Markov Chain Monte Carlo Methods and the Label Switching Problem in Bayesian Mixture Modelling

A. Jasra [1], C. C. Holmes and D. A. Stephens

Abstract. In the past ten years there has been a dramatic increase of interest in the Bayesian analysis of finite mixture models. This is primarily because of the emergence of Markov chain Monte Carlo (MCMC) methods. Whilst MCMC provides a convenient way to draw inference from complicated statistical models, there are many, perhaps under appreciated, problems associated with the MCMC analysis of mixtures. The problems are mainly caused by the nonidentifiability of the components under symmetric priors, which leads to so called *label switching* in the MCMC output. This will mean that ergodic averages of component specific quantities will be identical and thus useless for inference. We review the solutions to the label switching problem, such as artificial identifiability constraints (e.g. Diebolt & Robert (1994)), relabelling algorithms (Stephens 1997*a*) and label invariant loss functions (Celeux, Hurn & Robert 2000). We also review various MCMC sampling schemes that have been suggested for mixture models and discuss posterior sensitivity to prior specification.

Key words and phrases: Bayesian Statistics, Mixture Modelling, MCMC, Label Switching, Identifiability, Sensitivity Analysis.

1 Introduction

In their intrinsic form, mixture models provide a flexible way to model heterogeneous data. That is, if data are thought to belong to one of k classes (or components), but whose individual class memberships are unavailable, then mixture models provide a natural framework for statistical

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modelling. Moreover, due to the large class of functions that can be approximated by a mixture model, they are attractive for describing non-standard distributions. For a comprehensive list of the applications of mixture models see Titterington, Smith & Makov (1985) and for a recent overview see McLachlan & Peel (2000).

As a result of the early work of Newcomb (1886) and Pearson (1894) mixture models were established as a useful statistical tool. In addition, methodological advances in computational methods for frequentist mixture models including the maximum likelihood approach of Baum, Petrie, Soules & Weiss (1970) and more generally the expectation-maximisation (EM) algorithm (Dempster, Laird & Rubin 1977) added to their popularity. However, difficulties often arise in the application of mixture models. For example, in the context of frequentist mixtures with location-scale component distributions, the likelihood can become unbounded (see Aitkin (2001) for further details).

From the Bayesian perspective, before MCMC (Hastings (1970), Green (1995) and for a general introduction see Robert & Casella (1999) or Liu (2001)) mixture models were restricted to a few specialised cases: for example Bernardo & Giròn (1988). Following the work of Diebolt & Robert (1994) (data augmentation Gibbs sampler applied to mixtures), Bayesian mixture models could be applied routinely when the number of components is assumed known. Bayesian analysis via mixture models with an unknown number of components is now possible using the methods of Escobar & West (1995) (Dirichlet process mixtures), Mengersen & Robert (1996) (distributional distances), Richardson & Green (1997) (reversible jump MCMC) and Stephens (2000*a*) (Birth-and-Death MCMC). Due to the above developments, implementation of Bayesian mixtures has become increasingly popular in many academic disciplines, such as biological sequence analysis (Boys & Henderson 2004), econometrics (Frühwirth-Schnatter 2001), (Hurn, Justel & Robert 2003), machine learning (Beal, Ghahramani & Rasmussen 2002) and epidemiology (Green & Richardson 2002).

One of the main challenges of a Bayesian analysis using mixtures is the nonidentifiability of the components. That is, if exchangeable priors are placed upon the *parameters* of a mixture model, then the resulting posterior distribution will be invariant to permutations in the labelling of the parameters. As a result, the marginal posterior distributions for the parameters will be identical for each mixture component. Therefore, during MCMC simulation, the sampler encounters the symmetries of the posterior distribution and the interpretation of the labels switch. It is then meaningless to draw inference directly from MCMC output using ergodic averaging. Label switching significantly increases the effort required to produce a satisfactory Bayesian analysis of the data, but is a prerequisite of convergence of an MCMC sampler, and therefore must be addressed. Whilst convergence in MCMC simulation is a complex issue we regard a *minimum requirement* of convergence for a mixture posterior to be such that we have explored all possible labellings of the parameters. We will justify this choice in our examples in section 3. For a discussion of convergence issues see Robert & Casella (1999).

A difficulty in the Bayesian analysis of mixtures, when the number of components is unknown, is the sensitivity of the posterior distribution for the number of components to changes in the prior distribution for the parameters. Aitkin (2001) notes apparent difficulties in Bayesian analyses of mixture models and we discuss these concerns in this paper.

1.1 Interpretation of Mixture Models

In general, there are two ways in which mixture models can be interpreted.

First is the missing data formulation. We assume that data $\mathbf{x} = (x_1, \ldots, x_n)$ is i.i.d with distribution

$$x_i | z_i = j, \phi_j \quad \sim \quad f(x_i; \phi_j) \tag{1}$$

for $j = 1, \ldots, k$, the latent variables $\{z_n\}$ de-convolve the distribution of the data, with $p(z_i = j|\boldsymbol{\theta}) = \pi_j$ (with ϕ_j and $\boldsymbol{\theta}$ to be defined in the next section). However, if the i.i.d. assumption is relaxed, for example to Markovian dependence, we return the so-called hidden Markov model (HMM) see Baum & Petrie (1966) and Robert, Rydén & Titterington (2000). Therefore label switching is not restricted to 'standard' mixture models (e.g. Richardson & Green (1997)) but any model with conditional structure such as (1).

The second interpretation is through a semi-parametric construction. As noted above, due to the ability of a mixture model to approximate non-standard distributions, they can be seen as alternatives to non-parametric models. The missing data approach is appropriate in terms of clustering and the semi-parametric in areas such as density estimation.

1.2 An Illustrative Example: The Crab Data

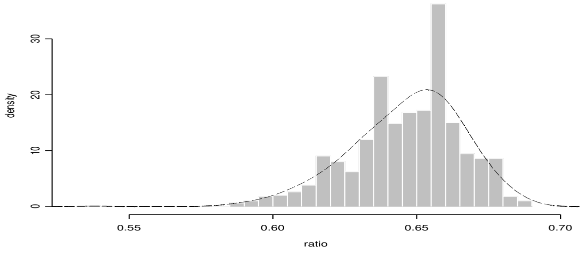
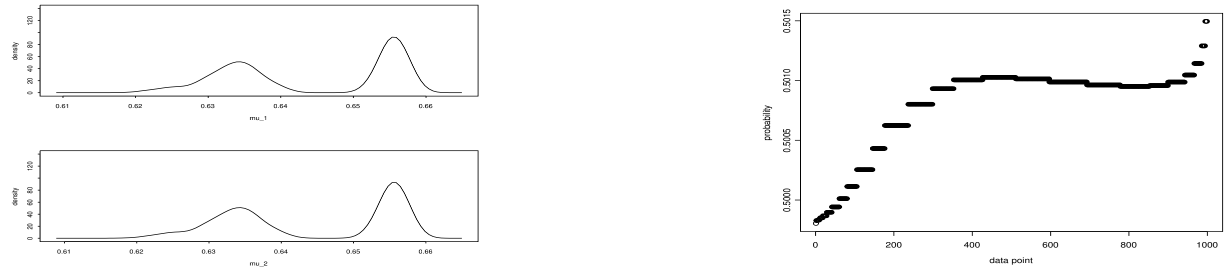


Figure 1: Histogram of the Crab Data with a kernel density estimate (dashed) overlaid.

To illustrate some of the issues discussed in section 1, we consider the famous crab data set analysed by Pearson (1894). The data is shown in Figure 1 and are comprised of measurements of the ratio of forehead to body length of 1000 crabs, and were the focus of one of the first major analyses of data by a mixture model. The measurements were provided to Pearson by W. F. R. Weldon, who speculated that there were two new subspecies present. Following Pearson (1894) we use a two component normal mixture model to analyse this data. Our priors for the parameters are described in section 2 and are exchangeable with respect to the labelling of the components.

In Figure 2 we observe the marginal posterior density estimates for the means (Figure 2a) and the classification probabilities (Figure 2b). The classification probability, for this example, is the probability that a data point is in component/class 1, based upon our MCMC output. The symmetries in the posterior distribution are immediately seen, with the posterior means being the same for each component, as well as the classification probabilities all being close to 1/2.

There appears, however, to be significant information in the output. This is because there are two modes in the posterior for the means, which represent the two possible populations in the data. Label switching masks this information and we need a way of dealing with it.



(a) Density Estimates.

(b) Classification Probabilities.

Figure 2: Marginal Posterior Density Estimates (a) and Classification Probabilities (b); Crab data. We fitted a two component mixture model to the data, the output is the last 88000 samples from a reversible jump sampler which were permuted for effect.

1.3 Solutions to the Label Switching Problem

For Bayesian mixtures the invariance of the likelihood to permutations in the labelling is not a problem that is as easily solved as in the frequentist approach. In the case of the latter, simple inequality constraints (artificial identifiability constraints (ICs)) on the parameter space can be used to break the symmetry in the likelihood (see McLachlan & Peel (2000)). For example, if the component parameters are θ_1 and θ_2 a possible constraint is $\theta_1 < \theta_2$. In the Bayesian context these constraints do not always perform adequately.

To demonstrate the above, consider the well-known Galaxy data (see for example Stephens (1997*a*)). The data set was first presented in Postman, Huchra & Geller (1986) and consists of the velocities (in 10^3km/s) of distant galaxies diverging from our own, from six well separated conic sections of the Corona Borealis: they can be observed in Figure 3. The data was originally of size 83, but we leave one observation out, in accordance with the analyses of Roeder (1990), Richardson & Green (1997) and Stephens (1997*a*). Since Richardson & Green (1997) found high posterior support for between $5 - 7$ components, we fit the random beta model (see section 2.2 for further details) of Richardson & Green (1997) with a fixed number of six components to the data. We ran a Gibbs sampler (the fixed dimensional updates in Richardson & Green (1997)) for 20000 iterations post burn in.

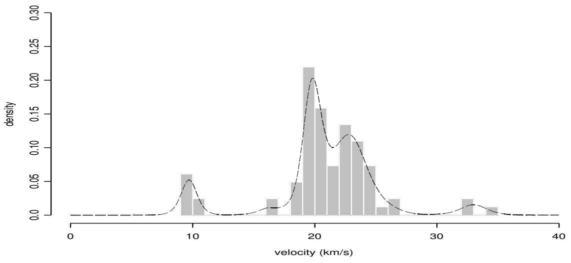


Figure 3: Histogram of the Galaxy Data. We overlaid the histogram with a kernel density estimate (dashed).

In Figure 4 we can observe the marginal posterior density estimates for the means under the identifiability constraint $\mu_1 < \cdots < \mu_6$, where μ_j denotes the mean parameter of the j^{th} normal component. We can see that there is evidence of multimodality in components two and five and it appears that the symmetry in the posterior has not been removed.

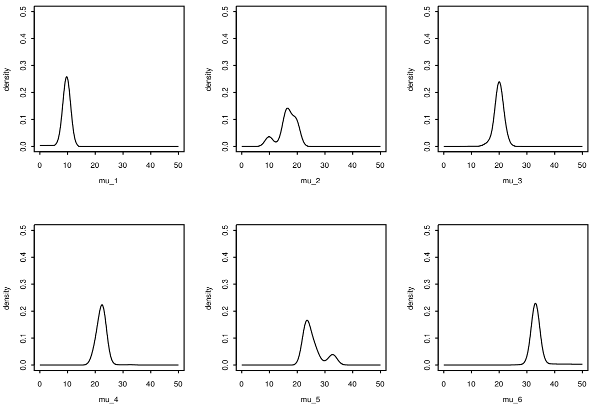


Figure 4: Marginal Posterior Density Estimates of the Sampled Means; Galaxy Data Set. The means were permuted to obey the constraint $\mu_1 < \cdots < \mu_6$. We fitted a six component normal mixture to the data, the output is the last 20000 iterations from the Gibbs sampler.

This problem is typical of MCMC mixture analysis and consequently there have been many ideas proposed to deal with label switching. Along with artificial identifiability constraints , Stephens

(1997a, 2000b) and Celeux (1998) developed *relabelling algorithms* to perform a k-means type clustering of the MCMC samples. Additionally Celeux et al. (2000) and Hurn et al. (2003) used *label invariant loss functions* - a decision theoretic procedure. Related to ICs is the *random permutation sampler* of Frühwirth-Schnatter (2001), which was designed both to improve the mixing of an MCMC sampler and a convenient way to apply identifiability constraints. In this article we provide a review of these methods.

One simple solution to the label switching problem is to adopt the *maximum a-posteriori* (MAP) estimator, which is equivalent to penalised maximum likelihood (see Ciuperca, Ridolfi & Idier (2003) for example). As a result, the label switching problem is only of concern during simulation. However, one of the main attractions of using a Bayesian approach, is the ability to reflect the uncertainties related to our inference. Clearly MAP estimation does not allow this. This aspect is of particular importance in mixture analysis, due to the likely genuine multimodality (modes which cannot be explained by permuting the labels of the parameters) of the posterior distribution (in our experience this occurs quite often). As a result, we do not believe that MAP estimates provide a general solution to the label switching problem, because of the inability of the estimate to accommodate competing explanations of the data.

1.4 Outline

The article is organised as follows. In section 2 we introduce some notation and a particular mixture model that we will be studying. In section 3 we review various MCMC sampling strategies for mixtures. When the number of components is fixed, it was established by Celeux et al. (2000) that the Gibbs sampler is not always appropriate to sample from a mixture posterior. This is because of the inability of the Gibbs sampler to traverse the support of highly multimodal distributions. We emphasise that we can simulate from a mixture posterior using Metropolis-Hastings updates without completion (simulation of the missing class labels), and that tempering MCMC (Neal 1996) may be used. We also consider reparameterisations, as discussed by Celeux et al. (2000), and variable dimension samplers. Next, we examine the existing solutions to the label switching problem. We begin in section 4 with identifiability constraints, then relabelling algorithms (section 5) and finally label invariant loss functions (section 6). In section 7 we discuss some of the potential problems with prior specification in Bayesian mixture models with an unknown number of components. In section 8 we conclude with our views on applying the methods reviewed as well as a future research area in Bayesian mixture modelling.

2 Notation and Mixture Models

Throughout this article we will use the following notation. We let $p(\cdot)$ represent a generic probability distribution. Denote data $\mathbf{x} = (x_1, \ldots, x_n)$ which is assumed to be independently and identically distributed (i.i.d.) with mixture distribution

$$p(x_i|\boldsymbol{\theta}, k) = \sum_{j=1}^{k} \pi_j f(x_i; \phi_j)$$

where f is some parametric component density/mass function, k is possibly unknown and finite, $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_k)$ are component specific parameters, $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_k)$ are the mixture proportions or weights and $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_k) = ((\pi_1, \phi_1), \ldots, (\pi_k, \phi_k))$. Denote the parameter space $\phi \in \Phi \subseteq \mathbb{R}^p$ with $\mathcal{S}^{k-1} \times \Phi^k = \Theta^k$, where $\mathcal{S}^{k-1} = \{(\pi_1, \ldots, \pi_{k-1}) : \pi_1, \ldots, \pi_{k-1} \geq 0 \cap \pi_1 + \cdots + \pi_{k-1} \leq 1\}$.

Define a *permutation* σ of the labels $1, \ldots, k$ of a parameter vector $\boldsymbol{\theta}$ as

$$\sigma(\boldsymbol{\theta}) = (\theta_{\sigma(1)}, \ldots, \theta_{\sigma(k)})$$

where $\sigma \in S_k$, the set of all $k!$ permutations of $1, \ldots, k$.

The nonidentifiability in the posterior arises as,

$$p(\mathbf{x}|\sigma(\boldsymbol{\theta}), k) = \prod_{i=1}^{n} \left\{ \sum_{j=1}^{k} \pi_{\sigma(j)} f(x_i; \phi_{\sigma(j)}) \right\}$$

is identical for all $\sigma \in S_k$. Hence if $p(\boldsymbol{\theta}) \equiv p(\sigma(\boldsymbol{\theta}))$ $\forall \sigma \in S_k$ then so is the posterior distribution, $p(\boldsymbol{\theta}|\mathbf{x})$. As a result, if there are k components in a mixture model, and one mode under a given labelling, there are $k!$ symmetric modes in the posterior distribution.

2.1 Random beta Model

A well known mixture model, that we will use for our examples, is the random beta model of Richardson & Green (1997). The model is as follows; data $x_1, \ldots, x_n$ are i.i.d with distribution

$$x_i|\boldsymbol{\theta}, k \quad \sim \quad \sum_{j=1}^{k} \pi_j \mathcal{N}(\mu_j, \lambda_j^{-1})$$

where $\mathcal{N}(\mu, \lambda^{-1})$ denotes the normal distribution with mean μ and precision λ. The priors, which are the same for each component $j = 1, \ldots, k$, are taken to be:

$$\begin{aligned} \mu_j &\sim \mathcal{N}(\xi, \kappa^{-1}) \\ \lambda_j|\beta &\sim \mathcal{G}a(\alpha, \beta) \\ \beta &\sim \mathcal{G}a(g, h) \\ \boldsymbol{\pi} &\sim \mathcal{D}(\delta) \end{aligned}$$

where $\mathcal{D}(\delta)$ is the symmetric Dirichlet distribution with parameter δ and $\mathcal{G}a(\alpha, \beta)$ is the gamma distribution, shape α, scale β. If k is unknown we assume $k \sim \mathcal{U}_{\{1,\ldots,k_{\max}\}}$ where $\mathcal{U}_{\{1,\ldots,k_{\max}\}}$ is the uniform distribution on the integers $1, \ldots, k_{\max}$ with $k_{\max}$ known.

The purpose of the hierarchical structure on the variances is to reduce the effect of the prior on the posterior; improper priors are generally unavailable for mixtures (see Gruet, Philippe & Robert (1999) for an example of improper priors in the mixture context). A problem with the above prior, when k is unknown, arises due to the Lindley-Bartlett paradox (Lindley 1957, Bartlett 1957). Jennison (1997) noted that, in the limit as $\kappa \to 0$ and $\beta \to \infty$, the posterior distribution for k favours models with fewer components. We illustrate this phenomenon in section 7.

Quantities in which we will often be interested are the classification probabilities, defined as:

$$p(z_i = j|\mathbf{x}, k) \quad = \quad \int_{\Theta} \frac{\pi_j f(x_i; \phi_j)}{\sum_{l=1}^{k} \pi_l f(x_i; \phi_l)} p(\boldsymbol{\theta}|\mathbf{x}) \mathrm{d}\boldsymbol{\theta}.$$

Then if we were interested in a single 'best' clustering we might take the groups which are formed by the maximal classification probabilities.

3 MCMC Samplers for Mixture Models.

As we saw in the section 1.2, label switching creates a problem at the inferential stage of analysis, however it does provide a useful convergence diagnostic at the simulation stage. That is, we know *a priori* that the mixture posterior has $k!$ symmetric modes; thus failure to visit them reveals that a MCMC sampler has not converged. Many different sampling schemes have been proposed for mixture models. We firstly review the most popular samplers that are available for simulating from standard mixtures with a known number of components.

3.1 The Gibbs Sampler

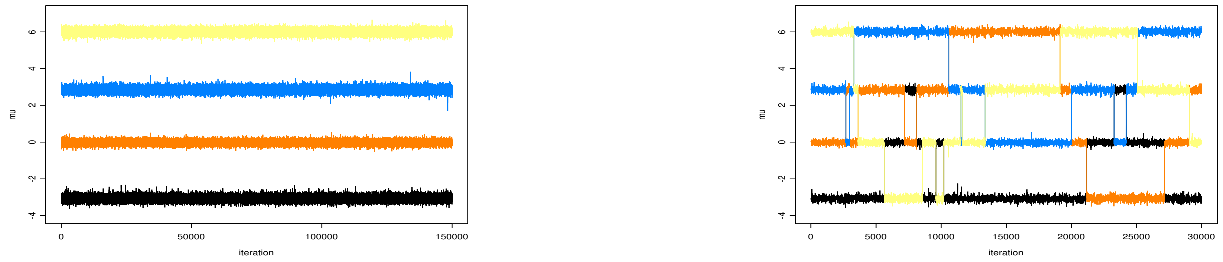
Following Diebolt & Robert (1994) perhaps the most popular methods to simulate from a mixture posterior distribution uses data augmentation and the Gibbs sampler. That is, by simulating the unobserved $\mathbf{z}$. However the highly multimodal nature of a mixture distribution often makes the Gibbs sampler inappropriate for this task. To illustrate such a case, we simulated 100 data points from $x_i \sim 1/4\{\mathcal{N}(-3, 0.55^2) + \mathcal{N}(0, 0.55^2) + \mathcal{N}(3, 0.55^2) + \mathcal{N}(6, 0.55^2)\}$ and then used the random beta model, with $k = 4$. We ran the sampler for 150000 iterations post burn in: the results of which are presented in Figure 5a.

The most striking feature of Figure 5a is that the sampler appears to be performing well, in the sense that it has picked out the means from the data. The apparent 'good' performance of the sampler is offset by the fact that it has only been able to visit one of the 4! symmetric modes in the posterior distribution. It may be the case that if we ran the sampler for more iterations that we would visit another symmetric mode. However, it is clear that the Gibbs sampler is unable to freely move around the space of this distribution. Such behaviour is highly undesirable since it is possible that there are many regions of the posterior support that are not being explored by the sampler.

We have shown that the Gibbs sampler cannot always visit the $k!$ symmetric modes of a posterior mixture distribution easily. We note that:

> From a statistical viewpoint, exploration of the $k!$ modal regions is redundant (Celeux et al. 2000).

Indeed if we wish to explore all of the $k!$ symmetric modes we could randomly permute the output from the sampler. That is, a simple addition of a Metropolis-Hastings move which proposes a random permutation of the labels, which is accepted with probability 1 (as used by Frühwirth-Schnatter (2001)). Clearly, this course of action is only appropriate if the posterior distribution is not genuinely multimodal (which would not be known *a priori* to simulation). This is because, if a Gibbs sampler is unable to move around the support of a multimodal distribution, and there exists genuine multimodality, then the sampler will not mix well (or at all) between the modes.



(a) Gibbs Sampling.

(b) Tempering.

Figure 5: Trace Plot of the Sampled Means; Simulated Data of Section 3.1. We fitted a four component normal mixture to the data, the output is the last 150000 iterations from the Gibbs sampler (a) and the last 150000 iterations from the tempering sampler (every fifth, b). The initial labelling is μ_1 (black), μ_2 (orange), μ_3 (blue) and μ_4 (yellow).

3.2 Metropolis-Hastings with Tempering updates

Since the Gibbs sampler cannot visit all of the modes of a mixture target, we need to consider alternative methods.

Cappé, Robert & Rydén (2001) state:

> We will not use completion to run our (MCMC) algorithm. That is to say, the latent variables $\{z_n\}$ is not to be simulated by the algorithm.... We believe that this choice is bound to accelerate convergence of the algorithm by the drastic reduction in the

dimensionality of the space.

We consider this approach by discarding the latent variables and updating the parameters using Metropolis-Hastings moves. Celeux et al. (2000) report that random walk proposal mechanisms are too local, in the sense that the sampler cannot move freely around the $k!$ symmetric modes. They use tempering MCMC, which was developed by Neal (1996). We will now introduce this method and apply it to the simulated data set of the previous section. We note that more advanced methods exist, for example Population or Evolutionary Monte Carlo (EMC) (Liang & Wong 2001). We shall not review these methods here, other than to note that population based MCMC works by embedding the target distribution of interest into a sequence of related distributions and sampling from $p^*(\cdot) \propto \prod_{j=0}^{m} p_j(\cdot)$, $p_0(\cdot)$ is the original target distribution: see Liu (2001) for a review and for an extension to the trans-dimensional case see Jasra, Holmes & Stephens (2004).

Tempering MCMC uses what is essentially a Metropolis-Hastings kernel to sample from the posterior distribution, in which case it is often beneficial to reparameterise the mixture proportions in the random beta model. This is because Metropolis-Hastings moves may not perform well on a constrained space such as the simplex of mixing proportions. We choose the reparameterisation $\pi_j = v_j / \sum_{l=1}^{k} v_l$ with $v_j > 0 \ \forall j$. We modify the prior for $\boldsymbol{\pi}$ as $v_j \sim \mathcal{G}(\delta, 1)$, with $v_j \perp\!\!\!\perp v_l \ \forall j \neq l$, where $A \perp\!\!\!\perp B$ means A is independent of B. As a result, our reparameterised model is equivalent to the original model.

We now describe the tempering MCMC method of Neal (1996).

3.2.1 Tempering MCMC

Suppose we have a target distribution $p_0(\boldsymbol{\theta})$ which has many isolated modes. Now suppose we have a sequence of m related distributions $p_1(\boldsymbol{\theta}), \ldots, p_m(\boldsymbol{\theta})$. The final distribution p_m is (potentially) quite different from p_0 but is thought to be easier to sample from. The objective is to use these distributions to assist in the movement around the support of the target.

In order to propose a new state in the chain $\boldsymbol{\theta}'$ we use an up-down scheme described with pseudocode in Figure 6 (note that $a \wedge b$ means $\min\{a, b\}$). The Figure tells us that we may need to draw from the intermediate distributions p_j via a Markov chain kernel. We note that this kernel itself may be a cycle of Metropolis-Hastings kernels; this is particularly useful if $\boldsymbol{\theta}$ is of high dimension.

To apply the method for mixtures we suppose $p_0(\cdot)$ is the posterior distribution. We then let $p_j(\cdot) \propto p_0(\cdot)^{\frac{1}{\zeta_j}}$, $j = 1, \dots, m$ where $1 > \zeta_1 > \cdots > \zeta_m > 0$ (the ζ's act as a temperature parameter). The objective is that during the first m simulations we flatten out the target allowing us to walk freely on the space. Then, for the next $m-1$ steps we return to a state that receives high posterior support under the target. To have sufficiently high acceptance probability the intermediate steps (i.e. the ζ's) should not have a large difference. We can add further simulations from $p_m(\cdot)$ to encourage movement between the modal regions.

```
Currently in state $\boldsymbol{\theta}$.
To propose a new state in the chain $\boldsymbol{\theta}'$

    Draw $\hat{\boldsymbol{\theta}}_1$ from $\boldsymbol{\theta}$ using $\hat{T}_1$.
    Draw $\hat{\boldsymbol{\theta}}_2$ from $\hat{\boldsymbol{\theta}}_1$ using $\hat{T}_2$.
                 $\vdots$
    Draw $\hat{\boldsymbol{\theta}}_m$ from $\hat{\boldsymbol{\theta}}_{m-1}$ using $\hat{T}_m$.
    Draw $\hat{\boldsymbol{\theta}}_{m-1}$ from $\hat{\boldsymbol{\theta}}_m$ using $\check{T}_{m-1}$.
                 $\vdots$
    Draw $\check{\boldsymbol{\theta}}_2$ from $\check{\boldsymbol{\theta}}_3$ using $\check{T}_2$.
    Draw $\boldsymbol{\theta}'$ from $\check{\boldsymbol{\theta}}_2$ using $\check{T}_1$.

where $\hat{T}_j$, $\check{T}_j$ is a transition kernel that
satisfies detailed balance with respect
to $p_j$, $j = 1, \dots, m$. Then the new state is
accepted with probability
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$$1 \quad \wedge \quad \frac{p_1(\boldsymbol{\theta})}{p_0(\boldsymbol{\theta})} \cdots \frac{p_m(\hat{\boldsymbol{\theta}}_{m-1})}{p_{m-1}(\hat{\boldsymbol{\theta}}_{m-1})} \frac{p_{m-1}(\hat{\boldsymbol{\theta}}_m)}{p_m(\hat{\boldsymbol{\theta}}_m)} \cdots \frac{p_0(\boldsymbol{\theta}')}{p_1(\boldsymbol{\theta}')}.$$

Figure 6: Transition Dynamics for Tempering MCMC.

3.2.2 Tempering for the Random Beta Model

To apply tempering MCMC for the reparameterised random beta model we will make some modifications to the algorithm.

Firstly we will add a Metropolis-Hastings step, so that with probability ω we perform a deterministic cycle of Metropolis-Hastings steps, implemented in the following manner. Draw a new $\boldsymbol{\mu}' = (\mu'_1, \ldots, \mu'_k)$ via an additive normal random walk. This move is accepted with probability $1 \wedge p(\boldsymbol{\mu}'|\cdots)/p(\boldsymbol{\mu}|\cdots)$, where

$$(2) \qquad p(\boldsymbol{\mu}|\cdots) \quad \propto \quad p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\lambda}, \boldsymbol{v})p(\boldsymbol{\mu})$$

and $|\cdots$ denotes conditioning on all other variables. For $\boldsymbol{\lambda}' = (\lambda'_1, \ldots, \lambda'_k)$ and $\boldsymbol{v}' = (v'_1, \ldots, v'_k)$ we use reflective proposals, that is, normal random walks bounced off a barrier at zero.

The second modification that will be made is to use tempering to simulate from the full conditionals, that is to sample from $p(\boldsymbol{\mu}|\cdots)$, $p(\boldsymbol{\lambda}|\cdots)$ and $p(\boldsymbol{v}|\cdots)$. We note that this is a valid MCMC sampler since any kernel (which is a cycle) that is invariant with respect to the (full) conditional distributions for all $\boldsymbol{\theta}_{-j} = (\theta_1, \ldots, \theta_{j-1}, \theta_{j+1}, \ldots, \theta_k)$ will have invariant distribution $p(\cdot)$ (Tierney 1994).

Our choice may seem odd, since the full conditionals may not be as multimodal as the full posterior. However if we consider equation (2) we can see that this is of mixture form, and is likely to have many modes.

Another reason why we do this is because in previous simulations, (on a hidden Markov model) we obtained huge rejection rates when sampling from the full posterior. It may be the case that a reduction in the dimensionality of the parameters may facilitate higher acceptance rates. Our approach may lead to longer computing time, than a single tempering move on $p(\boldsymbol{\mu}, \boldsymbol{\lambda}, \boldsymbol{v}|\beta, \mathbf{x})$, however it may also require fewer iterations to converge due to higher acceptance rates.

The intermediate steps will be performed using the same random walk proposal as above, also the levels will be taken to be the same for each full conditional. The Metropolis-Hastings steps allow us to explore a modal region, the tempering to move between modes. For all of our examples we set $\omega = \frac{1}{2}$.

Other proposals and reparameterisations that we have found to work well are as follows. For the precisions a multiplicative random walk with log normal proposals has been used. For the weights a reparameterisation onto the logit space, updating via an additive normal random walk can prove an effective strategy. Additionally, if the sampler exhibits slow movement around the state space, we often use heavy tailed (e.g. Cauchy) proposals to improve mixing.

3.3 Simulated Data Example

We now return to the simulated data at the beginning of the section, using the tempering sampler to draw from the posterior. We ran the MCMC sampler for sufficiently long post burn in (until the sampled parameters seemed to stabilise), with appropriate thinning to take into account rejections of our moves. The number of steps for the tempering was 55 starting at $\zeta_1 = 2$ increasing by 2 at each level. The choice of steps was tuned in prior simulations to achieve reasonable acceptance rates, which were (in the order $\boldsymbol{\mu}, \boldsymbol{\lambda}, \boldsymbol{v}$) for the Metropolis-Hastings moves $(0.15, 0.44, 0.23)$ and for the tempering moves $(0.007, 0.03, 0.016)$. The tempering acceptance rates appear to be quite low, but since they are used for global moves we are satisfied with the performance of our algorithm.

In Figure 5b we can observe the output. From this Figure we can see the correct label switching behaviour, the sampler visiting the majority (in fact, $(4! - 2)$) of the symmetric modes in the posterior distribution (mixing over colours). We note that for full convergence we would need to ensure the sampler visits all 4! modes, but the behaviour of the sampler is more than satisfactory. We now turn our attention to variable dimension samplers.

3.4 Variable Dimension Samplers

In this subsection we discuss variable dimension samplers.

Following Richardson & Green (1997) the standard way to simulate from a mixture with an unknown number of components is reversible jump MCMC (Green 1995) (for an up-to-date review see Green (2003)). Reversible jump is simply an extension of the Metropolis-Hastings method, with the measure theoretic construction necessary because of the lack of common dominating measure when jumping between distributions of differing dimension. Note, Stephens (2000*a*) and Cappé, Robert & Rydén (2003) have considered continuous time samplers. For continuous time samplers the standard accept-reject step of a reversible jump sampler is replaced by new states that are always accepted, but that occur via either a marked point process, or more generally a Markov jump process with appropriate stationary distribution.

In a comprehensive comparison between reversible jump and continuous time samplers, Cappé et al. (2003) demonstrated that there was little difference between the two. Theoretically, they showed that a sequence of reversible jump samplers converges to a continuous time sampler (in Skorohod topology). In terms of performance, they showed that the continuous time sampler was less efficient in that the CPU time, on average, was longer. The main differences appear that, firstly, the continuous time sampler can visit unlikely regions in the support of the posterior, thus yielding a sort of springboard between different modal regions (Cappé et al. 2003). Secondly that for the continuous time sampler there is a 'free' Rao-Blackwellisation to reduce the variance of the MC estimates of integrals. We have found that, in practice, these latter differences do not make a significant impact on the performance of the sampler (when compared to reversible jump) or the inference resulting from it.

3.4.1 Completion

Another aspect of interest is that of completion for variable dimension samplers. In our experience, for relatively small data sets, (e.g. the Galaxy data) the sampler which simulates the missing data comprehensively outperforms a sampler without completion. This is in terms of CPU time, mixing and convergence speed. For large data sets e.g. $n = 5000$, we found that the without completion sampler converged faster (we would generally expect this due to the reduction in size of the state space), but at a cost of longer CPU time.

As noted by Richardson & Green (1997) and Stephens ($2000a$), mixing within k is often improved by using variable dimension samplers. This is because the sampler now has the ability to move around the modes of a distribution (conditional on k) via a model of lower or higher dimension. That is, by jumping out of the k mixture model space, moving around in a model of different dimension, and then returning to a different region in the k space, thus escaping valleys in the posterior probability distribution that a fixed dimensional sampler is unable to scale. Indeed for the crab data example in section 1 we used a reversible jump sampler, since the fixed dimension sampler was unable to visit a genuine mode in the posterior. Therefore, variable dimension samplers provide an alternative method to sample from a mixture posterior with a known number of components. This is at the cost of extra programming effort and inefficiency due to the fact that the sampler will not necessarily stay in the model of interest for the entire run.

3.4.2 Multivariate Mixtures

Simulation from multivariate mixtures with an unknown number of components is also an issue of importance. Stephens (2000*a*) used a continuous time sampler to draw from a bivariate mixture posterior. More generally, Dellaportas & Papageorgiou (2004) have constructed a reversible jump sampler for multivariate mixtures of normals, with split/merge moves operating on the space of eigenvalues and eigenvectors of the covariance matrix. Dellaportas & Papageorgiou (2004) demonstrate their method on 2,3 and 5 dimensional data and report reasonable mixing properties for their algorithm.

3.5 Dirichlet Process Mixtures

An additional way of constructing a mixture with an unknown number of components is the Dirichlet process mixture (DPM): see for example Escobar & West (1995). In this approach the prior distribution for the parameters of the mixture is treated as unknown, say G, and a DP prior is placed upon it. The discreteness of G under the DP is exploited as follows. In any sample of parameters $(\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_n)$ (corresponding to the n possible components) there is positive probability of two or more points coinciding; thus reducing the components to k $(\leq n)$. Typically the full conditionals can be sampled from using Gibbs or possibly Metropolis-Hastings updates. West (1997) notes that DPMs are perhaps less general than the mixtures focused upon in this article, stating that the approach is “more geared towards density estimation and related objectives than mixture deconvolution or parameter estimation”.

3.6 Comments

We have considered samplers for mixtures. We have demonstrated that the Gibbs sampler is not always appropriate for sampling from a mixture posterior, though for some cases such as the Galaxy data example (section 1), the samples were more than adequate. We saw that tempering updates allowed full exploration of the mixture posterior.

In order to use tempering MCMC (as we have used it) we need to be able to calculate the marginal likelihood. Clearly, for standard mixtures this is straightforward. However, if the latent variables have special structure (for example Markovian) this calculation may be difficult. We have found that for HMMs that marginal update schemes (which requires the 'forward' step of the forwards-backwards algorithm of Baum et al. (1970)) can be computationally slow and sometimes leads to large autocorrelations and rejection rates in
Metropolis-Hastings moves (as found by Boys & Henderson (2003)).

There are other approaches for simulating from a mixture posterior, including perfect samplers: see Casella, Mengersen, Robert & Titterington (2002). Marin, Mengersen & Robert (2004) provide a review. Also work on exact simulation for changepoint problems via the forwards-backwards method can be found in Fearnhead (2004).

We now review the various ways of dealing with label switching, beginning with artificial identifiability constraints. To use the methods that we review, we recommend conditioning on k as argued by Robert (1997). Therefore we always consider label switching for mixtures with a fixed number of components. We will also assume that we have a sampler that can visit the $k!$ symmetric modes of the posterior.

4 Artificial Identifiability Constraints

4.1 The Method

We define an *identifiability constraint* as a condition on the parameter space Θ, such that only one permutation can satisfy it. An example of such a constraint is $\mu_1 < \cdots < \mu_k$ in the univariate random beta model. This identifiability constraint is *artificial*, as it not does arise from any genuine knowledge or belief about the model, but is rather an apparent inferential convenience.

We refer to ICs in the way they were initially used (as Diebolt & Robert (1994) or Dellaportas, Stephens, Smith & Guttman (1996)). In other words, at every iteration of the sampler, we permute the samples so they satisfy the constraint. When applying ICs, it is best to search for identifiability constraints that lead to density estimates of the parameters that are as unimodal as possible (as stated by Richardson & Green (1997)). Indications of inappropriate identifiability constraints include exaggerated skewness and multimodality in the density estimates.

The motivation behind imposing an IC is the following. Since the likelihood and prior are invariant to the labelling of the parameters, if we impose an identifiability constraint on the parameter space we break the symmetry in the posterior and the labelling problem should be solved. We would therefore focus on one of the $k!$ symmetric modes and output from the MCMC sampler can then be interpreted.

An identifiability constraint need not be imposed before any simulation takes place. Stephens (1997*a*) proved that inference conditional on an identifiability constraint can be performed when the constraint is imposed after the MCMC run (see proposition 3.1 and corollary 3.2 of Stephens (1997*a*)). Such procedures are equivalent to *changing the prior distribution.* That is, since the marginal posterior distributions are the same for each label and the likelihood is invariant to permutations, we define a new prior $p_n(\boldsymbol{\theta})$ such that

$$p_n(\boldsymbol{\theta}) \quad = \quad k!p(\boldsymbol{\theta})\mathbb{I}_{(\boldsymbol{\theta}\in C)}$$

where C is the constraint, $\mathbb{I}_{(\cdot)}$ is the indicator function and $p(\boldsymbol{\theta})$ is the unconstrained prior.

An alternative approach to identifiability constraints is provided by Frühwirth-Schnatter (2001). Frühwirth-Schnatter used a 'random permutation' sampler (RPS). That is, at every iteration of an MCMC sampler a Metropolis-Hastings move is used to propose a new permutation of the labels. This ensures the sampler visits all $k!$ symmetric modes. Frühwirth-Schnatter then applies exploratory data analysis on the MCMC output from the RPS by applying ICs; we search for constraints that give the clearest picture of all of the parameters (i.e. much same as the recommendations of Richardson & Green (1997) discussed above).

4.2 Comments on the Method

ICs have come under much scrutiny in the literature. Celeux (1997), Celeux et al. (2000), Stephens (1997a, 1997b, 2000b) have all voiced their concerns about imposing an identifiability constraint.

Much of the initial attention was confined to the effect on the MCMC sampler, such as the implications of truncating the support of the posterior in terms of simulation (as mentioned by Celeux (1997), Celeux et al. (2000)). However, as stated above, since identifiability constraints can be imposed after simulation, we can simulate from the unconstrained posterior distribution and then impose an IC. As a result there is no problem in terms of an adverse effect on simulation.

The use of exchangeable priors is normally an attempt to be weakly informative (e.g. Richardson & Green (1997)). However if the identifiability constraint used does not correctly isolate one of the $k!$ symmetric modes, we would hesitate to call such a specification weakly informative. This is because the prior will become highly influential on our inference, as demonstrated by Celeux et al. (2000). We note that they called this 'disturbing'; we contend that it is only to be *expected*, since different constraints correspond to different models.

One problem with identifiability constraints is the choice of constraint. Frühwirth-Schnatter (2001) suggests that "if the components of the state specific parameters have some physical meaning, then an expert in the field will have some idea in which way the groups or states differ and might be able to offer such an identifiability constraint". This seems reasonable, however we stress that if such expert opinion is available, an effort to produce subjective priors should be made. This may mean that there is no label switching at all; although label switching can still occur under subjective priors.

A more general difficulty of using ICs is in multivariate problems. Finding suitable identifiability constraints in such situations is almost impossible; moreover, it can be difficult to anticipate the overall effect of such an action.

We saw at the beginning of this paper, that identifiability constraints do not always work and we consider this example in more detail.

4.3 Example: Galaxy Data Revisited I

We now use the random beta model of Richardson & Green (1997) to illustrate that identifiability constraints can often induce informative priors that do not necessarily reflect the objective of their exchangeable versions. In order to do this we return to the output from the Galaxy data in section 1.3.

We computed the estimated means conditional on the identifiability constraint $\mu_1 < \cdots < \mu_6$, through ergodic averaging and compared them with the means estimated by the relabelling algorithm in Figure 8 (which we discuss in the next section and we believe the estimates to reflect one of the 6! symmetric modes of the posterior). The results of which can be seen in Table 1. For most of the means we can see that the new prior induced by the identifiability constraint produces very different results to the 'correct' clustering of the MCMC samples, and hence the constraint is more influential than was intended.

In the following section we review the method of relabelling algorithms.

Parameter	Constraint	KL
μ_1	8.07	9.71
μ_2	16.46	19.01
μ_3	19.90	19.88
μ_4	22.21	22.71
μ_5	25.62	22.86
μ_6	34.84	32.92

Table 1: Table of Estimated Means. The constraint column is the estimated means under the identifiability constraint $\mu_1 < \cdots < \mu_6$. The KL column is the estimated means under the relabelling algorithm in Figure 8.

5 Relabelling Algorithms

5.1 The Method

Relabelling algorithms were developed by Stephens (1997a, 1997b, 2000b) and Celeux (1998). The idea is as follows: suppose we define a loss function $L : \mathcal{A} \times \Theta \to [0, \infty)$ such that:

$$L(a, \boldsymbol{\theta}) \quad = \quad \min_{\sigma \in S_k} \{L_0(a, \sigma(\boldsymbol{\theta}))\}$$

where $\mathcal{A}$ is the action space. Then the optimal action a^* is :

$$a^* \quad = \quad \arg\min_a \int_\Theta L(a, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathbf{x}) \mathrm{d}\boldsymbol{\theta}. \tag{3}$$

Since the integral in equation (3) cannot be computed exactly we use an MC estimate. We suppose that we draw N samples from the posterior distribution (denote these $\boldsymbol{\theta}^{(t)}$, $t = 1, \ldots, N$) and then apply the algorithm in Figure 7 to remove label switching.

```
Intialise algorithm with permutations $\sigma_1, \ldots, \sigma_N$.
Repeat until a fixed point is reached.
1. Choose $\hat{a}$ to minimise $\sum_{t=1}^{N} L_0(a, \sigma_t(\boldsymbol{\theta}^{(t)}))$.
2. For $t = 1, \ldots, N$ choose $\sigma_t$ to minimise $L(\hat{a}, \sigma_t(\boldsymbol{\theta}^{(t)}))$.
```

Figure 7: A General Relabelling Algorithm.

The idea behind the algorithm is the following. Since the likelihood is invariant to permutations in the labelling, we seek to minimise the loss of performing an action a associated with $\boldsymbol{\theta}$ by selecting the permutation that minimises this loss and then minimising the posterior expected loss.

Stephens (2000*b*) derives an algorithm for clustering inference based upon reporting an $n \times k$ matrix, Q, of classification probabilities, i.e. q_{ij} is the probability that observation i is assigned to class j. Let $P(\boldsymbol{\theta})$ denote the true matrix of classification probabilities, where $p_{ij}(\boldsymbol{\theta}) = \pi_j f(x_i; \phi_j) / \sum_{l=1}^{k} \pi_l f(x_i; \phi_l)$. Stephens uses the Kullback-Liebler divergence to measure the loss of reporting Q when the true probabilities are $P(\theta)$. The algorithm is given in Figure 8: we refer to this algorithm as the KL algorithm.

```
Intialise algorithm with permutations $\sigma_1, \ldots, \sigma_N$.
Repeat until a fixed point is reached.
1. Choose $\hat{Q}$ to minimise
       $\sum_{t=1}^{N}\sum_{i=1}^{n}\sum_{j=1}^{k} p_{ij}\left\{\sigma_t(\boldsymbol{\theta}^{(t)})\right\}\log\left\{\frac{p_{ij}\{\sigma_t(\boldsymbol{\theta}^{(t)})\}}{q_{ij}}\right\}.$
2. For $t = 1, \ldots, N$ choose $\sigma_t$ to minimise
       $\sum_{i=1}^{n}\sum_{j=1}^{k} p_{ij}\left\{\sigma_t(\boldsymbol{\theta}^{(t)})\right\}\log\left\{\frac{p_{ij}\{\sigma_t(\boldsymbol{\theta}^{(t)})\}}{\hat{q}_{ij}}\right\}.$
```

Figure 8: Stephens' KL Algorithm for Clustering Inference.

In order to apply a relabelling algorithm, we must choose m (well dispersed) starting points, since the algorithm is only guaranteed to converge to a local minimum. We then select the permutations and quantities that give the optimal solution. If storage requirements are too substantial then an online version can be implemented. Additionally, step 2 of Figure 7 can be performed efficiently (for medium k) using the transportation algorithm: see Stephens (2000*b*) for details.

5.2 Comments on the Method

The form of a relabelling algorithm is exactly that of a k-means type clustering algorithm, with Stephens taking advantage of the special nature of the problem at hand. In our view, the method is an *automative way of applying (or inducing) an identifiability constraint.* That is, under an inferential objective the permutations of the labelling are induced or discovered so that all of the samples are labelled in the same way. We can then draw inference on any quantity by using ergodic averaging on the permuted samples.

We feel that the fact that the method is simply a way of applying an identifiability constraint (i.e. that the statistical model is changed) is under appreciated in the literature; it is not a fully decision theoretic method. That is, under a fully decision theoretic method, for every quantity of interest, we derive a loss function for estimation, which is not the case for relabelling algorithms (indeed, it would not be sensible since we may have different quantities that were estimated conditional on different identifiability constraints).

A method related to relabelling algorithms can be found in Marin et al. (2004). Marin et al. (2004) find the MAP estimate of the parameters based upon all of the MCMC samples. Then to permute the MCMC samples, they find the permutation that minimises the canonical scalar product between the MAP estimator and the sample. This method is simple to use, however has a one major drawback; when the parameter space features many genuine modes. In this case the MAP estimate will ignore minor modes, and may lead to inappropriate identifiability constraints being used.

We now demonstrate that relabelling algorithms applies or induces an identifiability constraint in the following example.

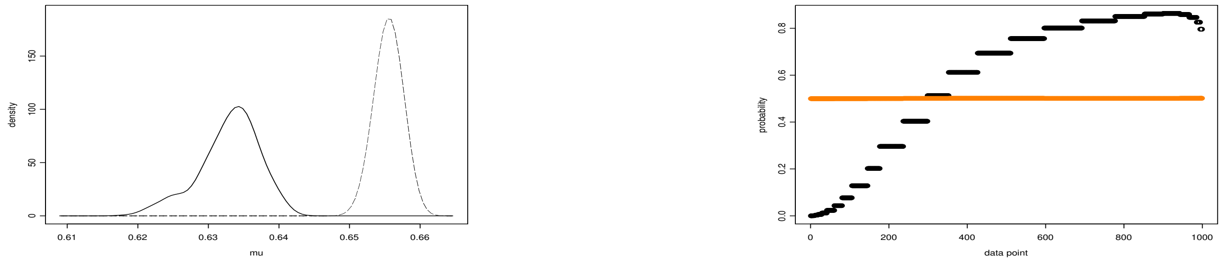
5.3 Example: Crab Data Revisited

We used Stephens KL algorithm to deal with the label switching of the Crab data example. The density estimates of the relabelled marginal posteriors and the classification probabilities can be seen in Figure 9.

Application of Stephens' KL algorithm has induced the identifiability constraint $\mu_1 < \mu_2$ (note that this was for this example, and is not a general mathematical result). This allows us to perform inference which is supported by Figure 9b which shows that the classification probabilities are far more discriminated under the relabelled samples.

We note that if we wanted to estimate the means say, it would be most sensible to take the estimate over the permuted MCMC samples. This is because, if we applied another algorithm with a different loss function, we may not obtain the same constraint (in this example it is unlikely another constraint would transpire). However, Stephens (2000*b*) reports that it is generally the case, when there is no genuine multimodality, that different relabelling algorithms often produce similar permutations.

Another potential problem with ICs (and hence relabelling algorithms), when the data in the components are poorly separated, is the following. Gruet et al. (1999) find that one of the components overwhelms the others, which become negligible. We explore this in the following example.



(a) Density Estimates.

(b) Classification Probabilities.

Figure 9: Marginal Posterior Density Estimates (a) (μ_1 (unbroken), μ_2 (dashed)) and Classification Probabilities (b); Crab data. We used Stephens' KL algorithm (Figure 8) to deal with the label switching. For (b) the orange dots are the classification probabilities under the unconstrained prior.

5.4 Example: Rao's Plant Data

For our next example we consider the plant data of Rao (1948). The data consist of the heights (in cm) of 454 plants of two different types. Rao (1948) used a two component normal mixture model to analyse the data. In Rao (1948) the data were presented in a frequency table, thus is essentially interval censored. To remove this effect, we added a $\mathcal{U}_{[-0.5,0.5]}$ random variable (where $\mathcal{U}_{[a,b]}$ is the continuous uniform distribution on $[a, b]$) to each data point (which we interpreted as the midpoint of each class interval).

The physical motivation for a mixture is clear, however let us observe the data, given in Figure 10. We can see that if the data is truly a two component mixture it is difficult to see evidence of this from the histogram (note that the sampling density/histogram need not be bimodal to be a two component mixture). Thus we would suggest that the data in the components are poorly separated.

To analyse this data we will use the random beta model, with $k = 2$ and use the KL algorithm to deal with label switching. We used tempering MCMC to sample from the posterior distribution. The trace plots of the parameters for 10000 iterations post burn in are given in Figure 11. From Figure 11a we can observe that there is significant label switching, since the plots for both components are similar.

We then used the KL algorithm to undo label switching. Whilst the object of inference is not clustering, we can observe in Figure 11b that the algorithm has worked well. This is because the algorithm appears to have isolated one of the 2 symmetric modes in the posterior distribution.

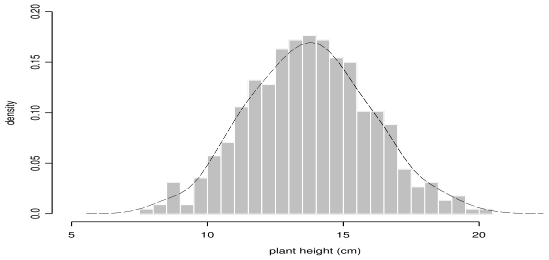


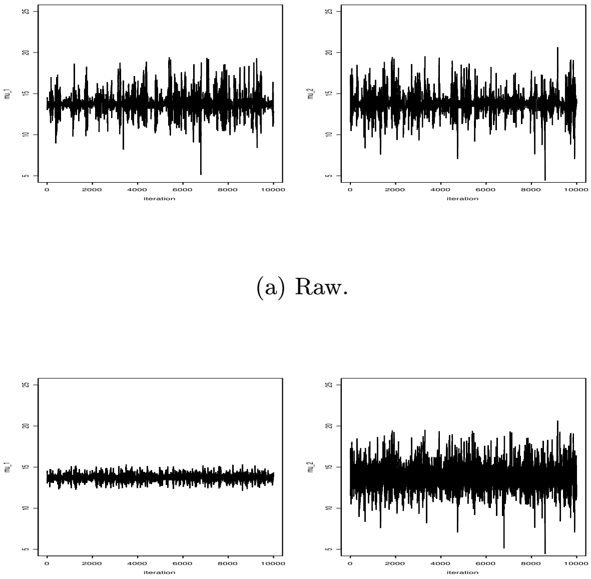
Figure 10: Histogram of Plant Data. We overlaid the histogram with a kernel density estimate (dashed).

We can see from the Table 2, that (for the relabelled samples) component 1 is dominating component 2 (since π=0.804). However we feel that this is *not* a defect of using a relabelling algorithm (and hence an IC). This is because the relabelled MCMC output appears to be correct (no bias of the constraint), as demonstrated by the fact that the relabelled components are so different, i.e. that the plot in Figure 11 (b) on the left has lower variance than the plot on the right. Whilst the inference from the mixture model (based upon the relabelled samples) appears to be incorrect: (for example, Rao estimated the mixture proportion as 0.566, we note, however, that our data may not give identical results to the original analysis as we have perturbed them) this does not matter from the perspective of dealing with label switching. The relabelling algorithm has performed well and exposed the view of the data that one component provides sufficient explanation of the data. In such cases, it may be more appropriate to determine subjective priors or different component densities.

We now consider the justifications for using relabelling algorithms.

Parameter	Raw Output	KL
μ_1	13.824	13.747
μ_2	13.819	13.897
λ_1^{-1}	3.773	4.690
λ_2^{-1}	3.66	3.075
π	0.519	0.804

Table 2: Table of Parameter Estimates for the Plant Data. The estimates (ergodic averages) are based upon the unconstrained prior and the permuted samples.



(a) Raw.

(b) Relabelled.

Figure 11: Tempering MCMC Trace Plots for Plant Data. Plot (a) displays the means as returned by our algorithm for 10000 iterations, plot (b) the relabelled means.

5.5 Justification of Relabelling Algorithms

Stephens (1997*a*) gives possible justifications of using relabelling algorithms.

The first justification was 'revisionist Bayes'. As stated in section 4.1 applying an identifiability constraint is equivalent to changing the prior distribution. Therefore, when we use a relabelling algorithm we are essentially changing the statistical model: How might we justify such an approach? Stephens suggests that we are returning to the modelling stage and forcing identifiability on the components of the mixture. Many Bayesians may find this explanation distinctly unsatisfactory, but we agree that it is a credible justification, as, if we seek to draw meaningful inference from the parameters of a mixture model, we need to be able to interpret them. If we use the extra information from the data (and hence the MCMC sampler), we can do so.

The second justification was 'mode hunter'. This is simply the view that we seek to find the permutations of the labelling which minimise the loss of computing the quantity of interest, and that we can calculate no other quantity.

Under the revisionist Bayes justification one actually believes in the permutations applied and is convinced that the model is representative of the real world problem. This is not the case under the mode hunter view.

5.6 Discussion

In this section we have shown that relabelling algorithms impose an IC. The exact nature of the constraint would depend both on the loss function chosen and the MCMC samples themselves.

We have stated that relabelling algorithms should be used with care when the data in the components are similar. Note that inference from the parameters in this case is not meaningless. There are many instances in the literature where analysis of data where the components are poorly separated has occurred, for example Rao (1948) and more recently Gruet et al. (1999). Additionally there may be situations that we do not know *a priori* that the components are poorly separated in the components, for example if we were analysing high dimensional data.

We now review the method of label invariant loss functions.

6 Label Invariant Loss Functions

6.1 The Method

Define a loss function $L : \mathcal{A} \times \Theta \to [0, \infty)$ such that:

$$L(a, \boldsymbol{\theta}) \;=\; L(a, \sigma(\boldsymbol{\theta}))\ \forall \sigma \in S_k.$$

Using such a loss function solves the labelling problem immediately. The way in which the method is applied (as in Celeux et al. (2000) and Hurn et al. (2003)) is the following. Compute the posterior expected loss

$$\begin{aligned} \mathbb{E}[L(a, \boldsymbol{\theta})|\mathbf{x}] &= \int_{\Theta} L(a, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathbf{x}) \mathrm{d}\boldsymbol{\theta} \\ &\approx \frac{1}{N} \sum_{i=1}^{N} L(a, \boldsymbol{\theta}^{(t)}) \end{aligned} \tag{4}$$

Normally equation (4) cannot be minimised analytically, and so stochastic optimisation methods (e.g. simulated annealing) are implemented.

An example of a particular loss function, used by Hurn et al. (2003), for clustering inference is:

$$\begin{aligned} L(a, \mathbf{z}) &= \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \{\mathbb{I}_{(z_i = z_j)}(1 - \mathbb{I}_{(a_i = a_j)}) \\ &\quad + \mathbb{I}_{(a_i = a_j)}(1 - \mathbb{I}_{(z_i = z_j)})\} \end{aligned}$$

where a_i is the allocation that we give for the i^{th} data point. This loss function is based upon a pairwise comparison of the allocation of data points. If the true pair of data points are in the same class and our decision is that they are not, then we lose one, conversely if we choose the correct allocation we lose zero. To compute the posterior expected loss, we have:

$$\begin{aligned} \mathbb{E}[L(a, \mathbf{z})|\mathbf{x}] &= \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \{p(z_i = z_j|\mathbf{x})(1 - \\ &\quad \mathbb{I}_{(a_i = a_j)}) + \mathbb{I}_{(a_i = a_j)} p(z_i \neq z_j|\mathbf{x})\}. \end{aligned} \tag{5}$$

We then estimate (5) from our MCMC output (it is invariant to the labelling) and then minimise with respect to a. For examples of other loss functions, see Celeux et al. (2000) and Hurn et al. (2003).

6.2 Comments on the Method

From the Bayesian point of view the method of label invariant loss functions is more satisfactory than identifiability constraints. That is, we draw inference conditional only on the data. The method is fully decision theoretic as for every quantity of interest we must construct a loss function and perform the expectation then minimisation procedure highlighted above. This approach acknowledges both that the marginal posteriors for the labels are the same and that there is significant information in the MCMC output. It is therefore a fully Bayesian procedure.

The main difficulty with this method is the computational cost. Performing a simulated annealing algorithm for many loss functions will often be computationally expensive and may not be feasible for some functions.

A second drawback is the fact that the method is restricted to a class of loss functions that may or may not make sense for the decision problem at hand. That is, the method requires that the loss functions be invariant to the labelling of the parameters and that it is computationally feasible to minimise the posterior expected loss. Whether a loss functions can be constructed, within this class, will depend upon the statistical objectives.

For our next section we discuss the role of the prior in Bayesian mixture modelling.

7 The Role of the Prior in Bayesian Mixture Modelling

One of the difficulties in Bayesian modelling is specifying a prior distribution when there is little information to be used. This is often the case in Bayesian analyses via mixture models with an unknown number of components and can lead to some additional (i.e. not label switching) inferential difficulties. We now demonstrate one such problem for the random beta model.

7.1 Example: Galaxy Data Revisited II

We reanalysed the Galaxy data, using the random beta model with k unknown. For 7 different settings of κ, (the normal prior precision on the component mean parameter) we ran a reversible jump sampler (similar to Richardson & Green (1997), except that we used a split/merge move that is much the same as described in Cappé et al. (2003) appendix C) for 500000 iterations, taking the burn in to be 100000 iterations. The results can be seen in Table 3.

In Table 3 we can observe Lindley's paradox. As we seemingly place less prior information on the component means (i.e. as $\kappa \to 0$) the prior becomes more informative for the number of components. Jennison (1997) notes that placing a prior on κ can help to reduce this effect (as used by Stephens (2000*a*)) and presumably is one of the reasons why Richardson & Green (1997) place a prior on β. In our opinion Lindley's paradox demonstrates that there is generally no natural way to represent 'prior ignorance' in this hierarchical modelling context. That is, it will often be the case that many reasonable prior specifications (for the parameters) will lead to differing inferences with respect to the number of components. This latter point is made by Aitkin (2001).

7.2 Further Discussion

Aitkin (2001) compiled a set of Bayesian analyses of the Galaxy data, ranging from the approach of Richardson & Green (1997) to Escobar & West (1995). Aitken notes that whilst each method has a sensible (weakly informative) prior specification, the posterior distributions for the number of components are markedly different. Indeed Aitkin (2001) notes

> The complexity of the prior structures needed for Bayesian analysis, the obscurity of their interaction with the likelihood, and the widely different conclusions they lead to over different specifications, leave the user completely unclear about 'what the data say' from a Bayesian point of view about the number of components in the mixture.

This is a traditional frequentist criticism of Bayesian inferential methods, but does illustrate the need for appropriate consideration of all elements of a Bayesian model. Of course, these concerns are only really of interest when performing clustering or discrimination analysis. In the case of

κ	Range of k with		$\max_k p(k\|\mathbf{x})$
	$p(k\|\mathbf{x}) \geq 0.05$	$p(k\|\mathbf{x}) \geq 0.001$	
$\frac{1}{R^2}$	$3-9$	$3-15$	6
$\frac{4}{R^2}$	$5-13$	$3-24$	8
$\frac{9}{R^2}$	$8-16$	$4-30$	10
$\frac{16}{R^2}$	$11-18$	$5-30$	14
$\frac{25}{R^2}$	$8-22$	$5-30$	19
$\frac{64}{R^2}$	$21-30$	$6-30$	30
$\frac{100}{R^2}$	$23-30$	$2-30$	30

Table 3: Sensitivity of the Posterior Distribution for k; Galaxy Data. Each row is based upon a reversible jump sampler run for 500000 iterations with a 100000 iteration burn in. The priors were set to be $\alpha = 2$, $\delta = 1$, $\xi = M$, $g = 0.2$, $h = 100g/\alpha R^2$ and $k_{\max} = 30$, where R and M denote the range and midpoint of the observed data.

the latter, Stephens (2000*a*) notes that priors should be set so that components are as different as possible, in order to avoid overfitting (too many components). When the objective of inference is prediction (for example computing density estimates) model averaging procedures may be used, and the influence of the prior on the number of components is of less concern.

We believe that meaningful data analysis can be performed using Bayesian mixture models, but an appreciation of the effect of the prior on the number of components is needed. Our general practice is to set priors according to the information available (e.g. data dependent as in Richardson & Green (1997)) and then to perform a sensitivity analysis in order to measure the influence of the prior specification on the number of components: especially using simulated data. Once we are certain we understand the implications of the prior on the posterior, we proceed with a data analysis, accepting that 'different priors will lead to different posteriors'.

Constructing priors for Bayesian mixture models is an area which still requires further research. We recommend the discussion of Richardson & Green (1997) and Stephens (2000*a*) as possible starting points.

We now discuss our recommendations for applying MCMC analysis to mixtures and the methods we use to deal with label switching. Finally we suggest an area of future reasearch for Bayesian mixture modelling.

8 Summary and Our Recommendations

In this article we have reviewed MCMC samplers for mixtures, solutions to the label switching problem and discussed the sensitivity of posterior inference for the number of mixture components to prior specifications.

When constructing an MCMC sampler for fixed dimensional, univariate mixtures, we generally use the following strategy. We begin by coding up a Metropolis-Hastings algorithm without completing the data (if we can compute the marginal likelihood). We will then seek to find the proposal densities and parameters that provide reasonable mixing (i.e. not too large autocorrelations in the chain). If the sampler is unable to move around the symmetric modes of the target we consider a couple of ideas.

First, if we are unsure as to the number of components in the mixture, we add reversible jump steps: this will normally provide adequate mixing. Secondly, we will try to use either tempering or evolutionary Monte Carlo (EMC). We have found that tempering is often effective, but in some difficult situations (highly separated modes in the posterior) we were often unable to tune the tempering sampler to enable the correct movement around the target space. In our experience, EMC works extremely well and we have never found an example where a properly tuned algorithm does not traverse the state space correctly.

We feel that the Gibbs sampler run with completion is often not worth programming (unless it can be quickly implemented, in BUGS for example) since the chance of it failing to converge is too high.

In order to choose a method to deal with label switching we have used the following criteria in our applied work. In situations for which we are only interested in a single inference from our mixture model (for example clustering the data) we often use a label invariant loss function. This choice is made as it will often need less programming effort than a relabelling algorithm. Conversely, if we are concerned with many label dependent quantities, we prefer the relabelling approach as this avoids performing a large number of simulated annealing algorithms. In our experience ICs (not through relabelling algorithms) are only of use in situations for which it is obvious on how to undo the label switching (for example Figure 5b).

In this article we have detailed the progress of Bayesian mixture modelling; so what challenges need to be addressed in the future? One area of current research in bioinformatics is gene clustering, (see for example Yeung, Fraley, Raftery & Ruzzo (2001)) which can be performed using mixture models. A drawback of using a Bayesian mixture model is the difficulty of simulating from a high-dimensional, variable dimensional target measure, which is characteristic of such problems (an example of a small data set is 2000 data points in 6 dimensions). Current reversible jump and continuous time samplers are unable to move efficiently around the sample space and new simulation methods are required to apply Bayesian methodology in such contexts: see Jasra et al. (2004) for a potential approach.

Acknowledgements

The first author was supported by an Engineering and Physical Sciences Research Council studentship. We also thank the executive editor and three referees for their comments on earlier versions.

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