman Professor, Department of Statistics, The Pennsylvania State University, University Park 16802 (E-mail: bgl@psu.edu). The authors are grateful to the associate editor, three referees, and the joint editor for insightful comments on the article. Their research was supported by NSF grant DMS-0405637.

1. INTRODUCTION

The m-component mixture models we consider here have densities of the form

$$p(x;\boldsymbol{\theta}) = \pi_1 f(x;\lambda_1) + \pi_2 f(x;\lambda_2) + \cdots + \pi_m f(x;\lambda_m)\ ,$$

where $\boldsymbol{\theta} = (\pi_1,\ldots,\pi_m,\lambda_1,\ldots,\lambda_m)^T$, $f(\cdot)$ is the density of a discrete or continuous random vector called the *component density*, λ_j is the component specific parameter, which can be scalar or vector, and π_j is the proportion of j^{th} subpopulation in the whole population with $\sum_{j=1}^{m}\pi_j = 1$. For a general introduction to mixture models, see Lindsay (1995), Böhning (1999), McLachlan and Peel (2000), and Mengersen (2009).

For any permutation $\boldsymbol{\sigma} = (\boldsymbol{\sigma}(1),\ldots,\boldsymbol{\sigma}(m))$ of the identity permutation $(1,\ldots,m)$, define the corresponding permutation of the parameter vector $\boldsymbol{\theta}$ by

$$\boldsymbol{\theta}^{\boldsymbol{\sigma}} = (\pi_{\boldsymbol{\sigma}(1)},\ldots,\pi_{\boldsymbol{\sigma}(m)},\lambda_{\boldsymbol{\sigma}(1)},\ldots,\lambda_{\boldsymbol{\sigma}(m)})^T.$$

Supposing that $\mathbf{x} = (x_1,\ldots,x_n)$ is a random sample from the m-component mixture density, the likelihood for $\mathbf{x}$ is

$$L(\boldsymbol{\theta};\mathbf{x}) = \prod_{i=1}^{n}\{\pi_1 f(x_i;\lambda_1) + \pi_2 f(x_i;\lambda_2) + \cdots + \pi_m f(x_i;\lambda_m)\}\ . \tag{1}$$

For any permutation $\boldsymbol{\sigma}$, $L(\boldsymbol{\theta}^{\boldsymbol{\sigma}};\mathbf{x})$ will be numerically the same as $L(\boldsymbol{\theta};\mathbf{x})$. Hence if $\hat{\boldsymbol{\theta}}$ is the maximum likelihood estimator (MLE), $\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}}$ is the MLE for any permutation $\boldsymbol{\sigma}$. In a technical sense, this means that the subscripts we assign to the π's and λ's are not identifiable unless we put additional restrictions on the model. This is the so-called *label switching* problem.

The label switching problem also occurs in Bayesian mixtures. Bayesian mixture analysis requires a prior distribution $\pi(\boldsymbol{\theta})$ for the parameters of the mixture model. If we do not have prior information that distinguishes between the components of a mixture model i.e. $\pi(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta}^{\boldsymbol{\sigma}})$ for any permutation $\boldsymbol{\sigma}$, the posterior distribution will be similarly symmetric and thus invariant to all the permutations of the component parameters and the marginal

posterior distributions for the parameters will also be identical for each mixture component. It is then meaningless to draw inference, relating to individual components, directly from Markov chain Monte Carlo (MCMC) samples using ergodic averaging before solving the label switching problem. For the illustrative examples of label switching, see Stephens (2000) and Jasra, Holmes, and Stephens (2005), among others.

Many methods have been proposed to deal with the labelling problem in Bayesian analysis. The easiest way to solve the label switching is to use an explicit parameter constraint so that only one permutation can satisfy it. This method is initially used by Diebolt and Robert (1994), Dellaportas, Stephens, Smith, and Guttman (1996), and Richardson and Green (1997). However, Celeux (1997), Celeux, Hurn, and Robert (2000), and Stephens (1997a,b, 2000) have all expressed their concerns about imposing an identifiability constraint. Another popular labelling method is to use a relabelling algorithm (Celeux 1998; Stephens 2000) that is designed to minimize a selected Monte Carlo risk. Stephens (2000) suggested a particular choice of loss function based on the Kullback-Liebler (KL) divergence. We will refer to this particular relabelling algorithm as the *KL algorithm*. Such risk based relabelling algorithms have two liabilities: They give results that can depend on the choice of starting labels and they require one to compare $m!$ permutations in each iteration. In addition, relabelling algorithms require batch processing, which can be computationally demanding on storage. Celeux (1998) and Stephens (2000) did provide some alternative on-line versions, designed to reduce the storage requirements.

There are many other labelling methods in the literature. See, for example, Celeux et al. (2000), Fruhwirth-Schnatter (2001), Hurn, Justel, and Robert (2003), Chung, Loken, and Schafer (2004), and Marin, Mengersen, and Robert (2005). Jasra et al. (2005) provided a good review about the existing methods to solve the label switching problem in Bayesian mixture modelling.

Our main proposed method PM(ALG) uses each MCMC sample as the starting value for an ascending algorithm generically denoted ALG. In our examples we will use the ECM (Meng and Rubin 1993) as the ascending algorithm. The samples are then relabelled ac-

cording to the posterior modes to which they converge. We will show that the PM(ALG) method is superior to other existing proposals in capturing the credible regions of highest posterior density (HPD). We will also show by example that it is computationally much faster than many other existing proposals when the number of components is larger. In addition, PM(ALG) is an online algorithm, which can reduce the storage requirements. Furthermore, risk based labelling methods have results that can depend on the choice of the initial labels for the samples. The PM(ALG) method does not require the initial labels, which can save considerable computation time.

The structure of the paper is as follows. Section 2 introduces our new labelling methods. In Section 3, we use two simulation examples and a real data set to compare the new labelling methods with two popular existing methods. We summarize our proposed labelling methods and discuss some future research work in Section 4.

2. INTRODUCTION OF NEW LABELLING METHODS

Given a smooth objective function, such as the posterior density $p(\boldsymbol{\theta})$, one can cluster points in $\boldsymbol{\theta}$ space by using an ascent algorithm (ALG) that monotonically increases the objective function. Each point $\boldsymbol{\theta}$ is then assigned to the critical point to which the algorithm converges when $\boldsymbol{\theta}$ is used as an initial value. Although there is the possibility of converging to a saddlepoint, in a typical posterior, the posterior modes will be the points of attraction for almost all starting values for the ascent algorithm, and so we are creating *modal clusters*. See Li, Ray, and Lindsay (2007) for the use of this idea in density based clustering.

2.1 Labelling Using Modal Clusters

The mixture labelling problem can be viewed as a clustering problem with a special structure. If we let the data set be all the MCMC samples $\boldsymbol{\theta}$ together with all their possible permutations $\boldsymbol{\theta}^{\boldsymbol{\sigma}}$, then the objective is to find $m!$ tight clusters, each containing exactly one permutation of each sample element $\boldsymbol{\theta}$. One can then choose any one of these tight clusters to be the newly labelled data set.

This relates to modal clustering as follows. If $\tilde{\boldsymbol{\theta}}$ is a mode, then so is $\tilde{\boldsymbol{\theta}}^{\boldsymbol{\sigma}}$ for any permutation $\boldsymbol{\sigma}$. If the chosen algorithm ascends from $\boldsymbol{\theta}$ to $\tilde{\boldsymbol{\theta}}^{\boldsymbol{\sigma}}$, we will say $\boldsymbol{\theta}$ has the same labelling as $\tilde{\boldsymbol{\theta}}^{\boldsymbol{\sigma}}$. If the algorithm is permutation symmetric we will also know that $\boldsymbol{\theta}^{\boldsymbol{\sigma}^{-1}}$, where $\boldsymbol{\sigma}^{-1}$ is the inverse permutation of $\boldsymbol{\sigma}$ such that $(\boldsymbol{\theta}^{\boldsymbol{\sigma}})^{\boldsymbol{\sigma}^{-1}} = \boldsymbol{\theta}$ for any $\boldsymbol{\theta}$ and $\boldsymbol{\sigma}$, will be given the same labelling as $\tilde{\boldsymbol{\theta}}$.

If the posterior density has a maximal mode at $\tilde{\boldsymbol{\theta}}$, it also has modes at all permutations of $\tilde{\boldsymbol{\theta}}$, and they are all maximal. We can pick one such mode to be our reference mode (hence the reference label), say by order constraint labelling on some parameter. Denote by $\hat{\boldsymbol{\theta}}$ the chosen reference maximal mode. If a sampled $\boldsymbol{\theta}$ converges to a maximal mode, say $\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}}$, then the natural label of $\boldsymbol{\theta}$ is $\boldsymbol{\sigma}^{-1}$ since $\boldsymbol{\theta}^{\boldsymbol{\sigma}^{-1}}$ would ascend to $\hat{\boldsymbol{\theta}}$. If the $\boldsymbol{\theta}$ converges to a minor mode, say $\boldsymbol{\theta}_*$, we could create a labelling system for all the samples $\boldsymbol{\theta}$ that are attracted to $\boldsymbol{\theta}_*$ (or its permutations) by creating a secondary reference mode $\hat{\boldsymbol{\theta}}_2$. If the reference mode $\hat{\boldsymbol{\theta}}_2$ was chosen so that it matched the label with the major mode $\hat{\boldsymbol{\theta}}$ using a risk based criterion that makes $\hat{\boldsymbol{\theta}}_2 = \boldsymbol{\theta}_*^{\boldsymbol{\sigma}}$ most similar to $\hat{\boldsymbol{\theta}}$ for some $\boldsymbol{\sigma}$, then we have a system that labels all points attracted to both the maximal and minor modes. One can extend this idea to any number of minor modes.

If one wishes to use this algorithm in a way that does not require storage of all the MCMC samples, one needs to find the reference maximal mode $\hat{\boldsymbol{\theta}}$ in advance of processing. Ascending algorithms are guaranteed only to find local modes, not global ones. In order to find one of the $m!$ maximal modes, we need to start from different initial values and choose the converged mode which has the largest posterior. Practically, the initial values can be chosen equally spaced from the burn-in samples of the MCMC sampling, such as choosing one from every 1000 (or more) burn-in samples. If one uses a burn-in of length 10,000 to 20,000, then, based on our experience, the resulting ten to twenty initial values will have every good chances of finding the maximal mode. (Suppose that the maximal mode garners 50% of the samples in posterior probability. If one were to take independent samples, then the chance it does not show up in 20 trials is about .000001 in probability.) If the MLE is not difficult to find, we can also include it as one of the initial values. (Although it is

possible that one finds a higher mode later in the sampling, it is unlikely to attract many of the samples, and so it might not be a wise choice to be the mode of reference.) Using above strategy, we successfully found all the maximal modes in the examples in Section 3. As an additional precaution, a general global search optimization technique, such as genetic algorithms (Holland 1975; Goldberg 1989; Davis 1991) and adaptive simulated annealing (Corana, Marchesi, Martini, Ridella 1992; Ingber and Rosen 1992), can be also used to find the maximal mode. For off-line version of our algorithm, one could also find the maximal mode at the end of the sampling. In our experience, the maximal mode is the one to which most of the samples converge when each MCMC sample is used as the starting value for the ascending algorithm.

Take the above found reference maximal mode $\hat{\boldsymbol{\theta}}$ and its associated minor modes as the reference modes (hence the reference labels). The aim of labelling is to find the labels $(\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_N)$ such that $\{\boldsymbol{\theta}_1^{\boldsymbol{\sigma}_1}, \ldots, \boldsymbol{\theta}_N^{\boldsymbol{\sigma}_N}\}$ have the same label meaning as $\hat{\boldsymbol{\theta}}$. Roughly speaking, this means that we would like this labelling to create a tight cluster around $\hat{\boldsymbol{\theta}}$. The algorithm of our proposed labelling method is as follows.

Algorithm 1: *Labelling based on posterior modes and an ascent algorithm (PM(ALG))*
Step 1: Taking each MCMC sample $\{\boldsymbol{\theta}_t, t = 1, \ldots, N\}$ as the initial value, find the corresponding converged mode $\{\mathbf{m}_t, t = 1, \ldots, N\}$ using the given ascent algorithm ALG.
Step 2: Apply to m_t the order constraint labelling used to define $\hat{\boldsymbol{\theta}}$, denoted by $\boldsymbol{\sigma}_t^*$ (hence $m_t^{\boldsymbol{\sigma}_t^*}$ has the same order constraint as $\hat{\boldsymbol{\theta}}$) and find the label $\boldsymbol{\sigma}_t$ of $\boldsymbol{\theta}_t$ based on the following situations.

a) If $\mathbf{m}_t^{\boldsymbol{\sigma}_t^*}$ is $\hat{\boldsymbol{\theta}}$, up to numerical error, then $\boldsymbol{\sigma}_t = \boldsymbol{\sigma}_t^*$.

b) If $\mathbf{m}_t^{\boldsymbol{\sigma}_t^*}$ is not $\hat{\boldsymbol{\theta}}$, but it is equivalent (up to a permutation) to a known reference minor mode, say $\hat{\boldsymbol{\theta}}_2$, assign the label $\boldsymbol{\sigma}_t$ such that $\mathbf{m}_t^{\boldsymbol{\sigma}_t} = \hat{\boldsymbol{\theta}}_2$.

c) If $\mathbf{m}_t^{\boldsymbol{\sigma}_t^*}$ is not $\hat{\boldsymbol{\theta}}$ and is not equivalent to a preexisting reference minor mode, create a new reference minor mode $\mathbf{m}_t^{\boldsymbol{\sigma}_t}$, where $\boldsymbol{\sigma}_t$ is based on a risk based criterion such as least

squares:

$$\boldsymbol{\sigma}_t = \arg\min_{\boldsymbol{\sigma}} (\mathbf{m}_t^{\boldsymbol{\sigma}} - \hat{\boldsymbol{\theta}})^T (\mathbf{m}_t^{\boldsymbol{\sigma}} - \hat{\boldsymbol{\theta}}) \,. \quad \square \tag{2}$$

The main idea of PM(ALG) is to explore the geometry of the mixture posterior by using each MCMC draw as a starting point for the ascent algorithm ALG and labelling the samples based on the modes of the posterior density they converge to. The natural assumption here is that *the samples converged to the same mode should have the same labels.*

2.2 The ECM Algorithm

The EM class of algorithms provide a natural ascent methodology for clustering because they are easy to use, requiring no choice of tuning parameters to maintain their ascent property. We can extend the modal clustering idea to the posterior density in order to label samples by constructing a Bayesian EM algorithm suitable in many mixture models. If the algorithm given below is not suitable in a given Bayesian mixture problem, it could be replaced with a gradient ascent algorithm that is suitably tuned to provide monotonic increases in the posterior.

Let us start by introducing an ascending algorithm to find the local posterior mode of Bayesian mixtures. Define the latent variable

$$Z_{ij} = \begin{cases} 1, & \text{if the } i^{th} \text{ observation is from } j^{th} \text{ component;} \\ 0, & \text{otherwise.} \end{cases}$$

Then the complete likelihood for $(\mathbf{x}, \mathbf{Z})$ is

$$L(\boldsymbol{\theta}; \mathbf{x}, \mathbf{Z}) = \prod_{i=1}^{n} \prod_{j=1}^{m} [\pi_j f(x_i; \lambda_j)]^{Z_{ij}},$$

where $\mathbf{Z} = \{Z_{ij}, 1 \le i \le n, 1 \le j \le m\}$, and the complete posterior distribution is

$$p(\boldsymbol{\theta}, \mathbf{Z} \mid \mathbf{x}) = \frac{1}{p(\mathbf{x})} \pi(\boldsymbol{\theta}) L(\boldsymbol{\theta}; \mathbf{x}, \mathbf{Z}),$$

where $p(\mathbf{x})$ is the marginal density for $\mathbf{x} = \{x_1 \cdots, x_n\}$.

Suppose that all the prior parameters are fixed and we are in a setting such that we can use Gibbs sampler to get the MCMC samples, i.e. there exists a partition of $\boldsymbol{\theta} = \{\boldsymbol{\theta}_{(1)}, \ldots, \boldsymbol{\theta}_{(p)}\}$ such that all the conditional complete posterior distributions $\{p(\boldsymbol{\theta}_{(i)} \mid ...), 1 \leq i \leq p\}$ are easily found, where $\boldsymbol{\theta}_{(i)}$ can be scalar or vector and |... denotes conditioning on all other parameters and the latent variable $\mathbf{Z}$. By combining the ideas of ECM (Meng and Rubin 1993), a class of GEM algorithm (Dempster, Laird, and Rubin 1977), and properties of Gibbs sampler, we propose the following algorithm to find the posterior modes of Bayesian mixtures.

Algorithm 2: *ECM algorithm for Bayesian mixtures (ECM(BM))*
Starting with the initial value of $\boldsymbol{\theta}$, iterate the following two steps until a fixed point is reached.

E-step: Find the conditional expectation of the latent variable $\mathbf{Z}$, i.e. the classification probability for each observation

$$p_{ij} = E(Z_{ij} \mid \mathbf{x}, \boldsymbol{\theta}) = \frac{\pi_j f(x_i; \lambda_j)}{\sum_{l=1}^{m} \pi_l f(x_i; \lambda_l)}.$$

M-step: Update $\boldsymbol{\theta}$ by maximizing the conditional complete posterior distribution $p(\boldsymbol{\theta}_{(i)} \mid ...), 1 \leq i \leq p$ sequentially with the latent variable Z_{ij} replaced by the classification probability p_{ij}. □

From the theory of ECM (Meng and Rubin 1993) and GEM (Dempster et al. 1977), we know that the posterior distribution $p(\boldsymbol{\theta})$ will increase after each iteration. Moreover, it is clear that the algorithm has a natural equivalence property. If $\boldsymbol{\theta}$ converges to $\boldsymbol{\theta}_*$, then $\boldsymbol{\theta}^{\boldsymbol{\sigma}}$ converges to ${\boldsymbol{\theta}_*}^{\boldsymbol{\sigma}}$. This will mean that if a modal cluster is formed by the algorithm, a fixed permutation of its elements will also be a cluster that ascends to the permuted mode.

2.3 Implementation Issues

One nice feature of PM(ALG) is that the algorithm does not depend on any initial choice of labels, which can save much computation time compared to other relabelling algorithms. In addition, PM(ALG) is an online algorithm, which does not require batch processing and thus reduces the amounts of storage.

Notice that the PM(ALG) method does not require one to compare $m!$ permutations to find each $\boldsymbol{\sigma}_t$ except for the initial discovery of a minor mode. In our experience most of the samples will converge to one of the $m!$ maximal modes. If $\mathbf{m}_t$ is one of the maximal modes i.e. there exists $\boldsymbol{\sigma}_t$ such that $\mathbf{m}_t^{\boldsymbol{\sigma}_t} = \hat{\boldsymbol{\theta}}$, the natural label of $\mathbf{m}_t$ is $\boldsymbol{\sigma}_t$ and it can be directly found by ordering $\mathbf{m}_t$ (based on any one dimensional component parameter such as a component mean) the same as the reference mode $\hat{\boldsymbol{\theta}}$.

For example, for a univariate normal mixture, suppose the reference maximal mode $\hat{\boldsymbol{\theta}}$ is ordered by the component means, so

$$\hat{\boldsymbol{\theta}} = (\hat{\pi}_1, \ldots, \hat{\pi}_m, \hat{\mu}_1, \ldots, \hat{\mu}_m, \hat{\sigma}_1, \ldots, \hat{\sigma}_m)$$

where $\hat{\mu}_1 < \hat{\mu}_2 < \ldots < \hat{\mu}_m$. Suppose $\mathbf{m}_t$ is one of the $m!$ maximal modes and we want to find $\boldsymbol{\sigma}_t$ such that $\mathbf{m}_t^{\boldsymbol{\sigma}_t} = \hat{\boldsymbol{\theta}}$. If the label $\boldsymbol{\sigma}^*$ is the one such that $\mathbf{m}_t^{\boldsymbol{\sigma}^*}$ is also ordered by the component means μ's, then we have $\boldsymbol{\sigma}^* = \boldsymbol{\sigma}_t$. Hence if $\mathbf{m}_t$ is one of the maximal modes, the labelling of $\mathbf{m}_t$ will be as easy as the order constraint labelling. This property makes PM(ALG) much faster, when m is large, than other risk based relabelling algorithms, which require $m!$ comparison in each iteration.

If $\mathbf{m}_t$ is a minor mode, we use the distance criteria (2) to find $\boldsymbol{\sigma}_t$ such that the distance between $\mathbf{m}_t^{\boldsymbol{\sigma}_t}$ and $\hat{\boldsymbol{\theta}}$ is minimized. Many other existing labelling methods can be also used to label the minor modes. For example, similar to the KL algorithm, we can also use the Kullback-Leibler divergence from the distribution on clusterings based on the reference mode

$\hat{\boldsymbol{\theta}}$, to the distribution on clusterings based on $\mathbf{m}_t^{\boldsymbol{\sigma}}$. Hence the criteria (2) can be replaced by

$$\boldsymbol{\sigma}_t = \arg\max_{\boldsymbol{\sigma}} \sum_{i=1}^{n} \sum_{j=1}^{m} p_{ij}(\hat{\boldsymbol{\theta}}) \log(p_{ij}(m_t^{\boldsymbol{\sigma}})) \,, \tag{3}$$

where $p_{ij}(\boldsymbol{\theta}) = \pi_j f(x_i; \lambda_j) / \sum_{l=1}^{m} \{\pi_l f(x_i; \lambda_l)\}$ is the classification probability of x_i from j^{th} component based on parameter $\boldsymbol{\theta}$. One nice feature of this criteria is its invariance to the scale effect of parameters. Notice that both of the above two criteria ((2) and (3)) require $m!$ comparisons to get the label $\boldsymbol{\sigma}_t$ for the minor mode $\mathbf{m}_t$.

2.4 HPD Labels and Labelling Credibility

In this section, we will describe one very attractive feature of PM(ALG) based on the new concept of "HPD label". This leads to a new method to assess the quality of the labels that have been assigned. To simplify the explanation, let us assume that the number of components is two (i.e. $m = 2$) and there are only one permutation class of modes (i.e. maximal modes).

Suppose that the parameter space is the full product space Ω (π's in the simplex, λ's in cross product space). Let us say that a subset S of Ω is an *identifiable subset* if there are no degenerate points in S and for every $\boldsymbol{\theta} \in S$, we have $\boldsymbol{\theta}^{\boldsymbol{\sigma}} \notin S$, where $\boldsymbol{\sigma} = (2, 1)$. If we restrict the parameters to lie in an identifiable subset S, then all the parameters have unique labels. For any identifiable subset S, we can create image set by permutation: $S^{\boldsymbol{\sigma}} = \{\boldsymbol{\theta}^{\boldsymbol{\sigma}} : \boldsymbol{\theta} \in S\}$. The image set is also identifiable.

Let us suppose that our goal is to build credible regions for the parameters, for any fixed credibility level $1 - \alpha$, using regions of highest posterior density (HPD). Such credible regions have the theoretical justification of being the smallest volume credible regions at a fixed level. To be specific, let the regions have the form $\psi_c = \{\boldsymbol{\theta} : p(\boldsymbol{\theta}) \geq c\}$, where $c = c_\alpha$ is chosen to give the target credibility level. For a given mode $\hat{\boldsymbol{\theta}}$, we define $S_c(\hat{\boldsymbol{\theta}})$ to be the maximal connected subset of the HPD region ψ_c that contains $\hat{\boldsymbol{\theta}}$. We will call $S_c(\hat{\boldsymbol{\theta}})$ the *modal region* defined by c and $\hat{\boldsymbol{\theta}}$. When $c = p(\hat{\boldsymbol{\theta}})$, $S_c(\hat{\boldsymbol{\theta}})$ is the single point $\{\hat{\boldsymbol{\theta}}\}$. As c

decreases, the size of $S_c(\hat{\boldsymbol{\theta}})$ increases. Note also that $S_c^{\boldsymbol{\sigma}}(\hat{\boldsymbol{\theta}})$, the permutation image of $S_c(\hat{\boldsymbol{\theta}})$, is automatically the maximal connected subset that contains $\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}}$, i.e. $S_c^{\boldsymbol{\sigma}}(\hat{\boldsymbol{\theta}}) = S_c(\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}})$. As long as c is sufficiently large, the set ψ_c will be the union of disjoint identifiable sets $S_c(\hat{\boldsymbol{\theta}})$ and $S_c(\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}})$. Assume that we have specified such a value of c. Then it is natural to use the identifiable (and hence well-labelled) set $S_c(\hat{\boldsymbol{\theta}})$ to describe the HPD region, as any other $S_c(\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}})$ is just the permuted (relabelled) image of $S_c(\hat{\boldsymbol{\theta}})$. In fact, if we view the problem asymptotically in n, these identifiable sets will eventually be disjoint for any c in accordance with the asymptotic identifiability of the labels.

Since the parameters have unique labels in $S_c(\hat{\boldsymbol{\theta}})$, the HPD region $S_c(\hat{\boldsymbol{\theta}})$ gives a natural labelling to all $\boldsymbol{\theta}$ values it contains. We will call these labels the *HPD labels*, and consider them to be the ideal labels. Note that not all points can be given HPD labels, as at some value of c, say c_0, the modal regions for $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}}$ intersect or they contain some degenerate points. For c larger than c_0, however, we can define unique HPD labels. We will let $\alpha_0 = \Pr(p(\boldsymbol{\theta}) > c_0)$ be the posterior probability of the points with HPD labels, and will call it the *labelling credibility*.

Assuming that the HPD region $S_c(\hat{\boldsymbol{\theta}})$ contains the single mode $\hat{\boldsymbol{\theta}}$, if we start an ascending algorithm at $\boldsymbol{\theta}$ within this HPD region, it necessarily climbs the posterior to $\hat{\boldsymbol{\theta}}$, and is so labelled. (The only way to leave the set is for the algorithm to decrease the posterior.) Hence the PM(ALG) method will assign the same labels to all the points of $S_c(\hat{\boldsymbol{\theta}})$ and thus PM(ALG) recovers all the ideal HPD labels, which is a primary motivation and essentially unique benefit of labelling based on an ascending algorithm. Specifically, if $\hat{\boldsymbol{\theta}}$ is the reference mode, then any point of HPD region $S_c(\hat{\boldsymbol{\theta}})$ has the label with identity permutation $(1, 2)$ and any point of region $S_c(\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}})$ has the label $\boldsymbol{\sigma}^{-1} = (2, 1)$.

If there are minor modes, the situation is somewhat more complex. Now each minor mode also creates a locally identifiable set that grows with index c shrinking. As c becomes small enough, the HPD region around one minor mode might begin to intersect with HPD regions from other minor or major modes. If we always take c to be sufficiently large that there is a single mode in the major modal regions, then the ALG always identifies the ideal

labels. If c is set low enough that there are one or more minor modes in $S_c(\hat{\boldsymbol{\theta}})$, then it is possible that our assignment method using a risk based criterion does not agree with the HPD region, which might cluster the minor modes differently. (While we would have liked for PM(ALG) to agree with HPD even for minor modal clusters, doing so would add considerable computational complexity to the problem).

Let c^* be the maximum posterior value among all the degenerate points. We define the *upper labelling credibility* to be $\alpha^* = \Pr(p(\boldsymbol{\theta}) > c^*)$. We will argue next that α^* provides an upper bound to, and a good approximation to the labelling credibility α_0. As such, it is a measure of how difficult the labelling problem is. It also indicates to us the level of arbitrariness involved in assigning labels to all sample points. (Small α^* implies that very few sample points will have HPD labels.)

When $c < c^*$, the modal region $S_c(\hat{\boldsymbol{\theta}})$ will contain one or more degenerate points and thus it is not identifiable. Hence $c_0 \geq c^*$ and the upper credibility level α^* is an *upper bound* for α_0, the proportion of points with ideal HPD labels. This upper bound becomes the actual labelling credibility if $S_c(\hat{\boldsymbol{\theta}})$ and $S_c(\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}})$ first connect at a degenerate point because when $c > c^*$, $S_c(\hat{\boldsymbol{\theta}})$ and $S_c(\hat{\boldsymbol{\theta}}^{\boldsymbol{\sigma}})$ are not connected and they do not contain any degenerate points. Unfortunately, it is difficult to verify whether this property holds in general, or even in a specific data analysis. Yao (2007) provided some graphical checking methods and the empirical evidence was that the upper bound α^* was indeed the labelling credibility α_0. We will therefore say that sample points with posterior greater than c^* are "likely" HPD labelled.

The value of c^* and hence the upper credibility level α^* can be easily estimated based on the ECM(BM) algorithm. When using ECM(BM), the updated point after each iteration from the degenerate point will be also the degenerate point. So the c^* value can be found by running the ECM(BM) algorithm starting from several degenerate points and choosing the converged degenerate mode with the largest posterior. In practice, one can make use of the maximum likelihood estimator (MLE) of $(m-1)$-component mixture when choosing the starting points. For example, suppose $m = 3$ and $((\hat{\pi}, 1-\hat{\pi}), (\hat{\lambda}_1, \hat{\lambda}_2))$ is the MLE of a two-component mixture. The parameter sets $((\hat{\pi}, 1-\hat{\pi}, 0), (\hat{\lambda}_1, \hat{\lambda}_2, \lambda_3))$, where λ_3 can be

any real value such as the one maximizing the prior for λ_3, can be included as one of the initial values for the ECM(BM) algorithm. Denote the estimate of c^* by $\hat{c}^*$. Then α^* can be estimated by the proportion of MCMC samples with posterior larger than $\hat{c}^*$.

2.5 The Classification MLE Method

From the asymptotic theory for the posterior distribution, see Walker (1969) and Fruhwirth-Schnatter (2006, sec. 1.3, 2.4.3, 3.3), we know that when sample size is large, the "correctly" labelled MCMC samples should, approximately, follow the normal distribution. Based on this property, we propose another method to do labelling based on minimizing the following negative log normal likelihood over $(\bar{\boldsymbol{\theta}}, \boldsymbol{\Sigma}, \boldsymbol{\sigma})$,

$$L(\bar{\boldsymbol{\theta}}, \boldsymbol{\Sigma}, \boldsymbol{\sigma}) = N \log(|\boldsymbol{\Sigma}|) + \sum_{t=1}^{N} (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}_t} - \bar{\boldsymbol{\theta}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}_t} - \bar{\boldsymbol{\theta}}) \tag{4}$$

where $\bar{\boldsymbol{\theta}}$ is the center value for the normal distribution, $\boldsymbol{\Sigma}$ is the covariance structure, and $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_N)$. This corresponds to applying the classification MLE clustering method to the full set of permuted $\boldsymbol{\theta}$-values. See Symons (1981), McLachlan (1982), and McLachlan and Basford (1988). As we shall see, this is a batch processing algorithm that comes close to matching the likely HPD labels.

If we assume $\boldsymbol{\Sigma}$ is diagonal i.e. all the parameters are orthogonal, this labelling method is exactly the same as Celeux (1998). We know that for the standard parametrization the parameters are not orthogonal. So here we use the general covariance matrix $\boldsymbol{\Sigma}$.

The algorithm to find labels by minimizing (4) is as follows.

Algorithm 3: *Labelling by normal likelihood (NORMLH)*

Starting with some initial values for $(\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_N)$ (setting them based on an order constraint, for example), iterate the following two steps until a fixed point is reached.

Step 1: Update $\bar{\boldsymbol{\theta}}$ and $\boldsymbol{\Sigma}$ by minimizing (4)

$$\bar{\boldsymbol{\theta}} = \frac{1}{N}\sum_{t=1}^{N} \boldsymbol{\theta}_t^{\boldsymbol{\sigma}_t} ,$$
$$\boldsymbol{\Sigma} = \frac{1}{N}\sum_{t=1}^{N} (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}_t} - \bar{\boldsymbol{\theta}})(\boldsymbol{\theta}_t^{\boldsymbol{\sigma}_t} - \bar{\boldsymbol{\theta}})^T .$$

Step 2: For $t = 1, \ldots, N$, choose $\boldsymbol{\sigma}_t$ by

$$\boldsymbol{\sigma}_t = \arg\min_{\boldsymbol{\sigma}} (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}} - \bar{\boldsymbol{\theta}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}} - \bar{\boldsymbol{\theta}}) . \quad \square$$

In step 2, after any change of $\boldsymbol{\sigma}_t$, we could also update $\bar{\boldsymbol{\theta}}$ and $\boldsymbol{\Sigma}$, thereby increasing the speed of convergence but increasing complexity. Since in each step of the above algorithm, the objective function (4) decreases, this algorithm must converge. However, like other general relabelling algorithms, this algorithm is only guaranteed to converge to a local minimum that depends on the initial labels. In order to get better results, we might choose a number of different starting labels.

The NORMLH method has a simple and nice explanation and runs very much faster than the PM(ALG) method if m is not large. As one referee pointed out, if m is too large or the dimension of the data is large, this method could have numerical problems due to the calculation of $\boldsymbol{\Sigma}^{-1}$. If this problem occurs, one could add a penalty function to the objective function. A penalty of the form $\lambda \times \text{Trace}(\boldsymbol{\Sigma}^{-1})$ creates a ridge type estimator for $\boldsymbol{\Sigma}$.

The dissertation of Yao (2007) described two other related labelling methods. Yao (2007) proposed to find the labels of the MCMC samples along with the mean $\bar{\boldsymbol{\theta}}$ by minimizing the determinant of the sample covariance matrix

$$L(\bar{\boldsymbol{\theta}}, \boldsymbol{\sigma}) = \det\left(\frac{1}{N}\sum_{t=1}^{N} (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}_t} - \bar{\boldsymbol{\theta}})(\boldsymbol{\theta}_t^{\boldsymbol{\sigma}_t} - \bar{\boldsymbol{\theta}})^T \right) , \tag{5}$$

where $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_N)$ and $\det(A)$ is the determinant of matrix A. The main idea of this method is to find the labels by minimizing the ellipsoidal volume of the labelled sample

clusters. Yao (2007) argued that NORMLH produces similar results to the above method but is much faster.

Without using the covariance $\boldsymbol{\Sigma}$ in step 2, the $\boldsymbol{\sigma}$ and $\bar{\boldsymbol{\theta}}$ found by Algorithm 3 in fact minimize $L(\bar{\boldsymbol{\theta}}, \boldsymbol{\sigma}) = \sum_{t=1}^{N} (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}^t} - \bar{\boldsymbol{\theta}})^T (\boldsymbol{\theta}_t^{\boldsymbol{\sigma}^t} - \bar{\boldsymbol{\theta}})$. This method is the K-means type labelling method introduced in the dissertation of Yao (2007). When $\boldsymbol{\theta}$ only contains m parameters (one for each component), say the m component means for one dimension data, this labelling method will be exactly the same as the order constraint labelling. However, unlike the order constraint labelling, this method can incorporate different component parameters together and can be easily extended to the multivariate case.

3. EXAMPLES

In this section, we will use two simulation examples and one real data set to compare our proposed two labelling methods (PM(ALG) and NORMLH) with order constraint labelling (OC) and Stephens' KL algorithm (KL). The OC method refers to ordering on the mean parameters. For PM(ALG), we used ECM(BM) for the ascent algorithm and we will refer to this particular modal cluster labelling method as PM(ECM). We used the MLE and twenty equally spaced samples from the 20,000 burn-in samples as the initial values to find the reference maximal mode. In all of our examples, we successfully found the maximal modes.

For comparison, we report the number of different labels for each method that differed from PM(ECM). We also report the newly defined upper labelling credibility level which can approximate the proportion of the HPD labels and measure how difficult the labelling problem is.

All the computations were done in Matlab 7.0 using a personal desktop with Intel Core 2 Quad CPU 2.40GHz. It is known that the OC method is the fastest one and it takes no more than several seconds in our examples. Hence, we only report the runtime for KL, NORMLH, and PM(ECM). We here have used PM(ECM) in batch mode so that we can determine its runtime in direct comparison with the others. Since the runtime for the NORMLH and KL algorithms depends on the number of starting points (i.e. the initial labels for all samples),

we only report the runtime of NORMLH and KL when using the PM(ECM) labels as the initial labels. (*The real runtime for NORMLH and KL could be much longer. If one used ten different initializations for the algorithm, it might take about ten times as long (generally longer than that since the runtime of NORMLH and KL depends on the quality of start values).*) Using these starts also ensures that the other methods are as similar to PM(ECM) as possible.

3.1 Simulation Studies

Example 3.1: We generated 400 data points from 0.3N(0,1)+0.7N(0.5,2). Based on this data set, we generated 20,000 MCMC samples (after initial burn-in) of component means, component proportions, and the unequal component variance. The MCMC samples are generated by Gibbs sampler with the priors given by Phillips and Smith (1996) and Richardson and Green (1997). That is to assume

$$\boldsymbol{\pi} \sim D(\delta, \delta),\ \mu_j \sim N(\xi, \kappa^{-1}),\ \sigma_j^{-2} \sim \Gamma(\alpha, \beta), \quad j = 1, 2\,,$$

where $D(\cdot)$ is Dirichlet distribution and $\Gamma(\alpha, \beta)$ is gamma distribution with mean α/β and variance α/β^2. Following the suggestion of Richardson and Green (1997), we let $\delta = 1$, ξ equal the sample mean of the observations, κ equal $1/R^2$, and $\alpha = 2$, where R is the range of the observations. Richardson and Green (1997) introduced an additional hierarchical model by allowing β to follow a gamma distribution, in order to reduce the influence of β on the posterior distribution of the number of components. Here we fix all the parameters in the prior distribution like Phillips and Smith (1996) and set $\beta = R^2/200$. Similar priors are used for the other two examples.

The upper labelling credibility level α^* was 98.5% and so almost all the samples likely have the ideal HPD labels. In this example, all the 20,000 samples, except for six, converged to the maximal modes. The other six samples converged to the same minor mode. Hence almost all the samples can be labelled directly by the converged maximal modes. The minor mode was labelled by the distance criterion (2).

The runtime for KL, NORMLH, and PM(ECM) were 66, 0.2, and 25 seconds, respectively. The total numbers of different labels between (OC, KL, NORMLH) and PM(ECM) were: 757, 212, and 0, respectively. On the subset above the labelling credibility c^*, the number of disagreements were 663, 203, and 0, respectively. (Note that NORMLH and PM(ECM) had the same labels in this example. Using the PM(ECM) labels as the initial values, NORMLH converged with just one iteration. If using the OC labels as the initial values, NORMLH converged in 3 iterations and the runtime was 3 seconds.)

Since there are only two components, we can easily use some parameter plots to check where the labelling differences occurred. Figure 1 gives the plots of $\sigma_1 - \sigma_2$ vs. π_1 for different labelling methods. Figure 2 gives the plots of $\sigma_1 - \sigma_2$ vs. $\mu_1 - \mu_2$. Note that the grey and black points represent the two permuted images of the labelled parameter values. From these plots, one can see that there are indeed relatively tight clusters around each posterior mode, and that OC and KL did not accurately recover these labels. The NORMLH and PM(ECM) methods clustered the two groups more naturally.

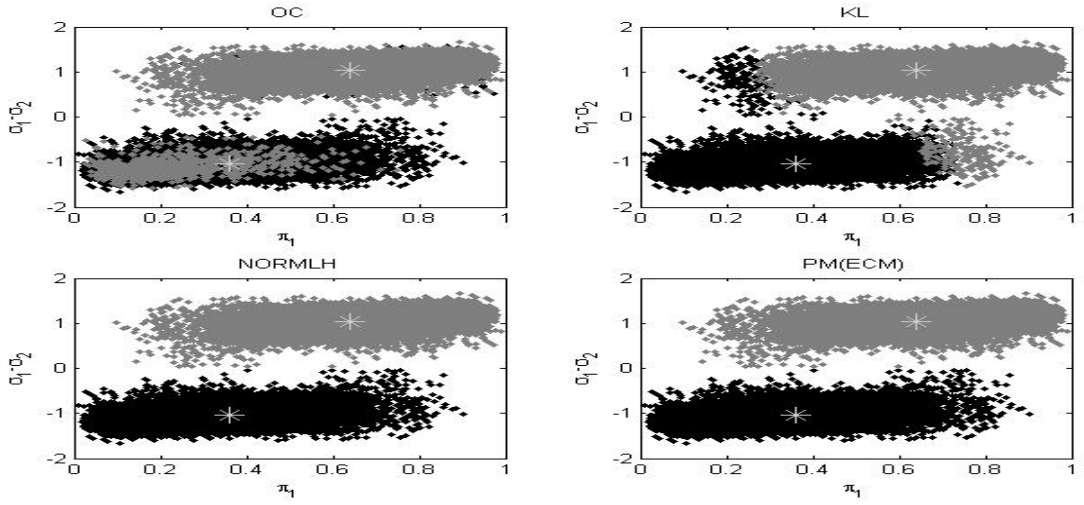


Figure 1: Plots of $\sigma_1 - \sigma_2$ vs. π_1 for the four labelling methods in Example 3.1. The black points represent one set of labels and the gray points are the permuted samples. The star points are the posterior modes.

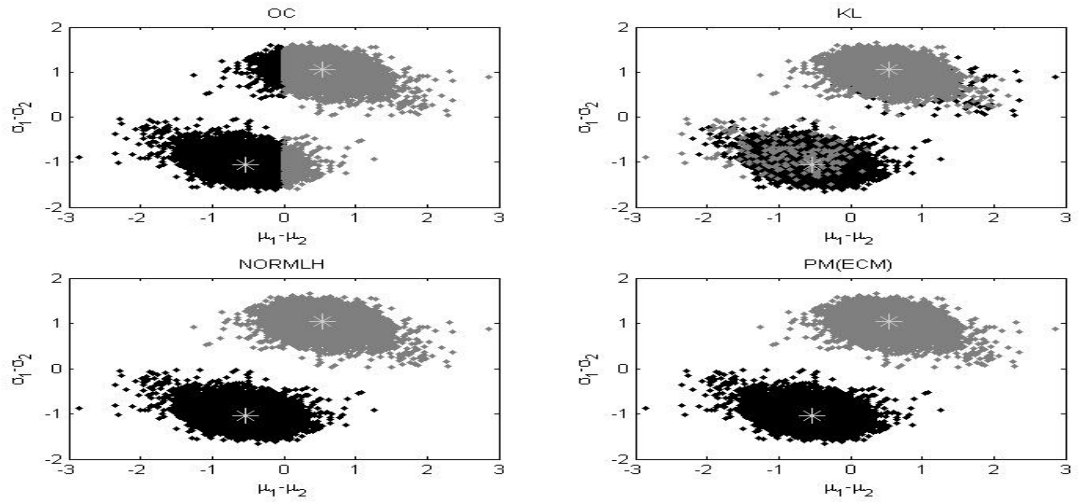


Figure 2: Plots of $\sigma_1 - \sigma_2$ vs. $\mu_1 - \mu_2$ for the four labelling methods in Example 3.1.

Example 3.2: We generated 400 data points from the eight-component normal mixture $\sum_{j=1}^{8} 0.125N(\mu_j, 1)$, where $\mu_j = 3(j-1)$. It is an example where, due to the constant weight parameters and variance parameters, we would expect the order constraint method to be very effective. The large number of components, however, will make labelling computationally difficult for relabelling algorithms. Based on this data set, we generated 5000 MCMC samples of component means, component proportions, and the equal component variance. (The personal computer used for the simulation did not have enough memory for the KL algorithm when we tried to label a large set of 10,000 samples, largely due to the storage of classification probabilities. Stephens (2000) did provide some alternative on-line versions for KL algorithm.)

The upper labelling credibility level was 58% and so at least 42% of the samples do not have ideal HPD labels. By our standards, the labels on these points are somewhat arbitrary (i.e. there is no natural/ideal way to label them). In this example, 95% of samples converged to the maximal modes. The other 5% of samples converged to four minor modes, three of which were degenerate modes.

The total number of different labels between (OC, KL, NORMLH) and PM(ECM) were: 109, 365, and 142, respectively. In this example, all the four methods had identical labels on

the subset above the labelling credibility c^*. Hence all the four methods recovered the likely HPD labels well and the labelling differences occurred for non-HPD labels.

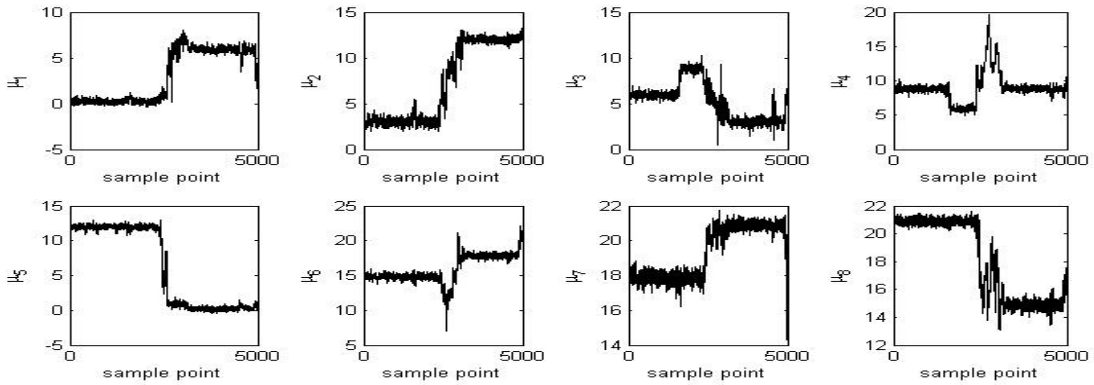
The runtime for KL, NORMLH, and PM(ECM) were 7.8629×10^4, 3.4394×10^4, and 79 seconds, respectively (The runtime for KL and NORMLH is based on one initialization). We can see that PM(ECM) was much faster than the other two methods since KL and NORMLH methods required one to compare $8! = 40320$ permutations in each iteration. From this example, we can see that if the number of components is large PM(ECM) will be much faster than KL and NORMLH.

It is difficult to graphically compare different labelling methods when the number of components is large. Instead, we provide the trace plots and the marginal density plots to illustrate the success of PM(ECM). (The OC, KL, and NORMLH methods had similar visual results for those plots.) Figure 3 provides the trace plots for the original Gibbs samples and the labelled samples by PM(ECM). Figure 4 provides the estimated marginal posterior density plots for the original samples and the labelled samples by PM(ECM). From these figures, we can see that PM(ECM) successfully removed the label switching in the raw output of the Gibbs sampler at a considerably lower computational expense than all but order constraint.

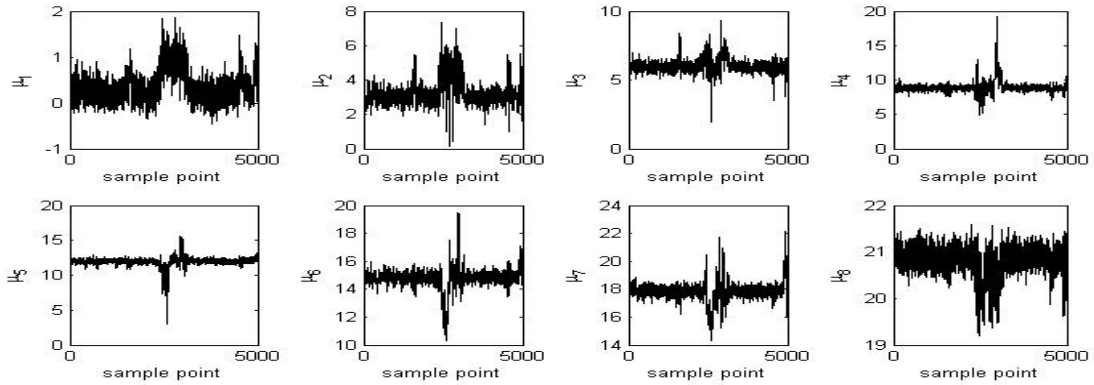
3.2 Real Data Application

We consider the acidity data set (Crawford, DeGroot, Kadane, and Small 1992; Crawford 1994). The data are shown in Figure 5. The observations are the logarithms of an acidity index measured in a sample of 155 lakes in north-central Wisconsin. This data set has been analyzed as a mixture of Gaussian distributions by Crawford et al. (1992), Crawford (1994), and Richardson and Green (1997). Based on the result of Richardson and Green (1997), the posterior for three components is largest. Hence, we fit this data set by a three-component normal mixture. We post processed the 20,000 Gibbs samples by the OC, KL, NORMLH, and PM(ECM) labelling methods.

The upper labelling credibility level was 71%. In this example around 91% of the 20,000



(a)

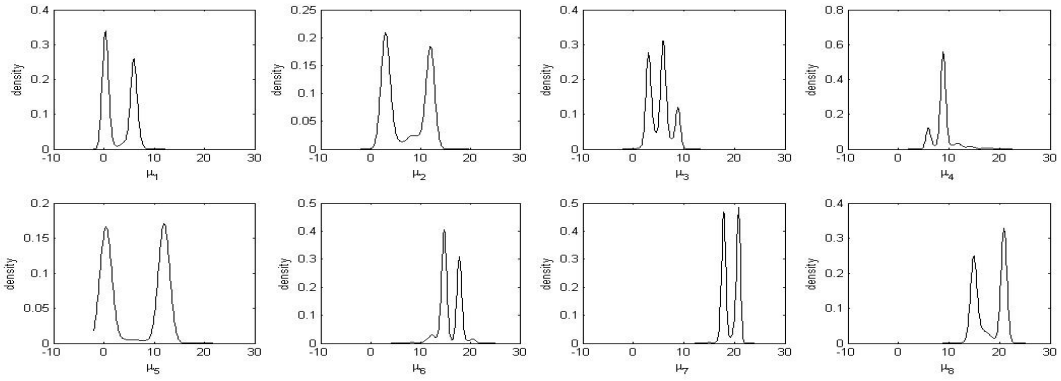


(b)

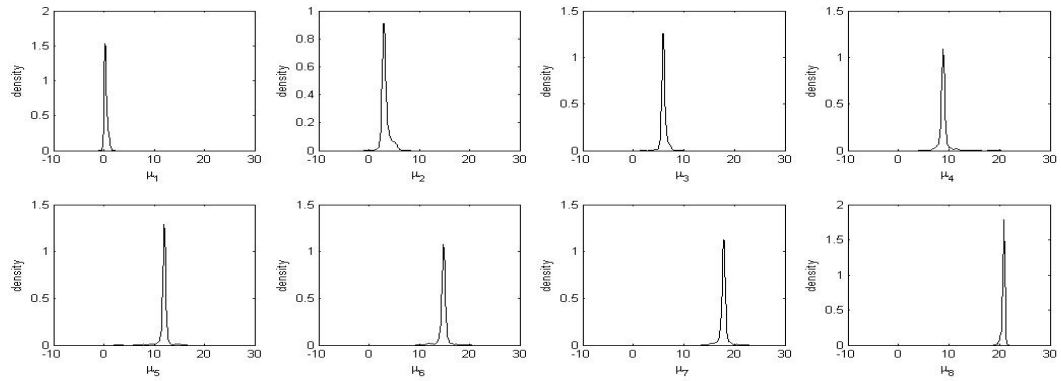
Figure 3: Trace plots of the Gibbs samples of component means for Example 3.2: (a) original Gibbs samples; (b) labelled samples by PM(ECM).

samples converged to the maximal modes. The other 9% of the samples converged to four minor modes. The runtime for KL, NORMLH, and PM(ECM) were 41, 5, and 60 seconds, respectively. The total numbers of different labels between (OC, KL, NORMLH) and PM(ECM) were: 103, 527, and 127, respectively. On the set of samples with posterior probability bigger than c^*, the number of disagreements were 4, 105, and 9, respectively. Hence both OC and NORMLH, but not the KL algorithm, recovered the likely HPD labels almost as well as PM(ECM) in this example.

Figure 6 shows the plots of $\sigma_2 - \sigma_3$ vs. $\mu_2 - \mu_3$ and its permutation image, between the second and third components, for all the labelled samples. Figure 7 shows the similar plots but only for the labelled samples with posterior larger than c^*. Note that, unlike the



(a)



(b)

Figure 4: Plots of estimated marginal posterior densities of component means for Example 3.2 based on: (a) original Gibbs samples; (b) labelled samples by PM(ECM).

two-component case, the points in the plots are not the same for all the methods. Whenever the labelling difference for one sample involves the label of the first component, the two permuted points, between the second and third components, in the plots will be different for different methods. (For example, supposing $(\mu_1^*, \mu_2^*, \mu_3^*, \sigma_1^*, \sigma_2^*, \sigma_3^*)$ is the labelled sample used by one method and $(\mu_3^*, \mu_2^*, \mu_1^*, \sigma_3^*, \sigma_2^*, \sigma_1^*)$ is the corresponding labelled sample used by another method, the two permuted points, between the second and third components, in the plots will be $(\mu_2^* - \mu_3^*, \sigma_2^* - \sigma_3^*)$ and $(\mu_3^* - \mu_2^*, \sigma_3^* - \sigma_2^*)$ for the first method and $(\mu_2^* - \mu_1^*, \sigma_2^* - \sigma_1^*)$ and $(\mu_1^* - \mu_2^*, \sigma_1^* - \sigma_2^*)$ for the second method.) From Figure 6 and 7, one can see that KL did not cluster the parameter points as well as the other three methods. Based on Figure 7, one can also see that all the methods, except for the KL algorithm, recovered the likely

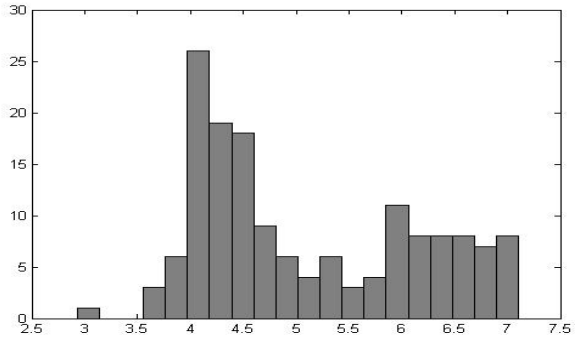


Figure 5: Histogram of acidity data. The number of bins used is 20.

HPD labels pretty well.

4. DISCUSSION

In this paper, we proposed two labelling methods: PM(ALG) and NORMLH. The PM(ALG) method uses each MCMC sample as the starting point for an ascending algorithm (such as the ECM(BM) algorithm introduced in Section 2.2) and assigns the label based on the mode to which the algorithm converges. Using one of the maximal modes as the reference mode, all other permuted maximal modes have clear labels. For the minor modes, we proposed to label them by comparing the minor modes with the reference mode based on the Euclidean distance (2) or Kullback-Leibler divergence criteria (3).

If the converged mode is a degenerate mode, meaning it corresponds to a mixture with at least one component less than the fitted model, then, as a referee pointed out, there really is no sensible labelling by PM(ALG) (or any other labelling method). We do not find this disturbing, as all sample points that converge to a degenerate mode do not have HPD labels, and so there is no single natural way to label them.

Due to the ascending property of ALG, the PM(ALG) method will reproduce the HPD labels in major modal groups. Hence the PM(ALG) method creates a natural and intuitive partition of the parameter space into labelled regions.

There are several other nice properties of the PM(ALG) method. Firstly, unlike a typical relabelling algorithm, the PM(ALG) method gives an answer that does not depend on a set of

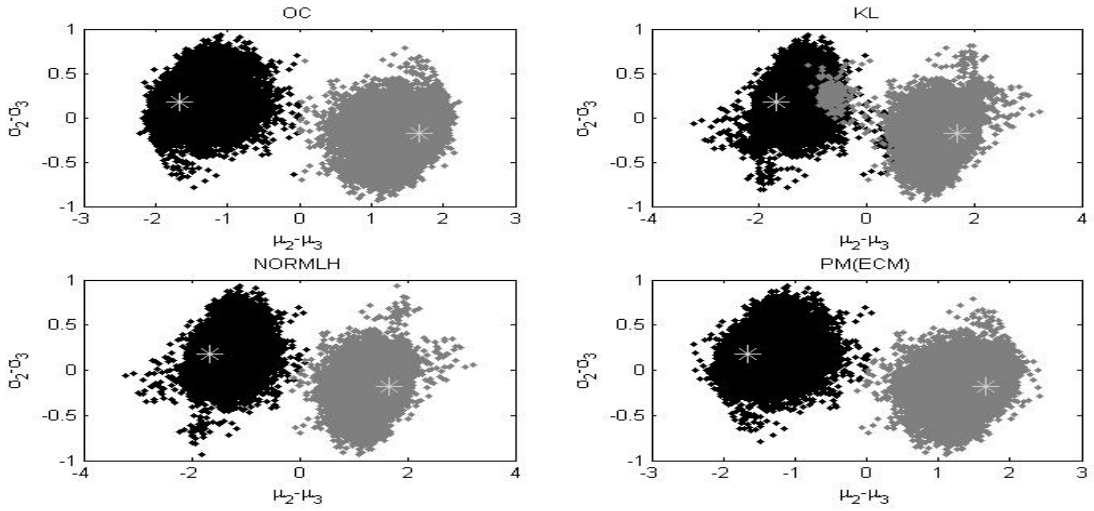


Figure 6: Plots of $\sigma_2 - \sigma_3$ vs. $\mu_2 - \mu_3$ for the acidity data. The black points represent one set of labels and the gray points are the permuted samples between the second and the third components. The star points are the posterior modes.

initial labels, the choice of which can change the labelling. Secondly, the PM(ALG) method is an online algorithm and it can do labelling along with the MCMC sampling process. Hence the storage requirements are reduced. Finally, the PM(ALG) method does not require one to compare $m!$ permutations when doing labelling except for the minor modes. This property can make PM(ALG) much faster than some other labelling methods when m is large, as shown in Example 2 in Section 3.

There are also some possible ways to further improve the computation speed of PM(ALG). One way is to find a faster ascending algorithm to find the local posterior mode. Another possibility when used in batch mode is to first cluster the samples by a method like K-means with large number of clusters K. Then, by assuming that the samples within each cluster have the same labels, we only need to find one converged mode for each cluster.

If a hierarchical Bayesian model is used, the marginal prior and the posterior distribution of $\boldsymbol{\theta}$ contains the integration with respect to the random prior parameters. If there is closed form for the marginal prior and hence the posterior distribution, we can still use the ECM(BM) to find the posterior modes. However, if there is no closed form for the posterior distribution, the ECM(BM) can not be used directly. One could, however, use the

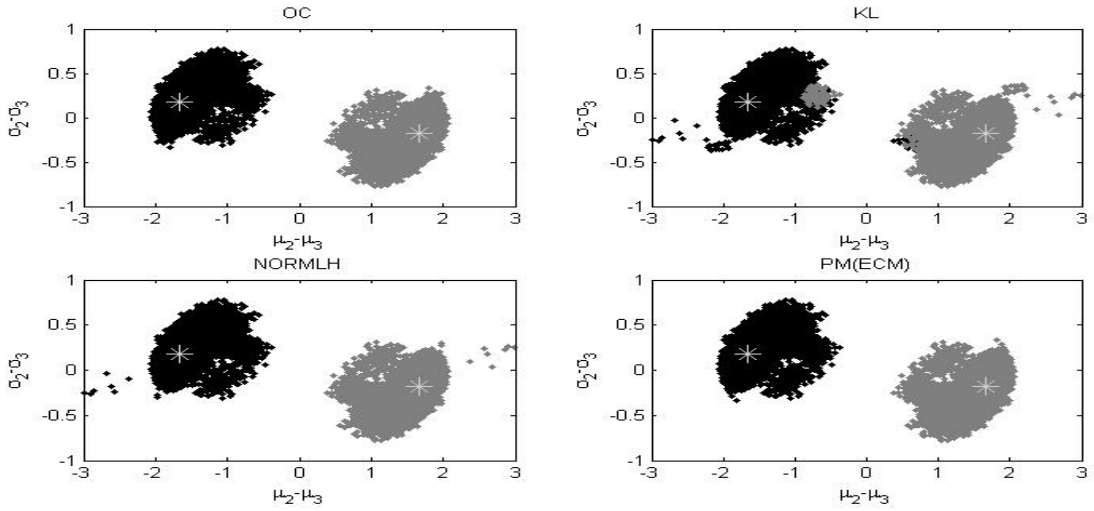


Figure 7: Plots of $\sigma_2 - \sigma_3$ vs. $\mu_2 - \mu_3$ for the samples with posterior higher than c^* for the acidity data.

ECM(BM) on the full posterior including hyperparameters. A second possibility, provided that the likelihood function dominates the prior distribution (the prior is relatively flat or the sample size is large), is to use the likelihood function to approximate the posterior. Then one could use the usual mixture EM algorithm to assign the labels based on the modes of the likelihood itself.

Our second proposed labelling method NORMLH is often computationally easy and fast when the number of components is not large. However this method might be nearly as slow as the KL algorithm when the number of components is large. In our examples, it performed somewhat better than the alternatives at recreating the PM(ECM) labels.

Finally, we introduced a new reliability measure called the "labelling credibility level" and an easy-to-compute approximation called the upper credibility level. This approximates the proportion of the samples that will have ideal HPD labels and measures how difficult the labelling problem is. It is estimated by the proportion of the samples with posterior larger than the maximum posterior of the degenerate modes. It can be used, as in the examples, to examine the clustering of the HPD regions.

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