Investigating the efficiency of marginalising over discrete parameters in Bayesian computations

Wen Zhang\textsuperscript{1}, Jeffrey Pullin\textsuperscript{1,2}, Lyle Gurrin\textsuperscript{3}, Damjan Vukcevic\textsuperscript{1,2,*}

\textsuperscript{1}School of Mathematics and Statistics, University of Melbourne, Australia
\textsuperscript{2}Melbourne Integrative Genomics, University of Melbourne, Australia
\textsuperscript{3}Melbourne School of Population and Global Health, University of Melbourne, Australia
*Corresponding author: Damjan Vukcevic, damjan.vukcevic@unimelb.edu.au

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Abstract

Bayesian analysis methods often use some form of iterative simulation such as Monte Carlo computation. Models that involve discrete variables can sometime pose a challenge, either because the methods used do not support such variables (e.g. Hamiltonian Monte Carlo) or because the presence of such variables can slow down the computation. A common workaround is to marginalise the discrete variables out of the model. While it is reasonable to expect that such marginalisation would also lead to more time-efficient computations, to our knowledge this has not been demonstrated beyond a few specialised models.

We explored the impact of marginalisation on the computational efficiency for a few simple statistical models. Specifically, we considered two- and three-component Gaussian mixture models, and also the Dawid-Skene model for categorical ratings. We explored each with two software implementations of Markov chain Monte Carlo techniques: JAGS and Stan. For JAGS, it was possible to compare marginalised and non-marginalised versions of the same model with the same samplers.

Our results show that marginalisation on its own does not necessarily boost performance. Nevertheless, the best performance was usually achieved with Stan, which requires marginalisation. We conclude that there is no simple answer to whether or not marginalisation is helpful. It is not necessarily the case that, when turned ‘on’, this technique can be assured to provide computational benefit independent of other factors, nor is it likely to be the model component that has the largest impact on computational efficiency.
1 Introduction

In a Bayesian framework, performing inference often involves the use of Markov chain Monte Carlo (MCMC) methods. Recently, MCMC methods based on Hamiltonian Monte Carlo (HMC), such as the ‘No U-Turn Sampler’ (NUTS) algorithm (Hoffman and Gelman, 2014) implemented in the probabilistic programming language Stan (Carpenter et al., 2017), have become popular, replacing methods based on Gibbs sampling in many domains. HMC-based methods require gradients of the likelihood function to be computed with respect to all parameters in the model. However, these gradients cannot be computed for discrete parameters, potentially limiting the use of HMC-based methods. One common approach to overcome this drawback is to marginalise the discrete parameters out of the model. HMC-based methods can then used to draw samples from the joint posterior distribution of the marginalised model. Today, marginalisation is the only way to fit models with discrete parameters in Stan. The widespread use of both Stan and models with discrete parameters has therefore made marginalisation a widely used technique in applied Bayesian modelling.

Recently, some of the authors of the current manuscript presented the R package rater, which implements Bayesian versions of several statistical models that allow analysis of repeated categorical rating data (Pullin et al., 2021). The models are based on, and include, the Dawid–Skene (DS) model (Dawid and Skene, 1979), and as such they include a discrete latent class parameter for each item. The rater package uses Stan to perform inference, and marginalised versions of the models are employed. The manuscript describing rater discusses in some detail the techniques of marginalisation and conditioning in an effort to explain the mathematical basis of the technique. In addition, other authors such as Joseph (2020) have sought to explain how to marginalise out discrete parameters in specific models.

While marginalisation requires substantial mathematical effort, folk wisdom in the Stan community suggests that fitting models with marginalisation is more efficient than using Gibbs sampling. Indeed, the Stan User’s Guide asserts that marginalisation can allow “more efficient sampling on an iteration-by-iteration basis” (Stan Development Team, 2022). To date, however, there has been little empirical evidence for the idea that marginalisation can improve computational efficiency. Recently, Yackulic et al. (2020) considered marginalising out latent states in a variety of Bayesian population models such as the Cormack–Jolly–Seber
(CJS) model. In particular, they demonstrated that marginalisation can improve computational performance by orders of magnitude in a CJS model. In their comparison, the fastest model—implemented using Stan—was more than one thousand times more efficient than the slowest non-marginalised model. These results highlight the potential of marginalisation, and Stan, to greatly increase the efficiency of Bayesian inference for models with discrete parameters. It is not clear however, whether the results presented by Yackulic et al. (2020) generalise to other models that contain discrete parameters.

Whether or not marginalisation makes computation more efficient is of both practical and theoretical interest. Practically, the efficiency of marginalisation would guide both whether marginalisation should be considered as a possible way to speed up generic Bayesian computations, and decisions about which software (i.e. JAGS vs Stan) and options within these software to use. Theoretically, it is of interest to determine whether the claimed improvements in efficiency suggested by the Rao–Blackwell Theorem actually hold in practice. Finally, this work could guide whether future probabilistic programming languages (such as SilcStan (Gorinova et al., 2019)) should implement automatic marginalisation for some, or even all, models.

In this paper, we explore the impact of marginalisation on computational efficiency for other models that contain discrete parameters: two- and three-component Gaussian mixture models and the Dawid–Skene model for categorical ratings. We implement various marginalised and non-marginalised version of the models in JAGS and marginalised versions of the models in Stan. We then compare the computational efficiency of the different inference approaches across various simulation scenarios.

2 Methods

2.1 Models and marginalisation

Here we describe the Gaussian mixture models and the Dawid–Skene model that we used for the generation and analysis of simulated data, including the prior distributions we chose for Bayesian inference. We include two versions of the likelihood functions: (i) ‘full’ versions, that include the discrete variables; and (ii) marginalised versions, where the discrete variables are marginalised out.

2.1.1 Gaussian mixture models

A Gaussian mixture model assumes that each observation is generated from one of a finite set of Gaussian distributions, referred to as the mixture components. The model uses a discrete latent variable as a category label to indicate the mixture component from which each observation was drawn. Suppose that we have $n$ continuously valued observations, $x_1, \ldots, x_n$. We assume that each observation $x_i$ belongs to one of $K$ mixture components. Associated with each $x_i$ is a discrete latent variable $z_i \in \{1, \ldots, K\}$ that indicates the mixture component from which $x_i$ was drawn. We assume that $z_1, \ldots, z_n$ are independent and identically distributed as follows. For $i = 1, \ldots, n$,

\[ z_i \sim \text{Categorical}(\pi_1, \ldots, \pi_K), \]

where $\pi_k \in [0, 1]$ for $k = 1, \ldots, K$ and $\sum_{k=1}^{K} \pi_k = 1$. The parameter $\pi_k$ specifies the proportion of the population of continuously valued observations (the $x_i$’s) belonging to the $k$th mixture component.

We assume that $x_1, \ldots, x_n$ conditional on $z_1, \ldots, z_n$ are independent and identically distributed as follows. For $i = 1, \ldots, n$ and $k = 1, \ldots, K$,

\[ x_i \mid z_i = k \sim \text{N} (\mu_k, \sigma^2). \]

The variance, $\sigma^2$, is assumed to be the same for all mixture components. For $k \in \{1, \ldots, K\}$, $\mu_k$ and $\sigma^2$ are unknown parameters.

For convenience, we combine the above quantities into vector formats: let $\mathbf{x} = (x_1, \ldots, x_n)$; $\mathbf{z} = (z_1, \ldots, z_n)$; $\mathbf{\pi} = (\pi_1, \ldots, \pi_K)$ and $\mathbf{\mu} = (\mu_1, \ldots, \mu_K)$. 

The full likelihood function (that includes $z$) for this model is

$$\Pr(x, z \mid \pi, \mu, \sigma^2) = \prod_{i=1}^{n} f(x_i \mid \mu_{zi}, \sigma^2) \cdot \pi_{zi},$$

where $f(x_i \mid \mu_{zi}, \sigma^2)$ is the probability density function of a Gaussian distribution with mean $\mu_{zi}$ and variance $\sigma^2$.

The marginalised likelihood function, where we marginalise over $z$, is

$$\Pr(x \mid \pi, \mu, \sigma^2) = \sum_z \Pr(x, z \mid \pi, \mu, \sigma^2)$$

$$= \sum_{z_1=1}^{K} \sum_{z_2=1}^{K} \cdots \sum_{z_n=1}^{K} \Pr(x, z \mid \pi, \mu, \sigma^2)$$

$$= \sum_{z_1=1}^{K} \sum_{z_2=1}^{K} \cdots \sum_{z_n=1}^{K} \prod_{i=1}^{n} f(x_i \mid \mu_{zi}, \sigma^2) \cdot \pi_{zi}$$

$$= \left( \sum_{z_1=1}^{K} f(x_1 \mid \mu_{z_1}, \sigma^2) \cdot \pi_{z_1} \right) \left( \sum_{z_2=1}^{K} f(x_2 \mid \mu_{z_2}, \sigma^2) \cdot \pi_{z_2} \right) \cdots \left( \sum_{z_n=1}^{K} f(x_n \mid \mu_{z_n}, \sigma^2) \cdot \pi_{z_n} \right)$$

$$= \prod_{i=1}^{n} \sum_{z_i=1}^{K} f(x_i \mid \mu_{z_i}, \sigma^2) \cdot \pi_{z_i}. \tag{1}$$

We place the following prior distributions on the parameters:

$$\pi \sim \text{Dirichlet}(\alpha),$$

$$\sigma \sim \text{Lognormal}(0, 1),$$

$$\mu_1 \sim \text{N}(0, 10^2),$$

$$\mu_k \sim \text{N}(0, 10^2, \mu_{k-1}), \quad \text{for } k = 2, \ldots, K,$$

where $\alpha$ is a vector of 1’s with length $K$, and $\text{N}(0, 10^2, \mu_{k-1})$ is the truncated normal distribution where we use the truncation $\mu_k > \mu_{k-1}$ to avoid label switching. We chose $10^2$ for the variance of the prior distribution after trying a range of values and selecting one that improved convergence.

### 2.1.2 Dawid–Skene model

The Dawid–Skene model for categorical ratings is applicable to scenarios where a set of items is classified into categories by one or more raters. Specifically, we have $I$ items and $J$ raters. We assume that each item belongs to one of $K$ categories. Associated with each item is a (discrete) latent parameter $z_i \in \{1, \ldots, K\}$ that indicates the true category for item $i$. Associated with each item–rater pair is a rating $y_{i,j}$ for item $i$ given by rater $j$\(^1\). Let $y$ be the vector of all ratings. We assume that $z_i, \ldots, z_I$ are independent and identically distributed as follows. For $i = 1, \ldots, I$,

$$z_i \sim \text{Categorical}(\pi_1, \ldots, \pi_K),$$

where $\pi_k \in [0, 1]$ for $k = 1, \ldots, K$ and $\sum_{k=1}^{K} \pi_k = 1$. One can consider $\pi_k$ as the prevalence of category $k$ in the population from which the items are sampled. We let $\pi = (\pi_1, \ldots, \pi_K)$ and $z = (z_1, \ldots, z_I)$.

For all possible pairs of $i, j$ where $i \in \{1, \ldots, I\}$, $j \in \{1, \ldots, J\}$, we assume that $y_{i,j}$ conditional on $z_i$ are independent and identically distributed as follows

$$y_{i,j} \mid z_i \sim \text{Categorical}(\theta_{j,z_i,1}, \ldots, \theta_{j,z_i,K})$$

\(^1\)For simplicity, we assume that each item is rated exactly once by each rater. The model naturally generalises to arbitrary numbers of ratings and more complex experimental designs, see Pullin et al. (2021).
where \( \theta_{j,z_i,k} \in [0, 1] \) for \( k = 1, \ldots, K \) and \( \sum_{k=1}^K \theta_{j,z_i,k} = 1 \). \( \theta_{j,z_i,k} \) is the probability that rater \( j \) rates an item of true category \( z_i \) as being in category \( k \). We let \( \theta \) be the vector of all possible \( \theta_{j,z_i,k} \)’s.

For this model, the full likelihood function that includes \( z \) is

\[
Pr(y, z | \theta, \pi) = \prod_{i=1}^I \left( \pi_{z_i} \cdot \prod_{j=1}^J \theta_{j,z_i,y_i,j} \right).
\]

The likelihood function where we marginalise over \( z \) is

\[
Pr(y | \theta, \pi) = \prod_{i=1}^I \left( \frac{1}{K} \sum_{k=1}^K \left( \pi_k \cdot \prod_{j=1}^J \theta_{j,k,y_i,j} \right) \right).
\]

We place weakly informative prior probability distributions on the parameters:

\[
\pi \sim \text{Dirichlet}(\alpha), \quad \theta_{j,k} \sim \text{Dirichlet}(\beta_k),
\]

where \( \alpha \) is a vector of length \( K \) with positive elements, \( \theta_{j,k} \) is the vector \((\theta_{j,k,1}, \ldots, \theta_{j,k,K})\), \( \beta \) is a \( K \times K \) matrix with positive elements, and \( \beta_k \) is the \( k \)th row of this matrix. Specifically, \( \beta \) contains the elements:

\[
\beta_{k,k'} = \begin{cases} 
Np & \text{if } k = k' \\
\frac{N(1-p)}{K-1} & \text{otherwise}
\end{cases} \quad \forall k, k' \in 1, \ldots, K.
\]

For the hyper-parameters \( \alpha, N \) and \( p \), we used the default values from the R package \texttt{rater} (Pullin et al., 2021): \( \alpha \) is a vector of 3’s, \( N = 8 \) and \( p = 0.6 \). See Pullin et al. (2021) for a description of how to interpret these parameters.

### 2.2 Data simulations

Here we describe how we simulated each test dataset. For each model and experimental scenario, we simulated 5 replicate datasets.

#### 2.2.1 Two-component Gaussian mixture model

We simulated observations from the following probability density function:

\[
g(x_i) = \pi_1 \cdot f(x_i | \mu_1, \sigma^2) + \pi_2 \cdot f(x_i | \mu_2, \sigma^2),
\]

where \( f(x_i | \mu, \sigma^2) \) is the probability density function of a Gaussian distribution with mean \( \mu \), variance \( \sigma^2 \) and mixture proportions \((\pi_1, \pi_2)\). We define the distance between components by \( |\mu_2 - \mu_1| \), and also \( \mu = (\mu_1, \mu_2) \) and \( \pi = (\pi_1, \pi_2) \).

For this model, we were interested in how the mixture proportions and distance between components modified the impact of marginalisation. We simulated four datasets, each of size 200. We set the values of \( \mu_1 \) and \( \mu_2 \) as in the second column of Table 1.

We paired the two options for the distances between components with three options for the mixture proportions: one with equal proportions, one with moderately imbalanced proportions and one with very imbalanced proportions. See the third and fourth columns of Table 1. The mixture proportion for Dataset 2 was set to be highly imbalanced. This allows us to investigate how discrete sampling for small probabilities impacts marginalisation. Plots of the density function for each dataset can be found in the first rows of Figure 1 and Figure 2.
We simulated a dataset with 5 raters and 100 items, where each item belongs to one of the 5 categories.

### 2.2.3 Dawid–Skene model

Plots of the density function for each dataset can be found in the first rows of Figure 3 and Figure 4.

For the three-component Gaussian mixture model, we index the simulations by both the maximal distance between components and whether the components are equidistant or not.

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We simulated eight datasets, each of size 200. We set the value of $\mu$ as in the second column of Table 2. The combinations of different mixture proportions, maximal distances between components and whether the components are equidistant or not gives us a $2 \times 2 \times 2$ balanced design, as shown in Table 2.

Plots of the density function for each dataset can be found in the first rows of Figure 3 and Figure 4.

### 2.2.2 Three-component Gaussian mixture model

Similar to the above, we simulated observations from the following the probability density distribution:

$$
g(x_i) = \pi_1 \cdot f(x_i \mid \mu_1, 2^2) + \pi_2 \cdot f(x_i \mid \mu_2, 2^2) + \pi_3 \cdot f(x_i \mid \mu_3, 2^2).
$$

We assume $\mu_1 < \mu_2 < \mu_3$ and define the maximal distance between components by $|\mu_3 - \mu_1|$. We consider two scenarios: (i) where the components are equidistant, $\frac{\mu_3 - \mu_2}{\mu_2 - \mu_1} = 1$; and (ii) where the components are non-equidistant, specifically $\frac{\mu_3 - \mu_2}{\mu_2 - \mu_1} = \frac{2}{5}$.

For the three-component Gaussian mixture model, we index the simulations by both the maximal distance between components and whether the three components are equidistant or not.

We simulated eight datasets, each of size 200. We set the value of $\mu$ as in the second column of Table 2. The combinations of different mixture proportions, maximal distances between components and whether the components are equidistant or not gives us a $2 \times 2 \times 2$ balanced design, as shown in Table 2.

Plots of the density function for each dataset can be found in the first rows of Figure 3 and Figure 4.

### 2.2.3 Dawid–Skene model

We simulated a dataset with 5 raters and 100 items, where each item belongs to one of the 5 categories ($J = 5$, $I = 100$, $K = 5$). We set the prevalence of each category to be uniform, i.e. $\pi = (\frac{5}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5})$.

For $j \in \{1, \ldots, 5\}$ and $k \in \{1, \ldots, 5\}$, we let $\theta_{j,k,k} = 0.7$ and $\theta_{j,k,l} = 0.075$ for all $l \neq k$. This means all raters classify the items correctly 70% of the time, and otherwise make errors uniformly amongst the other categories.

### 2.3 Software implementations

We explored the computational efficiency for each model–data pair using both JAGS and Stan. Specifically, we used the main R interfaces to each one: rstan (Stan Development Team, 2020) and rjags (Plummer, 2019). All of our models were coded ‘by hand’. We used the R package posterior (Bürkner et al., 2022) for summarising output from both JAGS and Stan.
JAGS supports direct sampling of discrete parameters. In contrast, Stan cannot be used when the posterior
distribution explicitly contains discrete parameters, so marginalisation is required. Using JAGS, we directly
compared marginalised and full versions of the same model (which we refer to as \textit{jags-full} and \textit{jags-marg}), and
also compared the performance of the JAGS models with the (necessarily marginalised) Stan model (which
we refer to as \textit{stan}). All implemented likelihood functions are described mathematically in Section 2.1.

Source code for reproducing all of the results in this manuscript is available on GitHub\textsuperscript{2}.

2.3.1 Gaussian mixture models with JAGS

For the two- and three-component Gaussian mixture models, we have two versions of each of the full and
marginalised models in JAGS, as follows.

Marginalised models:

1. The \textit{jags-marg-inbuilt} model is marginalised with the \texttt{dnormmix} distribution from the \texttt{mix}
module.
2. The \textit{jags-marg} model is marginalised manually as in Equation 1.

Full models:

1. The \textit{jags-full} model is unmarginalised and allowed to use any samplers from the \texttt{base}, \texttt{bugs}
and \texttt{mix} modules in JAGS.
2. The \textit{jags-full-restricted} model is unmarginalised but only allowed to use the following samplers:
   \begin{itemize}
   \item \texttt{base::Slice};
   \item \texttt{bugs::Dirichlet}.
   \end{itemize}

We selected this restricted set of samplers to try and force the \textit{jags-full-restricted} model to use the same set of
samplers as the \textit{jags-marg-inbuilt} and \textit{jags-marg} models. We did this to assess the impact of marginalisation
itself, rather than also the use of different samplers (which JAGS chooses automatically, based on the model
it is using). The set of samplers was selected by turning all samplers ‘off’ except for a candidate set and
looking for error messages when running the \textit{jags-marg-inbuilt} and \textit{jags-marg} models.

2.3.2 Dawid–Skene model with JAGS

We have the \textit{jags-marg} model which is marginalised manually and the unmarginalised \textit{jags-full} model which
is allowed to use any samplers from the \texttt{base} and \texttt{bugs} modules in JAGS. The \textit{jags-full-restricted} model is
unmarginalised but only allowed to use the same set of samplers as for the \textit{jags-full-restricted} for Gaussian
mixture models. We selected this restricted set of samplers by going through the same procedure for the
Dawid–Skene model as we did for the Gaussian mixture model (see above).

2.4 Evaluating computational efficiency

We evaluated computational efficiency by looking at four quantities of interest:

1. Computation time
2. Minimum effective sample size for the continuous parameters
3. Time per minimum effective sample
   (Computation time divided by Minimum effective sample size of continuous parameters)
4. The $\hat{R}$ statistic (Gelman and Rubin, 1992)

The way we measure these quantities is specified in Table 3.

\textsuperscript{2}https://github.com/katezhangwen/Efficiency-of-marginalising-over-discrete-latent-parameters
Table 3: Methods used for measuring the quantities to assess computational efficiency (see Section 2.4).

| Quantity                                      | JAGS                                                                 | Stan                                                                 |
|-----------------------------------------------|----------------------------------------------------------------------|----------------------------------------------------------------------|
| Computation time                              | Using the `system.time()` function to measure the time elapsed running `jags.model()` and `coda.samples()`. The quantity is the sum of the two computation times. | Using the `system.time()` function to measure the time elapsed running `stan()`. |
| Minimum effective sample size for the continuous parameters | (For both JAGS and Stan) Looking at `ess_bulk` and `ess_tail` for all continuous parameters of posterior’s `draws` object and taking the minimum. The numbers were similar, so we only present the `ess_bulk` measure in the result. |                                                            |
| Time per minimum effective sample             | (For both JAGS and Stan) Computation time divided by Minimum effective sample size of continuous parameters. |                                                            |
| $\hat{R}$                                     | (For both JAGS and Stan) Looking at `rhat` for all continuous parameters of posterior’s `draws` object and taking the maximum. |                                                            |

We ran the models on each of the 5 replicate datasets to obtain 5 observations of each of the quantities above for each model–data pair. The analysis was done with 3 chains, a total of 3000 iterations, with 1500 iterations of warm up.

3 Results

3.1 Gaussian mixture models

We used two plots to summarise results for two- and three-component Gaussian mixture models respectively. Figure 1 and Figure 3 shows results on the natural scale, while Figure 2 and Figure 4 shows results on a logarithmic scale (base 10) with common limits on the vertical axes. Figure 1 and Figure 3 highlight differences between models with the same dataset; Figure 2 and Figure 4 demonstrate the differences across different datasets.

The time per minimum effective sample measures the overall efficiency of each method. It is clear from Figure 1 and Figure 3 that `stan` usually outperformed all other models. Of the unrestricted JAGS models (i.e. all except `jags-full-restricted`), `jags-full` tended to outperform slightly when the (maximal) distance between components was large. When the (maximal) distance between components was small, the difference between `jags-full`, `jags-marg-inbuilt` and `jags-marg` was minor. The restricted model, `jags-full-restricted`, was consistently the worst performer across all scenarios.

Considering computation time and minimum effective sample size separately, although `stan`’s computation time was often higher than (in the two-component case) or comparable (in the three-component case) to those of the JAGS models, it had the highest minimum effective sample size in all cases, typically allowing it to be the most efficient overall. When the (maximal) distance between components was small, `jags-marg-inbuilt` and `jags-marg`, `jags-full` were significantly faster than `stan` when it comes to computation time (but they typically also had smaller effective sample sizes, thus did not typically outperform `stan` in overall efficiency).

The realised values of $\hat{R}$ demonstrate that `stan` converges the most consistently across all scenarios, whereas the JAGS models tend to perform inconsistently on many of the datasets.

The results in Figure 2 and Figure 4 suggest that is it ‘easier’ (in the sense that the time per minimum effective sample is lower) to draw posterior samples when using Data 1 and Data 2 for both the two- and three-
component Gaussian mixture models than for the other data structures. What distinguishes these datasets from the others is that their mixture components are distinct and well-separated (they have the largest distance between components, and in the three-component case the components are equidistant).

A highly imbalanced mixture proportion didn’t have any substantial impact on the relative performance of the models. This is evident from comparing Data 1 and Data 2 in Figure 2. Although Data 2 was ‘harder’ (in the sense that the time per minimum effective sample is higher) for all models, the relative difference between models, in time per minimum effective sample, is similar between the two datasets.
Figure 1: Time per minimum effective sample, computation time, minimum effective sample size and $\hat{R}$ when performing Bayesian inference of two-component Gaussian mixture models. The analysis is done with 3 chains, a total of 3000 iterations with 1500 iterations of warm up. Each box in the boxplot represents 5 results. The 5 results are obtained from 5 trials of analysis for each model–data pair. For each trial, we simulate one replicate of the dataset and run analysis for \texttt{stan}, \texttt{jags-full}, \texttt{jags-marg}, \texttt{jags-marg-inbuilt} and \texttt{jags-full-restricted} respectively. The horizontal line in the $\hat{R}$ plots is the conventional 1.1 threshold.
Figure 2: Same as Figure 1 but with results in each row shown on a common log_{10} scale to more easily compare across different datasets.
Figure 3: Same as Figure 1 but now showing the results for the three-component Gaussian mixture model.
Figure 4: Same as Figure 3 but with results in each row shown on a common log_{10} scale to more easily compare across different datasets.
3.2 Dawid–Skene model

Unlike the Gaussian mixture models, jags-full slightly outperformed stan as seen in the first row of Figure 5. The stan model had both a longer computation time and a larger minimum effective sample size compared to jags-full. However, the latter was so fast that its time per minimum effective sample size was smaller. The $\hat{R}$ values demonstrate that stan and jags-full converged the most consistently out of all models. The marginalised model, jags-marg, takes significantly longer computation time than all other models which makes it the worst performer when looking at time per minimum effective sample.

3.3 Main conclusions

Comparing the JAGS Gaussian mixture models, it is clear that marginalisation on its own does not necessarily boosts computational efficiency. The full model, jags-full, outperforms the two marginalised models (jags-marg-inbuilt and jags-marg) in almost all cases in terms of overall efficiency. Furthermore, the software implementations and choice of samplers had a much greater impact on computational efficiency. We can see this in two ways. First, by comparing the performance of jags-full and jags-full-restricted. The jags-full-restricted model consistently performed worse, and jags-full was the most efficient out of all JAGS models. This suggests that the boost from marginalisation is insufficient to overtake the boost from using a more efficient sampler. Second, we can compare the performance of stan against that of the marginalised JAGS models. The stan model (which is marginalised) was more efficient than the JAGS models, highlighting the difference due to choice of sampler and software implementation.

The results for Dawid–Skene suggest that marginalisation does not improve computational efficiency at all. Through comparing the performance of jags-marg and jags-full-restricted, the two models which we believe are using the same set of samplers, we see that the unmarginalised jags-full-restricted model performs better than the jags-marg model in terms of time per minimum effective sample. This means the unmarginalised model is in fact more computationally efficient even without the boost from the software implementation. In contrast, the fact that the marginalised stan model had computational efficiency similar to jags-full shows that, once again, the sampler and software implementation details are a more substantial factor in performance; in this case, the benefit was enough to counteract the seeming disadvantage of marginalisation.

4 Discussion

State-of-the-art software implementations of Markov chain Monte Carlo methods for Bayesian computation and optimisation currently use sampling techniques that require discrete parameters to be marginalised out of the full probability model whose joint posterior is the target distribution. Sampling from the model object that remains after marginalisation should be quicker and the process should reach convergence sooner, but we know of only one study that investigated this claim empirically. This question is important because overcoming the computational burden when using iterative simulation is a perennial challenge. If marginalisation of discrete parameters improves efficiency then it could be used more generally in models for which it is not strictly required. Marginalisation might then be viewed as one potential tool in the implementation of any data analysis. The posterior expectation of the marginalised discrete variable is often a quantity of interest in its own right, and many of the properties of the distribution of the marginalised parameter(s) can be identified and estimated from the sampled chains of values for the remaining model parameters.

We presented numerical results reflecting the impact of marginalisation on the computational efficiency for two- and three-component Gaussian mixture models and the Dawid–Skene model for categorical ratings. This investigation was robust to the extent that we explored two software implementations of Markov chain Monte Carlo techniques (JAGS and Stan) and directly compared marginalised and non-marginalised models while holding constant other aspects of the sampling procedure. Our results did not show that marginalisation on its own is sufficient to boost performance. Nevertheless, the most computationally efficient implementation of our models was usually Stan, which requires marginalisation.

One limitation of our study is that the models considered are either simple (normal mixtures) or of only
| Time per Min  | Effective Sample | Computation Time | Min Effective Sample | Rhat value |
|--------------|------------------|-----------------|----------------------|------------|
| 0.0          | 20               | 0.0             | 0.0                  | 1.02       |
| 0.5          | 40               | 0.5             | 0.5                  | 1.05       |
| 1.0          | 60               | 1.0             | 1.0                  | 1.08       |
| 1.5          | 80               | 1.5             | 1.5                  | 1.11       |

Figure 5: Time per minimum effective sample, computation time, minimum effective sample and $\hat{R}$ when performing Bayesian analysis on Dawid-Skene models for categorical ratings. Each box in the boxplot represents 5 results. The horizontal line in the $\hat{R}$ plots is the 1.1 threshold.
mid-level complexity (Dawid–Skene). The models are much more analytically tractable and therefore better understood than the Cormack–Jolly–Seber (CJS) model. This may be why an investigation of the CJS model showed that code for marginalised models was anywhere from five to more than 1,000 times faster than representations of the model that retained the discrete parameters while maintaining essentially identical inferences (Yackulic et al., 2020). The authors noted that “understanding how marginalisation works shrinks the divide between Bayesian and maximum likelihood approaches to population models [and] allows users to minimise the speed that is sacrificed when switching from a maximum likelihood approach”. That is, a wider appreciation of the benefits of marginalisation has the potential to promote the use of Bayesian statistical methods.

Another specific feature of the two- and three-component Gaussian mixture models is that we used only informal experiments to conclude that using $10^2$ as the variance of the prior distribution for the $\mu$’s would boost convergence performance. A more thorough investigation could and should be done to choose a value for the variance that provides the greatest improvement in convergence. We agree with Yackulic et al. (2020) that “widespread application of marginalisation in Bayesian population models will facilitate more thorough simulation studies, comparisons of alternative model structures, and faster learning”.

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