Transdimensional Transformation based Markov Chain Monte Carlo

Moumita Das and Sourabh Bhattacharya

Abstract

Variable dimensional problems, where not only the parameters, but also the number of parameters are random variables, offer quite challenging inferential tasks to the Bayesians. Although in principle the Reversible Jump Markov Chain Monte Carlo (RJMCMC) methodology, a general MCMC method which can jump between different dimensions, is a response to such challenges, the dimension-hopping strategies need not be always convenient for practical implementation, particularly because efficient “move-types” having reasonable acceptance rates are often difficult to devise.

In this article, we propose a novel and general dimension-hopping MCMC methodology that can update all the parameters as well as the number of parameters simultaneously using simple deterministic transformations of some low-dimensional (often one-dimensional) random variable. This methodology, which has been inspired by the recent Transformation based MCMC (TMCMC) (Dutta & Bhattacharya (2014)) for updating all the parameters simultaneously in general fixed-dimensional set-ups using low-dimensional (usually one-dimensional) random variables, facilitates great speed in terms of computation time and provides high acceptance rates, thanks to the low-dimensional random variables which effectively reduce the dimension dramatically. Quite importantly, our transformation based approach provides a natural way to automate the move-types in the variable dimensional problems. We refer to this methodology as Transdimensional Transformation based Markov Chain Monte Carlo (TTMCMC).

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We develop the theory of TTMCMC, illustrating it with normal mixtures with unknown number of components applied to three well-known real data sets. Moreover, in the context of density estimation, we propose a novel methodology to summarize the posterior distributions of the mixture densities, providing a way to obtain the mode of the posterior distribution of the densities and the associated highest posterior density credible regions. Based on our method we also propose a criterion to assess convergence of TTMCMC. These methods of summarization and convergence assessment are generally applicable to problems involving unknown functions such as nonparametric regression and functional data analysis.

**Keywords:** Block update; Distance between densities; Mixture; Move type; Posterior distribution of densities with random number of components; Transdimensional Transformation based Markov Chain Monte Carlo.

1. **INTRODUCTION**

Simultaneous inference on both model and parameter space is an issue that is fundamental to modern statistical practice (Sisson (2005)). Examples of such problems arise in mixture analysis where the parameters associated with the mixture components as well as the number of mixture components are unknown (see, for example, Richardson & Green (1997)); in change point analysis where the locations and the number of change points are unknown (see, for example, Green (1995)); in variable selection problems where the number of covariates and the associated coefficients are unknown (Dellaportas, Forster & Ntzoufras (2002), Dellaportas & Forster (1999)); in spline smoothing where the location and the number of knots are unknown (see Denison, Mallick & Smith (1998) for instance); in continuous wavelet representation of unknown functions with a finite, but unknown number of wavelet basis functions and the corresponding parameters (Chu, Clyde & Liang (2009)); in autoregressive time series models where the order of the autoregression and the associated parameters are unknown (Vermaak, Andrieu, Doucet & Godsill (2004)); in factor analysis where the dimension of the latent factor loading matrix and the associated parameters are unknown (Lopes & West (2004)); in spatial point processes where the locations and the number of points are random (see Møller & Waagepetersen (2004)); to name only a few.
A general Markov Chain Monte Carlo (MCMC) strategy which can explore variable dimensional spaces by jumping between different dimensions has been proposed by Green (1995), which is well-known as Reversible Jump MCMC (RJMCMC).

1.1 A simple example for illustration of the basic concept of RJMCMC

To illustrate the key idea with a simple example, note that if the current state \( x = (x_1, \ldots, x_k) \in \mathbb{R}^k \), then a new move in \( \mathbb{R}^{k+1} \) may be constructed by first selecting one of \( x_1, \ldots, x_k \) at random; if \( x_{i'} \) denotes the chosen co-ordinate where \( i' \in \{1, \ldots, k\} \), then \( x_{i'} \) can be split into \( x_{i'} + u \) and \( x_{i'} - u \), where \( u \sim q(\cdot) \), where \( q \) is any arbitrary density. Thus, the new “birth” move with dimension \( k + 1 \) is \( x' = (x_1, x_2, \ldots, x_{i'-1}, x_{i'} + u, x_{i'} - u, x_{i'+1}, \ldots, x_k) = (x'_1, x'_2, \ldots, x'_{k+1}) \), after re-labeling for convenience. For returning from \( x' \) to \( x \), one can select \( x_{i'}' \) and \( x_{i'+1}' \) at random without replacement, and simply take the average of the selected elements. This constitutes an instance of the “death” move balancing the birth move. The proposed birth and death moves are accepted with appropriate probabilities which satisfy the detailed balance condition.

In the above, we implicitly assumed that in the birth move other than \( x_{i'} \) all other co-ordinates of \( x \) remain unchanged. Similarly, in the death move, we implicitly assumed that except \( x_{i'}' \) and \( x_{i'+1}' \), which are are averaged, the remaining co-ordinates of \( x' \) remain unchanged. In fact, at each iteration, after one performs either the birth or the death move, the dimension (the number of parameters) is then either \( k + 1 \) or \( k - 1 \), which remains fixed for the current iteration. Hence, for the current iteration, one can then update all the co-ordinates sequentially (or some co-ordinates using random scan) following the traditional fixed dimensional Metropolis-Hastings method. It is also possible, in principle, to change dimension and propose change to the remaining co-ordinates and accept or reject all the changed co-ordinates simultaneously in a single block. That is, if the current state \( x = (x_1, \ldots, x_k) \in \mathbb{R}^k \) then we can split the randomly chosen \( x_{i'} \) into \( x_{i'} + u \) and \( x_{i'} - u \) and also use the random walk proposals to propose, for \( i \in \{1, \ldots, k\}\setminus\{i'\} \), \( x'i = x_i + v_i \); \( v_i \sim N(0, \sigma_i^2) \) independently. We can then accept or reject \( x' = (x'_1, x'_2, \ldots, x'_k) = (x_1 + v_1, x_2 + v_2, \ldots, x'_{i'-1} + v_{i'-1}, x_{i'} + u, x_{i'} - u, x'_{i'+1} + v_{i'+1}, \ldots, x_k + v_k) \) jointly, in a single block. Similar joint updating can be done if the death move results, balancing the jointly proposed birth move.
1.2 Brief discussion on efficiency of block updating proposals involving dimension change

Gained wisdom from MCMC for fixed dimensions lead us to prefer joint updating strategies since these strategies are not affected by the posterior cross-correlations between the parameters and are known to improve mixing. Also, joint updating strategies can significantly reduce computational burden since the acceptance rate needs to be computed only once in each iteration, whereas sequentially updating $k$ parameters (which is usually the default choice compared to random scan), requires such acceptance ratio computation $k$ times. However, it is also well-known that even for moderately large number of parameters, the acceptance probability for the joint proposal tends to be very small, rendering such algorithms very inefficient. The problem is only aggravated in joint proposals involving dimension changes as efficient dimension changing moves are more difficult to construct compared to fixed dimensional moves. There have been many attempts of creating automatic RJMCMC samplers which also maintain high acceptance rates; see, for example, Brooks, Giudici & Roberts (2003), Robert (2003), Green (2003), Godsill (2003), Sisson (2005) and the references therein. However, in spite of the commendable attempts, these ideas are perhaps relevant in quite specific models with several restrictive assumptions; see Sisson (2005).

1.3 Our proposition: change dimension and update all parameters simultaneously using deterministic transformations of a single random variable

The issues discussed above point towards the need to develop general and natural move types that can change dimensions as well as update the other parameters simultaneously, while maintaining reasonably high acceptance rates. In this regard, the transformation based MCMC (TMCMC) approach of Dutta & Bhattacharya (2014) in the fixed dimensional set-up provides the necessary motivation. The key concept of TMCMC is to simulate a single, one-dimensional random variable from some arbitrary distribution and propose simple deterministic transformations to all the parameters using the one-dimensional random variable. The proposed set of parameters will then be accepted with an appropriate acceptance probability that satisfies the detailed balance condition. Needless to mention, since the dimension is effectively reduced to one, due to deterministic transformations of a single random variable, the acceptance rate remains reasonably high even if the
entire set of high-dimensional parameters is updated in a single block. For the complete details, see Dutta & Bhattacharya (2014).

In this article we show that the same concept of deterministic transformations of a single random variable can be exploited to construct, for any general variable dimensional problem, a generic and effective dimension-hopping sampler which can change dimensions and update all the remaining parameters in a single block while maintaining high acceptance rates. We refer to this generic variable dimensional MCMC sampler as Transdimensional Transformation based Markov Chain Monte Carlo (TTMCMC). But before we formally introduce TTMCMC it is necessary to provide a brief overview of the basic concept of TMCMC involving transformations and one-dimensional random variables; we do this in Section 2. We introduce TTMCMC in Section 3. In Section 4 we extend our proposed methodology to more general situations where one wishes to jump more than one dimension at a time. In Section 5 we extend TTMCMC to situations where different sets of parameters are related so that changing dimension of one of such sets makes appropriate dimension changing imperative for all the remaining sets.

We illustrate TTMCMC with normal mixtures with unknown number of components; the basic premise is provided in Section 6. In this context, we develop a methodology for summarizing the posterior distributions of densities, using ideas similar to those of Mukhopadhyay, Bhattacharya & Dihidar (2011) who first introduce the ideas for summarizing the posterior distribution of clusterings, rather than the posterior distribution of densities. In particular, in Section 7 we develop a method of obtaining the modes and the highest posterior density regions of the posterior distribution of the mixture densities with random number of components. Furthermore, again following the ideas of Mukhopadhyay et al. (2011) in the clustering context, in Section 8 we develop a method to assess convergence of TTMCMC.

With these developments, in Section 9 we then apply our methods to analyse three well-studied real data sets, namely, the enzyme, acidity and the galaxy data; Richardson & Green (1997). Finally, we make concluding remarks in Section 10.
2. A BRIEF OVERVIEW OF THE KEY IDEA OF TMCMC

In order to obtain a valid algorithm based on transformations, Dutta & Bhattacharya (2014) design appropriate move types so that detailed balance and irreducibility hold. We first illustrate the basic idea on transformation based moves with a simple example. Given that we are in the current state \( x \), we may propose the “forward move” \( x' = x + \epsilon \), where \( \epsilon > 0 \) is a simulation from some arbitrary density \( g(\cdot) \) which is supported on the positive part of the real line. To move back to \( x \) from \( x' \), we need to apply the “backward transformation” \( x' - \epsilon \). In general, given \( \epsilon \) and the current state \( x \), we shall denote the forward transformation by \( T(x, \epsilon) \), and the backward transformation by \( T^b(x, \epsilon) \). For fixed \( \epsilon \) the forward and the backward transformations must be one-to-one and onto, and must satisfy \( T^b(T(x, \epsilon), \epsilon) = x = T(T^b(x, \epsilon), \epsilon) \); see Dutta & Bhattacharya (2014) for a detailed discussion regarding these.

The simple idea discussed above has been generalized to the multi-dimensional situation by Dutta & Bhattacharya (2014). Remarkably, for any dimension, the moves can be constructed by simple deterministic transformations of the one-dimensional random variable \( \epsilon \), which is simulated from any arbitrary distribution on some relevant support. We provide some examples of such moves in the next section after introducing some necessary notation borrowed from Dutta & Bhattacharya (2014).

2.1 Notation

Suppose now that \( \mathcal{X} \) is a \( k \)-dimensional space of the form \( \mathcal{X} = \prod_{i=1}^{k} \mathcal{X}_i \) so that \( T = (T_1, \ldots, T_k) \) where each \( T_i : \mathcal{X}_i \times D \rightarrow \mathcal{X}_i \), for some set \( D \), are the component-wise transformations. Let \( z = (z_1, \ldots, z_k) \) be a vector of indicator variables, where, for \( i = 1, \ldots, k \), \( z_i = 1 \) and \( z_i = -1 \) indicate, respectively, application of forward transformation and backward transformation to \( x_i \), and let \( z_i = 0 \) denote no change to \( x_i \). Given any such indicator vector \( z \), let us define \( T_z = (g_1,z_1, g_2,z_2, \ldots, g_k,z_k) \) where

\[
g_{i,z_i} = \begin{cases} 
T_i^b & \text{if } z_i = -1 \\
x_i & \text{if } z_i = 0 \\
T_i & \text{if } z_i = 1.
\end{cases}
\]
Corresponding to any given \( z \), we also define the following ‘conjugate’ vector \( z^c = (z_1^c, z_2^c, \ldots, z_k^c) \), where

\[
   z_i^c = \begin{cases} 
   1 & \text{if } z_i = -1 \\
   0 & \text{if } z_i = 0 \\
   -1 & \text{if } z_i = 1.
   \end{cases}
\]

With this definition of \( z^c \), \( T_{z^c} \) can be interpreted as the conjugate of \( T_z \).

Since \( 3^k \) values of \( z \) are possible, it is clear that \( T \), via \( z \), induces \( 3^k \) many types of ‘moves’ of the forms \( \{T_{z_i}; i = 1, \ldots, 3^k\} \) on the state-space. Suppose now that there is a subset \( \mathcal{Y} \) of \( \mathcal{D} \) such that the sets \( T_{z_i}(x, \mathcal{Y}) \) and \( T_{z_j}(x, \mathcal{Y}) \) are disjoint for every \( z_i \neq z_j \). In fact, \( \mathcal{Y} \) denotes the support of the distribution \( g(\cdot) \) from which \( \epsilon \) is simulated.

2.2 Examples of transformations on two-dimensional state-space using single \( \epsilon \)

Although for the sake of illustration we provide below examples pertaining to two-dimensional cases it is important to remark at the outset that these examples can be easily generalized to any dimension; see Dutta & Bhattacharya (2014).

1. **Additive transformation:** Suppose \( \mathcal{X} = \mathcal{D} = \mathbb{R}^2 \). With two positive scale parameters \( a_1 \) and \( a_2 \), we can then consider the following additive transformation: \( T_{(1,1)}(x, \epsilon) = (x_1 + a_1 \epsilon, x_2 + a_2 \epsilon) \), \( T_{(-1,1)}(x, \epsilon) = (x_1 - a_1 \epsilon, x_2 + a_2 \epsilon) \), \( T_{(1,-1)}(x, \epsilon) = (x_1 + a_1 \epsilon, x_2 - a_2 \epsilon) \) and \( T_{(-1,-1)}(x, \epsilon) = (x_1 - a_1 \epsilon, x_2 - a_2 \epsilon) \). We may choose \( \mathcal{Y} = (0, \infty) \times (0, \infty) \). Observe that none of the above moves \( z \) contains 0 as one of its elements. Indeed, as shown in Dutta & Bhattacharya (2014), moves \( z \) which includes 0 as at least one of its elements are not necessary for the validity of the additive transformation.

2. **Multiplicative transformation:** Suppose \( \mathcal{X} = \mathcal{D} = \mathbb{R} \times (0, \infty) \). Then we may consider the following multiplicative transformation: \( T_{(1,1)}(x, \epsilon) = (x_1 \epsilon, x_2 \epsilon) \), \( T_{(-1,1)}(x, \epsilon) = (x_1 / \epsilon, x_2 \epsilon) \), \( T_{(1,-1)}(x, \epsilon) = (x_1 \epsilon, x_2 / \epsilon) \), \( T_{(-1,-1)}(x, \epsilon) = (x_1 / \epsilon, x_2 / \epsilon) \). We may let \( \mathcal{Y} = \{(-1,1) - \{0\}\} \times (0,1) \). Note that moves \( z \) which
includes 0 as at least one of its elements are not required for the additive transformation, even though non-additive transformations need these moves for their validity. However, since \( z = (0, 0) \) does not propose any change to the current \((x_1, x_2)\), we will typically discard this move in a way that does not affect convergence of the algorithm; see Dutta & Bhattacharya (2014) for details regarding this.

3. *Additive-multiplicative transformation:* Suppose \( \mathcal{X} = \mathcal{D} = \mathbb{R} \times (0, \infty) \). It is possible to combine additive and multiplicative transformations in the following manner:

\[
\begin{align*}
T_{(1,1)}(x, \epsilon) &= (x_1 + \epsilon, x_2 \epsilon), \quad T_{(-1,1)}(x, \epsilon) = (x_1 - \epsilon, x_2 \epsilon), \quad T_{(1,-1)}(x, \epsilon) = (x_1 + \epsilon, x_2 / \epsilon), \quad T_{(-1,-1)}(x, \epsilon) = (x_1 - \epsilon, x_2 / \epsilon), \\
T_{(1,0)}(x, \epsilon) &= (x_1 + \epsilon, x_2), \quad T_{(-1,0)}(x, \epsilon) = (x_1 - \epsilon, x_2), \quad T_{(0,1)}(x, \epsilon) = (x_1, x_2 \epsilon), \\
T_{(0,-1)}(x, \epsilon) &= (x_1, x_2 / \epsilon), \quad T_{(0,0)}(x, \epsilon) = (x_1, x_2). 
\end{align*}
\]

We may let \( \mathcal{Y} = (0, \infty) \times (0, 1) \). Again, we will discard \( z = (0, 0) \) in our resulting algorithm.

It is clearly possible to construct valid transformations in high-dimensional spaces using combinations of valid transformations on one-dimensional spaces. Moreover, mixtures of additive and multiplicative transformations have been advocated by Dey & Bhattacharya (2014a). These transformations remain valid even in the case of TTMCMC, which we detail in the next section.

3. TTMCMC FOR UPDATING THE DIMENSION AND THE PARAMETERS IN A SINGLE BLOCK USING DETERMINISTIC TRANSFORMATIONS OF A SINGLE RANDOM VARIABLE

First we illustrate the main idea of TTMCMC informally using the additive transformation.

3.1 Illustration of the key idea of TTMCMC with a simple example

Assume that the current state is \( x = (x_1, x_2) \in \mathbb{R}^2 \). We first randomly select \( u = (u_1, u_2, u_3) \sim \text{Multinomial}(w_b, w_d, w_{nc}) \), where \( w_b, w_d, w_{nc} (> 0) \) such that \( w_b + w_d + w_{nc} = 1 \) are the probabilities of birth, death, and no-change moves, respectively. That is, if \( u_1 = 1 \), then we increase the dimensionality from 2 to 3, if \( u_2 = 1 \), then we decrease the dimensionality from 2 to 1, and if \( u_3 = 1 \), then we keep the dimensionality unchanged. In the latter case, when the dimensionality is
unchanged, the acceptance probability remains the same as in TMCMC, as provided in Algorithm 3.1 of Dutta & Bhattacharya (2014).

If \( u_1 = 1 \), we can increase the dimensionality by first selecting one of \( x_1 \) and \( x_2 \) with probability \( 1/2 \); assuming for clarity that \( x_1 \) has been selected, we then construct the move-type \( T_{b,z}(x,\epsilon) = (x_1 + a_1\epsilon, x_1 - a_1\epsilon, x_2 + z_2a_2\epsilon) = (g_{1,z_1=1}(x_1,\epsilon), g_{1,z_1=-1}(x_1,\epsilon), g_{2,z_2}(x_2,\epsilon)) \), say. Here, as in TMCMC, we draw \( \epsilon \sim g(\cdot) \), where \( g(\cdot) \) is supported on the positive part of the real line, and draw \( z = (z_1, z_2) \) where \( z_i = 1 \) with probability \( p_i \) and \( z_i = -1 \) with probability \( 1 - p_i \). Also, as before, \( z^c = (z_1^c, z_2^c) \) is the conjugate of \( z \), where \( z_1^c = 1 \) if \( z_1 = -1 \) and \( z_1^c = -1 \) if \( z_1 = 1 \). We re-label \( x' = T_{b,z}(x,\epsilon) = (x_1 + a_1\epsilon, x_1 - a_1\epsilon, x_2 + z_2a_2\epsilon) \) as \( (x'_1, x'_2, x'_3) \). Thus, \( T_{b,z}(x,\epsilon) \) increases the dimension from 2 to 3.

We accept this birth move with probability

\[
a_b(x,\epsilon) = \min \left\{ 1, \frac{1}{3} \times \frac{w_d}{w_b} \times \frac{I_2^{(z_1)}(z_2^c)}{I_2^{(z_1)}(z_2)} \frac{I_2^{(-1)(z_2)}}{I_2^{(-1)(z_2)}} \right. \\
\times \left. \frac{\pi(x_1 + a_1\epsilon, x_1 - a_1\epsilon, x_2 + z_2a_2\epsilon)}{\pi(x_1, x_2)} \times \left| \frac{\partial(T_{b,z}(x,\epsilon))}{\partial(x,\epsilon)} \right| \right\}. \tag{3.1}
\]

In (3.1),

\[
\left| \frac{\partial(T_{b,z}(x,\epsilon))}{\partial(x,\epsilon)} \right| = \left| \frac{\partial(x_1 + a_1\epsilon, x_1 - a_1\epsilon, x_2 + z_2a_2\epsilon)}{\partial(x_1, x_2, \epsilon)} \right| = \left| \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \\ a_1 & -a_1 & z_2a_2 \end{pmatrix} \right| = 2a_1. \tag{3.2}
\]

Now let us illustrate the problem of returning to \( = (x_1, x_2) \) (\( \in \mathbb{R}^2 \)) from \( T_{b,z}(x,\epsilon) = (x_1 + a_1\epsilon, x_1 - a_1\epsilon, x_2 + z_2a_2\epsilon) \) (\( \in \mathbb{R}^3 \)). For our purpose, we can select \( x_1 + a_1\epsilon \) with probability \( 1/3 \); then select \( x_1 - a_1\epsilon \) from the remaining two elements with probability \( 1/2 \), and form the average \( x_1^* = ((x_1 + a_1\epsilon) + (x_1 - a_1\epsilon))/2 = x_1 \). For non-additive transformations we can consider the averages of the backward moves of each of the selected elements. Even in this additive transformation example, after simulating \( \epsilon \) as before we can consider the respective backward moves of \( x_1 + a_1\epsilon \) and \( x_1 - a_1\epsilon \), both yielding \( x_1 \), and then take the average denoted by \( x_1^* \). For the remaining element \( x_2 + z_2a_2\epsilon \), we need to simulate \( z_2^c \) and then consider the move \( (x_2 + z_2a_2\epsilon) + z_2^ca_2\epsilon = x_2 \). Thus, we can return to \( (x_1, x_2) \) using this strategy.
Letting $x' = (x'_1, x'_2, x'_3)$, and denoting the average involving the first two elements by $x^*_1$, the death move is then given by $x'' = T_{d,2}(x', \epsilon) = (x^*_1, x'_3 + z_2^* a_2 \epsilon) = (x^*_1, x'_3 + z_2^* a_2 \epsilon)$. Now observe that for returning to $(x'_1, x'_2)$ from $x^*_1$, we must have $x^* + a_1 \epsilon = x'_1$ and $x^* - a_1 \epsilon = x'_2$, which yield $\epsilon^* = (x'_1 - x'_2)/2a_1$. Hence, the Jacobian associated with the death move in this case is given by

$$
\left| \frac{\partial (T_{d,2}(x', \epsilon), \epsilon^*, \epsilon)}{\partial (x', \epsilon)} \right| = \left| \frac{\partial \left( \frac{x'_1 + x'_2}{2}, x'_3 + z_2^* a_2 \epsilon, \frac{x'_1 - x'_2}{2}, \epsilon \right)}{\partial (x'_1, x'_2, x'_3, \epsilon)} \right| = \left| \begin{array}{cccc}
\frac{1}{2} & 0 & \frac{1}{2a_1} & 0 \\
\frac{1}{2} & 0 & -\frac{1}{2a_1} & 0 \\
0 & 1 & 0 & 0 \\
0 & z_2^* a_2 & 0 & 1 \\
\end{array} \right| = \frac{1}{2a_1}.
$$

(3.3)

We accept this death move with probability

$$
a_d(x'', \epsilon, \epsilon^*) = \min \left\{ 1, 3 \times \frac{w_b}{w_d} \times \frac{P(z^{\epsilon})}{P(z)} \frac{\pi(x'')}{\pi(x')} \left| \frac{\partial (T_{d,2}(x', \epsilon), \epsilon^*, \epsilon)}{\partial (x', \epsilon)} \right| \right\} = \min \left\{ 1, 3 \times \frac{w_b}{w_d} \times \frac{p_{I(1)}(z_2^*)}{p_{I(1)}(z_2)} \frac{q_{I(-1)}(z_2^*)}{q_{I(-1)}(z_2)} \times \frac{\pi(x'')}{\pi(x')} \times \frac{1}{2a_1} \right\}. \quad (3.4)
$$

In the general situation, we shall make the birth, death and no-change probabilities $w_b$, $w_d$, $w_{nc}$ depend upon the current dimension $k$, and denote them by $w_{b,k}$, $w_{d,k}$ and $w_{nc,k}$, respectively, satisfying $w_{b,k} + w_{d,k} + w_{nc,k} = 1$ for every $k \geq 1$. Note that when the current dimension $k = 1$, then $w_{d,k} = 0$, because $k \geq 1$. Similarly, if in some cases there is reason to assume that the number of parameters can not exceed some finite quantity denoted by $k_{max}$, then $w_{b,k_{max}} = 0$.

### 3.2 General TTMCMC algorithm for jumping one dimension at a time

We now provide the TTMCMC algorithm in the general case, as follows.

**Algorithm 3.1** General TTMCMC algorithm based on a single $\epsilon$.

- Let the initial value be $x^{(0)} \in \mathbb{R}^k$.
- For $t = 0, 1, 2, \ldots$
  1. Generate $u = (u_1, u_2, u_3) \sim \text{Multinomial}(1; w_{b,k}, w_{d,k}, w_{nc,k})$. 


2. If \( u_1 = 1 \) (increase dimension), then
   
   (a) Randomly select a co-ordinate from \( \mathbf{x}^{(t)} = (x_1^{(t)}, \ldots, x_k^{(t)}) \) assuming uniform probability \( 1/k \) for each co-ordinate. Let \( j \) denote the chosen co-ordinate.
   
   (b) Generate \( \epsilon \sim g(\cdot) \) and for \( i = 1, \ldots, k; \ i \neq j \) simulate

   \[
   z_i \sim \text{Multinomial}(1; p_i, q_i, 1 - p_i - q_i)
   \]

   independently.

   (c) Propose the following birth move:

   \[
   \mathbf{x}' = T_{b,z}(\mathbf{x}^{(t)}, \epsilon) = (g_{1,z_1}(x_1^{(t)}, \epsilon), \ldots, g_{j-1,z_{j-1}}(x_{j-1}^{(t)}, \epsilon), g_{j,z_j}(x_j^{(t)}, \epsilon), g_{j+1,z_{j+1}}(x_{j+1}^{(t)}, \epsilon), \ldots, g_{k,z_k}(x_k^{(t)}, \epsilon)).
   \]

   Re-label the elements of \( \mathbf{x}' \) as \( (x_1', x_2', \ldots, x'_{k+1}) \).

   (d) Calculate the acceptance probability of the birth move \( \mathbf{x}' \):

   \[
   a_b(\mathbf{x}^{(t)}, \epsilon) = \min \left\{ 1, \frac{1}{k+1} \frac{w_{d,k+1}}{w_{b,k}} \frac{P_j(\zeta^c)}{P_j(\zeta)} \frac{\pi(\mathbf{x}')}{\pi(\mathbf{x}^{(t)})} \left| \frac{\partial(T_{b,z}(\mathbf{x}^{(t)}, \epsilon))}{\partial(\mathbf{x}^{(t)}, \epsilon)} \right| \right\},
   \]
   
   where
   
   \[
   P_j(\zeta) = \prod_{i \neq j=1}^{k} p_{i}^{I_{(1)}(z_i)} q_{i}^{I_{(-1)}(z_i)},
   \]
   
   and
   
   \[
   P_j(\zeta^c) = \prod_{i \neq j=1}^{k} p_{i}^{I_{(1)}(z_i^c)} q_{i}^{I_{(-1)}(z_i^c)}.
   \]

   (e) Set
   
   \[
   \mathbf{x}^{(t+1)} = \begin{cases}
   \mathbf{x}' & \text{with probability } a_b(\mathbf{x}^{(t)}, \epsilon) \\
   \mathbf{x}^{(t)} & \text{with probability } 1 - a_b(\mathbf{x}^{(t)}, \epsilon).
   \end{cases}
   \]

3. If \( u_2 = 1 \) (decrease dimension), then
   
   (a) Generate \( \epsilon \sim g(\cdot) \).
(b) Randomly select co-ordinate \( j \) with probability \( 1/k \), and randomly select co-ordinate \( j' \) from the remaining co-ordinates with probability \( 1/(k-1) \). Let \( x_j^* = \left( g_{j,z_j=-1}(x_j,\epsilon) + g_{j',z_j'=1}(x_{j'},\epsilon) \right)/2 \). Replace the co-ordinate \( x_j \) drawn first by the average \( x_j^* \), and delete \( x_{j'} \).

(c) Simulate \( z \) by generating independently, for \( i = 1,\ldots,k \), but \( i \neq j,j' \), \( z_i \sim Multinomial(1;p_i,q_i,1-p_i-q_i) \). For \( i \neq j,j' \), apply the transformation \( x_i' = g_{i,z_i}(x_i(t),\epsilon) \).

(d) Propose the following death move:

\[
x' = T_{d,z}(x^{(t)},\epsilon) = (g_{1,z_1}(x_1^{(t)},\epsilon),\ldots,g_{j-1,z_{j-1}}(x_{j-1}^{(t)},\epsilon),x_j^*,g_{j+1,z_{j+1}}(x_{j+1}^{(t)},\epsilon),\ldots,g_{j'-1,z_{j'-1}}(x_{j'-1}^{(t)},\epsilon),g_{j'+1,z_{j'+1}}(x_{j'+1}^{(t)},\epsilon),\ldots,g_{k,z_k}(x_k^{(t)},\epsilon)).
\]

Re-label the elements of \( x' \) as \( (x_1',x_2',\ldots,x_{k-1}') \).

(e) Solve for \( \epsilon^* \) from the equations \( g_{j,z_j=1}(x_j^*,\epsilon^*) = x_j \) and \( g_{j,z_j=-1}(x_j^*,\epsilon^*) = x_{j'} \) and express \( \epsilon^* \) in terms of \( x_j \) and \( x_{j'} \).

(f) Calculate the acceptance probability of the death move:

\[
a_d(x^{(t)},\epsilon,\epsilon^*) = \min\left\{ 1, k \times \frac{w_{b,k-1}}{w_{d,k}} \times \frac{P_{(j,j')}(z^*)}{P_{(j,j')}(z)} \times \frac{\pi(x')}{\pi(x^{(t)})} \left| \frac{\partial(T_{d,z}(x^{(t)},\epsilon,\epsilon^*),\epsilon^*)}{\partial(x^{(t)},\epsilon)} \right| \right\},
\]

where

\[
P_{(j,j')}(z) = \prod_{i \neq j,j'}^k \frac{P_i^{I_{(1)}(z_i)} I_{(-1)}(z_i)}{P_i^{I_{(1)}(z_i)}},
\]

and

\[
P_{(j,j')}(z') = \prod_{i \neq j,j'}^k \frac{P_i^{I_{(1)}(z_i') I_{(-1)}(z_i')}}{P_i^{I_{(1)}(z_i') I_{(-1)}(z_i')}}.
\]

(g) Set

\[
x^{(t+1)} = \begin{cases} 
    x' & \text{with probability } a_d(x^{(t)},\epsilon,\epsilon^*) \\
    x^{(t)} & \text{with probability } 1 - a_d(x^{(t)},\epsilon,\epsilon^*)
\end{cases}
\]

4. If \( u_3 = 1 \) (dimension remains unchanged), then implement steps (1), (2), (3) of Algorithm 3.1 of Dutta & Bhattacharya (2014).
A few observations regarding Algorithm 3.1 are in order.

- Note that the acceptance probabilities are independent of the proposal density $g(\cdot)$ irrespective of its form, just as in TMCMC.

- In the acceptance probabilities, 
  
  \[ \frac{P(j)(z^c)}{P(j)(z)} = 1 \quad \text{and} \quad \frac{P(j,j')(z^c)}{P(j,j')(z)} = 1 \]
  
  if $p_i = q_i$ for each $i$, resulting in simplification of the acceptance ratio computation. The birth, death and the no-change probabilities given by $w_{b,k}$, $w_{d,k}$ and $w_{nc,k}$ can also be chosen to be equal for every $k > 1$, which will result in further simplification of the computation of the acceptance ratio.

- Splitting a parameter into two and merging two parameters are naturally accomplished in our transformation based approach through the forward and backward transformations. This, in conjunction with the use of single $\epsilon$ which effectively reduces the variable dimensional problem to a one-dimensional problem, maintains high acceptance rate. Thus, in this sense, some degree of automation of the move-types is achieved.

3.3 Irreducibility and aperiodicity

It is easy to see that our TTMCMC algorithm is irreducible and aperiodic. Assume that $x \in \mathbb{R}^k$, with $k \geq 1$. For $k' > 0$ with $k' \neq k$, let $(k', A_{k'})$ have positive probability under the target distribution, that is, $\pi(k', A_{k'}) > 0$; here $A_{k'}$ is a Borel set associated with $\mathbb{R}^{k'}$. Then $\mathbb{R}^{k'}$ can be reached from $x \in \mathbb{R}^k$ in a finite number of steps using the birth and the death moves, accordingly as $k' > k$ or $k' < k$. Thus, if $k' > k$, $\mathbb{R}^{k'}$ can be reached in $(k' - k)$ steps by applying the birth move, and if $k' < k$, then $\mathbb{R}^{k'}$ can be reached in $(k - k')$ steps using the death move. Once $\mathbb{R}^{k'}$ is reached the non-change move-type and the transformations can be used to reach $A_{k'}$ in $k'$ steps. For the proof of the latter see Dutta & Bhattacharya (2014) and Dey & Bhattacharya (2014a). Thus, $(k', A_{k'})$ can be reached from $x \in \mathbb{R}^k$ in $(|k' - k| + k')$ steps with positive probability. Since the set $(k', A_{k'})$ is arbitrary, aperiodicity also follows.
3.4 Detailed balance for Algorithm 3.1

To see that detailed balance is satisfied for the birth and death moves, note that associated with the birth move, the probability of transition $x \in \mathbb{R}^k \mapsto T_{b,z}(x,\epsilon) \in \mathbb{R}^{k+1}$ is given by:

$$
\pi(x) \times \frac{1}{k} \times w_{b,k} \times g(\epsilon) \times \prod_{i \neq j = 1}^{k} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)}
$$

$$
\times \min \left\{ 1, \frac{1}{k+1} \times \frac{w_{d,k+1}}{w_{b,k}} \times \prod_{i \neq j = 1}^{k} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \pi(T_{b,z}(x,\epsilon)) \times \left| \frac{\partial(T_{b,z}(x,\epsilon))}{\partial(x(t),\epsilon)} \right| \right\} .
$$

Here we assume that $x_j$ was selected, and was split into $g_{j,z_j = 1}(x_j,\epsilon)$ and $g_{j,z_j = -1}(x_j,\epsilon)$. Hence, it is not necessary to simulate $z_j$. For the remaining co-ordinates we need to simulate $z_i; \ i \neq j = 1, \ldots, k$.

At the reverse death move we must be able to return to $x \in \mathbb{R}^k$ from $T_{b,z}(x,\epsilon) \in \mathbb{R}^{k+1}$.

We select $g_{j,z_j = 1}(x_j,\epsilon)$ with probability $1/(k+1)$, then select $g_{j,z_j = -1}(x_j,\epsilon)$ without replacement with probability $1/k$, take their respective backward transformations and finally take the resultant average. Thus, although it is not necessary to simulate $z_j$ here, we must simulate $z_i; \ i \neq j = 1, \ldots, k$ for the co-ordinates after re-labelling them appropriately to correspond to the remaining $(k+1) - 2 = k - 1$ co-ordinates and $z_i; \ i \neq j = 1, \ldots, k$, the latter simulated in the balancing birth move. The transition probability of the death move is hence given by:

$$
\pi(x) \times w_{d,k+1} \times g(\epsilon) \times \prod_{i \neq j = 1}^{k} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \times \frac{1}{k+1} \times \frac{1}{k} \times \left| \frac{\partial(T_{d,z}^{-1}(x(t),\epsilon),\epsilon^*)}{\partial(x(t),\epsilon)} \right| 
$$

$$
\times \min \left\{ 1, (k+1) \times \frac{w_{b,k}}{w_{d,k+1}} \times \prod_{i \neq j = 1}^{k} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \pi(T_{b,z}(x,\epsilon)) \times \left| \frac{\partial(T_{d,z}(x(t),\epsilon),\epsilon^*)}{\partial(x(t),\epsilon)} \right| \right\} 
$$

$$
= g(\epsilon) \times \min \left\{ \pi(T_{b,z}(x,\epsilon)) \times w_{d,k+1} \times \prod_{i \neq j = 1}^{k} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \times \frac{1}{k+1} \times \left| \frac{\partial(T_{d,z}^{-1}(x(t),\epsilon),\epsilon^*)}{\partial(x(t),\epsilon)} \right| , 
$$

$$
\frac{1}{k} \times w_{b,k} \times \prod_{i \neq j = 1}^{k} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \times \pi(x) \right\} .
$$

(3.6)
Noting that 
\[
\left| \frac{\partial (T_d^{-1}(x^{(i)}, \epsilon^*))}{\partial (x^{(i)}, \epsilon)} \right| = \left| \frac{\partial (T_d(x^{(i)}, \epsilon))}{\partial (x^{(i)}, \epsilon)} \right|,
\]
it follows that (3.5) = (3.6), showing that detailed balance holds for the birth and the death moves. The proof of detailed balance for the no-change move type where the dimension remains unchanged is the same as that of TMCMC, and has been proved in the supplement of Dutta & Bhattacharya (2014).

### 3.5 Dependence structure on the distribution of z

In Algorithm 3.1 we have assumed that for \(i \in \{1, \ldots, k\} \setminus \{j\}\) and for \(i \in \{1, \ldots, k\} \setminus \{j,j'\}\) (accordingly as the move-type is birth move or death move), \(z_i\) are independently simulated in every iteration. Although the co-ordinate-wise moves are dependent since the same \(\epsilon\) is used for updating them, more flexible and structured dependence can be induced within the moves in the same way as Algorithm S-4.1 of the supplement of Dutta & Bhattacharya (2014) in the TMCMC context. Such structured dependence allows for selecting the co-ordinate-wise forward or backward transformations in ways that take account of the posterior correlation between the parameters, thus facilitating more efficient moves.

Briefly, at each iteration, for \(i = 1, \ldots, k\), we can reparameterize \(p_i\) and \(q_i\) as
\[
\begin{align*}
    p_i &= \frac{\exp(\psi_{1i})}{\sum_{j=1}^{3} \exp(\psi_{ji})}; \\
    q_i &= \frac{\exp(\psi_{2i})}{\sum_{j=1}^{3} \exp(\psi_{ji})}; \\
    1 - p_i - q_i &= \frac{\exp(\psi_{3i})}{\sum_{j=1}^{3} \exp(\psi_{ji})},
\end{align*}
\]
for \(j = 1, 2, 3\),
\[
(\psi_{1j}, \psi_{2j}, \ldots, \psi_{jk}) \sim N_k (\mu_j, \Sigma_j)
\] (3.8)

independently, where \((\mu_j, \Sigma_j); j = 1, 2, 3\) are to be chosen appropriately by the user. At each iteration of TTMCMC we then first simulate \((\psi_{1j}, \psi_{2j}, \ldots, \psi_{jk}); j = 1, 2, 3\) using (3.8), obtain \(\{p_i, q_i, 1-p_i-q_i; i = 1, \ldots, k\}\) using (3.7); then given \(\{p_i, q_i, 1-p_i-q_i; i = 1, \ldots, k\}\) we simulate \(z_i \sim \text{Multinomial}(1; p_i, q_i, 1-p_i-q_i)\) independently as before, where \(i \in \{1, \ldots, k\} \setminus \{j\}\) or \(i \in \{1, \ldots, k\} \setminus \{j,j'\}\).

As in the case of TMCMC, it can be easily verified that our modified TTMCMC algorithm with this hierarchical dependence structure for the distribution of \(z\) satisfied detailed balance.
4. JUMPING MORE THAN ONE DIMENSIONS AT A TIME

We now consider the situations where instead of jumping one dimension, one wishes to jump several dimensions at a time. That is, we now consider the more general framework where \( x = (x_1, \ldots, x_k) \in \mathbb{R}^k \) and that we wish to increase the dimension to \( k + m \), or to decrease the dimension from \( k + m \) to \( k \), where \( 1 \leq m \leq 2k \).

For an illustrative example, assume that \( k = 3 \) and \( m = 2 \), so that it is required to jump from \( \mathbb{R}^3 \) to \( \mathbb{R}^5 \). Also assume for simplicity the additive transformation. One may anticipate that this can be accomplished by simulating a single positive \( \epsilon \sim g(\cdot) \), selecting, say, \( x_1 \) and \( x_2 \) at random without replacement from \( x = (x_1, x_2, x_3) \), simulating \( z_3 \), and then constructing the birth move \( x' = T_{b,z_3}(x, \epsilon) = (x_1 + a_1 \epsilon, x_1 - a_1 \epsilon, x_2 + a_2 \epsilon, x_2 - a_2 \epsilon, x_3 + z_3 a_3 \epsilon) = (x_1', x_2', x_3', x_4', x_5') \). However, dimension matching is not achieved by this move since the dimension of \( (x, \epsilon) = (x_1, x_2, x_3, \epsilon) \) is 4, while that of \( x' = (x_1', x_2', x_3', x_4', x_5') \) is 5. In other words, the Jacobian \( \frac{\partial(T_{b,z_3}(x, \epsilon))}{\partial(x, \epsilon)} \) is not well-defined.

To get past the dimension-matching problem, we need to simulate two \( \epsilon \)'s from \( g(\cdot) \): \( \epsilon_1 \) for splitting \( x_1 \) into \( x_1 + a_1 \epsilon_1 \) and \( x_1 - a_1 \epsilon_1 \), and \( \epsilon_2 \) for splitting \( x_2 \) into \( x_2 + a_2 \epsilon_2 \) and \( x_2 - a_2 \epsilon_2 \), and to update \( x_3 \) to \( x_3 + z_3 a_3 \epsilon_2 \). Hence the birth move takes the form \( x' = T_{b,z_3}(x, \epsilon_1, \epsilon_2) = (x_1 + a_1 \epsilon_1, x_1 - a_1 \epsilon_1, x_2 + a_2 \epsilon_2, x_2 - a_2 \epsilon_2, x_3 + z_3 a_3 \epsilon_2) = (x_1', x_2', x_3', x_4', x_5') \). Now the dimensions of both \( x' = (x_1', x_2', x_3', x_4', x_5') \) and \( (x, \epsilon_1, \epsilon_2) = (x_1, x_2, x_3, \epsilon_1, \epsilon_2) \) are the same and equals 5; hence the Jacobian

\[
\frac{\partial(T_{b,z_3}(x, \epsilon_1, \epsilon_2))}{\partial(x, \epsilon_1, \epsilon_2)} = \frac{\partial(x_1 + a_1 \epsilon_1, x_1 - a_1 \epsilon_1, x_2 + a_2 \epsilon_2, x_2 - a_2 \epsilon_2, x_3 + z_3 a_3 \epsilon_2)}{\partial(x_1, x_2, x_3, \epsilon_1, \epsilon_2)} = 4a_1 a_2,
\]

is well-defined. The acceptance probability of the birth move in this example is given by

\[
a_b(x, \epsilon_1, \epsilon_2) = \min \left\{ 1, \frac{1}{(3 + 2)(3 + 1)} \times \frac{w_{d,5}}{w_{b,3}} \times \frac{p_3^{I_{(1)}(z_3)} q_3^{I_{(-1)}(z_3)}}{p_3^{I_{(1)}(z_3)} q_3^{I_{(-1)}(z_3)}} \times \frac{\pi(x')}{{\pi(x)}} \times \left| \frac{\partial(T_{b,z_3}(x, \epsilon_1, \epsilon_2))}{\partial(x, \epsilon_1, \epsilon_2)} \right| \right\}
= \min \left\{ 1, \frac{1}{20} \times \frac{w_{d,5}}{w_{b,3}} \times \frac{p_3^{I_{(1)}(z_3)} q_3^{I_{(-1)}(z_3)}}{p_3^{I_{(1)}(z_3)} q_3^{I_{(-1)}(z_3)}} \times \frac{\pi(x')}{{\pi(x)}} \times 4a_1 a_2 \right\}.
\]

(4.1)

For the corresponding death move, that is, for moving from \( x' = (x_1', x_2', x_3', x_4', x_5') \) to \( x'' = \)
equations yield \( \epsilon \) death move, \( x \) general TTMCMC algorithm for jumping \( m \), \( \epsilon \), \( T \), \( z \) • • •

Thus, in general, for moving from dimension \( t \), \( m \) •, we must have, for the reverse of this death move, \( x'' + a_1 \epsilon_1 = x'_1, x'' - a_1 \epsilon_1 = x'_2, x'' + a_2 \epsilon_2 = x'_3, x'' - a_2 \epsilon_2 = x'_4 \). The first two equations yield \( \epsilon_1 = \frac{x'_1 - x''}{2a_1} \) and the last two equations yield \( \epsilon_2 = \frac{x'_2 - x''}{2a_2} \). The Jacobian is given by

\[
\left| \frac{\partial (T_{d,z1}(x', \epsilon_1'; \epsilon_1, \epsilon_2, \epsilon_2, \epsilon_1))}{\partial (x', \epsilon_2, \epsilon_1)} \right| = \frac{1}{4a_1 a_2}.
\]

We accept this death move with probability

\[
a_d(x'', \epsilon_1, \epsilon_2, \epsilon_1^*, \epsilon_2^*) = \min \left\{ 1,5 \times 4 \times \frac{w_{b,3}}{w_{d,5}} \times \frac{P(z^c)}{P(z^a)} \frac{\pi(x'')}{\pi(x')} \left| \frac{\partial (T_{d,z1}(x', \epsilon_2); \epsilon_1^*, \epsilon_2, \epsilon_1)}{\partial (x', \epsilon_2, \epsilon_1)} \right| \right\}
\]

\[
= \min \left\{ 1,20 \times \frac{w_{b,3}}{w_{d,5}} \times \frac{p_3}{p_{13}} \frac{I_{03}(z_3)}{I_{-13}(z_3)} \frac{q_3}{q_{33}} \frac{I_{-13}(z_3)}{I_{-13}(z_3)} \times \frac{\pi(x'')}{\pi(x')} \times \frac{1}{4a_1 a_2} \right\}.
\]

Thus, in general, for moving from dimension \( k \) to dimension \( k + m \), we need to simulate \( \epsilon_1, \ldots, \epsilon_m \) for updating \( x = (x_1, \ldots, x_k) \) to \( x' = (x'_1, x'_2, \ldots, x'_{k+1}, x'_{k+2}, \ldots, x'_{k+m}) \). The associated general TTMCMC algorithm for jumping \( m \) dimensions is provided as Algorithm 4.1

**Algorithm 4.1 General TTMCMC algorithm for jumping \( m \) dimensions.**

- Let the initial value be \( x^{(0)} = R^k \), where \( k \geq m \).

- For \( t = 0,1,2, \ldots \)

1. Generate \( u = (u_1, u_2, u_3) \sim \text{Multinomial}(1; w_{b,k}, w_{d,k}, w_{nc,k}) \).

2. If \( u_1 = 1 \) (increase dimension from \( k \) to \( k + m \)), then
   (a) Randomly select \( m \) co-ordinates from \( x^{(t)} = (x_1^{(t)}, \ldots, x_k^{(t)}) \) without replacement. Let \( j_m = (j_1, \ldots, j_m) \) denote the chosen co-ordinates.

   (b) Generate \( \epsilon_m = (\epsilon_1, \ldots, \epsilon_m) \sim g(\cdot) \) and for \( i = 1, \ldots, k; \ i \neq j_1, \ldots, j_m \), simulate \( z_i \sim \text{Multinomial}(1; p_i, q_i, 1 - p_i - q_i) \) independently.

   (c) Propose the birth move as follows: apply the transformation \( x_i^{(t)} \rightarrow g_{i,z_i}(x_i^{(t)}, \epsilon_1) \) for \( i \in \{1, \ldots, k\} \setminus j_m \) and, for each \( \ell \in j_m \),
split $x^{(t)}_\ell$ into $g_{\ell,z_\ell=1}(x^{(t)}_\ell, \epsilon_\ell)$ and $g_{\ell,z_\ell=-1}(x^{(t)}_\ell, \epsilon_\ell)$. In other words, the birth move is given by:

$$x' = T_{b,z}(x^{(t)}, \epsilon_m) = (g_{1,z_1}(x^{(t)}_1, \epsilon_1), \ldots, g_{j_1-1,z_{j_1-1}}(x^{(t)}_{j_1-1}, \epsilon_1),$$

$$g_{j_1,z_{j_1}=1}(x^{(t)}_{j_1}, \epsilon_1), g_{j_1,z_{j_1}=-1}(x^{(t)}_{j_1}, \epsilon_1), g_{j_1+1,z_{j_1+1}}(x^{(t)}_{j_1+1}, \epsilon_1), \ldots,$$

$$g_{j_2-1,z_{j_2-1}}(x^{(t)}_{j_2-1}, \epsilon_1), g_{j_2,z_{j_2}=1}(x^{(t)}_{j_2}, \epsilon_2), g_{j_2,z_{j_2}=-1}(x^{(t)}_{j_2}, \epsilon_2),$$

$$g_{j_2+1,z_{j_2+1}}(x^{(t)}_{j_2+1}, \epsilon_1), \ldots, g_{j_m-1,z_{j_m-1}}(x^{(t)}_{j_m-1}, \epsilon_1), g_{j_m,z_{j_m}=1}(x^{(t)}_{j_m}, \epsilon_m),$$

$$g_{j_m,z_{j_m}=-1}(x^{(t)}_{j_m}, \epsilon_m), g_{j_m+1,z_{j_m+1}}(x^{(t)}_{j_m+1}, \epsilon_1), \ldots, g_{k,z_k}(x^{(t)}_k, \epsilon_1)).$$

Re-label the $k+m$ elements of $x'$ as $(x'_1, x'_2, \ldots, x'_{k+m})$. Notice that except for the co-ordinates $x^{(t)}_{j_1}, x^{(t)}_{j_2}, \ldots, x^{(t)}_{j_m}$, for which we use $\epsilon_1, \epsilon_2, \ldots, \epsilon_m$ respectively for updating, for all the remaining co-ordinates we use only $\epsilon_1$.

(d) Calculate the acceptance probability of the birth move $x'$:

$$a_b(x^{(t)}, \epsilon_m) = \min \left\{ 1, \frac{1}{(k + m)_m} \times \frac{w_{d,k+m}}{w_{b,k}} \times \frac{P_{(j_m)}(z^c)}{P_{(j_m)}(z)} \times \frac{\pi(x')}{\pi(x^{(t)})} \left| \frac{\partial(T_{b,z}(x^{(t)}, \epsilon_m))}{\partial(x^{(t)}, \epsilon_m)} \right| \right\},$$

where for integers $a > 0$ and $r > 0$ with $a > (r-1)$, we define $(a)_r = a \times (a - 1) \times (a - r + 1)$. Also,

$$P_{(j_m)}(z) = \prod_{i \in \{1,\ldots,k\} \setminus j_m} p_i^{I^{(1)}(z_i)} q_i^{I^{(-1)}(z_i)},$$

and

$$P_{(j_m)}(z^c) = \prod_{i \in \{1,\ldots,k\} \setminus j_m} p_i^{I^{(1)}(z_i^c)} q_i^{I^{(-1)}(z_i^c)}.$$

(e) Set

$$x^{(t+1)} = \begin{cases} x' & \text{with probability} \quad a_b(x^{(t)}, \epsilon) \\ x^{(t)} & \text{with probability} \quad 1 - a_b(x^{(t)}, \epsilon). \end{cases}$$

3. If $u_2 = 1$ (decrease dimension from $k$ to $k - m$, for $k \geq 2m$), then
(a) Generate $\epsilon_m = (\epsilon_1, \ldots, \epsilon_m) \sim g(\cdot)$.

(b) Randomly, without replacement, select co-ordinates $j_m = (j_1, \ldots, j_m)$ and $j'_m = (j'_1, \ldots, j'_m)$ from $x = (x_1, \ldots, x_k)$. For $\ell = 1, \ldots, m$, let $x_{\ell}^* = (g_{\ell,j_e^*} = 1(x_{\ell}, \epsilon_\ell) + g_{\ell,j'_e^*} = 1(x_{\ell}', \epsilon_\ell))/2$; replace the co-ordinate $x_{\ell}^*$ by the average $x_{\ell}'$ and delete $x_{\ell}'$.

(c) Simulate $z$ by generating independently, for $i \in \{1, \ldots, k\} \setminus j_m$, $z_i \sim \text{Multinomial}(1; p_i, q_i, 1 - p_i - q_i)$.

(d) For $i \in \{1, \ldots, k\} \setminus j_m$, apply the transformation $x_i' = g_{i,z_i}(x_i^{(t)}, \epsilon_1)$.

(e) Propose the following death move:

$$x' = T_{d,z}(x^{(t)}, \epsilon_m) = (g_{1,z_1}(x_1^{(t)}, \epsilon_1), \ldots, g_{j_1-1,z_{j_1-1}}(x_{j_1-1}^{(t)}, \epsilon_1), x_{j_1}^*, g_{j_1+1,z_{j_1+1}}(x_{j_1+1}^{(t)}, \epsilon_1), \ldots, g_{j_2-1,z_{j_2-1}}(x_{j_2-1}^{(t)}, \epsilon_1), x_{j_2}^*, g_{j_2+1,z_{j_2+1}}(x_{j_2+1}^{(t)}, \epsilon_1), \ldots, g_{j_m-1,z_{j_m-1}}(x_{j_m-1}^{(t)}, \epsilon_1), x_{j_m}^*, g_{j_m+1,z_{j_m+1}}(x_{j_m+1}^{(t)}, \epsilon_1), \ldots, g_{k,z_k}(x_k^{(t)}, \epsilon_1)).$$

Re-label the elements of $x'$ as $(x'_1, x'_2, \ldots, x'_{k-m})$.

(f) For $\ell = 1, \ldots, m$, solve for $\epsilon_\ell^*$ from the equations $g_{\ell,z_\ell}(x_{\ell}^*, \epsilon_\ell^*) = x_{\ell}^*$ and $g_{\ell,z'_\ell}(x_{\ell}', \epsilon_\ell^*) = x_{\ell}'$ and express $\epsilon_\ell^*$ in terms of $x_{\ell}^*$ and $x_{\ell}'$. Let $\epsilon_m^* = (\epsilon_1^*, \ldots, \epsilon_m^*)$.

(g) Calculate the acceptance probability of the death move:

$$a_d(x^{(t)}, \epsilon_m, \epsilon_m^*)$$

$$= \min \left\{ 1, (k)_m \times \frac{w_{k-m}}{w_{d,k}} \times \frac{P(j_m,j'_m)(z^c)}{P(j_m,j'_m)(z)} \left| \frac{\partial(T_{d,z}(x^{(t)}, \epsilon_m), \epsilon_m^*, \epsilon_m)}{\partial(x^{(t)}, \epsilon_m)} \right| \right\},$$

where

$$P(j_m,j'_m)(z) = \prod_{i \in \{1, \ldots, k\} \setminus \{j_m,j'_m\}} \frac{\prod_{l=1}^d I_{l(z_i)} q_i}{I_{l-1}(z_i)} p_i^{I_{l+1}(z_i)},$$

and

$$P(j_m,j'_m)(z^c) = \prod_{i \in \{1, \ldots, k\} \setminus \{j_m,j'_m\}} \frac{\prod_{l=1}^d I_{l(z_i^c)} q_i}{I_{l-1}(z_i^c)} p_i^{I_{l+1}(z_i^c)}.$$
(h) Set
\[ x^{(t+1)} = \begin{cases} 
  x' & \text{with probability } a_d(x^{(t)}, \epsilon_m, \epsilon_m^*) \\
  x^{(t)} & \text{with probability } 1 - a_d(x^{(t)}, \epsilon_m, \epsilon_m^*) 
\end{cases} \]

4. If \( u_3 = 1 \) (dimension remains unchanged), then implement steps (1), (2), (3) of Algorithm 3.1 of Dutta & Bhattacharya (2014).

- End for

### 4.1 Detailed balance for Algorithm 4.1

To see that detailed balance is satisfied for the birth and death moves, note that associated with the birth move, the probability of transition \( x \in \mathbb{R}^k \mapsto T_{b,z}(x, \epsilon_m) \in \mathbb{R}^{k+m} \), with \( k \geq m \), is given by:

\[
\pi(x) \times \frac{1}{(k)_m} \times w_{b,k} \times \prod_{i=1}^{m} g(\epsilon_i) \times \prod_{i \in \{1, \ldots, k\} \setminus j_m} p_i^{I_{(1)}(z_i) I_{(-1)}(z_i)} q_i^{I_{(1)}(z_i) I_{(-1)}(z_i)} \\
\times \min \left\{ 1, \frac{1}{(k + m)_m} \times \prod_{i \in \{1, \ldots, k\} \setminus j_m} p_i^{I_{(1)}(z_i^c) I_{(-1)}(z_i^c)} q_i^{I_{(1)}(z_i) I_{(-1)}(z_i)} \\
\times \frac{\pi(T_{b,z}(x, \epsilon_m))}{\pi(x)} \times \left| \frac{\partial(T_{b,z}(x^{(t)}, \epsilon_m))}{\partial(x^{(t)}, \epsilon_m)} \right| \right\} \\
= \prod_{i=1}^{m} g(\epsilon_i) \times \min \left\{ \pi(x) \times w_{b,k} \times \frac{1}{(k)_m} \times \prod_{i \in \{1, \ldots, k\} \setminus j_m} p_i^{I_{(1)}(z_i) I_{(-1)}(z_i)} q_i^{I_{(1)}(z_i) I_{(-1)}(z_i)} , \frac{1}{(k)_m} \times \frac{1}{(k + m)_m} \right. \\
\times w_{d,k+m} \times \prod_{i \in \{1, \ldots, k\} \setminus j_m} p_i^{I_{(1)}(z_i^c) I_{(-1)}(z_i^c)} q_i^{I_{(1)}(z_i^c) I_{(-1)}(z_i^c)} \pi(T_{b,z}(x, \epsilon_m)) \times \left| \frac{\partial(T_{b,z}(x^{(t)}, \epsilon_m))}{\partial(x^{(t)}, \epsilon_m)} \right| \left. \right\}. \tag{4.4} \]
The transition probability of the reverse death move is given by:

\[
\pi(x) \times w_{d,k+m} \times \prod_{i=1}^{m} g(\epsilon_i) \times \prod_{i \in \{1,...,k\} \setminus J_m} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \\
\times \frac{1}{(k+m)m} \times \frac{1}{(k)m} \times \left| \frac{\partial(T_{d,k}^{-1}(x^{(t)}, \epsilon_m), \epsilon^*_m, \epsilon_m)}{\partial(x^{(t)}, \epsilon_m)} \right| \\
\times \min \left\{ 1, \frac{w_{b,k}}{w_{d,k+m}} \times \prod_{i \in \{1,...,k\} \setminus J_m} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \times \frac{\pi(T_{b,z}(x, \epsilon_m))}{\pi(T_{b,z}(x, \epsilon_m))} \times \left| \frac{\partial(T_{d,k}^{-1}(x^{(t)}, \epsilon_m), \epsilon^*_m, \epsilon_m)}{\partial(x^{(t)}, \epsilon_m)} \right| \right\} \\
= \prod_{i=1}^{m} g(\epsilon_i) \times \min \left\{ \pi(T_{b,z}(x, \epsilon_m)) \times w_{d,k+m} \times \prod_{i \in \{1,...,k\} \setminus J_m} p_i^{I(1)(z_i)} q_i^{I(-1)(z_i)} \times \frac{1}{(k)m} \times \frac{1}{(k+m)m} \times \left| \frac{\partial(T_{d,k}^{-1}(x^{(t)}, \epsilon_m), \epsilon^*_m, \epsilon_m)}{\partial(x^{(t)}, \epsilon_m)} \right| \right\},
\]

(4.5)

Noting that \( \left| \frac{\partial(T_{d,k}^{-1}(x^{(t)}, \epsilon_m), \epsilon^*_m, \epsilon_m)}{\partial(x^{(t)}, \epsilon_m)} \right| = \left| \frac{\partial(T_{b,z}(x^{(t)}, \epsilon_m))}{\partial(x^{(t)}, \epsilon_m)} \right| \), it follows that (4.4) = (4.5), showing that detailed balance holds for the birth and the death moves.

Note that exactly as discussed in Section 3.5 we can incorporate a hierarchical dependence structure on the distribution of \( z \) in Algorithm 4.1, which does not hamper the detailed balance condition.

5. Jumping More Than One Dimensions at a Time When There Several Sets of Parameters Are Related

It is often the case that changing dimension of one set of parameters forces changing dimension of the other sets of parameters accordingly. For instance, in a mixture problem with unknown number of components (see, for example, Richardson & Green (1997)), where the \( i \)-th component is characterized by the mean and standard deviation \( (\mu_i, \sigma_i) \), when the dimension of the current \( k \)-dimensional mean vector \( (\mu_1, \ldots, \mu_k) \) is increased by one, then one must simultaneously increase...
the dimension of the current \(k\)-dimensional vector of standard deviations \((\sigma_1, \ldots, \sigma_k)\) by one. In this section we extend TTMC to general situations of this kind.

For an illustrative example, assume that the Markov chain is currently at the state \((\mu_1, \log(\sigma_1)), (\mu_2, \log(\sigma_2))\) \((\mu_1, \mu_2, \log(\sigma_1), \log(\sigma_2)) \in \mathbb{R}^2 \times \mathbb{R}^2\). Let \(x = (x_1, x_2, x_3, x_4) = (\mu_1, \mu_2, \log(\sigma_1), \log(\sigma_2))\). Suppose that it is required to increase the dimension to \(\mathbb{R}^3 \times \mathbb{R}^3\) using the additive transformation.

To achieve dimension matching in this problem, as in Section 4 here also we need to simulate two \(\epsilon\)’s from \(g(\cdot)\): \(\epsilon_1\) for splitting \(x_1\) into \(x_1 + a_1 \epsilon_1\) and \(x_1 - a_1 \epsilon_1\) and \(\epsilon_2\) for splitting \(x_3\) into \(x_3 + a_3 \epsilon_2\) and \(x_3 - a_3 \epsilon_2\). With the same \(\epsilon_1\) we can also update \(x_2\) to \(x_2 + z_2 a_2 \epsilon_1\) and \(x_4\) to \(x_4 + z_4 a_4 \epsilon_1\). Note that it is possible to use \(\epsilon_2\) to split \(x_3\) into \(x_3 + a_3 \epsilon_2\) and \(x_3 - a_3 \epsilon_2\) and update \(x_4\) to \(x_4 + z_4 a_4 \epsilon_2\), instead of using \(\epsilon_1\) to update \(x_4\) to \(x_4 + z_4 a_4 \epsilon_1\). That is, we can use \(\epsilon_1\) and \(\epsilon_2\) for updating the sub-blocks \((\mu_1, \mu_2)\) and \((\log(\sigma_1), \log(\sigma_2))\), respectively. However, using \(\epsilon_1\) for both the sub-blocks induce dependence between the updates through the common \(\epsilon_1\) and hence may be desirable since we are updating all the sub-blocks in a single block. Hence, in this article, we confine ourselves to using a common \(\epsilon_1\) across the sub-blocks.

Hence, in this example, the birth move takes the form \(x' = T_{b_{22}, z}(x, \epsilon_1, \epsilon_2) = (x_1 + a_1 \epsilon_1, x_1 - a_1 \epsilon_1, x_2 + z_2 a_2 \epsilon_1, x_3 + a_3 \epsilon_2, x_3 - a_3 \epsilon_2, x_4 + z_4 a_4 \epsilon_1, x_4 - z_4 a_4 \epsilon_1) = (x_1', x_2', x_3', x_4', x_5', x_6')\). Now the dimensions of both \(x' = (x_1', x_2', x_3', x_4', x_5', x_6')\) and \((x, \epsilon_1, \epsilon_2) = (x_1, x_2, x_3, x_4, \epsilon_1, \epsilon_2)\) is 6, and so the Jacobian

\[
\left| \frac{\partial (T_{b_{22}, z}(x, \epsilon_1, \epsilon_2))}{\partial (x, \epsilon_1, \epsilon_2)} \right| = \left| \frac{\partial (x_1 + a_1 \epsilon_1, x_1 - a_1 \epsilon_1, x_2 + z_2 a_2 \epsilon_1, x_3 + a_3 \epsilon_2, x_3 - a_3 \epsilon_2, x_4 + z_4 a_4 \epsilon_1)}{\partial (x_1, x_2, x_3, x_4, \epsilon_1, \epsilon_2)} \right| = 4a_1 a_3,
\]

is well-defined. The acceptance probability of the birth move in this example is given by

\[
a_b(x, \epsilon_1, \epsilon_2) = \min \left\{ \frac{1}{3} \times \frac{w_{d, 6}}{w_{b, 4}} \times \prod_{i=2,4} \frac{p_{i}}{q_{i}} \frac{I_{1}(z_{i}^{\prime})}{I_{1}(z_{i})} \frac{I_{-1}(z_{i})}{I_{-1}(z_{i})} \times \frac{\pi(x')}{\pi(x)} \times \left| \frac{\partial (T_{b_{22}, z}(x, \epsilon_1, \epsilon_2))}{\partial (x, \epsilon_1, \epsilon_2)} \right| \right\}
= \min \left\{ \frac{1}{3} \times \frac{w_{d, 6}}{w_{b, 4}} \times \prod_{i=2,4} \frac{p_{i}}{q_{i}} \frac{I_{1}(z_{i}^{\prime})}{I_{1}(z_{i})} \frac{I_{-1}(z_{i})}{I_{-1}(z_{i})} \frac{\pi(x')}{\pi(x)} \times 4a_1 a_3 \right\}.
\]

(5.1)

For the corresponding death move, that is, for moving from \(x' = (x_1', x_2', x_3', x_4', x_5', x_6')\) to \(x'' = T_{d, z}(x', \epsilon_2) = (\frac{x_1' + x_2'}{2}, \frac{x_3' + x_5'}{2}, x_4' + z_4 a_4 \epsilon_2)\), we must have, for the reverse of this death move, \(x_1'' = x_1', x_1'' - a_1 \epsilon_1 = x_2', x_2'' + a_3 \epsilon_2 = x_4', x_3'' - a_3 \epsilon_2 = x_5'\).
We accept this death move with probability

\[
\frac{a_d(x'', \epsilon_1, \epsilon_2, \epsilon_1^*, \epsilon_2^*)}{\min \left\{ 1, 3 \times \frac{w_{b,4}}{w_{d,6}} \times \frac{P(z'') \pi(x'') \pi(x')}{P(z) \pi(x')} \right\}} = \min \left\{ 1, 3 \times \frac{w_{b,4}}{w_{d,6}} \times \prod_{i=2,4} \frac{p_i^{I_1(z_i)} q_i^{I_{-1}(z_i)}}{p_i^{I_1(z_i)} q_i^{I_{-1}(z_i)}} \times \frac{\pi(x'')}{\pi(x')} \times \frac{1}{4a_1a_3} \right\}.
\]

(5.3)

Note that for given \(k\), in general mixture problems we would need to update \( (\mu_1, \mu_2, \ldots, \mu_k), (\log(\sigma_1), \log(\sigma_2), \ldots, \log(\sigma_k)), (\omega_1, \omega_2, \ldots, \omega_k) \), where, for \( j = 1, \ldots, k\), \( \omega_j \) correspond to the mixing proportion \( \pi_j \), where \( \sum_{j=1}^k \pi_j = 1 \), as \( \pi_j = \exp(\omega_j)/\sum_{\ell=1}^k \exp(\omega_j) \). If \( (a_{\mu_1}, \ldots, a_{\mu_k}), (a_{\sigma_1}, \ldots, a_{\sigma_k}), (a_{\omega_1}, \ldots, a_{\omega_k}) \) are the scales associated with the three sub-blocks, then the Jacobian for the birth move, if the \( j \)-th component is selected, is given by \( 8a_{\mu_j} a_{\sigma_j} a_{\omega_j} \), and that for the death move is \( (8a_{\mu_j} a_{\sigma_j} a_{\omega_j})^{-1} \). See Section 9 where we apply TTMCMC to normal mixtures with unknown number of components, illustrated with three real data sets.

In general, \( x \in \mathbb{R}^{mk} \) may be of the form \( \left( x_1, x_2, \ldots, x_m \right) \), where \( x_\ell = (x_{\ell,1}, x_{\ell,2}, \ldots, x_{\ell,k}) \) for \( \ell = 1, 2, \ldots, m \), where \( m \geq 1 \) is an integer. Let us assume that if the dimension of any one \( x_\ell \) is changed, then the dimensions of all other \( x_{\ell'} \); \( \ell' \neq \ell \) must also change accordingly, as in the above example. We then have the following general TTMCMC algorithm provided as Algorithm 5.1.

**Algorithm 5.1** General TTMCMC algorithm for jumping \( m \) dimensions with \( m \) related sets of co-ordinates.

- Let the initial value be \( x^{(0)} \in \mathbb{R}^{mk} \), where \( k \geq m \).
- For \( t = 0, 1, 2, \ldots \)
  1. Generate \( u = (u_1, u_2, u_3) \sim \text{Multinomial}(1; w_{b,k}, w_{d,k}, w_{nc,k}) \).
2. If \( u_1 = 1 \) (increase dimension from \( mk \) to \( (m+1)k \)), then

(a) Randomly select one co-ordinate from \( x_1^{(t)} = (x_{11}^{(t)}, \ldots, x_{1k}^{(t)}) \) without replacement. Let \( j \) denote the chosen co-ordinate.

(b) Generate \( \epsilon_m = (\epsilon_1, \ldots, \epsilon_m) \overset{iid}{\sim} g(\cdot) \) and for \( i \in \{1, \ldots, k\} \setminus \{j\} \) simulate \( z_{\ell,i} \sim \text{Multinomial}(1;p_{\ell,i}, q_{\ell,i}, 1-p_{\ell,i}-q_{\ell,i}) \) independently, for every \( \ell = 1, \ldots, m \).

(c) Propose the birth move as follows: for each \( \ell = 1, \ldots, m \), apply the transformation \( x_{\ell,i}^{(t)} \rightarrow g_{\ell,z_{\ell,i}}(x_{\ell,i}^{(t)}, \epsilon_1) \) for \( i \in \{1, \ldots, k\} \setminus \{j\} \) and, for each \( \ell \in \{1, \ldots, m\} \), split \( x_{\ell,j}^{(t)} \) into \( g_{\ell,z_{\ell,j}=1}(x_{\ell,j}^{(t)}, \epsilon_\ell) \) and \( g_{\ell,z_{\ell,j}=-1}(x_{\ell,j}^{(t)}, \epsilon_\ell) \). In other words, let \( x' = T_{b,z}(x^{(t)}, \epsilon_m) = (x_1', \ldots, x_m') \) denote the complete birth move, where, for \( \ell = 1, \ldots, m \), \( x'_\ell \) is given by

\[
x'_\ell = (g_{\ell,z_{\ell,1}}(x_{\ell,1}^{(t)}, \epsilon_1), \ldots, g_{j-1,z_{\ell,j-1}}(x_{\ell,j-1}^{(t)}, \epsilon_1), g_{j,z_{\ell,j}=1}(x_{\ell,j}^{(t)}, \epsilon_\ell), g_{j,z_{\ell,j}=-1}(x_{\ell,j}^{(t)}, \epsilon_\ell), g_{j+1,z_{\ell,j+1}}(x_{\ell,j+1}^{(t)}, \epsilon_1), \ldots, g_{k,z_{\ell,k}}(x_{\ell,k}^{(t)}, \epsilon_1)).
\]

Re-label the \( k+1 \) elements of \( x'_\ell \) as \( (x'_{\ell,1}, x'_{\ell,2}, \ldots, x'_{\ell,k+1}) \). Notice that, following the discussion presented in the illustrative example in the beginning of this section, we use \( \epsilon_\ell \) only for splitting \( x_{\ell,j}^{(t)} \) into \( g_{j,z_{\ell,j}=1}(x_{\ell,j}^{(t)}, \epsilon_\ell) \) and \( g_{j,z_{\ell,j}=-1}(x_{\ell,j}^{(t)}, \epsilon_\ell) \). To update the remaining co-ordinates, we use \( \epsilon_1 \) for all the blocks.

(d) Calculate the acceptance probability of the birth move \( x' \):

\[
a_b(x^{(t)}, \epsilon_m) = \min \left\{ 1, \frac{1}{k+1} \times \frac{w_{d,k+1}}{w_{b,k}} \times \frac{P_{(j)}(z^c)}{P_{(j)}(z)} \times \frac{\pi(x')}{\pi(x^{(t)})} \left| \frac{\partial(T_{b,z}(x^{(t)}, \epsilon_m))}{\partial(x^{(t)}, \epsilon_m)} \right| \right\},
\]

where

\[P_{(j)}(z) = \prod_{\ell=1}^{m} \prod_{i \in \{1, \ldots, k\} \setminus \{j\}} P_{\ell,i}^{I_{(1)}(z_{\ell,i})} q_{\ell,i}^{I_{(-1)}(z_{\ell,i})},\]
and

\[ P_j(z^c) = \prod_{\ell=1}^{m} \prod_{i \in \{1,\ldots,k\}\setminus\{j\}} p_{\ell,i}^{I_\ell(\varepsilon^c_{\ell,i})} q_{\ell,i}^{I_{\ell-1}(\varepsilon^c_{\ell,i})}. \]

(e) Set

\[ x^{(t+1)} = \begin{cases} 
  x' & \text{with probability } a_b(x^{(t)}, \varepsilon_m) \\
  x^{(t)} & \text{with probability } 1 - a_b(x^{(t)}, \varepsilon_m).
\end{cases} \]

3. If \( u_2 = 1 \) (decrease dimension from \( k \) to \( k - m \), for \( k \geq 2m \)),
then

(a) Generate \( \varepsilon_m = (\varepsilon_1, \ldots, \varepsilon_m) \overset{\text{iid}}{\sim} g(\cdot). \)

(b) Randomly, without replacement, select co-ordinates \( j \) and \( j' \) from \( x_1 = (x_{1,1}, \ldots, x_{1,k}) \). For \( \ell = 1, \ldots, m \), let

\[ x_{\ell,j}^* = \left( g_{j,z_{\ell,j}=1}(x_{\ell,j}, \varepsilon_\ell) + g_{j',z_{\ell,j'}=1}(x_{\ell,j'}, \varepsilon_\ell) \right) / 2; \]

replace the co-ordinate \( x_{\ell,j} \) by the average \( x_{\ell,j}^* \) and delete \( x_{\ell,j'} \).

(c) Simulate \( z \) by generating independently, for \( \ell = 1, \ldots, m \) and for \( i \in \{1, \ldots, k\}\setminus\{j, j'\} \), \( z_{\ell,i} \sim \text{Multinomial}(1; p_{\ell,i}, q_{\ell,i}, 1 - p_{\ell,i} - q_{\ell,i}). \)

(d) For \( \ell = 1, \ldots, m \) and for \( i \in \{1, \ldots, k\}\setminus\{j, j'\} \), apply the transformation

\[ x_{\ell,i}' = g_{i,z_{\ell,i}}(x_{\ell,i}^{(t)}, \varepsilon_1). \]

(e) Propose the following death move \( x' = T_{d,z}(x^{(t)}, \varepsilon_m) = (x_1', \ldots, x_m') \)
where for \( \ell = 1, \ldots, m \), \( x_\ell' \) is given by

\[ x_{\ell,j}' = \left( g_{1,z_{\ell,1}}(x_{\ell,1}^{(t)}, \varepsilon_1), \ldots, g_{j-1,z_{\ell,j-1}}(x_{\ell,j-1}^{(t)}, \varepsilon_1), x_{\ell,j}^*, g_{j+1,z_{\ell,j+1}}(x_{\ell,j+1}^{(t)}, \varepsilon_1), \ldots, g_{k,z_{\ell,k}}(x_{\ell,k}^{(t)}, \varepsilon_1) \right). \]

Re-label the elements of \( x'_\ell \) as \( (x_{\ell,1}', x_{\ell,2}', \ldots, x_{\ell,k-1}') \).

(f) For \( \ell = 1, \ldots, m \), solve for \( \varepsilon^*_{\ell} \) from the equations \( g_{\ell,z_{\ell,j}=1}(x_{\ell,j}^*, \varepsilon^*_{\ell}) = x_{\ell,j} \) and \( g_{\ell,z_{\ell,j'}=-1}(x_{\ell,j'}^*, \varepsilon^*_{\ell}) = x_{\ell,j'} \) and express \( \varepsilon^*_{\ell} \) in terms of \( x_{\ell,j} \) and \( x_{\ell,j'} \). Let \( \varepsilon^*_m = (\varepsilon^*_1, \ldots, \varepsilon^*_m). \)
(g) Calculate the acceptance probability of the death move:

\[ a_d(x^{(t)}, \epsilon_m, \epsilon^*_m) = \min \left\{ 1, k \times \frac{w_{b,k-m}}{w_{d,k}} \times \frac{P_{(j,j')} (z^c)}{P_{(j,j')} (z)} \times \frac{\pi(x')}{\pi(x^{(t)})} \left| \frac{\partial (T_{d,z} (x^{(t)}, \epsilon_m, \epsilon^*_m), \epsilon_m, \epsilon^*_m)}{\partial (x^{(t)}, \epsilon_m)} \right| \right\}, \]

where

\[ P_{(j,j')} (z) = \prod_{\ell=1}^m \prod_{i \in \{1, \ldots, k\} \setminus \{j, j'\}} p_{\ell,i}^{I_{\{1\}}(z_{\ell,i})} q_{\ell,i}^{I_{\{-1\}}(z_{\ell,i})}, \]

and

\[ P_{(j,j')} (z^c) = \prod_{\ell=1}^m \prod_{i \in \{1, \ldots, k\} \setminus \{j, j'\}} p_{\ell,i}^{I_{\{1\}}(z_{c,\ell,i})} q_{\ell,i}^{I_{\{-1\}}(z_{c,\ell,i})}. \]

(h) Set

\[ x^{(t+1)} = \begin{cases} 
  x' & \text{with probability } a_d(x^{(t)}, \epsilon_m, \epsilon^*_m) \\
  x^{(t)} & \text{with probability } 1 - a_d(x^{(t)}, \epsilon_m, \epsilon^*_m). 
\end{cases} \]

4. If \( u_3 = 1 \) (dimension remains unchanged), then implement steps (1), (2), (3) of Algorithm 3.1 of Dutta & Bhattacharya (2014).

- End for

It can be easily checked that detailed balance is satisfied for Algorithm [5.1].

ALgorithms 3.1, 4.1 and 5.1 provide concrete ways to implement our TTMCMC procedure, in general variable dimensional problems. The additive and the multiplicative transformations, and combinations of them can be effectively utilized, in conjunction with just a few, fixed number of \( \epsilon \)’s to accomplish transdimensional movement. The methodology reduces the variable dimensional problem to effectively fixed dimensional, indexed by a fixed and small number of \( \epsilon \)’s. The fixed and low-dimensional nature of \( \epsilon \) (or the set \( \{\epsilon_1, \ldots, \epsilon_m\} \)) ensures reasonably high acceptance rate. Thus, our algorithms can be viewed as providing valid, automated schemes for Bayesian inference in general variable dimensional problems.

It is now time to illustrate TTMCMC with challenging practical examples – the normal mixture set-up with unknown number of components provide an important and interesting premise in this regard. In the next section we provide details of the set-up.
6. THE NORMAL MIXTURE SET UP WITH UNKNOWN NUMBER OF COMPONENTS

We illustrate TTMCMC on mixture models with unknown number of components with application to the well-studied enzyme, acidity and the galaxy data sets. Richardson & Green (1997) modeled these data sets using parametric normal mixtures and applied RJMCMC for Bayesian inference. On the other hand, Bhattacharya (2008) (see also Escobar & West (1995)) proposed a semiparametric normal mixture model based on Dirichlet process and used Gibbs sampler for Bayesian inference.

6.1 Normal mixture

Let the data points \(y_1, \ldots, y_n\) be independently and identically (\(iid\)) distributed as the normal mixture of the following form: for \(i = 1, \ldots, n\)

\[
f(y_i|\nu_k, \tau_k, \pi_k, k) = \sum_{j=1}^{k} \pi_j \sqrt{\frac{\tau_j}{2\pi}} \exp\left\{-\frac{\tau_j}{2} (y_i - \nu_j)^2\right\},
\]

(6.1)

where \(\nu_k = (\nu_1, \ldots, \nu_k)\), \(\tau_k = (\tau_1, \ldots, \tau_k)\), \(\pi_k = (\pi_1, \ldots, \pi_k)\). Given \(k > 0\), for each \(j\), \(-\infty < \nu_j < \infty\), \(\tau_j > 0\), \(0 < \pi_j < 1\) such that \(\sum_{j=1}^{k} \pi_j = 1\). We allow \(k\) to be random, so that the dimension of the model (that is, the number of the component parameters) is random.

6.2 Prior structure

Note that the semiparametric mixture model of Bhattacharya (2008) can be viewed as a parametric model when the scale parameter associated with the base distribution of the Dirichlet process prior tends to infinity. Hence, from that perspective, the base distribution of \(\nu_j\) and \(\tau_j\) may be regarded as the respective priors for our current parametric mixture context. Thus, motivated by Bhattacharya (2008), we consider the following prior for \(\nu\) and \(\tau\):

\[
[\tau_j] \sim \mathcal{G} \left( \frac{s}{2}, \frac{S}{2} \right)
\]

(6.2)

\[
[\nu_j|\tau_j] \sim N \left( \nu_0, \frac{\psi}{\tau_j} \right).
\]

(6.3)

In the above, by \(\mathcal{G}(a, b)\) we mean a gamma distribution with mean \(a/b\) and variance \(a/b^2\) and \(N(\mu, \sigma^2)\) denotes the normal distribution with mean \(\mu\) and variance \(\sigma^2\). Specifications of the values of the hyperparameters \(s, S, \nu_0, \psi\) are discussed in the context of applications.
For the implementation purpose, we reparameterize \( \tau_j \) as \( \exp(\tau_j^*) \), where \( \tau_j^* \sim \log (G(s/2, S/2)) \). Since \(-\infty < \tau_j^* < \infty\), this reparameterization frees the parameter space from any restrictions, allowing TTMCMC to move freely. We denote \( (\tau_1^*, \ldots, \tau_k^*) \) by \( \tau_k^* \).

For \( \pi \) we propose the following prior based on reparameterization: for \( j = 1, \ldots, k \),

\[
\pi_j = \frac{\exp(\omega_j)}{\sum_{\ell=1}^k \exp(\omega_\ell)}; \quad \omega_1, \ldots, \omega_k \overset{iid}{\sim} \mathcal{N}(\mu_\omega, \sigma_\omega^2). \tag{6.4}
\]

Thus, we need to update \( \omega_k = (\omega_1, \ldots, \omega_k) \), instead of \( \pi \), using TTMCMC. Note that, for the normal prior on \( \omega_j \), the induced prior on \( \pi \) is not the traditional Dirichlet distribution. However, if \( \omega_j \sim \log (G(\alpha_j, 1)) \) independently, for \( \alpha_j > 0; \ j = 1, \ldots, k \), then \( \pi \sim \mathcal{D}(\alpha_1, \ldots, \alpha_k) \), the Dirichlet distribution with parameters \( \alpha_1, \ldots, \alpha_k \). For our applications we consider both kinds of distributions for \( \omega \).

As regards the prior on \( k \), we consider the uniform distribution on \( \{1, 2, \ldots, 30\} \), the truncated Poisson distribution on \( \{1, 2, \ldots, 30\} \) and the discretized normal with mean \( \mu_k \) and variance \( \sigma_k^2 \) on \( \{1, 2, \ldots, 30\} \).

6.3 Label switching

It is well-known that the mixture likelihood is invariant to permutations (labels) of the component parameters; hence, the mixture parameters are not identifiable. This problem is often known as label-switching. So, if inference on the parameters is of interest, then proper labeling of the components is necessary. Richardson & Green (1997) considered ordering the mean parameters; see also Stephens (2000) for other methods for tackling label switching. However, Lee, Marin, Mengersen & Robert (2009) argue and demonstrate that putting constraints on the prior parameter space can have severe ill effects on both inference and computation. Moreover, there seems to be a subtle question if identifiability is at all desirable when inference regarding clustering of the data is of interest. To consider a simple example, suppose that clustering the dataset \( \{y_1, y_2, y_3, y_4\} \) using a two-component normal mixture model is of interest. Assume that \( \{y_1, y_3\} \) are associated with \( \nu_1 \) and \( \{y_2, y_4\} \) are associated with \( \nu_2 \), where \( \nu_1 < \nu_2 \). But because of this imposed constraint, the clusterings \( \{\{y_1, y_3\}, \{y_2, y_4\}\} \) and \( \{\{y_2, y_4\}, \{y_1, y_3\}\} \) can not be regarded as identical. In
This article our goal is to demonstrate TTMCMC with inference regarding posterior distributions of densities. Since inference on densities is not affected by label switching, we do not concern ourselves with the problem of label switching.

7. SUMMARIZATION OF THE POSTERIOR DISTRIBUTION OF MIXTURE DENSITIES

Note that the mixture setup induces a posterior distribution on mixture densities of the form (6.1). In other words, the set-up provides a way to make Bayesian inference regarding the unknown density of the observed data $y_1, \ldots, y_n$. An obvious candidate of such density estimate is the unconditional posterior expectation of the function

$$f(x|k, \nu_k, \tau_k, \pi_k) = \sqrt{\tau_j} \pi_j \exp\left\{-\frac{\tau_j}{2} (x - \nu_j)^2\right\}; \quad -\infty < x < \infty,$$

with respect to the posterior of $k, \nu, \tau_k, \pi_k$. For empirical purposes, one can just average $f(x|k, \nu_k, \tau_k, \pi_k)$ over TTMCMC samples of $k, \nu, \tau_k, \pi_k$.

Note, however, that the posterior expectation (or the corresponding empirical average) fails to retain the finite mixture form of the resultant density estimate (see also Richardson & Green (1997)). More importantly, although this averaging yields a point density estimate, hitherto there does not seem to be any attempt to quantify the uncertainty of the posterior distribution of the densities having the mixture form with unknown number of components.

Motivated by Mukhopadhyay et al. (2011) who propose a methodology for obtaining the modes and any desired highest posterior density credible regions associated with the posterior distribution of clusterings, here we attempt the same for the posterior distribution of densities having form (6.1). Following Mukhopadhyay et al. (2011) here we propose a definition of “central density”:

**Definition 1** A density $f_0$ is “central” which, for any $\epsilon > 0$ satisfies the following equation:

$$P(\{f : d(f_0, f) < \epsilon\}) = \sup_g P(\{f : d(g, f) < \epsilon\}),$$

for some suitable metric $d$. 

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In this article, we consider the sup-norm metric between any two density functions \( f \) and \( g \), given by
\[
d(f, g) = \sup_{-\infty < x < \infty} |f(x) - g(x)|.
\]
For empirical purpose we evaluate this metric at discrete equidistant points \( x_0, x_1, \ldots, x_m \) covering the effective support of the densities in question.

Observe that \( f_0 \) is the global mode of the posterior distribution of densities as \( \epsilon \to 0 \). If the distribution of \( f \) is unimodal, then the central density remains the same for all \( \epsilon > 0 \). However, for multimodal distributions, the central density varies with \( \epsilon \), signifying existence of local modes, which we define as follows.

**Definition 2** We define \( f_{\text{loc}} \) to be a local mode if
\[
\lim_{\epsilon \downarrow 0} \sup_{g \in \mathcal{N}(f_{\text{loc}}, \eta)} \frac{P \left( \{ f \in \mathcal{N}(f_{\text{loc}}, \eta) : d(f, g) < \epsilon \} \right)}{P \left( \{ f \in \mathcal{N}(f_{\text{loc}}, \eta) : d(f, f_{\text{loc}}) < \epsilon \} \right)} = 1,
\]
where \( \mathcal{N}(f_{\text{loc}}, \eta) = \{ f : f(f_{\text{loc}}, f) < \eta \} \) for some \( \eta > 0 \).

Note that unlike the distribution of clusterings considered by Mukhopadhyay et al. (2011), which is discrete, the distribution of the mixture densities of the form (7.1) is continuous; this is clear since although \( k \), the number of mixture components is at most countable, the parameters \( \nu \), \( \tau \) and \( \pi \) are continuous. Hence, although obtaining the global mode in the case of clusterings is an arduous task, here our problem is relatively easier.

It is nevertheless clear that without the aid of empirical methods the central density function defined in (7.2) cannot be obtained. Using available TTMCMC samples \( \{ f(j) ; j = 1, \ldots, N \} \) of length \( N \), the latter sufficiently large, useful empirical methods can be devised, as we demonstrate in the next section.

### 7.1 Empirical definition of central density function

We define that density \( f^{(j)} \) as “approximately central,” which, for a given small \( \epsilon > 0 \), satisfies the following equation:
\[
f^{(j)} = \arg\max_{1 \leq i \leq N} \frac{1}{N} \# \left\{ f^{(\ell)} ; 1 \leq \ell \leq N : d(f^{(i)}, f^{(\ell)}) < \epsilon \right\}.
\]

The central density \( f^{(j)} \) is easily computable and the ergodic theorem ensures convergence of \( f^{(j)} \) almost surely to the true central density \( f_0 \).
7.2 Construction of desired credible regions of densities

Given a central density \( f^{(j)} \), an approximate 95% posterior density credible region is given by the set \( \{ f^{(\ell)} ; 1 \leq \ell \leq N : d(f^{(\ell)}, f^{(j)}) < \epsilon^* \} \), where \( \epsilon^* \) is such that

\[
\frac{1}{N} \# \{ f^{(\ell)} ; 1 \leq \ell \leq N : d(f^{(\ell)}, f^{(j)}) < \epsilon^* \} \approx 0.95. \tag{7.5}
\]

In (7.5) \( \epsilon^* \) can be chosen adaptively by starting with \( \epsilon^* = 0 \) and then slightly increasing \( \epsilon^* \) by a quantity \( \zeta \) until (7.5) is satisfied. In our applications, we chose \( \zeta = 10^{-5} \). Approximate highest posterior density (HPD) regions can be constructed by taking the union of the highest density regions. Following Mukhopadhyay et al. (2011) we next discuss an adaptive methodology for constructing HPD regions.

7.3 Construction of desired HPD regions of densities

Assume that there are \( \ell \) modes, \( \{ f_1^*, \ldots, f_\ell^* \} \), obtained by varying \( \epsilon \) of the neighborhoods \( \{ f : d(f, f^{(i)}) < \epsilon \}; i = 1, \ldots, N \). Consider the regions \( S_j = \{ f : d(f_j^*, f) < \epsilon_j^* \}; j = 1, \ldots, \ell \). Set, initially, \( \epsilon_1^* = \epsilon_2^* = \cdots = \epsilon_\ell^* = 0 \).

(i) For \( i = 1, \ldots, N \), if the \( i \)-th TTMCMC realization \( f^{(i)} \) does not fall in \( S_j \) for some \( j \), then increase \( \epsilon_j^* \) by a small quantity, say, \( \zeta \).

(ii) Calculate the probability of \( \bigcup_{j=1}^{\ell} S_j \) as \( P = \#\{\bigcup_{j=1}^{\ell} S_j\} / N \).

(iii) Repeat steps (i) and (ii) until \( P \approx 0.95 \) or any desired probability.

In step (i) we implicitly assume that, since \( f^{(i)} \notin S_j \), \( S_j \) must be a region with low probability, so its expansion is necessary to increase the probability. We achieve this expansion by increasing \( \epsilon_j^* \) by \( \zeta \). Thus the sets \( S_j \) are selected adaptively, by adaptively increasing \( \epsilon_j^* \). The desired approximate HPD region is then the final union of the \( S_j \)'s.

8. TTMCMC CONVERGENCE DIAGNOSTICS FOR THE MIXTURE PROBLEM

It is a really challenging task to provide adequate convergence diagnostics for variable dimensional problems. However, armed with our metric-based methodology we can now provide a convergence
diagnostic method for the challenging variable dimensional mixture problem. Following the same principle as Mukhopadhyay et al. (2011), we divide our TTMCMC sample of size $N$ into $m$ equal parts, each part having the same size $N/m$, assuming divisibility of $N$ by $m$. For each such subsample of size $m$, we compute a central density function and the corresponding approximate 95% credible region. If the $m$ credible regions thus obtained are close to each other, one can safely infer that the $m$ subsamples arose from the same stationary distribution.

Analogous to the convergence diagnostic method Mukhopadhyay et al. (2011), the method below can assess if two credible regions corresponding to two separate subsamples are close to each other. Let $(CR_{ε_1}, ε_1)$ and $(CR_{ε_2}, ε_2)$ denote the 95% credible regions and the corresponding radii obtained from any two subsamples. Suppose that $η_1 > 0$ is the least positive value such that $CR_{ε_1 + η_1} ⊃ CR_{ε_2}$, and also suppose that $η_2 > 0$ is the least positive value such that $CR_{ε_2 + η_2} ⊃ CR_{ε_1}$. Then, if both the increments $η_1, η_2$ are sufficiently small, then the 95% credible regions $CR_{ε_1}$ and $CR_{ε_2}$ can be said to be “close”.

We now present our applications of TTMCMC to the three real data sets modeled by mixtures with unknown number of components.

### 9. APPLICATION OF TTMCMC TO REAL DATA SETS MODELED BY NORMAL MIXTURES WITH UNKNOWN NUMBER OF COMPONENTS

To fit mixture models to each of the three data sets – enzyme, acidity, and galaxy, we implement Algorithm 5.1 updating $(k, ν, τ, ω)$ simultaneously in a single block using the additive transformation. For every iteration of TTMCMC we chose equal move-type probabilities of birth, death and no-change strategies. Also, for the underlying additive transformation, we chose equal probabilities of forward and backward transformations. The forms of the Jacobian for the birth and the death moves are given by $8a_{ν_j}a_{τ_j}a_{ω_j}$ and $(8a_{ν_j}a_{τ_j}a_{ω_j})^{-1}$ respectively, where $a_{ν_j}, a_{τ_j}$ and $a_{ω_j}$ are the scales for additive TTMCMC updating of $ν_j, τ_j$ and $ω_j$ respectively.

All our TTMCMC codes are written in C (optimality of the codes are not attempted) and implemented on a 32 bit, dual core (2.53 GHz × 2) laptop with 2.8 GiB memory.

Specific details of inference and implementation of our methodologies follow.
9.1 Enzyme data

Following Bhattacharya (2008) we set $s = 4.0$; $S = 2 \times (0.2/1.22) = 0.3278689$; $\nu_0 = 1.45$; $\psi = 33.3$. Rather than assuming $\omega_j \sim \log \left( \mathcal{G}(\alpha_j, 1) \right)$ which induce the traditional Dirichlet distribution for $\pi$ here we assume that $\omega_j \sim N \left( \mu_{\omega_j}, \sigma_{\omega_j}^2 \right)$, with $\mu_{\omega} = 0$ and $\sigma_{\omega}^2 = 0.25$. We chose zero mean and somewhat small variance to reflect our belief that $\omega_j$’s are relatively close to 1, so that a priori the mixing probabilities $\pi$ are approximately the same. We specify the uniform distribution on $\{1, \ldots, 30\}$ as the prior on $k$.

For implementing TTMCMC it is necessary to select the scales $a_{\nu_j}, a_{\tau_j}, a_{\omega_j}$ appropriately for each $j = 1, \ldots, k$. Rather than selecting the scales in order to optimize the acceptance rate (see Dey & Bhattacharya (2014b) for optimal scaling theory in the context of additive TMCMC), here we choose the scales by directly quantifying convergence of the TTMCMC chain using the convergence diagnostic procedure proposed in Section 8. We experimented by setting, for every $j = 1, \ldots, k$, the scale values $a_{\nu_j} = a_{\nu}$, $a_{\tau_j} = a_{\tau}$, and $a_{\omega_j} = a_{\omega}$, with $a_{\nu}, a_{\tau}, a_{\omega}$ being one of the trial values 0.05, 0.1, 0.15, 0.20, 0.25. With every trial value, we ran our TTMCMC algorithm for a burn-in of 300,000 iterations, and a further 15,000,000 iterations, storing one in 150 iterations, thus obtaining a total of 10,000 realizations from the posterior distribution. For each trial run we assessed convergence of our TTMCMC chain using the method proposed in Section 8. We divided our TTMCMC samples into two parts, one part consisting of the first 5,000 realizations and the other part containing the next 5,000 realizations. Constructing the approximate 95% credible regions as prescribed, we obtained $\eta_1$ and $\eta_2$ associated with the convergence diagnostic. We selected that trial value which yielded the smallest $\eta_1$ and $\eta_2$ among the trial runs. Indeed, the smallest $\eta_1$ and $\eta_2$ turned out to be $\eta_1 = 0.09146$ and $\eta_2 = 0.07816$, which corresponded to $a_{\nu} = a_{\tau} = a_{\omega} = 0.05$. Hence, we report our results with respect to these trial values. Moreover, since both these quantities are small, we conclude that convergence has taken place appropriately.

Our TTMCMC implementation with the scales selected as above took 2 minutes and 51 seconds.

We also verified convergence of our TTMCMC chain with informal trace plots. Figure 9.1
displays the trace plots of $k$, $\nu_1$, $\tau_1$ and $\omega_1$. As seen in panel (a) of Figure 9.1, the posterior distribution of $k$ placed full mass on 2 components. Whenever birth or death moves were proposed after the sufficiently long burn-in period, they got rejected, thus the parameters $(\nu, \tau, \omega)$ were updated only when the no-change move is proposed and accepted. Although somewhat unusual, this issue is hardly surprising since the data strongly supports bimodality. The information regarding bimodality is particularly strong thanks to the small range on which the data are supported and the large size of the data (the data set contains 245 observations on an effective support $(0, 3)$). We experimented with many starting values of $k$, but every time the results remained unchanged. That the mixing of our TTMCMC chain is adequate can be more clearly visualized from the trace plots of $\nu_1$, $\tau_1$ and $\omega_1$ since $(k, \nu, \tau, \omega)$ are updated simultaneously in a single block. Panels (b), (c) and (d) of Figure 9.1 show adequate mixing properties of the chain. Thus, the mixing information provided by these trace plots supports the conclusion obatained by our proposed credible region based convergence assessment method.

The mode of the posterior distribution of mixture densities turned out to be the density function corresponding to the 8463-th iteration, consisting of 2 components. This corresponds to selecting $\epsilon = 0.1$ in (7.4). Note that for small values of $\epsilon$ the empirical probabilities may be quite small just because of the finite number of TTMCMC samples. Hence it takes care to find the appropriate modal density function. For greater reliability, we evaluated the right hand side of (7.4) for $\epsilon = 0.001, 0.005, 0.01, 0.05, 0.1, 0.15$. For each mode, we obtained the corresponding 95% HPD region, and compared the radii of the HPD regions. We chose that mode for which the radius is the smallest. For both $\epsilon = 0.1$ and 0.15 the results remained the same and did not suggest strong evidence of multimodality. Indeed, the radius of the 95% HPD region centered around the mode is 0.4474; since this is adequately small, unimodality seems to be the case even from this perspective.

Figure 9.2 shows the modal density (thick, black curve), along with some other densities within the 95% HPD region overlapped on the histogram of the data. Quite good fit of the posterior distribution of the densities to the data is indicated by the diagram.
Figure 9.1: **Enzyme data:** Trace plots of $k$, $\nu_1$, $\tau_1$ and $\omega_1$. It is incorrect to interpret panel (a) “the chain for $k$ did not move” – in fact, many no-change move-types got accepted, and because $(k, \nu, \tau, \omega)$ are updated simultaneously in a single block, that also explains why the parameters $\nu$, $\tau$ and $\omega$ moved freely.
Figure 9.2: **Enzyme data:** Goodness of fit of the posterior distribution of densities (coloured curved) to the observed data (histogram). The thick black curve is the modal density and the other coloured curves are some densities contained in the 95% HPD.
9.2 Acidity data

Again following Bhattacharya (2008) we set $s = 4.0$; $S = 2 \times (0.2/0.573) = 0.6980803$; $\nu_0 = 5.02$; $\psi = 33.3$. Here also we assume that $\omega_j \sim N\left(\mu_{\omega_j}, \sigma^2_{\omega_j}\right)$, with $\mu_{\omega_j} = 0$ and $\sigma^2_{\omega_j} = 0.25$. Again, we put the uniform prior distribution on $\{1, \ldots, 30\}$ on $k$.

Following the convergence diagnostic method detailed above for choosing appropriate scales here we obtain $a_{\nu_j} = a_{\tau_j} = a_{\omega_j} = 0.05$ for $j = 1, \ldots, k$. For these scales we obtained $\eta_1 = 0.02542$ and $\eta_2 = 0.03318$, which are also small enough, indicating good convergence.

With the chosen scales our implementation took 1 minute and 39 seconds to yield 10,000 realizations following a burn-in of 300,000 iterations, after storing one in 150 iterations out of further 15,000,000 iterations after the burn-in period.

The trace plots of $k, \nu_1, \tau_1$ and $\omega_1$, shown in Figure 9.3, again indicate good mixing properties and are consistent with the conclusions of our proposed credible region based convergence assessment criterion.

With our prior structure here the posterior distribution of $k$ again strongly favored 2 components, taking the values 2 and 3 with posterior probabilities 0.997 and 0.003 respectively. Thus, compared to the enzyme data, here the posterior of $k$ has somewhat greater variability due to the larger effective support and smaller data size (the acidity data consists of 155 observations on the effective support $(2, 8)$).

The mode of the posterior distribution of mixture densities, which correspond to taking $\epsilon = 0.05$, turned out to be the mixture density associated with the 7160-th iteration, consisting of two components. Here we followed the same principle of mode selection as detailed in the case of the enzyme data. Once again we did not find strong evidence of multimodality of the posterior of the densities. The radius of the 95% HPD region centered around the modal density is 0.46416. This is relatively small and seems to be consistent with unimodality.

The modal density and sample densities falling in the 95% HPD region, overlapped on the histogram of the observed data are shown in Figure 9.4. Once again, good fit to the data is indicated.
Figure 9.3: **Acidity data**: Trace plots of $k$, $\nu_1$, $\tau_1$ and $\omega_1$. As with the enzyme data, here also it is wrong to interpret from panel (a) that “the chain for $k$ moved very little”. Even for this acidity data, many no-change move-types got accepted, and because $(k, \nu, \tau, \omega)$ are updated simultaneously in a single block, the parameters $\nu$, $\tau$ and $\omega$ could move freely.
Figure 9.4: **Acidity data:** Goodness of fit of the posterior distribution of densities (coloured curved) to the observed data (histogram). The thick black curve is the modal density and the other coloured curves are some densities contained in the 95% HPD.
9.3 Galaxy data

In contrast with the previous two cases of the enzyme and the acidity data, here a similar prior structure failed to provide good fit to the far more challenging galaxy data, which is much more sparse and seems to exhibit far greater number of modes.

Here, following Bhattacharya (2008) we set $s = 4.0; S = 2; \nu_0 = 20; \text{but } \psi = 33.3$ did not seem appropriate as in the previous two situations. Here $\psi = 0.0005$ turned out to be much more appropriate. This implies that the prior of $\nu_j$ has relatively small variation – this makes sense since the data consists of many local modes each concentrated on small regions. Also, unlike in the previous two cases here we assume that $\omega_j \sim \log(G(5, 1))$, so that $\pi$ follows the Dirichlet distribution with all the parameters equal to 5. The prior mean and mode of $\pi_j$ associated with this Dirichlet distribution are $1/k$ and the variance is $(k - 1)/6k^2$. Note that the mean and the variance of the uniform Dirichlet distribution, which corresponds to taking all the parameters equal to 1, are $1/k$ and $(k - 1)/\{k(k + 1)\}$, respectively. Hence, for large $k$, the variance of our prior distribution is about $1/6$ times that of the uniform Dirichlet. This lesser variability ensures that the minor local modes receive non-negligible prior weights, and hence makes sense in this galaxy data scenario. As regards the prior on $k$, here we chose a discretized normal distribution on $\{1, \ldots, 30\}$ with mean 15 and variance 50. This reflects our belief that although all the values in $\{1, \ldots, 30\}$ receive significant prior masses, relatively large number of components is preferable in this application where many local modes are exhibited by the data.

In this application, following the previous convergence diagnostic method, we found the appropriate scales to be $a_{\nu_j} = a_{\tau_j} = a_{\omega_j} = 1$ for $j = 1, \ldots, k$. These scales correspond to $\eta_1 = 0.02022$ and $\eta_2 = 0.0151$, which indicate good convergence.

The implementation of TTMCMC in this application took 7 minutes and 50 seconds to yield 10,000 realizations after discarding a burn-in of 300,000 iterations, and then storing one iteration in every 150 iterations out of further 15,000 iterations following the burn-in period.

Note that, even in this challenging galaxy data application, the trace plots turned out to be quite reasonable, as shown in Figure 9.5. Thus, reasonable overall mixing behavior of the TTM-
CMC chain is indicated by the trace plots, consistent with the results of our credible region based convergence assessment criterion.

In this problem the posterior distribution of $k$ turned out to be much more variable than in the previous two cases. Here $k \in \{9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29\}$ with respective probabilities $\{0.0001, 0.0009, 0.0018, 0.0069, 0.0159, 0.0294, 0.0484, 0.0759, 0.1066, 0.1268, 0.1278, 0.1143, 0.1084, 0.0828, 0.0695, 0.0366, 0.0243, 0.0136, 0.0062, 0.0027, 0.0011\}$. Thus most of the possible values of $k$ received positive posterior masses. It is also difficult to single out any particular value of $k$ that is very strongly favored by the posterior, unlike in the previous two applications.

The mode of the posterior distribution of mixture densities turned out to be associated with the 6268-th iteration having 20 components, and corresponds to taking $\epsilon = 0.05$. As before, we did not obtain strong evidence of multimodality of the posterior distribution of the densities. As such, the radius of the 95% HPD region turned out to be 0.08641, which is relatively small, and hence encouraging, not providing strong evidence of multimodality.

Figure 9.6 depicts the modal density and sample densities falling in the 95% HPD region, overlapped on the histogram of the observed data. The fit to the data seems to be quite encouraging with the sample densities capturing even the minor modes located at the extreme ends of the support of the data.

10. CONCLUSION

The transformation based concepts of TMCMC in the fixed-dimensional set-up has led to the interesting variable-dimensional counterpart TTMCMC, just as the traditional Metropolis-Hastings methodology led to RJMCMC. Consequently, the advantages of TMCMC over Metropolis-Hastings (see Dutta & Bhattacharya (2014), Dey & Bhattacharya (2014a), Dey & Bhattacharya (2014b)) are expected to carry over to TTMCMC as compared to RJMCMC. As we demonstrated in this paper, TTMCMC is simple to implement, can update all the (variable number of) parameters in a single block while maintaining reasonable acceptance rates thanks to drastic effective reduction of the dimensionality. Indeed, TTMCMC effectively reduces the variable dimensional problem into a fixed
Figure 9.5: **Galaxy data**: Trace plots of $k$, $\nu_1$, $\tau_1$ and $\omega_1$. Good mixing behavior of the TTMCMC chain is exhibited by the above panels.
Figure 9.6: **Galaxy data:** Goodness of fit of the posterior distribution of densities (coloured curved) to the observed data (histogram). The thick black curve is the modal density and the other coloured curves are some densities contained in the 95% HPD.
dimensional problem involving a single $\epsilon$ or just a few, fixed number of $\epsilon$’s. The block updating strategy of TTMCMC using $\epsilon$ or a few $\epsilon$’s also ensures huge computational savings. Importantly, the move-types of TTMCMC seems to have the natural automation property based on the available deterministic transformation and their inverses. Our illustrations of TTMCMC in the set up of the challenging problem involving normal mixtures with unknown number of components, and applied to three real data sets, vindicate the advantages of TTMCMC. Although in this paper, due to lack of space we confine ourselves to application of TTMCMC only to mixtures, applications of TTMCMC to various other problems are being carried out by these authors and their colleagues. Das & Bhattacharya (2014) have successfully applied TTMCMC in the context of a novel spatio-temporal model involving a random sum with unknown number of terms and a large number of other fixed-dimensional parameters, all of which are updated in a single block. Specifically, the dimension of that spatio-temporal problem varies randomly between 3000 and 3100. TTMCMC exhibited excellent performance even in this extremely challenging set-up. In another new spatio-temporal model development scenario, which also includes a random sum with random number of terms, along with many other fixed-dimensional parameters, Mr. Arnab Hazra is developing a TTMCMC based methodology for Bayesian inference. Mr. Prakash Chakraborty and Mr. Prosenjit Kundu are applying TTMCMC in the context of variable selection in regression problems and factor analysis where the dimension of the latent factor loading matrix is unknown.

Apart from developing TTMCMC, based on Mukhopadhyay et al. (2011) we have also proposed a methodology for summarizing the posterior distributions of mixture densities. In particular, we have prescribed a procedure for obtaining the modes and desired HPD regions of the posterior of mixture density functions. Using the ideas we have proposed a convergence diagnostic criterion for the underlying TTMCMC algorithm. The performances of these procedures are demonstrated in the three real data examples. These developments, in our opinion, can play important roles in various applications involving random basis function expansions, for instance, in nonparametric regression and functional data analysis. Since basis function expansions typically involve unknown number of summands, TTMCMC based inference along with our procedure for summarizing posterior distribution of functions, are expected to constitute a very interesting and
important combination for such challenging data analysis. Convergence of TTMCMC in such class
of problems can be assessed using our proposed diagnostic based on credible regions of functions
associated with sub-samples of the entire set of TTMCMC realizations. Since convergence in
variable dimensional problems is particularly difficult to assess, our methodology, which seems
to provide a reliable convergence assessment criterion, perhaps provides a significant advance, at
least in the large class of problems involving unknown functions.
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