A note on Metropolis-Hasting for sampling across mixed spaces

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Abstract

We are concerned with the Metropolis-Hastings algorithm for sampling across so-called mixed spaces. The most important example of a mixed space is a space that consists of real vectors of different lengths. Sampling within this space is called trans dimensional sampling and enjoys an enormous popularity across many statistical communities. However, the ubiquitous literature is completely divided over the abilities of the Metropolis-Hastings algorithm in these scenarios. This lead to the success of the reversible jump algorithm as the quasi gold standard. Unfortunately, the actual contribution of reversible jump is consistently misunderstood. Thus, this paper gives a dense overview of the theory that builds the mathematical foundations of sampling within mixed spaces, discusses a changepoint example and finally clears up any misunderstandings.

Keywords: MCMC, trans dimensional sampling
1 Introduction

The foundation of MCMC sampling is that under some circumstances Markov chains converge towards their invariant distribution, say $\pi$, regardless of their initial state. Thus, by simulating such a chain for a longer while we obtain an approximate sample of $\pi$. MCMC methods provide schemes to build Markov chains with a predefined invariant distribution. A thorough treatment of the convergence of Markov chains in regards to MCMC can be found in Tierney (1994).

There is a tremendous number of scientific articles and books about MCMC available. I recommend Bishop and Mitchell (2014) for a practical introduction. My writings about MCMC were mainly inspired, in accordance to this ordering, by Bishop and Mitchell (2014); Koenig
The Gibbs sampler is a primal MCMC method. It builds a Markov chain by decomposing $\pi$ into simpler conditional versions. This facilitates sampling of complex joint distributions, but is somewhat restricted in its ability to explore $\mathcal{S}$. However, this strategy is employed intensively in more sophisticated MCMC algorithms as well.

The well-known Metropolis-Hastings algorithm is capable of incorporating user defined proposal distributions. They enable the exploration of the state space in any desired fashion. That way, the Metropolis-Hastings algorithm even allows us to explore only parts of the state space accurately w.r.t. $\pi$. This greatly facilitates the handling of conditional versions of $\pi$.

We consider Bayesian changepoint models to illustrate the considered sampling approaches. They are composed of a likelihood, i.e. the distribution of the data, and the prior that models the parameters the model relies on. This prior usually comprises the changepoint locations and segment heights. Given an observed data set, we may be interested into the distribution of the changepoints given the data. This distribution is the product of a marginalization over the segment heights and its functional form may thus be completely unknown. Hence, for an analysis of changepoint data by means of a Bayesian changepoint model, we may be compelled to rely on samples exclusively.

However, changepoint models add a considerable complexity to the sampling algorithm. If the number of changepoints is unknown, the state space contains vectors of segment heights with varying lengths. This is an example of a mixed space. Proposals that transition through those spaces are usually defined as mixtures. Their components describe transitions either within the same or across different dimensions.

Similar scenarios arise in regression (Mitchell and Beauchamp, 1988) and also in point processes (Geyer and Moller, 1994). In regression models we often want to find a small subset of relevant covariates out of the mixed space of all possible subsets of covariates together with their effect sizes. This is referred to as subset selection, feature selection, variable selection, attribute selection or regularization. In turn, point processes live in a mixed space too, that is the space of all possible finite point configurations. Each configuration consists of the number of points together with their positions.
Generally, the design of proposals is the key for the efficiency of the Metropolis-Hastings algorithm and is often pursued by means of suitable distance measures to imitate certain random walk behaviors. Since there are no natural choices for distances between points of different dimensions, in this case, we rely on functions to establish links between those spaces.

Even though this can readily be realized with the Metropolis-Hastings algorithm, there are sophisticated proposals whose direct design and use turns out to be cumbersome in practice. To this end, the reversible-jump algorithm represents a specialization of the Metropolis-Hastings algorithm that facilitates the handling of an important family of those proposals.

During my research consistently reappearing wrong statements came to my attention. They claim that the Metropolis-Hastings algorithm was not capable of trans dimensional sampling or that the reversible-jump algorithm generalized MCMC methods to general state spaces. Since these views seem to be ubiquitous, I find it important to consider them thoroughly and to verify their true content.

In the following we briefly explain the Gibbs sampler (Section 2) and consider a primal version of the Metropolis-Hastings algorithm (Section 4), investigate the reversible-jump algorithm (Section 5) and elaborate a changepoint example (Section 6). Thereafter, we look at the Metropolis-Hastings algorithm for general state spaces (Section 7), mixture proposals (Section 8) and mixed spaces (Section 9). In the discussion we give a critical analysis of the public perception towards reversible-jump and its actual contribution (Section 10).

2 The Gibbs Sampler

The Gibbs sampler (Geman and Geman, 1984) is a primal MCMC sampling algorithm which is based on a decomposition of the objective distribution into conditional versions. It is mainly used to sample from the joined distribution of a set of random variables. Thereby each step involves sampling from a subgroup of the random variables given the remaining random variables conditioned on the last sample. In the following we elaborate the Gibbs sampler in a slightly more general manner.

We are given a probability space \((\mathcal{S}, \mathcal{A}, \pi)\). Let \(S\) be a random variable which is distributed according to \(\pi\). We draw independent samples from \(\pi\) in a stepwise manner. In each step we condition \(S\) on the outcome of a function. Given a set of functions \(f_0, \ldots, f_{n-1}\) from \(\mathcal{S}\) into another
unspecified space $\mathcal{D}$, in step $i = 1, 2, ...$ we gather a sample $s_i$ from $(S \mid f_j(S) = f_j(s_{i-1}))$. $j$ is chosen either randomly or by following a scheme, for example $j = i - 1 \ mod \ n$ and the initial sample $s_0$ has to be specified manually.

Assume that the distribution of $(S \mid f_j(S) = f_j(s'))$ is described by the Markov kernel $\kappa_j(s', ds)$.

**Lemma 1.** $\pi$ is an invariant distribution of $\kappa_j$.

**Proof.** For $A \in \mathcal{A}$ we know that

$$\kappa_j(s', A) = \mathbb{P}(S \in A \mid f_j(S) = f_j(s')) = \mathbb{E}\{1 \{S \in A\} \mid f_j(S) = f_j(s')\}$$

With this we further conclude

$$\pi \otimes \kappa_j(\mathcal{S} \times A) = \int \kappa_j(s', A) \pi(ds')$$

$$= \int \mathbb{E}\{1 \{S \in A\} \mid f_j(S) = f_j(s')\} \pi(ds')$$

$$\stackrel{*}{=} \int 1 \{s' \in A\} \pi(ds') = \pi(A)$$

Whereby we have used the properties of the conditional expectation in $*$. □

However, are $\kappa_j$’s are generally not irreducible or aperiodic. This is a requirement to be justified by $\pi$ and the $f_j$’s together with their call sequence.

A famous and quite old application of the Gibbs sampler is the Ising model (Ising, 1925). There, $\mathcal{S}$ consists of the positive or negative values of the grid points of a finite grid, whereby independence is induced by spatial separation. This yields very simple sampling steps, each conducted on a single grid point given all the other, but essentially only its neighboring grid points. Higdon (1998) provides very vivid and more sophisticated treatments of the Ising model.

### 3 The detailed balance condition

Now we introduce a sufficient condition for a Markov kernel $\kappa$ to have a given distribution $\pi$ as an invariant distribution. It is called the detailed balance condition and greatly facilitates the invariance proofs for the MCMC algorithms in the subsequent sections.

Let $\pi$ and $\kappa$ be defined on the measurable space $(\mathcal{S}, \mathcal{A})$. 

**Definition 1.** The Markov kernel $\kappa$ preserves the detailed balance condition w.r.t. $\pi$ if
$$\pi \otimes \kappa(A \times B) = \pi \otimes \kappa(B \times A)$$
for all elements $A, B \in \mathcal{A}$.

If $\kappa$ preserves the detailed balance condition with respect to $\pi$, $\pi$ is an invariant distribution of $\kappa$ since $\pi \otimes \kappa(\Omega \times \cdot) = \pi \otimes \kappa(\cdot \times \Omega) = \pi$. The opposite implication does not generally hold.

**Definition 2.** For a probability measure $\mu$ over the product of one and the same measurable space $(\mathcal{S}, \mathcal{A})$, we define the probability measure $\mu^t$ as the transpose of $\mu$ through
$$\mu^t(A) = \mu(A^t)$$
for all $A \in \mathcal{A} \otimes \mathcal{A}$ whereby $A^t = \{(s, s') \mid (s', s) \in A\}$. In the following, with $\pi \otimes \kappa^t$ we refer to the transpose of the entire product measure $\pi \otimes \kappa$.

**Corollary 1.** $\pi$ and $\kappa$ meet the detailed balance condition if and only if $\pi \otimes \kappa = \pi \otimes \kappa^t$ applies.

**Proof.** The proof of “$\Leftarrow$” is straightforward. Let $\mu = \pi \otimes \kappa$. Since the sets $A \times B$ with $A, B \in \mathcal{A}$ generate $\mathcal{A} \otimes \mathcal{A}$ and are closed under intersections, $\mu$ is the unique measure with values $\mu(A \times B)$ over those sets. The detailed balance of $\kappa$ w.r.t. $\pi$ thus implies that $\mu = \mu^t$. \(\square\)

Once it is in equilibrium, these sort of Markov chains exhibit same probabilities in forward and backward direction and therefore, they are called reversible. Thus, MCMC methods that preserve the detailed balance condition are called reversible. This should not be mixed up with the reversible-jump algorithm of Green (1995).

### 4 The Metropolis-Hastings algorithm

In the following we want to elaborate the well-known Metropolis-Hastings algorithm and some of its derivatives. It is an MCMC sampler that traverses through the state space by means of a user defined proposal. Characteristic for this sampler is that each proposed value undergoes an accept-reject step which decides whether the proposed value or the previous sample is chosen to be the next sample. This acceptance step alone secures the detailed balance of the Metropolis-Hastings kernel and thus, gives the user great freedom in designing proposals.
A primal version was first published in [Metropolis et al. (1953)] and then extended in [Hastings (1970)]. [Tierney (1994)] combines the latest findings about Markov chains in general state spaces and put them into context with Metropolis-Hastings and MCMC. [Geyer and Moller (1994)] elaborates the Metropolis-Hastings algorithm for spatial point processes. [Green (1995)] presents the reversible-jump algorithm that facilitates the use of a certain family of specific proposals which are mainly used to sample across spaces of different dimensions. [Tierney (1998)] generalizes the Metropolis-Hastings algorithm in a reaction to a hype on Metropolis-Hastings in more sophisticated scenarios. [Roodaki et al. (2011)] addresses mixtures of proposals used in the Metropolis-Hastings algorithm exhaustively.

In the ubiquitous literature, the Metropolis-Hastings algorithm is usually introduced on the basis of densities. For the time being, we shall motivate the algorithm in the same manner. We are given a measure space \((\mathcal{S}, \mathcal{A}, \lambda)\) and a probability measure \(\pi\) with a density \(p\) such that 
\[
\pi(ds) = p(s)\lambda(ds).
\]

In its primal form, the Metropolis-Hastings algorithm requires the user to provide a Markov kernel \(\kappa\) from \((\mathcal{S}, \mathcal{A})\) to \((\mathcal{S}, \mathcal{A})\) in form of a conditional density \(k(s', s)\) such that \(\kappa(s', ds) = k(s', s)\lambda(ds)\). This Markov kernel is referred to as the proposal.

**Algorithm 1** (Metropolis-Hastings). (I) Choose an initial state \(s_0 \in \mathcal{S}\) (II) In step \(i = 1, 2, \ldots\) propose a new state \(s\) according to \(\kappa(s_{i-1}, \cdot)\) and set \(s_i = s\) with probability
\[
a_{s_{i-1}s} = \min \left\{ 1, \frac{p(s)k(s, s_{i-1})}{p(s_{i-1})k(s_{i-1}, s)} \right\}
\]
otherwise set \(s_i = s_{i-1}\). We agree that dividing by 0 and in particular 0/0 yields 0 here.

We shall refer to the term \(p(s)k(s, s_{i-1})/p(s_{i-1})k(s_{i-1}, s)\) as the acceptance ratio. It roughly represents the density of \(\pi \otimes \kappa\) w.r.t. \(\pi \otimes \kappa\). Let 
\[
\mu(s', \cdot) = \int a_{x's} \delta_x(\cdot) + (1 - a_{x's})\delta_{x'}(\cdot)k(s', ds)
\]
\(\mu\) is the Markov kernel that is applied in each step in the Metropolis-Hastings algorithm.

**Lemma 2.** \(\mu\) preserves the the detailed balance condition w.r.t. \(\pi\).

**Proof.** There is nothing to prove for \(A, B \in \mathcal{A}\) with \(A = B\). Since \(A \times B\) is the disjoint union of \((A \cap B) \times (A \cap B), (A \setminus B) \times (B \setminus A), (A \setminus B) \times (A \cap B)\) and \((A \cap B) \times (B \setminus A)\) we can w.l.o.g. assume...
that $A \cap B = \emptyset$. We get
\[
\int_B \mu(s',A)\pi(ds') = \int_B \int a_{s's} \delta_s(A)k(s',s)p(s')\lambda(ds)\lambda(ds')
\]
\[
\overset{\ast}{=} \int_A \int a_{ss'} \delta_s(B)k(s,s')p(s)\lambda(ds)\lambda(ds) = \int_A \mu(s,B)\pi(ds)
\]
whereby we have used that $a_{s's}k(s',s)p(s') = a_{ss'}k(s,s')p(s)$ and Fubini’s theorem in $\ast$. 

By looking into $a_{s's}$, we see that normalization constants w.r.t. $p$ would cancel out. Thus, by using a suitable proposal, the algorithm is capable of producing approximate samples of conditional versions of $\pi$ without knowing the normalization constants w.r.t. $p$. This is one of the great advantageous of the Metropolis-Hastings algorithm.

It is important to note that the irreducibility and aperiodicity of the Metropolis-Hastings kernel $\mu$ has to be met by the acceptance probability together with the proposal. Equation (1) shows, that we can only perform a transition if the corresponding backward transition is also feasible, more precisely, if $p(s)k(s,s_{i-1})$ is positive. In the most extreme case this could mean that we apply an irreducible and aperiodic proposal, but the resulting Metropolis-Hastings kernel is just a point mass concentrated on the last sample.

## 5 The reversible-jump algorithm

The famous reversible-jump algorithm is mainly used to sample between real spaces of varying dimensions which are endowed with their corresponding Lebesgue measure. Therefore, it matches the dimensions of the spaces by embedding them into a superordinate space of higher dimension. Green (1995) introduces this as *dimension matching*. Diffeomorphisms are applied to translate between this superordinate space and the target space.

Let now $\mathcal{J}_i = \mathbb{R}^i$ be equipped with the standard Borel $\sigma$-algebra $\mathcal{A}_i$ and the $i$ dimensional Lebesgue measure $\lambda_i$. The distribution $\pi$ is defined over the union of all these spaces and exhibits a density $p$ w.r.t. $\sum_{i=1}^\infty \lambda_i \circ id_i$, whereby $id_i : \mathcal{J}_i \to \bigcup_{j=1}^\infty \mathcal{J}_j$ with $id_i(s) = s$.

In order to transition from $\mathcal{J}_j$ to $\mathcal{J}_i$ the user provides:

- a $k \geq \max\{i,j\}$.

- a diffeomorphism $(s,u)_{ji} : \mathcal{J}_j \times \mathcal{J}_{k-j} \to \mathcal{J}_i \times \mathcal{J}_{k-i}$ with its inverse $(s,u)_{ij} : \mathcal{J}_i \times \mathcal{J}_{k-i} \to \mathcal{J}_j \times \mathcal{J}_{k-j}$.
• kernel densities $k_{ji}$ and $k_{ij}$ from $S_j$ to $S_{k-j}$ and from $S_i$ to $S_{k-i}$ respectively. Both are densities w.r.t. their corresponding Lebesgue measures.

• measurable functions $q_i : S \rightarrow [0, 1]$ for $i = 1, 2, \ldots$ with $\sum_{i=1}^{\infty} q_i(s') = 1$ for all $s' \in S$

Given an $s' \in S_j$, we choose the target space $S_i$ according to the probabilities $q_i(s')$ and sample an $u' \in S_{k-j}$ according to $k_{ji}(s', u')$ to obtain the newly proposed sample $s$ through $s = s_{ji}(s', u')$.

**Lemma 3.** Let $|(s, u)_{ji}|$ be the absolute value of the Jacobi determinant of $(s, u)_{ji}$. For $s' \in S_j$ and $u' \in S_{k-j}$, we may use

$$r_{s'u'} = \begin{cases} 1, & q_j(s_{ij})k_{ij}(s_{ij}, u_{ij})p(s_{ij}) \\ q_i(s')k_{ji}(s', u')p(s') & |(s, u)_{ji}| \end{cases}$$

as the acceptance probability in the Metropolis-Hastings algorithm, whereby the detailed balance is preserved w.r.t. $\pi$.

**Proof.** Let $A \in \mathcal{A}_j$ and $B \in \mathcal{A}_i$

$$\int_A \int r_{s'u'} q_i(s') \delta_{s_{ji}}(B) k_{ji}(s', u') p(s') du' ds' = \int \delta_{s_{ij}}(A) \int r_{(s,u)_{ij}} q_i(s_{ij}) \delta_{s}(B) k_{ji}(s_{ij}, u_{ij}) p(s_{ij}) |(s, u)_{ij}| duds = \int \int r_{su} q_j(s) \delta_{s_{ij}}(A) k_{ij}(s, u) p(s) duds$$

whereby we have used integration by substitution for multiple variables in $\ast$.

$k$ is the dimension of the superordinate state space. The dimension of $u'$ is complementary to the dimension of the old sample within the superordinate $k$ dimensional space. Thus, we are allowed to produce samples by generating random numbers within a space of a different dimension as the target space. The diffeomorphism finally combines the old sample with $u'$ in order to propose a new sample.

The reversible-jump algorithm can also be applied to the purely discrete spaces. There it is sufficient to use a bijection. The acceptance probability would look the same, with the difference that the Jacobi determinant is skipped.
A changepoint example

Now we want to consider a simple changepoint example. We compare two different proposals for the trans dimensional sampling part, a tightly adapted proposal using a sophisticated diffeomorphism and a very loosely adapted proposal.

Figure 1 shows an artificial dataset. The $n = 550$ data points were drawn independently from Gaussian distributions having a constant variance of 1 and mean values that are subject to successive changes. The data shown in Figure 1 exhibits around 7 to 9 such changepoints.

To build an exemplary Bayesian model here, we choose a prior for the changepoint locations and mean values: The time from one changepoint to the next is geometrically distributed with $q = 3/550$ and the mean values in case of a jump are distributed according to $\mathcal{N}(0, 25)$.

The sampling starts with no changepoints and an overall mean of 0. Thus, we start with a single segment and a single mean (also called segment height). Throughout the sampling, new changepoint locations may be found or discarded. Consequently, segments and their corresponding heights may be inserted or removed by what is usually called birth and death moves. Additionally, we also allow shift moves that shift single changepoints and adjust moves that adjust the height of single segments.

Remark 1. These moves have to be understood as Gibbs sampling like moves, whereby in each step we decide for certain segments and heights to change, but keep all the rest constant. The difference to Gibbs sampling is that we do not sample exactly from the conditional distributions, instead we perform a Metropolis-Hastings like step with it. Detailed balance is therefore preserved here, but the irreducibility and aperiodicity can only be ensured by an accumulation of different steps.

An adjust move relocates the height of a uniformly chosen segment according to $\mathcal{N}(h', 10^{-5})$, whereby $h'$ is the old height. This is used for fine tuning the segment heights. A shift move shifts
the location of a uniformly chosen changepoint uniformly to a new position within the neighboring
changepoints.

Let $\phi$ be the density of the normal distribution. In the adjust move that moves the height $h'$ of
a segment $S$ to $h$ we get an acceptance ratio of
\[
\frac{\phi(h, 0, 25) \prod_{j \in S} \phi(y_j; h, 1)}{\phi(h', 0, 25) \prod_{j \in S} \phi(y_j; h', 1)}
\]
Note that the probabilities of choosing the adjust move, the segment and the density values of the
data points within the untouched segments cancel out. Furthermore, since the normal distribution
is symmetric w.r.t. its mean, the proposal densities cancel out as well. What remains are the
density values for the data points within the adjusted segment and the priors for the segment
heights.

We agree that 1 and $n + 1$ are considered as (artificial) changepoints. However, they cannot
be shifted. In the shift move we shift a changepoint at location $i$ to location $j$. Let $\ell$ and $k$ are
the changepoints to the left and right of the changepoint at $i$ and let $h_1$ respectively $h_2$ be the
corresponding segment heights. The acceptance ratio reads
\[
\frac{\prod_{m=\ell}^{j-1} \phi(y_m; h_1, 1) \prod_{m=j}^{h-1} \phi(y_m; h_2, 1)\prod_{m=\ell}^{i-1} \phi(y_m; h_1, 1) \prod_{m=i}^{k-1} \phi(y_m; h_2, 1)}
\]
Here, the probabilities of choosing the move and the changepoint and also the priors for the heights
cancel out.

The probabilities for the moves were all set to 0.25, except in the boundary cases. If there is
only one segment, birth and adjust have the same probability of 0.5 and if each timepoint has a
changepoint then death and adjust have the probabilities 0.5 respectively 0.25.

### 6.1 A loosely adapted implementation of birth and death

In the death move we choose a changepoint uniformly, remove it and choose a new height for
the remaining segment according to $\mathcal{N}(0, 25)$. In the birth move we choose a new changepoint
uniformly among the timepoints without a changepoint. The two heights left and right of the new
changepoint are then updated independently according to $\mathcal{N}(0, 25)$. 
Let $p_d$ respectively $p_b$ be the probabilities to choose a death or a birth move. Further, let $i$ be the timepoint of the changepoint we want to remove in a death move and let $\ell$ and $k$ are the changepoints to the left and right of the changepoint at $i$ and let $h_1$ respectively $h_2$ be the corresponding segment heights. Finally, let $h$ be the height of the resulted segment. The acceptance ratio for the death move reads

$$\frac{c + 1}{n - c} \cdot \frac{p_b}{p_d} \cdot \frac{\prod_{m=\ell}^{k-1} \phi(y_m; h, 1)}{\prod_{m=\ell}^{i-1} \phi(y_m; h_1, 1) \prod_{m=i}^{k-1} \phi(y_m; h_2, 1)}$$

whereby $c + 1$ is the number of changepoints whereby we leave $1$ and $n + 1$ aside.

Since a birth move can only be reversed by a death move, their corresponding acceptance ratios are reciprocal to each other.

### 6.2 A tightly adapted implementation of birth and death

This time we design birth and death moves that are better adapted to the changepoint problem. A good estimator for the mean value (or height) that applies to a segment is the mean of the observations belonging to it. If $\mu$ is this mean and we split the segment into two parts such that the lengths of the resulting segments are $n_1$ and $n_2$ and their corresponding mean values are $\mu_1$ and $\mu_2$, we see that $\mu = \frac{n_1 \mu_1 + n_2 \mu_2}{n_1 + n_2}$. Reversely, we can choose $\mu_1 = \mu + u/n_1$ and $\mu_2 = \mu - u/n_2$ whereby $u = \frac{n_1 \mu_1 - n_2 \mu_2}{n_1 + n_2}$. Thus, $(\mu, u)$ describes a diffeomorphism whose Jacobi determinant is $-\frac{n_1 n_2}{n_1 + n_2}$.

That means in a death move we would just use $h = \frac{n_1 h_1 + n_2 h_2}{n_1 + n_2}$. In the birth move we sample a $u$ from, say $\mathcal{N}(0, 3)$ and set $h_1 = h + u/n_1$ and $h_2 = h - u/n_2$. Therefore, the acceptance ratio for the death move reads

$$\frac{n_1 n_2}{n_1 + n_2} \cdot \frac{c + 1}{n - c} \cdot \frac{p_b}{p_d} \cdot \frac{\phi(u; 0, 3) \phi(h; 0, 25) \prod_{m=\ell}^{k-1} \phi(y_m; h, 1)}{\phi(h_1; 0, 25) \phi(h_2; 0, 25) \prod_{m=\ell}^{i-1} \phi(y_m; h_1, 1) \prod_{m=i}^{k-1} \phi(y_m; h_2, 1)}$$

### 6.3 Results

We now compare both proposals empirically in terms of their runtime and acceptance rates. The acceptance rates are an indicator for the speed of mixing (how fast the Markov chain converges).
| Acceptance rates | adjust moves | shift moves | death moves | birth moves |
|------------------|--------------|-------------|-------------|-------------|
| Loosely adapted  | 0.993278     | 0.0558759   | 0.00151519  | 0.00152487  |
| Tightly adapted  | 0.992897     | 0.0567016   | 0.0255789   | 0.0257372   |

Figure 2: The fractions of accepted moves.

Lower rates can indicate that the Markov chain struggles with exploring the state space and thus, would mix more slowly.

We computed $10^7$ successive samples. On my computer (AMD 64 with 3200 GHZ CPU) the sampling that utilises the loosely adapted proposals needed 13530 milliseconds and the tightly adapted ones 13288 milliseconds. Table 2 shows the acceptance rates for the individual moves. The loosely adapted proposals have much bigger problems in finding alternate changepoint configurations through death and birth moves. They succeed over 10 times less often than the tightly adapted ones.

## 7 A general representation of the Metropolis-Hastings algorithm

The drawback of the primal Metropolis-Hastings algorithm of Section 4 is that we require $\kappa$ to have a density w.r.t. a given measure. Thus, [Tierney (1998)] extends the Metropolis-Hastings algorithm to work with arbitrary choices of $\pi$ and $\kappa$. We will summarize its main outcomes in this section.

We are given an arbitrary probability space $(\mathcal{S}, \mathcal{A}, \pi)$ and a Markov kernel $\kappa$ from $(\mathcal{S}, \mathcal{A})$ to $(\mathcal{S}, \mathcal{A})$. This time we do not require densities of $\pi$ or $\kappa$ nor do we presume an underlying measure $\lambda$. The idea is to use $a_{s,s'} = \min \left\{ 1, \frac{\pi \otimes \kappa'(ds', ds)}{\pi \otimes \kappa(ds', ds)} \right\}$ as the acceptance probability in the Metropolis-Hastings algorithm. $\frac{\pi \otimes \kappa'(ds', ds)}{\pi \otimes \kappa(ds', ds)}$ represents the density of $\pi \otimes \kappa'$ w.r.t. $\pi \otimes \kappa$ evaluated at $(s', s) \in \mathcal{S} \times \mathcal{S}$. This is in accordance with the acceptance probability introduced by Equation (1).

However, the density $\frac{\pi \otimes \kappa'(ds', ds)}{\pi \otimes \kappa(ds', ds)}$, which is also referred to as the acceptance ratio, may not exist everywhere. Furthermore, in order to prove the detailed balance of this Metropolis-Hastings kernel, we also require that $\frac{\pi \otimes \kappa'(ds', ds)}{\pi \otimes \kappa(ds', ds)} = 1 / \frac{\pi \otimes \kappa(ds', ds)}{\pi \otimes \kappa'(ds', ds)}$. 

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Let $\xi$ be a symmetric measure such that $\pi \otimes \kappa$ and $\pi \otimes \kappa'$ are absolutely continuous w.r.t. $\xi$, for example $\xi = \lambda \otimes \lambda$ as in the primal Metropolis-Hastings algorithm or $\xi = \pi \otimes \kappa + \pi \otimes \kappa'$. Whilst the former is only eligible in scenarios where $\pi$ and $\kappa$ are defined through densities w.r.t. an underlying measure $\lambda$, the latter is always eligible. The theorem of Radon-Nikodym ensures that the densities $\frac{\pi \otimes \kappa(ds', ds)}{\xi(ds', ds)}$ and $\frac{\pi \otimes \kappa'(ds', ds)}{\xi(ds', ds)}$ exist.

**Definition 3.** Let

$$ R = \left\{ (s', s) \mid \frac{\pi \otimes \kappa(ds', ds)}{\xi(ds', ds)} > 0, \frac{\pi \otimes \kappa'(ds', ds)}{\xi(ds', ds)} > 0 \right\} $$

**Lemma 4.** On $R \cap A \otimes A$ the densities $\frac{\pi \otimes \kappa}{\pi \otimes \kappa}$ and $\frac{\pi \otimes \kappa'}{\pi \otimes \kappa}$ exist and equal to

$$ \frac{\pi \otimes \kappa(ds', ds)}{\xi(ds', ds)} \frac{\pi \otimes \kappa'(ds', ds)}{\xi(ds', ds)} $$

**Proof.** This holds since for $(s', s) \in R$ we may write

$$ \pi \otimes \kappa(ds', ds) = \frac{\pi \otimes \kappa(ds', ds)}{\xi(ds', ds)} \xi(ds', ds) $$

$$ = \frac{\pi \otimes \kappa(ds', ds)}{\xi(ds', ds)} \frac{\pi \otimes \kappa'(ds', ds)}{\xi(ds', ds)} \xi(ds', ds) $$

$$ = \frac{\pi \otimes \kappa(ds', ds)}{\xi(ds', ds)} \frac{\pi \otimes \kappa'(ds', ds)}{\xi(ds', ds)} \pi \otimes \kappa'(ds', ds) $$

$\square$

**Lemma 5.** We may use

$$ a_{s's} = \begin{cases} \min \left\{ 1, \frac{\pi \otimes \kappa'(ds', ds)}{\pi \otimes \kappa(ds', ds)} \right\} & (s', s) \in R \\ 0 & \text{otherwise} \end{cases} $$

(2)

as the acceptance probability in the Metropolis-Hastings algorithm, whereby the detailed balance is preserved w.r.t. $\pi$.

**Proof.** As in Lemma 2 w.l.o.g. we only consider transitions between disjoint sets. Thus, for $(s', s) \in R$ with $s \neq s'$ we see that

$$ a_{s's} \pi \otimes \kappa(ds', ds) = a_{s's} \frac{\pi \otimes \kappa(ds', ds)}{\pi \otimes \kappa'(ds', ds)} \frac{\pi \otimes \kappa'(ds', ds)}{\pi \otimes \kappa(ds', ds)} \pi \otimes \kappa(ds', ds) $$

$$ = a_{s's} \pi \otimes \kappa'(ds', ds) \pi \otimes \kappa'(ds', ds) = a_{s's} \pi \otimes \kappa'(ds', ds) = a_{s's} \pi \otimes \kappa(ds', ds) $$

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whereby we have used that \( a_{s's'} \pi \otimes \kappa(ds',ds) = a_{s's} \). Since \((s',s) \in R\) implies \((s,s') \in R\), in the above equation the left hand side and right hand sight will both be zero for \((s',s) \notin R\). \(\square\)

The above formulation of the Metropolis-Hastings algorithm captures a vast range of possible choices of \(\kappa\). However, it gives only little guidance on how to compute the acceptance ratios, which might sometimes be infeasible whatsoever. However, the theoretical construction that relies on the mutual densities of the forward and backward transitions defined on a suitable set \(R\) may prove instrumental in practice.

In the following to keep the notation uncluttered, we do not explicitly mention the set \(R\) in the acceptance probability anymore. Instead, we may safely set the acceptance ratio to 0 wherever it is not defined.

### 8 Mixture proposals

Now we consider the case where the proposal \(\kappa\) decomposes into a mixture

\[
\kappa(s',ds) = \sum_{i \in \mathcal{M}} q_i(s') \kappa_i(s',ds)
\]

whereby \(\mathcal{M}\) is a finite or countable set, \(\kappa_i\) a Markov kernel from \((\mathcal{S},\mathcal{A})\) to \((\mathcal{S},\mathcal{A})\) and \(q_i : \mathcal{S} \to [0,1]\) is a measurable function with \(\sum_{i \in \mathcal{M}} q_i(s') = 1\) for all \(s' \in \mathcal{S}\). For \(i \in \mathcal{M}\) we refer to \(\kappa_i\) as the \(i\)-th move. The probability of choosing move \(i\) while being in \(s'\) is given by \(q_i(s')\).

Let’s assume that move \(i\) has its corresponding backward (or reverse) move \(r_i \in \mathcal{M}\). The question is, when is it possible to perform the Metropolis-Hastings algorithm on the basis of the moves, i.e. when are we allowed to use

\[
a_{s's'} = \min \left\{ 1, \frac{\pi \otimes \kappa_r(ds',ds')}{\pi \otimes \kappa_i(ds',ds)} \cdot \frac{q_r(s)}{q_i(s')} \right\}
\]

as the acceptance probability in the Metropolis-Hastings algorithm, whereby the detailed balance is preserved w.r.t. \(\pi\)? [Roodaki et al. (2011)] provides a thorough treatment of this scenario. Its main result can be stated as follows.

**Lemma 6.** If for each \(i \in \mathcal{M}\) there exists a disjoint \(Z_i \in (\mathcal{A} \otimes \mathcal{A})\) and a unique \(r_i \in \mathcal{M}\) with

\[
(I) \int_{Z_i} q_i(s') \pi \otimes \kappa_i(ds',ds) = 0 \quad \text{and} \quad (II) Z_{ri} = Z_i^\dagger
\]
we may use (3) as the acceptance probability in the Metropolis-Hastings algorithm, whereby the
detailed balance is preserved w.r.t. $\pi$.

Proof. W.l.o.g. choose $(s', s) \in Z_i$ with $s' \neq s$. We see that

$$a_{s's'} \pi \otimes \kappa(ds', ds) = a_{s's'} q_i(s') \pi \otimes \kappa_i(ds', ds)$$

$$= a_{s's'} q_i(s) \pi \otimes \kappa_i(ds, ds') = a_{s's'} \pi \otimes \kappa(ds, ds')$$

This is correct because (I) and (II) state that we can safely set $a_{s's'} q_j(s') \pi \otimes \kappa_j(ds', ds) = 0$ and $a_{s's'} q_j(s) \pi \otimes \kappa_j(ds, ds') = 0$ for all $j \neq i$.

9 Mixture state spaces

In the trans dimensional case as introduced in Section $5$ we sample across homogeneous spaces of
different dimensions. Now we want to elaborate sampling across arbitrary measurable spaces.

Let $\mathcal{D}$ be a finite or countable set and let $(\mathcal{S}_i, \mathcal{A}_i)_{i \in \mathcal{D}}$ be a family of arbitrary but disjoint
measure spaces. The mixture $(\mathcal{S}, \mathcal{A})$ of $(\mathcal{S}_i, \mathcal{A}_i)_{i \in \mathcal{D}}$ is defined as

$$\mathcal{S} = \bigcup_{i \in \mathcal{D}} \mathcal{S}_i, \quad \mathcal{A} = \sigma \left( \bigcup_{i \in \mathcal{D}} \mathcal{A}_i \right)$$

whereby $\mathcal{A}$ is the smallest $\sigma$-algebra that comprises all $\mathcal{A}_i$'s. We want to sample from $\pi$
which is defined on $\mathcal{A}$. A natural choice for the proposal $\kappa$ is a mixture with components that
solely transition between pairs of the spaces, i.e.

$$\kappa(s', \cdot) = \sum_{\ell \in \mathcal{M}} q_\ell(s') \kappa_\ell(s', \cdot)$$

whereby $\mathcal{M} \subseteq \mathcal{D} \times \mathcal{D}$ with $\mathcal{M}^t = \mathcal{M}$. For $(j, i) \in M$ we agree that $\kappa_{ji}(s', \mathcal{S}_i) = 1$ and

$$\sum_{i \in \mathcal{D}} q_{ji}(s') = \begin{cases} 1 & s' \in \mathcal{S}_j \\ 0 & \text{otherwise} \end{cases}$$

for all $s' \in \mathcal{S}_j$. The form of the kernel $\kappa_{ji}(s', \cdot)$ is irrelevant whenever $q_{ji}(s') = 0$.

In order to meet the conditions of Lemma $6$ it is sufficient to choose $Z_{ji} = \mathcal{S}_j \times \mathcal{S}_i$ and
$r_{ji} = (i, j)$ for all $(j, i) \in M$. Thus, we may compute the acceptance probabilities solely based on
the $\kappa_{ji}$'s.
A special case arises if each measurable space $(\mathcal{I}_i, \mathcal{A}_i)$ is endowed with a measure $\lambda_i$, such that $\pi$ exhibits a density $p$ w.r.t. $\lambda = \sum_{i \in \mathcal{I}} \lambda_i \circ \text{id}$. If each component $\kappa_{ji}$ is chosen such that it exhibits a density w.r.t. to $\lambda_i$, the acceptance probabilities are straightforward to compute. Furthermore, for $\mathcal{I} = \mathbb{R}^i$ this leads to the most simple trans dimensional Metropolis-Hastings algorithm. An example is represented by the loosely adapted proposals of Section 6. There, we transition into $\mathbb{R}$ respectively $\mathbb{R}^2$ by means of densities w.r.t the one respectively two dimensional Lebesgue measure.

We have seen that mixture proposals allow for sampling across arbitrary spaces in the fashion of the Metropolis-Hastings algorithm. A reversible-jump proposal can also be assembled into a mixture kernel. Using the notation of Section 5 the component that transitions from $\mathbb{R}^j$ to $\mathbb{R}^i$ reads

$$\kappa_{ji}(s', \cdot) = \int \delta_{sji}(\cdot) k_{ji}(s', u') du'$$

Thus, according to Lemma 5 and 6 the Metropolis-Hastings acceptance probabilities for this kernel exist.

Let $r_{s',u'}$ be the acceptance probability of an arbitrary instance of the reversible-jump algorithm for transitions from $\mathbb{R}_j$ to $\mathbb{R}_i$. Since the corresponding Metropolis-Hastings acceptance probability has to be independent of $u'$, the idea is to somehow average $r_{s', \cdot}$ wherever $s_{ji}(s', \cdot)$ is constant.

**Lemma 7** (Siems 2018). The Metropolis-Hastings acceptance probability in Equation 3 for the move $(j, i)$ in the reversible-jump algorithm reads

$$a_{s's} = \mathbb{E}\{r_{s'u} \mid s_{ji}(s', U) = s\} \tag{4}$$

whereby $U$ is a random variable that is distributed according to the distribution which is determined through $k_{ji}(s', \cdot)$.

**Proof.** Since $\mathbb{E}\{r_{s'u} \mid s_{ji}(s', U)\} = a_{s's_{ji}(s', U)}$, the properties of the conditional expectation yield

$$\int_A a_{s's_{ji}(s', u')}k_{ji}(s', u') du' = \int_A r_{s'u}k_{ji}(s', u') du' \tag{5}$$

for all $A \in \sigma(\{s_{ji}(s', \cdot)\})$. Thus, for $A \in \mathcal{A}_j$ and $B \in \mathcal{A}_i$ we get

$$\int_A \int \delta_{s}(B)a_{s's}k_{ji}(s', ds)\pi(ds') = \int_A \int \delta_{s_{ji}(B)}a_{s's_{ji}(B)}k_{ji}(s', u')p(s')du'ds'$$

$$\overset{*}{=} \int_A \int \delta_{s_{ji}(B)}r_{s'u'}k_{ji}(s', u')p(s')du'ds' = \int_B \int \delta_{s_{ij}}(A)r_{su}k_{ij}(s,u)p(s)duds$$

$$\overset{*}{=} \int_B \int \delta_{s_{ij}}(A)a_{ss_{ij}}k_{ij}(s,u)p(s)duds = \int_B \int \delta_{s}(A)a_{ss'}k_{ij}(s,ds')\pi(ds)$$
whereby we have used (5) in \(*\).

The computation of the conditional expectation in (4) might be infeasible even if the acceptance probabilities of the reversible-jump algorithm are readily available. Thus, the reversible-jump algorithm is potentially capable of sampling by means of certain proposals which are not directly accessible through the Metropolis-Hastings algorithm of Section 7. However, if \(s_{ji}(s', \cdot)\) is injective, as in the changepoint example in Section 6, we get \(a_{s', s} = r_{s', u'}\) whereby \(u'\) can be chosen uniquely such that \(s_{ji}(s', u') = s\).

**Reversible jump Markov chain Monte Carlo computation and Bayesian model determination**

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\[
\alpha_m(x, x') = \min \left\{ 1, \frac{\pi(dx')q_m(x', dx)}{\pi(dx)q_m(x, dx')} \right\}. \tag{6}
\]

For straightforward cases, the dimension-matching requirement can be imposed fairly simply.

Figure 3: An excerpt from Green (1995)

10 Discussion

Now we want to discuss some misunderstandings related to the reversible-jump algorithm. Green (1995) claims: “Our framework provides a natural generalisation of Hastings methods to general parameter spaces.”. Unfortunately, this statement is deceptive. Indeed Green (1995) is convinced that the Metropolis-Hastings algorithm is incapable of sampling across spaces of different dimensions. Figure 3 depicts his false reasoning. He states that the density used to perform the move \(m\) must also be used for the backward transition. As we have seen in Section 8 this is wrong. In Chen et al. (2012) you can find a further false reasoning to prove this stubborn belief.
There is now unfortunately a tremendous amount of papers which support these false conclusions without scrutinizing them. Important examples are Sisson (2005); Green (2003); Green and Hastie (2009); Carlin and Chib (1995); Sambridge et al. (2006)). According to Google scholar Green (1995) has been cited over 5000 times until now.

The overemphasis of the dimension of the space has led to an oversimplification of the mathematical language. Therefore, the literature partially reads like science fiction. By this, reversible-jump was raised to the de facto gold-standard in the trans dimensional case. This is somehow paradox, because reversible-jump is a fairly complicated method itself.

As we have seen, the dimension can conveniently be abstracted by means of mixture spaces. By this, sampling across different spaces becomes an ordinary task for the conventional Metropolis-Hastings algorithm. A thorough search for papers which share this stance revealed only Godsill (2001); Tierney (1998); Roodaki et al. (2011); Geyer and Moller (1994); Jannink and Fernando (2004) and Andrieu et al. (2001).

The name reversible-jump stems from Green’s conviction that he constructed a method which overcomes the non-reversibility of trans dimensional moves in the Metropolis-Hastings algorithm. In this context the reversibility of a move means that the backward move in the opposite direction is feasible. Unfortunately, this name collides with the notion of reversible MCMC methods. Here, the word reversible indicates that the Markov chain created by the MCMC method is reversible, i.e. it meets the detailed balance condition. Thus, the name reversible-jump is highly misleading and lacks a proper meaning. Conversely, the name reversible MCMC is potentially used ambiguously.

Even though Tierney (1998) and Roodaki et al. (2011) generalize the Metropolis-Hastings algorithm such that it captures the proposals utilized in the reversible-jump algorithm, Lemma 7 shows that in order to compute the acceptance probability in Equation 3 we would still need to incorporate the diffeomorphism that acts on the superordinate space of higher dimension. Therefore, the reversible-jump algorithm greatly facilitates the design and implementation of a family of proposals which are otherwise cumbersome or even impossible to use directly inside the Metropolis-Hastings acceptance probability of Equation (3).

Ultimately, the literature around reversible jump and trans dimensional sampling is pervaded with misleading claims and poor mathematical language. In addition, the outshining popularity of Green (1995) exacerbates this situation even further. Nevertheless, the reversible-jump algorithm
makes an important contribution to trans dimensional sampling and in particular to Bayesian
disciplines like changepoint analysis, regression and point processes.

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