IID Sampling from Posterior Dirichlet Process Mixtures

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Abstract

The influence of Dirichlet process mixture is ubiquitous in the Bayesian nonparametrics literature. But sampling from its posterior distribution remains a challenge, despite the advent of various Markov chain Monte Carlo methods. The primary challenge is the infinite-dimensional setup, and even if the infinite-dimensional random measure is integrated out, high-dimensionality and discreteness still remain difficult issues to deal with.

In this article, exploiting the key ideas proposed in Bhattacharya (2021b), we propose a novel methodology for drawing \( \text{iid} \) realizations from posteriors of Dirichlet process mixtures. We focus in particular on the more general and flexible model of Bhattacharya (2008), so that the methods developed here are simply applicable to the traditional Dirichlet process mixture.

We illustrate our ideas on the well-known enzyme, acidity and the galaxy datasets, which are usually considered benchmark datasets for mixture applications. Generating 10,000 \( \text{iid} \) realizations from the Dirichlet process mixture posterior of Bhattacharya (2008) given these datasets took 19 minutes, 8 minutes and 5 minutes, respectively, in our parallel implementation.

Keywords: Dirichlet process mixture; Ellipsoid; Minorization; Parallel computing; Perfect sampling; Residual distribution.

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1 Introduction

The Bayesian nonparametric literature is heavily dominated by Dirichlet process (DP) mixtures, which go back to Antoniak (1974) and Ferguson (1983). The basic premise is given by the following setup: for observed data \( y_i : i = 1, \ldots, n \), the conditional distribution of \( y_i \) given parameters \( \theta_i \) is \( [y_i|\theta_i] \sim f(\cdot | \theta_i) \), where \( f(\cdot | \theta) \) is a parametric distribution with parameters \( \theta \), and \( \theta_i \sim G \) independently, where \( G \) is a random distribution on which some appropriate prior must be assigned. The DP mixture model considers the following prior for \( G \): \( G \sim DP(\alpha G_0) \), the Dirichlet process prior introduced in Ferguson (1973); here \( \alpha > 0 \) is a scale parameter and \( G_0 \) is the base (expected) distribution of \( G \). Thus, conditionally on \( G \), the distribution of \( y_i \) is a mixture of \( f(\cdot | \theta) \) over the distribution \( G \) of \( \theta \). Usually a prior is placed on the scale parameter \( \alpha \).

Although DP mixtures have already seen applications in almost all areas of statistics, its journey began with the recognition of its versatility with respect to clustering, nonparametric regression and nonparametric density estimation. Of course, the beginning of the computer era in the 1990s played a very significant role in the development of the computational aspects of posterior DP mixtures. Escobar (1994), Escobar and West (1995), West et al. (1994), MacEachern (1994), Müller et al. (1996), MacEachern and Müller (1998), etc. seem to recognize the practical and computational aspects of such models and developed various Gibbs sampling algorithms based on a Pólya urn scheme obtained after integrating out the infinite-dimensional random measure \( G \). Neal (2000) provided a comprehensive overview of the various Markov chain Monte Carlo (MCMC) algorithms used for sampling from posterior DP mixtures, and also provided algorithms for non-conjugate setups, that is, when \( f(\cdot | \theta) \) and \( G_0(\theta) \) are non-conjugate. Green and Richardson (2001), Jain and Neal (2004) and Jain and Neal (2007) propose split-merge moves embedded in reversible jump (Green (1995), Richardson and Green (1997)) and Metropolis-Hastings procedures to implement DP mixtures, in conjugate and non-conjugate setups.

Ishwaran and James (2001) (see also Ishwaran and James (2000)) proposed a block Gibbs sampling algorithm when \( G \) is retained in the model; their key idea is to truncate \( G \) to a finite-dimensional random measure such that the latter is almost indistinguishable from the original random measure. On the other hand, Papaspiliopoulos and Roberts (2008) proposed a retrospective MCMC method which does not require truncation of \( G \); an alternative method based on slice sampling is proposed by Walker (2007).

All the existing MCMC sampling methods for DP mixtures have their advantages and disadvantages with respect to mixing and implementation time, and it is difficult to single out any MCMC method that is guaranteed to outperform the others in all situations. The ideal scenario, although it might seem “too ambitious” to the statistical and probabilistic community, is to devise an \( iid \) sampling procedure. Indeed, our objective in this article is to propose a novel methodology for generating \( iid \) realizations from the posterior of DP mixtures. We specifically focus on the much more flexible and efficient model proposed by Bhattacharya (2008), which includes the traditional DP mixture as a special case. Hence, although we develop the \( iid \) sampling method with respect to Bhattacharya (2008), it is simply applicable to the traditional DP mixture. Our idea is to first truncate \( G \) to render it finite-dimensional, but such that the truncated version is practically indistinguishable from the original one. Indeed, we obtain an upper bound for the \( L_1 \)-distance between the predictive distributions of the original and truncated versions which is very significantly smaller than the bound obtained by Ishwaran and James (2001).
for the traditional DP mixture. Such a bound ensures that the posterior realizations under the original random measure and the truncated one, are identical in practice. The key to our highly efficient upper bound is the bounded number of components of the mixture model for the observations, which are mixed with respect to the DP.

Once such truncation is established, we invoke the general iid sampling strategy on finite-dimensional Euclidean spaces proposed by Bhattacharya (2021b). In a nutshell, the idea is to create an infinite sequence of closed, concentric ellipsoids, representing the target distribution as an infinite mixture on the ellipsoids and the annuli (regions between successive concentric ellipsoids), drawing a mixture component with the appropriate probability and finally simulating perfectly from the mixture component using a novel strategy. In our DP context, although the parameters associated with the truncated random measure can be represented in a finite-dimensional Euclidean space, the parameters of the mixture distribution of the observations coincide with each other with positive probabilities, and hence the method of Bhattacharya (2021b) can not be directly applied here. We thus extend his procedure by including the truncated random measure in the proposal associated with perfect sampling strategy, so that once its parameters are simulated aided by a suitable diffeomorphic transformation for efficiency, the rest of the parameters are simply drawn from the truncated measure, in a way that the entire procedure of iid sampling remains “perfect”.

We apply our iid sampling method to three well-known datasets, namely, the enzyme, acidity and galaxy data, which are are usually considered to be benchmarks for mixture applications. Generation of 10,000 iid realizations from the posterior of Bhattacharya (2008) for these datasets took 19 minutes, 8 minutes and 5 minutes, respectively, with parallel implementation on 80 cores. The resultant Bayesian inferences turned out to be very encouraging.

The rest of our article is organized as follows. In Section 2 we begin with a brief description of the DP mixture model of Bhattacharya (2008). The iid sampling idea for such DP mixture is detailed in Section 3. In Section 4 we provide details on the application of our iid sampling procedure to the three benchmark datasets. We summarize our ideas and make concluding remarks in Section 5.
2 The DP mixture with bounded number of components for the observational mixture model

2.1 Model description

Letting $y = (y_1, \ldots, y_n)$ denote the data of size $n$, a slightly extended version of the DP mixture model of Bhattacharya (2008) is as follows:

\[
[y|\xi, \pi] \overset{iid}{\sim} \sum_{j=1}^{M} \pi_j f(\cdot|\xi_j); \tag{1}
\]

\[
[\xi_1, \ldots, \xi_M|G] \overset{iid}{\sim} G; \tag{2}
\]

\[
G \sim DP(\alpha G_0); \tag{3}
\]

\[
\pi_j = \frac{\exp(\psi_j)}{\sum_{k=1}^{M} \exp(\psi_k)}; \quad j = 1, \ldots, M; \tag{4}
\]

\[
\psi_j \overset{iid}{\sim} f_\psi, \tag{5}
\]

where $\xi = (\xi_1, \ldots, \xi_M)$, $\pi = (\pi_1, \ldots, \pi_M)$ and $f_\psi$ denotes any appropriate prior distribution for the $\psi_j$.

Note that (1) shows that the model for the individual observations is a mixture with a maximum of $M$ components. Also observe that under the above model, given $G$, for any value of $M$, the prior predictive distribution is given by

\[
f_G(y) = \sum_{i=1}^{M} \pi_i \int f(y|\xi_i) \prod_{j=1}^{M} dG(\xi_j)
\]

\[
= \sum_{i=1}^{M} \pi_i \int f(y|\xi_i) dG(\xi_i)
\]

\[
= \int f(y|\xi) dG(\xi),
\]

so that the marginal distribution of any data point given $G$ is the same as that of the traditional DP mixture. However, given $G$, $y_1, \ldots, y_n$ are not independent, as their joint distribution conditional on $G$, shows below:

\[
[y|G, \pi] = \int \left\{ \prod_{i=1}^{n} \left[ \sum_{j=1}^{M} \pi_j f(y_i|\xi_j) \right] \right\} \prod_{j=1}^{M} dG(\xi_j).
\]

Thus, the DP mixture model of Bhattacharya (2008) is very significantly different from the traditional DP mixture, and is perhaps much more realistic in terms of the dependence structure. Further note that if $M = n$, $\pi_j = \frac{1}{M}$ for $j = 1, \ldots, M$ and for each $i$, $y_i$ is set to come from $f(\cdot|\xi_i)$, then the above model reduces to the traditional DP model. Thus, the traditional DP model is a special case of Bhattacharya (2008). Numerous theoretical, asymptotical, computational and application-wise advantages of DP mixture of Bhattacharya (2008) over the traditional DP mixture are noted in Bhattacharya (2008), Mukhopadhyay et al. (2011), Mukhopadhyay et al. (2012), Mukhopadhyay and Bhattacharya (2021).
2.2 Truncation of the infinite-dimensional random measure

It holds almost surely (see, for example, Sethuraman (1994)), that

\[ G = \sum_{i=1}^{\infty} w_i \delta_{\phi_i}, \]  

(6)

where \( w_1 = V_1 \) and for \( i = 2, 3, \ldots \), \( w_i = V_i \prod_{j<i} (1 - V_j) \), \( \phi_i \sim \text{G}_0 \) and \( V_i \sim \text{Beta}(1, \alpha) \).

As in Ishwaran and James (2001) (see also Ishwaran and James (2000)), we consider the following truncation of (6): \( w_1 = V_1 \) and \( w_i = V_i \prod_{j<i} (1 - V_j) \), for \( j = 2, \ldots, N \). We set \( V_N = 1 \) so that \( \sum_{i=1}^{N} w_i = 1 \). Let \( G_N \) denote the truncated probability measure corresponding to (6) with \( N \) summands. That is,

\[ G_N = \sum_{i=1}^{N} w_i \delta_{\phi_i}, \]  

(7)

Let \( \varphi_N = (\alpha, \psi_1, \ldots, \psi_M, \phi_1, \ldots, \phi_N, V_1, \ldots, V_{N-1}) \) and \( \varphi = (\alpha, \psi_1, \ldots, \psi_M, \phi_1, \phi_2, \ldots, V_1, V_2, \ldots) \).

Let \( \mathbf{z} = (z_1, \ldots, z_n) \) denote the allocation variables corresponding to \( \mathbf{y} \), that is, for \( i = 1, \ldots, n \), and \( j = 1, \ldots, M \), \( z_i = j \) indicates that \( [y_i | z_i = j, \xi] \sim f(\cdot | \xi_j) \). The probability of the event \( z_i = j \) is given by \( [z_i = j] = \pi_j \). With these, consider the marginal distribution of \( \mathbf{y} \) corresponding to \( G_N \) as follows:

\[ m_N(\mathbf{y}) = \sum_{\mathbf{z}} [\mathbf{z}] \int \prod_{i=1}^{n} [y_i | z_i, \xi] d\xi [\varphi_N] [\varphi_N] d\varphi_N \]

\[ = \sum_{\mathbf{z}} [\mathbf{z}] \int \prod_{i=1}^{n} [y_i | z_i, \xi] \pi_N(d\xi), \]  

(8)

where \( \pi_N(\xi) = \int [\xi | \varphi_N] [\varphi_N] d\varphi_N \) stands for the marginal distribution of \( \xi \) corresponding to \( G_N \). The marginal distribution of \( \mathbf{y} \) corresponding to \( G \) is given by

\[ m_\infty(\mathbf{y}) = \sum_{\mathbf{z}} [\mathbf{z}] \int \prod_{i=1}^{n} [y_i | z_i, \xi] d\xi [\varphi] [\varphi] d\varphi \]

\[ = \sum_{\mathbf{z}} [\mathbf{z}] \int \prod_{i=1}^{n} [y_i | z_i, \xi] \pi_\infty(d\xi), \]  

(9)

where \( \pi_\infty(\xi) = \int [\xi | \varphi] [\varphi] d\varphi \) stands for the marginal distribution of \( \xi \) corresponding to \( G \).

Theorem 1.

\[ \int |m_N(\mathbf{y}) - m_\infty(\mathbf{y})| d\mathbf{y} \leq 2 \left[ 1 - E \left( \left( \sum_{i=1}^{N-1} w_i \right)^M \right) \right] \approx 4M \exp(-(N-1)/\alpha). \]

Proof. Note that

\[ |m_N(\mathbf{y}) - m_\infty(\mathbf{y})| \leq \sum_{\mathbf{z}} [\mathbf{z}] \int \prod_{i=1}^{n} [y_i | z_i, \xi] \pi_N(d\xi) - \pi_\infty(d\xi), \]  

(10)
so that
\[ \int |m_N(y) - m_\infty(y)| dy \leq 2D(\pi_N, \pi_\infty), \] (11)
where \( D(\pi_N, \pi_\infty) \) is the total variation distance between the probability measures \( \pi_N \) and \( \pi_\infty \). The rest of the proof follows in the similar lines as that of Ishwaran and James (2000).

\[ \square \]

**Remark 2.** The crucial advantage of the upper bound of Theorem 1 is that the bound depends only upon \( M, N \) and \( \alpha \), and not upon \( n \), the sample size. Although \( n \) may be very large, \( M \) is usually chosen to be much smaller, and hence our upper bound is significantly smaller than the corresponding upper bound of Ishwaran and James (2001) in the traditional DP mixture context, given by \( 4n \exp \{-(N-1)/\alpha\} \).

To illustrate the differences between the two different upper bounds, note that with \( M = 30 \) and \( N = 50 \), for \( \alpha = 3 \) for instance, our upper bound is given by \( 9.676 \times 10^{-6} \), whereas for the traditional DP mixture model, for \( n = 245 \), the size of the enzyme dataset, the corresponding upper bound of Ishwaran and James (2001) is \( 4n \exp \{-(N-1)/\alpha\} = 7.902 \times 10^{-5} \). For the sizes \( n = 155 \) and \( n = 82 \) for the acidity and the galaxy datasets, the upper bound for the Bhattacharya (2008) model remains the same for the same \( M, N \) and \( \alpha \), but for the traditional DP mixture, the upper bounds are \( 4.999 \times 10^{-5} \) and \( 2.645 \times 10^{-5} \), respectively. Thus, the upper bound for our model is an order of magnitude smaller than for the traditional DP mixture.

### 2.3 Reparameterization

For our convenience, for \( i = 1, \ldots, N-1 \), let us reparameterize \( V_i \) as \( V_i = \frac{\exp(\xi_i)}{1 + \exp(\xi_i)} \) and \( \alpha \) as \( \alpha = \exp(\tilde{\alpha}) \). Let \( \theta = (\xi, \vartheta) \), where \( \vartheta = (\tilde{\alpha}, \psi_1, \ldots, \psi_M, \phi_1, \ldots, \phi_N, \zeta_1, \ldots, \zeta_N) \). Then the reparameterized version of the joint posterior, proportional to likelihood times prior becomes
\[ \pi(\theta|y) \propto \prod_{i=1}^{n} \left[ \sum_{j=1}^{M} \pi_j f(y_i|x_j) \right] \times \prod_{j=1}^{M} [\psi_j] \times \prod_{j=1}^{M} G_N(\xi_j) \times \prod_{i=1}^{N} [\phi_i] \times \prod_{i=1}^{N} [\zeta_i] \times [\tilde{\alpha}]. \] (12)

We shall henceforth consider this reparameterized setup for our purpose.

### 3 The iid sampling idea

Note that our DP mixture posterior distribution can be represented as
\[ \pi(\theta|y) = \sum_{i=1}^{\infty} \pi(B_i \times A_i|y) \pi_i(\theta|y), \] (13)
where \( A_i \) are disjoint compact subsets of \( \mathbb{R}^d \) with \( d = 2N + M + 1 \) such that \( \bigcup_{i=1}^{\infty} B_i \times A_i = \mathbb{R}^{d+M} \). Here \( B_i \)'s correspond to \( \xi \) and \( A_i \)'s correspond to \( \vartheta \). In (13),
\[ \pi_i(\theta|y) = \frac{\pi(\theta|y)}{\pi(B_i \times A_i|y)} I_{B_i \times A_i}(\theta), \] (14)
is the distribution of \( \theta \) restricted on \( B_i \times A_i; I_{B_i \times A_i} \) being the indicator function of \( B_i \times A_i \). Also, \( \pi(B_i \times A_i|y) = \int_{B_i \times A_i} \pi(d\theta|y) \geq 0 \). Clearly, \( \sum_{i=1}^{\infty} \pi(B_i \times A_i|y) = 1. \)
The key idea of generating iid realizations from \( \pi(\theta | y) \) is to randomly select \( \pi_i(\cdot | y) \) with probability \( \pi_i(B_i \times A_i | y) \) and then to perfectly simulate from \( \pi_i(\cdot | y) \). Note that due to (7), \( \xi_i \)'s must take one of the \( \phi_i \) values. Hence, the choice of the sets \( A_i \) determine the sets \( B_i \). Hence, it is sufficient to adequately choose \( A_i \), the method of which we discuss next.

### 3.1 Choice of the sets \( A_i \) and estimation of \( \pi(B_i \times A_i | y) \)

For some appropriate \( d \)-dimensional vector \( \mu \) and \( d \times d \) positive definite scale matrix \( \Sigma \), we shall set \( A_i = \{ \vartheta : c_{i-1} \leq (\vartheta - \mu)^T \Sigma^{-1} (\vartheta - \mu) \leq c_i \} \) for \( i = 1, 2, \ldots, \), where \( 0 = c_0 < c_1 < c_2 < \cdots \). Note that \( A_i = \{ \vartheta : (\vartheta - \mu)^T \Sigma^{-1} (\vartheta - \mu) \leq c_i \} \), and for \( i \geq 2 \), \( A_i = \{ \vartheta : (\vartheta - \mu)^T \Sigma^{-1} (\vartheta - \mu) \leq c_i \} \setminus \bigcup_{j=1}^{i-1} A_j \).

To obtain reliable estimates of \( \mu \) and \( \Sigma \), well-mixing MCMC algorithms may be employed. However, although a Gibbs sampling algorithm is available for our DP mixture model, it is difficult to get it converged in practice. To elucidate, note that as \( \alpha \rightarrow \infty \), a simple application of the Borel-Cantelli lemma in conjunction with the Markov inequality shows that \( V_i \) converges to 0 almost surely for each \( i \). This entails that \( w_j \), for \( j = 1, \ldots, N - 1 \), converge to zero, almost surely. Hence, conditional on the rest of the unknowns, \( \xi_1 = \xi_2 = \cdots = \xi_M \). That is, when all the \( \xi_i \) are expected to be distinct, there is, in fact, only one common distinct value (or a small number of distinct values) for these parameters in the relevant Gibbs sampling strategy, when \( \alpha \) is large. Although theoretically the Gibbs sampler is still irreducible, in practice, reliability of the chain in highly compromised, at least in our experience.

We completely avoid the aforementioned problem by implementing transformation based Markov Chain Monte Carlo (TMCMC) of Dutta and Bhattacharya (2014) instead of the Gibbs sampler. In fact, additive TMCMC turned out to be adequate for all the examples that we considered. In our TMCMC algorithm we updated \( \vartheta \) using TMCMC and \( \xi \) by direct simulation from \( G_N \). We set \( \mu \) and \( \Sigma \) to be the mean and covariance of the TMCMC realizations of \( \vartheta \).

### 3.2 Estimation of \( \pi(B_i \times A_i | y) \)

Recall that the key idea of iid sampling from \( \pi(\theta | y) \) is to randomly select \( \pi_i(\cdot | y) \) with probability \( \pi(B_i \times A_i | y) \) and then to exactly simulate from \( \pi_i(\cdot | y) \). However, the mixing probabilities \( \pi(B_i \times A_i | y) \) are not available to us. Note that the TMCMC realizations are not useful for estimating these probabilities, since there can be only a finite number of such realizations in practice, whereas the number of the mixing probabilities is infinite. In this regard, we extend the Monte Carlo based estimation idea of Bhattacharya (2021b) to suit our purpose, assuming for the while that an infinite number of parallel processors are available, and that the \( i \)-th processor is used to estimate \( \pi(B_i \times A_i | y) \) using Monte Carlo sampling up to a constant.

To elaborate, let \( \pi(\theta | y) = C \hat{\pi}(\theta | y) \), where \( \hat{\pi}(\theta | y) \) is the right hand side of (12) and \( C > 0 \) is the unknown normalizing constant. Then for any Borel set \( A \) in the Borel
where $p$ is the uniform probability measure corresponding to (17), and 

\[ \sigma \mathcal{P} \quad \theta \quad \mathcal{B} \quad \text{those probability for} \quad \pi \]

For further details regarding the usefulness of this proposal, see Bhattacharya (2021b).

3.3 Minorization for $\pi_i(\cdot | y)$

As in Bhattacharya (2021b), here we consider the following uniform independence proposal distribution on $A_i$ embedded in a Metropolis-Hastings framework for $\pi_i(\cdot | y)$ to update the entire block $\phi$:

\[ q_i(\phi) = \frac{1}{\mathcal{L}(A_i)} I_{A_i}(\phi). \]  

(17)

For further details regarding the usefulness of this proposal, see Bhattacharya (2021b).

For $\theta \in B_i \times A_i$, for any Borel set $\mathbb{B} \times \mathbb{A}$ in the Borel $\sigma$-field of $\mathbb{R}^r$, where $r = d + M$, let $P_i(\theta, \mathbb{B} \cap B_i \times \mathbb{A} \cap A_i)$ denote the corresponding Metropolis-Hastings transition probability for $\pi_i(\cdot | y)$. Note that this transition probability is strictly positive only for those $\mathbb{B}$ such that $\mathbb{B} \cap B_i$ corresponds to $\mathbb{A} \cap A_i$. Let $s_i = \inf_{\theta \in B_i \times A_i} \frac{\hat{\pi}(\theta | y)}{\prod_{j=1}^M G_N(\xi_j)}$ and

\[ S_i = \sup_{\theta \in B_i \times A_i} \frac{\hat{\pi}(\theta | y)}{\prod_{j=1}^M G_N(\xi_j)}; \]

Then, with (17) as the proposal density we have, for any $\theta \in B_i \times A_i$:

\[ P_i(\theta, \mathbb{B} \cap B_i \times \mathbb{A} \cap A_i) \geq \int_{\mathbb{B} \cap B_i \times \mathbb{A} \cap A_i} \min \left\{ 1, \frac{\hat{\pi}(\theta' | y)}{\hat{\pi}(\theta | y)} \times \frac{\prod_{j=1}^M G_N(\xi_j)}{\prod_{j=1}^M G_N(\xi'_j)} \right\} p_i(\theta') d\theta' \prod_{j=1}^M G_N(d\xi'_j) \]

\[ \geq \left( \frac{s_i}{S_i} \right) \times \frac{\mathcal{L}(\mathbb{A} \cap A_i)}{\mathcal{L}(A_i)} \times G_N(\xi' \in \mathbb{B} \cap B_i) \]

\[ = p_i Q_i(\theta' \in \mathbb{A} \cap A_i) \times G_N(\xi' \in \mathbb{B} \cap B_i) \],  

(18)

where $p_i = s_i / S_i$,

\[ Q_i(\theta' \in \mathbb{A} \cap A_i) = \frac{\mathcal{L}(\mathbb{A} \cap A_i)}{\mathcal{L}(A_i)} \]

is the uniform probability measure corresponding to (17), and

\[ G_N(\xi' \in \mathbb{B} \cap B_i) = \int_{\mathbb{B} \cap B_i} \prod_{j=1}^M G_N(d\xi'_j). \]
Since (18) holds for all \( \theta \in B_i \times A_i \), the entire set \( B_i \times A_i \) is a small set.

Let \( \hat{s}_i \) and \( \hat{S}_i \) denote the minimum and maximum of \( \frac{\hat{\pi}(\theta|x)}{\prod_{j=1}^M g_N(\xi_j)} \) over the Monte Carlo samples drawn uniformly from \( B_i \times A_i \) in course of estimating \( \hat{\pi}(B_i \times A_i | y) \). Then \( \frac{\hat{s}_i}{\hat{S}_i} \leq \frac{s_i}{S_i} \). Hence, there exists \( \eta_i > 0 \) such that \( 1 \geq \frac{\hat{s}_i}{\hat{S}_i} \geq \frac{s_i}{S_i} - \eta_i > 0 \). Let \( \tilde{p}_i = \frac{\hat{s}_i}{\hat{S}_i} - \eta_i \). Then it follows from (18) that

\[
P_i(\theta, B \cap B_i \times A \cap A_i) \geq \tilde{p}_i \; Q_i(\theta' \in A \cap A_i) \times G_N(\xi' \in B \cap B_i),
\]

which we shall consider for our purpose. Recall that in practice, \( \eta_i \) is expected to be very close to zero, since the Monte Carlo sample size would be sufficiently large. Thus, \( \tilde{p}_i \) is expected to be very close to \( p_i \).

### 3.4 Split chain

Due to the minorization (19), the following decomposition holds for all \( \theta \in B_i \times A_i \):

\[
P_i(\theta, B \cap B_i \times A \cap A_i) = \tilde{p}_i \; Q_i(\theta' \in A \cap A_i) \times G_N(\xi' \in B \cap B_i) + (1 - \tilde{p}_i) \; R_i(\theta, B \cap B_i \times A \cap A_i),
\]

where

\[
R_i(\theta, B \cap B_i \times A \cap A_i) = \frac{P_i(\theta, B \cap B_i \times A \cap A_i) - \tilde{p}_i \; Q_i(\theta' \in A \cap A_i) \times G_N(\xi' \in B \cap B_i)}{1 - \tilde{p}_i}
\]

(20)

is the residual distribution.

Therefore, to implement the Markov chain \( P_i(\theta, B \cap B_i \times A \cap A_i) \), rather than proceeding directly with the uniform proposal based Metropolis-Hastings algorithm, we can use the split (20) to generate realizations from \( P_i(\theta, B \cap B_i \times A \cap A_i) \). That is, given \( \theta \), we can simulate from \( Q_i \times G_N \) with probability \( \tilde{p}_i \), and with the remaining probability, can generate from \( R_i(\theta, \cdot) \).

To simulate from the residual density \( R_i(\theta, \cdot) \) we devise the following rejection sampling scheme. Let \( \tilde{R}_i(\theta, \theta') \) and \( \tilde{P}_i(\theta, \theta') \) denote the densities of \( \theta' \) corresponding to \( R_i(\theta, \cdot) \) and \( P_i(\theta, \cdot) \), respectively. Then it follows from (20) and (21) that for all \( \theta \in B_i \times A_i \),

\[
\tilde{R}_i(\theta, \theta') = \frac{\tilde{P}_i(\theta, \theta') - \tilde{p}_i \; q_i(\theta') \prod_{j=1}^M g_N(\xi_j)}{1 - \tilde{p}_i} \leq \frac{\tilde{P}_i(\theta, \theta')}{1 - \tilde{p}_i}
\]

(21)

\[
\Leftrightarrow \frac{\tilde{R}_i(\theta, \theta')}{\tilde{P}_i(\theta, \theta')} \leq \frac{1}{1 - \tilde{p}_i}, \text{ for all } \theta' \in B_i \times A_i.
\]

Hence, given \( \theta \) we can continue to simulate \( \theta' \sim \tilde{P}_i(\theta, \cdot) \) using the uniform proposal distribution (17) and generate \( U \sim U(0, 1) \) until

\[
U < \frac{(1 - \tilde{p}_i) \tilde{R}_i(\theta, \theta')}{\tilde{P}_i(\theta, \theta')}
\]

(22)

is satisfied, at which point we accept \( \theta' \) as a realization from \( \tilde{R}_i(\theta, \cdot) \).
Now

\[
\hat{P}_i(\theta, \theta') = q_i(\theta') \prod_{j=1}^{M} G_N(\xi'_j) \times \min \left\{ 1, \frac{\hat{\pi}(\theta'|y)}{\pi(\theta'|y)} \times \frac{\prod_{j=1}^{M} G_N(\xi'_j)}{\prod_{j=1}^{M} G_N(\xi_j)} \right\} + r_i(\theta) I_0(\theta')
\]

\[= \frac{1}{\mathcal{L}(A_i)} \prod_{j=1}^{M} G_N(\xi'_j) \times \min \left\{ 1, \frac{\hat{\pi}(\theta'|y)}{\pi(\theta'|y)} \times \frac{\prod_{j=1}^{M} G_N(\xi'_j)}{\prod_{j=1}^{M} G_N(\xi_j)} \right\} + r_i(\theta) I_0(\theta'),
\]

where

\[
r_i(\theta) = 1 - \int_{B_i \times A_i} \min \left\{ 1, \frac{\hat{\pi}(\theta'|y)}{\pi(\theta'|y)} \times \frac{\prod_{j=1}^{M} G_N(\xi'_j)}{\prod_{j=1}^{M} G_N(\xi_j)} \right\} q_i(\theta') d\theta' \prod_{j=1}^{M} G_N(d\xi'_j)
\]

\[= 1 - \int_{B_i \times A_i} \min \left\{ 1, \frac{\hat{\pi}(\theta'|y)}{\pi(\theta'|y)} \times \frac{\prod_{j=1}^{M} G_N(\xi'_j)}{\prod_{j=1}^{M} G_N(\xi_j)} \right\} \frac{1}{\mathcal{L}(A_i)} d\theta' \prod_{j=1}^{M} G_N(d\xi'_j). \tag{23}
\]

Let \(\hat{r}_i(\theta)\) denote the Monte Carlo estimate of \(r_i(\theta)\) obtained by simulating \(\theta'\) from the uniform distribution on \(A_i, \xi'_j\) from \(\prod_{j=1}^{M} G_N(\xi'_j)\) given \(\theta'\) and finally taking the average of \(\min \left\{ 1, \frac{\hat{\pi}(\theta'|y)}{\pi(\theta'|y)} \times \frac{\prod_{j=1}^{M} G_N(\xi'_j)}{\prod_{j=1}^{M} G_N(\xi_j)} \right\}\) in (23). In our implementation, we shall consider the following:

\[
\hat{P}_i(\theta, \theta') = \frac{1}{\mathcal{L}(A_i)} \prod_{j=1}^{M} G_N(\xi'_j) \times \min \left\{ 1, \frac{\hat{\pi}(\theta'|y)}{\pi(\theta'|y)} \times \frac{\prod_{j=1}^{M} G_N(\xi'_j)}{\prod_{j=1}^{M} G_N(\xi_j)} \right\} + \hat{r}_i(\theta) I_0(\theta'),
\]

\[\hat{R}_i(\theta, \theta') = \frac{\hat{P}_i(\theta, \theta') - \hat{p}_i q_i(\theta') \prod_{j=1}^{M} G_N(\xi'_j)}{1 - \hat{p}_i}.
\]

In all practical implementations, for sufficiently large Monte Carlo sample size, (22) holds if and only if

\[U < \frac{(1 - \hat{p}_i) \hat{R}_i(\theta, \theta')}{\hat{P}_i(\theta, \theta')} \tag{24}\]

holds; see Bhattacharya (2021b) for details. Consequently, as in Bhattacharya (2021b), we shall carry out our implementations with (24).

### 3.5 Perfect sampling from \(\pi_i(\cdot|y)\)

From (20) it follows that (see Bhattacharya (2021b)) at any given positive time \(T_i = t, \theta'\) will be drawn from \(Q_i \times G_N\) with probability \(\hat{p}_i\). Hence, the distribution of \(T_i\) is geometric, having the form

\[P(T_i = t) = \hat{p}_i(1 - \hat{p}_i)^{t-1}; \quad t = 1, 2, \ldots \tag{25}\]

Due to (25), first \(T_i\) can be drawn from the geometric distribution and then one may simulate \(\theta^{i-T_i} \sim Q_i \times G_N\). Subsequently, the chain only needs to be carried forward in time till \(t = 0\), using \(\theta^{i+1} = g_i(\theta^i, U_i^{(t+1)})\), where \(g_i(\theta^i, U_i^{(t+1)})\) is the deterministic function corresponding to the simulation of \(\theta^{i+1}\) from \(\hat{R}_i(\theta^i, \cdot)\). Here \(\{U_i^{(t)}, t = 0, -1, -2, \ldots\}\) is an appropriate sequence of random numbers assumed to be
available before beginning the perfect sampling implementation. The realization $\theta^{(0)}$ obtained at time $t = 0$ is a perfect draw from $\pi_i$.

In practice, storing the uniform random numbers $\{U_i^t; t = 0, -1, -2, \ldots\}$ or explicitly considering the deterministic relationship $\theta^{(t+1)} = \varrho_i(\theta^{(t)}, U_i^t)$, are not required. These would be required only if we had taken the search approach, namely, iteratively starting the Markov chain at all initial values at negative times and carrying the sample paths to zero.

The complete algorithm for $iid$ sample generation from $\pi(\cdot|y)$ is of the same form as Algorithm 1 of Bhattacharya (2021b), and hence we do not provide the explicit algorithm here.

### 3.6 Diffeomorphism

It is obvious that small values of $\hat{p}_i$ would lead to large values of $T_i$, which would make the perfect sampling algorithm inefficient. To solve this problem, Bhattacharya (2021b) proposed inversion of a diffeomorphism proposed in Johnson and Geyer (2012) to flatten the posterior distribution in a way that its infimum and the supremum are reasonably close (so that $\hat{p}_i$ are adequately large) on all the relevant ellipsoids and annuli.

The issue of small values of $\hat{p}_i$ persists even the current DP mixture context, and hence the diffeomorphism fix is again of great value. Here it is of interest to render the posterior $\pi(\xi, \vartheta|y)$ thick-tailed using the inverse of the diffeomorphic transformation of Johnson and Geyer (2012). Note, however, that since $\xi$ depends directly on $\vartheta$ through $G_N$, it is sufficient to consider the inverse diffeomorphic transformation for $\vartheta$ only.

Thus, setting $\gamma = h^{-1}(\vartheta)$, where $h$ is a diffeomorphism, the density of $(\xi, \gamma)$ is given by

$$\pi_{\xi, \gamma}(\xi, \gamma|y) = \pi(\xi, h^{-1}(\gamma)|y) |\det \nabla h(\gamma)|^{-1}$$

where $\nabla h(\gamma)$ denotes the gradient of $h$ at $\gamma$ and $\det \nabla h(\gamma)$ stands for the determinant of the gradient of $h$ at $\gamma$. The details of the transformation are provided below.

As in Bhattacharya (2021b), here we consider the following isotropic function $h : \mathbb{R}^d \mapsto \mathbb{R}^d$ of Johnson and Geyer (2012):

$$h(\gamma) = \begin{cases} f(\|\gamma\|) \frac{2}{b\|\gamma\|}, & \gamma \neq 0 \\ 0, & \gamma = 0, \end{cases}$$

for some function $f : (0, \infty) \mapsto (0, \infty)$, $\|\cdot\|$ being the Euclidean norm. Johnson and Geyer (2012) consider isotropic diffeomorphisms, that is, functions of the form $h$ where both $h$ and $h^{-1}$ are continuously differentiable, with the further property that $\det \nabla h$ and $\det \nabla h^{-1}$ are also continuously differentiable. Specifically, they define $f : [0, \infty) \mapsto [0, \infty)$ given by

$$f(x) = \begin{cases} e^{bx} - e^{\frac{b}{2}}, & x > \frac{1}{b} \\ x^3 + x^2, & x \leq \frac{1}{b}, \end{cases}$$

where $b > 0$.

We apply the same transformation to the uniform proposal density (17), so that the new proposal density becomes

$$q_i(\gamma) = \frac{1}{L(A_i)} I_{A_i}(h^{-1}(\gamma)) |\det \nabla h(\gamma)|^{-1}.$$
Now, for any set \( A \), let \( h_{\omega}(A) = \{ h(\vartheta) : \vartheta \in A \} \) and for any set \( B \), let \( h_{\xi}(B) = \{ h(\xi) : \xi \in B \} \). Also, let 
\[ s_i = \inf_{\xi \in h(B_i), \gamma \in h(A_i)} \frac{\tilde{\pi}_{e,\gamma}(\xi, \gamma | y)}{\pi(\gamma) \prod_{j=1}^N G_N(\xi_j)} \quad \text{and} \quad S_i = \sup_{\xi \in h(B_i), \gamma \in h(A_i)} \frac{\tilde{\pi}_{e,\gamma}(\xi, \gamma | y)}{\pi(\gamma) \prod_{j=1}^N G_N(\xi_j)}, \]
where \( \tilde{\pi}_{e,\gamma}(\xi, \gamma | y) \) is the same as (26) but without the normalizing constant. Then, with (29) as the proposal density, we have
\[
P_i((\xi, \gamma), h_{\xi}(B \cap B_i) \times h_{\vartheta}(A \cap A_i)) 
\geq \int_{h_{\xi}(B \cap B_i) \times h_{\vartheta}(A \cap A_i)} \min \left\{ 1, \frac{\tilde{\pi}_{e,\gamma}(\xi', \gamma | y)}{\tilde{\pi}_{e,\gamma}(\xi, \gamma | y)} \times \frac{q_i(\vartheta)}{q_i(\vartheta')} \times \prod_{j=1}^N \frac{G_N(\xi_j)}{G_N(\xi'_j)} \right\} q_i(\gamma') d\gamma' \prod_{j=1}^M G_N(d\xi'_j),
\]
where \( p_i = s_i / S_i \), \( Q_i \) is the probability measure corresponding to (29) and \( G_N \) is given by
\[
G_N(\xi' \in h_{\xi}(B \cap B_i)) = \int_{h_{\xi}(B \cap B_i)} \prod_{j=1}^M G_N(d\xi'_j).
\]
With \( \hat{p}_i = \hat{s}_i / \hat{S}_i - \eta_i \), where \( \hat{s}_i \) and \( \hat{S}_i \) are Monte Carlo estimates of \( s_i \) and \( S_i \) and \( \eta_i > 0 \) is adequately small, the rest of the details remain the same as before with necessary modifications pertaining to the new proposal density (29) and the new Metropolis-Hastings acceptance ratio with respect to (29) incorporated in the subsequent steps. Once \( \gamma \) is generated from (26) we transform it back to \( \vartheta \) using \( \vartheta = h^{-1}(\gamma) \) and accordingly reset the values of \( \xi \).

4 Applications

We now illustrate our iid sampling idea on posterior DP mixture of normal mixture models with unknown but bounded number of components with application to the well-studied enzyme, acidity and the galaxy data sets. Richardson and Green (1997) and Das and Bhattacharya (2019) modeled these data sets using parametric normal mixtures and applied reversible jump Markov chain Monte Carlo and transdimensional transformation based Markov chain Monte Carlo, respectively, for Bayesian inference.

On the other hand, Bhattacharya (2008) modeled these data using the DP mixture of the form given in Section 2 with an \( M \)-component mixture of normal densities. In other words, \( f(\cdot | \xi_j) \) is taken as the density of \( N(\nu_j, \sigma_j^2) \), the normal distribution with mean \( \nu_j \) and variance \( \sigma_j^2 \), the latter primarily parameterized by \( \lambda_j = \sigma_j^{-2} \). Further, he set \( \pi_j = 1/M \), for \( j = 1, \ldots, M \); this choice may be advantageous in real data setups, as aptly demonstrated in Majumdar et al. (2013). Integrating out \( G \), Bhattacharya (2008) arrived at a Pólya-urn scheme, which he used to construct a Gibbs sampler for Bayesian inference.

For our illustration, we consider the same model and priors as Bhattacharya (2008) but implement the iid sampling method for the three aforementioned datasets. It is to be noted that the Pólya-urn based Gibbs sampling procedure will not serve our purpose of estimating \( \mu \) and \( \Sigma \) needed for \( A_i \), as the random measure \( G \) is integrated out. Indeed, recall from Section 3.1 that \( A_i \) are based upon \( \vartheta \), which includes parameters associated with \( G \). In the same section we argued that Gibbs sampling including \( G_N \) is laden with difficulties, and that such difficulties can be completely bypassed using TMCMC, which we employ and generally recommend for estimating \( \mu \) and \( \Sigma \).
All our \textit{iid} simulations are based on the diffeomorphic transformation detailed in Section 3.6, since without this substantially large values of $\hat{p}_i$ could not be ensured.

All our codes are written in C using the Message Passing Interface (MPI) protocol for parallel processing. We implemented our codes on a 80-core VMWare provided by Indian Statistical Institute. The machine has 2 TB memory and each core has about 2.8 GHz CPU speed.

Below we provide details on \textit{iid} sampling for the three datasets, along with comparisons with TMCMC.

4.1 Enzyme data

This dataset concerns the distribution of enzymatic activity in the blood, for an enzyme involved in the metabolism of carcinogenic substances, among a group of $n = 245$ unrelated individuals. We model this data using normal mixture of a maximum of $M = 30$ components, where the parameters are assumed to arise from $G_N$, with $N = 50$. The choice of $M$ is the same as in Bhattacharya (2008), Das and Bhattacharya (2019), Mukhopadhyay and Bhattacharya (2012), Richardson and Green (1997), while that of $N$ is based upon Remark 2.

As in Bhattacharya (2008), we assume that under $G_0$, $\tau_j \sim G(s/2, S/2)$ and given $\tau_j$, $\nu_j \sim N(\nu_0, \frac{c}{\tau_j})$, where for $a > 0$, $b > 0$, $G(a,b)$ stands for the gamma distribution with mean $a/b$ and variance $a/b^2$, and $c > 0$ is an appropriate constant. In this example, following Bhattacharya (2008) we set $s = 4$, $S = 2 \times (0.2/1.22) = 0.328$, $\nu_0 = 1.45$, $c = 33.3$ For the prior of $\alpha$ we considered $G(a_\alpha,b_\alpha)$ with $a_\alpha = 2$ and $b_\alpha = 4$, as in Bhattacharya (2008).

To estimate $\mu$ and $\Sigma$ for $A_i$, we implemented additive TMCMC with scaling constants in the additive transformation for $\vartheta$ set to $\sqrt{0.5}$, while $\xi$ are simulated from $\prod_{j=1}^M G_N$, given $\vartheta$. We discarded the first $10^6$ iterations as burn-in and stored one in $10^6$ iterations in the next $10^6$ iterations, to yield $10,000$ realizations for our purpose. This exercise took 25 minutes on a single core.

To complete specification of $A_i$, we set $\sqrt{c_1} = 8.0$ and $\sqrt{c_i} = \sqrt{c_1} + 0.0005 \times (i - 1)$, for $i = 1, \ldots, 10^4$. These choices ensured adequate coverage of the parameter space of $\vartheta$ and significantly large values of $\hat{p}_i$ as we chose the diffeomorphism parameter $b = 0.01$. We sampled 5000 Monte Carlo realizations uniformly from $A_i$ to reliably estimate the corresponding probabilities and to compute $\hat{s}_i$ and $\hat{S}_i$; we set $\eta_i = 10^{-10}$. In the Monte Carlo context, we replaced the computationally inefficient rejection sampling method of uniformly sampling from $A_i$ with the efficient algorithm proposed in Bhattacharya (2021b), completely bypassing rejection sampling.

With these, we simulated 10,000 \textit{iid} realizations from the posterior $\pi(\xi, \vartheta | y)$ on 80 cores, which took 19 minutes. Using these \textit{iid} realizations we obtained the key results presented diagrammatically in Figure 1. Panel (a) of Figure 1 compares the posterior predictive densities obtained using TMCMC and \textit{iid} sampling, showing that they are almost identical and well-capture the details of the histogram of the observed data. Panel (b) compares 20 times pointwise posterior predictive variances associated with panel (a) computed using TMCMC and \textit{iid} realizations. Although \textit{iid}-based variances are expected to be non-negligibly larger than those based on TMCMC, here they are only slightly larger than those of TMCMC, in spite of scaling up by 20. The reason for such close agreement between \textit{iid} and TMCMC realizations is excellent mixing of the TMCMC
chain, as summarized by the typical autocorrelation plots of $\nu_{30}$ and $\tau_{30}$, provided in panels (c) and (d), respectively.

Letting $K$ denote the number of mixture components, with respect to iid sampling, the sample-based posterior probabilities of $K = 2, 3, 4, 5, 6$ are 0.2758, 0.4462, 0.2280, 0.0461, 0.0039, respectively and zero for the other values of $K$. On the other hand, the TMCMC based posterior probabilities of the same values of $K$ are 0.2743, 0.4468, 0.2313, 0.0443, 0.0033 and zero for the other values of $K$. Thus, a strong agreement is exhibited between iid sampling and TMCMC even with respect to the posterior of $K$.

4.2 Acidity data

The acidity data set is on an acidity index measured in a sample of $n = 155$ lakes in north-central Wisconsin. With the same model and prior structure as for the enzyme data, here we set $s = 4, S = 2 \times (0.2/0.573) = 0.698, \nu_0 = 5.02, c = 33.3, a_\alpha = 2, b_\alpha=4, M = 30$ and $N = 50$.

The TMCMC details remain essentially the same as in the enzyme case. Only here we discarded the first $1.5 \times 10^6$ iterations as burn-in and stored one in $150$ iterations in the next $1.5 \times 10^6$ iterations, to yield $10,000$ realizations. The scaling constants for additive transformation for $\theta$ here are $\sqrt{0.05}$. This exercise took 28 minutes on a single core.

The iid sampling details are also essentially the same as in the enzyme data; only here we set $\sqrt{c_1} = 7.0$ and $\sqrt{c_i} = \sqrt{c_1} + 0.0005 \times (i - 1)$, for $i = 1, \ldots, 10^4$. On 80 cores, the time taken is only 8 minutes to generate $10,000$ iid realizations.

Figure 2 presents the results of iid sampling for the acidity data, along with comparison with TMCMC. Panel (a) shows close agreement between iid and TMCMC sampling, but not as close as for enzyme. Indeed, panel (b) shows that the TMCMC based pointwise posterior predictive variances, multiplied by 38, are uniformly non-negligibly smaller than those based on iid realizations. The reason for this difference can be attributed to the TMCMC autocorrelations. Although the location parameters have negligible autocorrelations, exemplified by $\nu_{30}$, shown in panel (c), the scale parameters $\tau$ do not have negligible autocorrelations for many lags, as shown in panel (d) for $\tau_{30}$ as an instance.

Here the number of components $K = 2, 3, 4, 5$ has the empirical posterior probabilities 0.7810, 0.2111, 0.0078, 0.0001 and zero for other values of $K$ with respect to iid sampling and 0.7289, 0.2590, 0.0121, 0.0000 and zero for other values of $K$ with respect to TMCMC, which are not in disagreement.

4.3 Galaxy data

The galaxy data consists of the velocities of $n = 82$ distant galaxies, diverging from our own galaxy. With the same model and prior structure as before, here we set $s = 4, S = 2, \nu_0 = 20, c = 33.3, a_\alpha = 2, b_\alpha=4, M = 30$ and $N = 50$.

The TMCMC details here are the same as in the acidity case, except that here we set the scaling constants for additive transformation of $\theta$ to be 1. The time taken is 21 minutes on a single core for this TMCMC algorithm for the galaxy data.

The iid sampling details are essentially the same as the previous two examples, except that here $\sqrt{c_1} = 9.0$ and $\sqrt{c_i} = \sqrt{c_1} + 0.0005 \times (i - 1)$, for $i = 1, \ldots, 10^4$ and the diffeomorphism parameter is $b = 0.001$. The time taken for generating $10,000$ iid realizations is only 5 minutes on our 80 cores.
Figure 1: IID and TMCMC sampling for the enzyme data.
Figure 2: IID and TMCMC sampling for the acidity data.
Figure 3 presents the results of iid sampling and TMCMC for the galaxy data. Here again panel (a) shows close agreement between iid and TMCMC sampling; the only slight disagreement being at the left-most mode. Panel (b) shows that the TMCMC based pointwise posterior predictive variances, again multiplied by 38, are non-negligibly smaller than those based on iid realizations, except at a few points in the left-most modal region. The reason for this difference can be attributed to the TMCMC autocorrelations. Although both location and scale parameters seem to have small autocorrelations, shown in panels (c) and (d), these are of course somewhat high in comparison with the iid case where no autocorrelation is present, and have hence contributed to the slight disagreement in panel (a).

The posterior probabilities of the number of components $K = 1, 2, 3, 4, 5$ are 0.0265, 0.2725, 0.4994, 0.1965, 0.0051 and zero for other values of $K$ with respect to the iid sampling procedure and those with respect to TMCMC are 0.0229, 0.2517, 0.5185, 0.2045, 0.0024 and zero for other values of $K$. That is, with respect to the number of components as well, the posterior probabilities are in agreement.

Now, we anticipate that there may arise the question that if smooth density estimators as shown in panel (a) of Figure 3 reflect a model that fails to capture the minor details of the histogram. Our response would be that the purpose of model-based analysis is to smooth the histogram, and capturing minor details may be artifacts of the method employed to implement the model. To demonstrate, we implement our additive TM-CMC algorithm once again for the galaxy data, but now with the scaling constants set to $\sqrt{0.006}$. The corresponding TMCMC based density estimate, pointwise posterior predictive variances with respect to TMCMC and the autocorrelation plots are provided in Figure 4. Panel (a) shows that the posterior predictive density based on the TMCMC realizations captures all the minor details of the histogram, and panel (b) shows that the pointwise posterior predictive variances based on this TMCMC algorithm are much larger compared to panel (b) of Figure 3. Although the location parameters do not exhibit substantial autocorrelations, as exemplified by panel (c), the scale parameters have high autocorrelations which refuse to die down even at lag 40.

Such high autocorrelations are, in fact, responsible for the high pointwise posterior predictive variances of panel (b) and the deceptively accurate density estimate of panel (a). The latter warrants further explanation. Note that high autocorrelation of $\tau_k$, for any $k = 1, \ldots, 30$, implies that the realizations of $\tau_k$ are not much different from each other. Hence, the correlation between $\tau_j$ and $\tau_k$, for $j \neq k$, will tend to be close to zero. This would effectively imply many distinct $\tau_k$, which would enforce the same number of distinct $\nu_k$. The square roots of the inverse of these $\tau_k$ act as bandwidths for the density estimation, and so there would be many distinct locations and the corresponding bandwidths. Together they reach out to every minor bump of the histogram and create the impression of great accuracy of the resultant density estimate. As we argued, such accuracy is nothing but an artifact of poor mixing of TMCMC taking small steps in each iteration, and hence must be considered spurious. Hence, Figure 3 and not Figure 4, represents the correct Bayesian inference. Also note that the posterior probability of the number of components $K = 2, 3, 4, 5, 6, 7, 8$ here are 0.0021, 0.0414, 0.1988, 0.3688, 0.3020, 0.0860, 0.0009, respectively. Thus, this TMCMC algorithm supports more components than the correct iid method or the efficient TMCMC method, which is in keeping with the above discussion with respect to autocorrelations.
(a) TMCMC and iid-based posterior predictive density for galaxy.

(b) Pointwise variances with TMCMC and iid sampling.

(c) TMCMC autocorrelation plot for $\nu_{30}$.

(d) TMCMC autocorrelation plot for $\tau_{30}$.

Figure 3: IID and TMCMC sampling for the galaxy data.
Figure 4: TMCMC sampling for the galaxy data with small scaling constant.
5 Summary and conclusion

MCMC sampling from posterior DP mixtures offers substantial challenges in terms of both mixing and implementation time. Despite the existence of a plethora of MCMC algorithms for DP mixtures, it is extremely difficult to single out any algorithm for general application. More disconcertingly, it is not possible to rigorously address if the underlying Markov chain has at all converged to the target DP mixture posterior. The ideal situation of iid sampling is usually perceived as inconceivable and impractical by the statistical and probabilistic community, even in finite-dimensional setups. In finite-dimensional situations, as well as in multimodal and variable-dimensional contexts, and even for doubly intractable target distributions, we attempted to come up with efficient iid sampling procedures (Bhattacharya (2021b), Bhattacharya (2021c), Bhattacharya (2021a)). In this article, we have attempted to provide a novel iid sampling procedure for DP mixtures in general, focussing particularly on the more general, flexible and efficient DP mixture model of Bhattacharya (2008). The key idea is of course a generalization of our aforementioned works on iid sampling, but the infinite-dimensional and discrete nature of DP called for some significant modification of our existing theory to create a valid iid sampling procedure for DP mixtures. Our theory does not depend upon conjugate or non-conjugate setups and works equally well for both situations. Application of our iid method to three benchmark datasets revealed excellent performance, including very fast parallel computation.

It is important to note that Mukhopadhyay and Bhattacharya (2012) had already created a novel perfect sampling procedure for the DP mixture of Bhattacharya (2008), integrating out the random measure $G$ and creating appropriate bounding chains associated with an efficient Gibbs sampling procedure. The method encompasses both conjugate and non-conjugate cases, and so, is highly relevant and comparable with our current work. However, the theory requires compact parameter space, which is not required in this current work. Moreover, the computation required by Mukhopadhyay and Bhattacharya (2012) seems to be too intensive for generating a large number of iid realizations. For instance, application of their method to the galaxy data with $M = 10$ took 11 days to generate a single perfect realization! Parallelizing their method would only halve the time, which still would not serve the purpose of generating adequate number of iid realizations. In contrast, in our current work, we have been able to generate 10,000 realizations for the galaxy data in just 5 minutes, even with $M = 30$! Although our procedure is based on truncating the random measure $G$, the upper bound of Theorem 1, illustrated in detail in Remark 2, shows almost indistinguishable agreement of the truncated model with the original one. Indeed, for all practical purposes, simulations from the original and the truncated DP mixture models of Bhattacharya (2008) would be identical.

Although various advantages of Bhattacharya (2008) over the traditional DP mixture model are established, Theorem 1 and Remark 2 bring out yet another great advantage of the former with respect to truncation. Indeed, the truncated DP mixture model of Bhattacharya (2008) is in much closer agreement with the original one compared to that in the case of the traditional DP mixture model.

In fine, we remark that although DP mixtures clearly dominate the literature on Bayesian nonparametrics, there are various other classes of nonparametric Bayesian models as well, for instance, those based on Pólya trees. In our future work, we intend to further generalize our iid sampling procedure to encompass all nonparametric Bayesian models.
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