Non-reversible guided Metropolis–Hastings kernel

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Abstract

We construct a non-reversible Metropolis–Hastings kernel as a multivariate extension of the guided-walk kernel proposed by Gustafson (1998) by introducing a projection from state space to a locally compact topological group. As a by-product, we construct an efficient reversible Metropolis–Hastings kernel based on the Haar measure which is of interest in its own right. The proposed non-reversible kernel was 10-40 times better than the random-walk Metropolis kernel or the Hamiltonian Monte Carlo kernel for the Gaussian process classification example in terms of effective sample size.

1 Introduction

1.1 Non-reversible Metropolis–Hastings kernel

Markov chain Monte Carlo methods have become essential tools in Bayesian computation. Bayesian statistics have been strongly influenced by the evolution of these methods. This influence was well expressed in Robert and Casella (2011), Green et al. (2015). However, the applicability of traditional Markov chain Monte Carlo methods is limited for some statistical problems involving large data sets. This motivated researchers to work on new kinds of Monte Carlo methods, such as piecewise deterministic Monte Carlo methods (Bouchard-Côté et al., 2018, Bierkens et al., 2019), divide-and-conquer methods (Wang and Dunson, 2013, Neiswanger et al., 2014, Scott et al., 2016), approximate subsampling methods (Welling and Teh, 2011, Ma et al., 2015), and non-reversible Markov chain Monte Carlo methods.

In this paper, we focus on non-reversible Markov chain Monte Carlo methods. Reversibility refers to the sophisticated balancing condition (detailed-balance condition) which makes the Markov kernel invariant with respect to the probability measure of interest. Although reversible Markov kernels form a nice class (Kipnis and Varadhan, 1986, Roberts and Rosenthal, 1997, Roberts and Tweeddle, 2001, Kontoyiannis and Meyn, 2011), the condition is not necessary for the invariance. Breaking reversibility sometimes improves the convergence properties of Markov chains (Diaconis and Saloff-Coste, 1993, Diaconis et al., 2000, Andrieu and Livingstone, 2019).

However, without the sophisticated balancing condition, constructing a Markov chain Monte Carlo method is not an easy task. There are many efforts working in this direction but still there is a large gap between the theory and practice. The guided-walk method for a probability measure in a one-dimension Euclidean space proposed by Gustafson (1998) sheds some light in this direction. A multivariate extension was studied in Ma et al. (2019), but that extension was still based on the one-dimensional Markov kernel. In this paper, we consider a general multivariate extension of Gustafson (1998), termed the guided Metropolis–Hastings kernel.

The main idea of our method is to introduce a projection which maps state space $E$ to a totally ordered group. The ordering provides a global topological information to the Markov kernels.
Using this ordering, we can decompose any Markov kernel into a sum of positive (+) and negative (−) directional sub-Markov kernels. By employing rejection sampling, two sub-Markov kernels are normalised to be positive and negative directional Markov kernels. Then we can construct a non-reversible Markov kernel on \( E \times \{-, +\} \) by applying the systematic-scan Gibbs sampler.

Usually, the total masses of the two sub-Markov kernels are quite different, which results in inefficiency of rejection sampling. To avoid this issue, we focus on the case where the total masses are the same. However, it is nontrivial to find such a Markov kernel. By using the Haar measure, we introduce a novel Markov kernel termed the Haar-mixture reversible kernel that has the desired property. Our proposed method, the guided Metropolis–Hastings kernel, is constructed by using the Haar-mixture reversible kernel as the proposal kernel. Using this method, we introduce many non-reversible guided Metropolis–Hastings kernels which are of practical interest.

1.2 Literature review

Here we briefly review the existing literature which has studied non-reversible Markov kernels that modify reversible Metropolis–Hastings kernels. First of all, products of reversible Markov kernels are not reversible in general. For example, the systematic-scan Gibbs sampler is usually non-reversible.

The so-called lifting method was considered in, for example, Diaconis et al. (2000), Turitsyn et al. (2011), Vucelja (2016). In this method, a Markov kernel is lifted to an augmented state space by splitting the Markov kernel into two sub-Markov kernels. An incidental variable chooses which kernel should be followed. The guided-walk kernel Gustafson (1998) and the method we are proposing are classified into this category. Another approach is preparing two Markov kernels in advance and constructing a systematic-scan Gibbs sampler as in Ma et al. (2019).

The Hamiltonian Monte Carlo kernel has an incidental variable by construction. Therefore, a systematic-scan Gibbs sampler can naturally be defined, as in Horowitz (1991). Also, Tripuraneni et al. (2017) constructed a different non-reversible kernel which twists the original Hamiltonian Monte Carlo kernel. See also Sherlock and Thiery (2017), Ludkin and Sherlock (2018).

An important exception which does not introduce incidental variables is Bierkens (2016), which introduced an anti-symmetric part into the acceptance probability so that the kernel becomes non-reversible while preserving \( \Pi \)-invariance. See also Neal (2020), which avoids requiring an additional incidental variable by focusing on the uniform distribution that is implicitly used for the acceptance-rejection procedure in the Metropolis–Hastings algorithm.

1.3 Reversibility and Metropolis–Hastings kernel

Before analysing the non-reversible Markov kernel, we first recall the definition of reversibility. Reversibility is important throughout the paper since our construction of a non-reversible Markov kernel is based on a class of reversible Markov kernels. A Markov kernel \( P \) on a measurable space \((E, \mathcal{E})\) is \( \mu \)-reversible for a \( \sigma \)-finite measure \( \mu \) if

\[
\int_A \mu(dx)Q(x, B) = \int_B \mu(dx)Q(x, A)
\]

for any \( A, B \in \mathcal{E} \). If \( Q \) is \( \mu \)-reversible, then \( Q \) is \( \mu \)-invariant. There is a strong connection between ergodicity and \( \mu \)-reversibility. See Kipnis and Varadhan (1986, 1997), Roberts and Tweedie (2001), Kontogiannis and Meyn (2011).

As we mentioned above, our non-reversible Markov kernel is based on a class of reversible kernels. Suppose that \( \mu \) is a probability measure on an abelian group \((E, +)\). A simple approach to construct a reversible kernel is to first describe \( \mu \) as a convolution of probability measures \( \mu_Y, \mu_Z \),
and then define independent random variables \( Y_1, Y_2 \sim \mu_Y \) and \( Z \sim \mu_Z \). Finally, construct \( Q \) as the conditional distribution of \( X_2 = Y_2 + Z \) given \( X_1 = Y_1 + Z \). Then the probabilities in (1.1) are \( \Pr(X_1 \in A, X_2 \in B) \) and \( \Pr(X_1 \in B, X_2 \in A) \) which are the same by construction. Examples 2.10 and 2.14 follow this approach, and construction of Example 1.1 is based on Example 2.14.

Let \( \mathbb{R}_+ = (0, \infty) \).

**Example 1.1 (Chi-squared kernel).** Let \( L \in \mathbb{N} \) and \( \rho \in (0, 1) \). Consider a Markov kernel \( Q(x, dy) \) on \( \mathbb{R}_+ \) defined by the update

\[
y = \left[ \left( (1 - \rho) x \right)^{1/2} + \rho^{1/2} w_1 \right]^2 + \sum_{l=2}^{L} \rho^{1/2} w_l^2,
\]

where \( w_1, \ldots, w_L \) are independent and follow the standard normal distribution \( \mathcal{N}(0, 1) \). The conditional distribution of \( y/\rho \) given \( x \) is the non-central chi-squared distribution with \( L \) degrees of freedom and non-central parameter \( (1 - \rho)x/\rho \). Suppose that \( x \sim \mathcal{G}(L/2, 1/2) \), where \( \mathcal{G}(\nu, \alpha) \) is the Gamma distribution with shape parameter \( \nu \) and rate parameter \( \alpha \). By the properties of the non-central chi-squared distribution, \( (x, y) \) has the same law as that of

\[
\left( \sum_{l=1}^{L} v_l^2, \sum_{l=1}^{L} \left( (1 - \rho)^{1/2} v_l + \rho^{1/2} w_l \right)^2 \right),
\]

where \( v_1, \ldots, v_L, w_1, \ldots, w_L \sim \mathcal{N}(0, 1) \) are independent. Both \( (v_l, (1 - \rho)^{1/2} v_l + \rho^{1/2} w_l) \) and \( ((1 - \rho)^{1/2} v_l + \rho^{1/2} w_l, v_l) \) have the same law. Hence, \( (x, y) \) and \( (y, x) \) have the same law. Therefore, the kernel is \( \mathcal{G}(L/2, 1/2) \)-reversible.

Although the above construction of a reversible Markov kernel is simple, by far the most popular scheme for such constructions is using the Metropolis–Hastings method. Here we recall the definition of the Metropolis–Hastings kernel. This definition is a little wider than the usual one as in that we do not assume a particular form for the acceptance probability.

**Definition 1.2.** Let \( Q \) be a Markov kernel and let \( \Pi \) be a probability measure on \( E \). The acceptance probability is a joint measurable function \( \alpha : E^2 \rightarrow [0, 1] \) such that

\[
\alpha(x, y)\Pi(dx)Q(x, dy) = \alpha(y, x)\Pi(dy)Q(y, dx).
\]  

A Markov kernel \( P \) is called a Metropolis–Hastings kernel of \( (Q, \Pi, \alpha) \) if

\[
P(x, dy) = Q(x, dy)\alpha(x, y) + \delta_x(dy) \left\{ 1 - \int_E Q(x, dy)\alpha(x, y) \right\}.
\]

A Metropolis–Hastings kernel \( P \) is \( \Pi \)-reversible. Also, if \( Q \) is \( \mu \)-reversible and a probability measure \( \Pi \) has a density \( \pi \) with respect to \( \mu \), then by taking

\[
\alpha(x, y) = \min \left\{ 1, \frac{\pi(y)}{\pi(x)} \right\},
\]

the triplet \( (Q, \Pi, \alpha) \) satisfies (1.2).
2 Guided kernel

2.1 Unbiasedness

In this section, we introduce the $\Delta$-guided Metropolis–Hastings kernel, which is the non-reversible Markov kernel that we want to propose in this article. A measurable map $\Delta : E \rightarrow G$ is called a statistic, where $G = (G, \leq)$ is a totally ordered set. Here, a totally ordered set is a set $G$ equipped with a binary relation $\leq$ which satisfies three properties: (a) $a \leq b$ and $b \leq a$ implies $a = b$, (b) if $a \leq b$ and $b \leq c$, then $a \leq c$, (c) $a \leq b$ or $b \leq a$ for all $a, b \in G$. We write $a < b$ if $a \leq b$ and $a \neq b$.

Example 2.1 (Lexicographical order). For $x = (x_1, \ldots, x_d)$, let $s(x)_i = x_i + \cdots + x_d$ be a partial sum of the vector $x$ from the $i$th element to the $d$th element. Euclidean space $\mathbb{R}^d$ is a totally ordered set by introducing a version of lexicographical order $\leq$, where $x < y$ if and only if $s(x)_i = s(y)_i$ for $i = 1, \ldots, d$, or

$$s(x)_1 = s(y)_1, \ldots, s(x)_i = s(y)_i, s(x)_{i+1} < s(y)_{i+1}$$

for some $i = 0, \ldots, d - 1$.

A statistic $\Delta$ will guide a Markov kernel $Q(x, dy)$ according to the incidental directional variable $i \in \{-, +\}$ as in [Gustafson (1998)]. When the positive direction $i = +$ is selected, then $y$ is sampled according to $Q(x, dy)$ unless $\Delta x \leq \Delta y$ by rejection sampling. If the negative direction $i = -$ is selected, $y$ is sampled unless $\Delta y \leq \Delta x$. It is typical that one of the rejection sampling directions has high rejection probability (see Example 2.3). To avoid this inefficiency, we consider a class of Markov kernels $Q$ such that the probabilities of the events $\Delta x \leq \Delta y$ and $\Delta y \leq \Delta x$ measured by $Q(x, \cdot)$ are the same. We say $Q$ is unbiasedness if this property is satisfied. If unbiasedness is violated, then the rejection sampling can be inefficient due to the high rejection probability.

Definition 2.2. Let $\Delta : E \rightarrow G$ be a statistic. We say a Markov kernel $Q$ on $E$ is $\Delta$-unbiased if

$$Q(x, \{y \in E : \Delta x \leq \Delta y\}) = Q(x, \{y \in E : \Delta y \leq \Delta x\})$$

for any $x \in E$. Also, we say that two statistics $\Delta$ and $\Delta'$ from $E$ to possibly different totally ordered sets are equivalent if

$$Q(x, \{y \in E : \Delta x \leq \Delta y\} \ominus \{y \in E : \Delta' x \leq \Delta' y\}) = 0,$$

$$Q(x, \{y \in E : \Delta y \leq \Delta x\} \ominus \{y \in E : \Delta' y \leq \Delta' x\}) = 0$$

for $x \in E$, where $A \ominus B = (A \cap B^c) \cup (A^c \cap B)$.

If $\Delta$ and $\Delta'$ are equivalent, then $\Delta$-unbiasedness implies $\Delta'$-unbiasedness. Let $v^\top$ be the transpose of $v \in \mathbb{R}^d$.

Example 2.3 (Random-walk kernel). Let $\Gamma$ be a probability measure on $\mathbb{R}^d$ which is symmetric about the origin, that is, $\Gamma(A) = \Gamma(-A)$ for $-A = \{x \in E : -x \in A\}$. Let $Q(x, A) = \Gamma(A - x)$. Then $Q$ is $\Delta$-unbiased for $\Delta x = v^\top x$ for some $v \in \mathbb{R}^d$ since

$$Q(x, \{y : \Delta x \leq \Delta y\}) = \Gamma(\{x : 0 \leq v^\top x\}) = \Gamma(\{x : v^\top x \leq 0\}).$$

On the other hand, $Q$ is not $\Delta'$-unbiased for $\Delta' x = x_1^2 + \cdots + x_d^2$, where $x = (x_1, \ldots, x_d)$, if $\Gamma$ is not the Dirac measure centred on $(0, \ldots, 0)$. In particular, if $\Gamma(\{(0, \ldots, 0)\}) = 0$, then $Q(x, \Delta'y \leq \Delta'x) = 0$ for $x = (0, \ldots, 0)$. 

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where $p$ Metropolis–Hastings kernel of variance corresponding to the central limit theorem. The inner product

$$
\langle f, g \rangle = \int f(x)g(x)\Pi(dx)
$$

With this property, it is straightforward to check that $\Delta$-unbiased Markov kernel $Q$ on $E$ and a measurable function $\alpha : E \times E \to [0,1]$ satisfy (1.3). We say a Markov kernel $P_G$ on $E \times \{-,+\}$ is the $\Delta$-guided Metropolis–Hastings kernel of $(Q, \Pi, \alpha)$ if

$$
P_G(x,+,dy,+) = Q_+(x,dy)\alpha(x,y)
$$

$$
P_G(x,+,dy,-) = \delta_x(dy) \left\{ 1 - \int_E Q_+(x,dy)\alpha(x,y) \right\}
$$

$$
P_G(x,-,dy,-) = Q_-(x,dy)\alpha(x,y)
$$

$$
P_G(x,-,dy,+) = \delta_x(dy) \left\{ 1 - \int_E Q_-(x,dy)\alpha(x,y) \right\},
$$

where

$$
Q_+(x,dy) = 2Q(x,dy)1_{\{\Delta x < \Delta y\}} + Q(x,dy)1_{\{\Delta x = \Delta y\}},
$$

$$
Q_-(x,dy) = 2Q(x,dy)1_{\{\Delta y < \Delta x\}} + Q(x,dy)1_{\{\Delta x = \Delta y\}}.
$$

The Markov kernel $P_G$ satisfies the so-called $\Pi_G$-skew-reversible property

$$
\Pi_G(dx,+P_G(x,+,dy,+)) = \Pi_G(dy,-P_G(y,-,dx,-),
$$

$$
\Pi_G(dx,+P_G(x,+,dy,-)) = \Pi_G(dy,-P_G(y,-,dx,+),
$$

where

$$
\Pi_G = \Pi \otimes (\delta_- + \delta_+)/2.
$$

With this property, it is straightforward to check that $P_G$ is $\Pi_G$-invariant.

Example 2.5 (Guided-walk kernel). The $\Delta$-guided Metropolis–Hastings kernel corresponding to a random-walk kernel $Q$ on $\mathbb{R}$ is called the guided-walk in [Gustafson (1998)]. For a multivariate target distribution, $\Delta x = v^\top x$ for some $v \in \mathbb{R}^d$ was considered in [Gustafson (1998), Ma et al. (2019)].

We now see that $P_G$ is always expected to be better than $P$ in the sense of the asymptotic variance corresponding to the central limit theorem. The inner product $\langle f, g \rangle = \int f(x)g(x)\Pi(dx)$ and the norm $\|f\| = (\langle f, f \rangle)^{1/2}$ can be defined on the space of $\Pi$-square integrable functions. Let $(X_0, X_1, \ldots)$ be a Markov chain with Markov kernel $P$ and $X_0 \sim \Pi$. Then we define the asymptotic variance

$$
\text{var}(f, P) = \lim_{N \to \infty} \text{var} \left( N^{-1} \sum_{n=1}^N f(X_n) \right)
$$

if the right-hand side exists. The existence of the right-hand side limit is a kernel-specific problem and not addressed here. Let $\lambda \in [0,1)$. As in [Andrieu (2016)], to avoid a kernel-specific argument, we consider a pseudo asymptotic variance

$$
\text{var}_\lambda(f, P) = \|f_0\|^2 + 2 \sum_{n=1}^{\infty} \lambda^n \langle f_0, P^n f_0 \rangle,
$$

where $f_0 = f - \Pi(f)$, which always exists. Under some conditions, $\lim_{\lambda \to 1^-} \text{var}_\lambda(f, P) = \text{var}(f, P)$. We can also define $\text{var}_\lambda(f, P_G)$ for $\Pi$-square integrable function $f$ on $E$ by considering $f((x,i)) = f(x)$.

Proposition 2.6 (Theorem 3.17 of [Andrieu and Livingstone (2019)]). Suppose that $f$ is $\Pi$-square integrable. Then for $\lambda \in [0,1]$, $\text{var}_\lambda(f, P_G) \leq \text{var}_\lambda(f, P)$.

By taking $\lambda \rightarrow 1-$, we can expect that the non-reversible kernel $P_G$ is better than $G$ in the sense of smaller asymptotic variance.
2.2 Random-walk property

Constructing a $\Delta$-unbiased Markov kernel is a crucial step for our approach. However, determining how to construct a $\Delta$-unbiased Markov kernel is nontrivial. The random-walk property is the key for this construction.

Let $G$ be a topological group; that is, $G$ is a group and its group actions $(x,y) \mapsto xy$ and $x \mapsto x^{-1}$ are continuous. The topological group $E$ is equipped with a Borel $\sigma$-algebra. Let $A^{-1} = \{ g \in G : g^{-1} \in A \}$ for a Borel set $A$ of $G$.

**Definition 2.7.** Markov kernel $Q(x,dy)$ has the $(\Delta, \Gamma)$-random-walk property if there is a statistic $\Delta : E \to G$ with a probability measure $\Gamma$ on a topological group $G$ such that $\Gamma(A) = \Gamma(A^{-1})$ for any Borel set $A$ of $G$ and

$$Q(x, \{y \in E : \Delta y \in A\} = \Gamma((\Delta x)^{-1} A).$$

A typical example of a Markov kernel with the $(\Delta, \Gamma)$-random-walk property is Example 2.3.

Let $(G, \leq)$ be an ordered group; that is, $G$ is a group and $\leq$ is a total ordering such that $a \leq b$ implies $ca \leq cb$ and $ac \leq bc$ for $a, b, c \in G$.

**Proposition 2.8.** If $Q$ has the $(\Delta, \Gamma)$-random-walk property with ordered group $G$, then $Q$ is $\Delta$-unbiased.

**Proof.** Let $A = [\Delta x, +\infty) = \{ g \in A : \Delta x \leq g \}$. Then for the unit element $e$,

$$Q(x, \{ y \in E : \Delta x \leq \Delta y \}) = Q(x, \{ y \in E : \Delta y \in A \}) = \Gamma((\Delta x)^{-1} A) = \Gamma([e, +\infty)).$$

Similarly, $Q(x, \{ y \in E : \Delta y \leq \Delta x \}) = \Gamma([-\infty, e])$. Since $[e, +\infty)^{-1} = (-\infty, e]$, $Q$ is $\Delta$-unbiased. $\square$

2.3 Haar-mixture reversible kernel

There seems to be no obvious way of constructing a Markov kernel with the random-walk property. We introduce Markov kernels which are reversible with respect to the Haar measure. The Haar measure enables us to construct a random walk on a locally compact topological group, which is a crucial step towards obtaining the random-walk property. The connection between the Markov kernels and the random-walk property will be made clear in the next section.

Let $(G, \times)$ be a locally compact topological group equipped with the Borel $\sigma$-algebra. Let $(E, +)$ be a left $G$-module, which is an abelian topological group with left-group action $(g, x) \mapsto gx$ from $G \times E$ to $E$. We assume that $E$ is equipped with a Borel $\sigma$-algebra $\mathcal{E}$ and the left-group action is jointly measurable. Let $Q$ be a $\mu$-reversible Markov kernel on $(E, \mathcal{E})$, where $\mu$ is a $\sigma$-finite measure. Let

$$Q_g(x, A) = Q(gx, gA) \ (x \in E, A \in \mathcal{E}, g \in G).$$

Then $Q_g$ is $\mu_g$-reversible where

$$\mu_g(A) = \mu(gA).$$

Let $\nu$ be the right Haar measure on $G$, that is, $\nu(Ag) = \nu(A)$. Set

$$\mu_\ast(A) = \int_{g \in G} \mu_g(A) \nu(dg) \ (A \in \mathcal{E}). \quad (2.2)$$

Assume that $\mu_\ast$ is $\sigma$-finite. Then $\mu_\ast$ is a left-invariant measure. Indeed,

$$\mu_\ast(a A) = \int_{b \in G} \mu_b(aA) \nu(db) = \int_{b \in G} \mu(bA) \nu(db) = \int_{b \in G} \mu(bA) \nu(db) = \mu_\ast(A).$$

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Suppose that $\mu$ is absolutely continuous with respect to $\mu_*$. Then $(g, x) \mapsto d\mu_g/d\mu_*(x)$ is jointly measurable. This is because $d\mu_g/d\mu_*(x) = d\mu/d\mu_*(gx)$ by the left-invariance of $\mu_*$, and $(g, x) \mapsto gx$ is assumed to be jointly measurable. Let

$$K(x, dg) = \frac{d\mu_g}{d\mu_*}(x)\nu(dg)$$

By the Radon–Nikodym theorem, $K(x, G) = 1$ $\mu_*$-almost surely. Define

$$Q_*(x, A) = \int_{g \in G} K(x, dg)Q_g(x, A).$$

(2.3)

**Definition 2.9.** The Markov kernel $Q_*$ defined by (2.3) is called the Haar-mixture reversible kernel of $Q$.

**Example 2.10** (Beta-gamma kernel). Beta-gamma (autoregressive) kernel $Q(x, dy)$ on $E = \mathbb{R}_+$ is defined by

$$y = bx + c, \ b \sim \mathcal{B}_\epsilon(k, k(1 - \rho)), \ c \sim \mathcal{G}(k(1 - \rho), 1),$$

where $b, c$ are independent, $k > 0$ is a constant, and $\mathcal{B}_\epsilon(\alpha, \beta)$ is the Beta distribution with shape parameters $\alpha$ and $\beta$. The kernel is $\mu = \mathcal{G}(k, 1)$-reversible. See Lewis et al. (1989). The Metropolis–Hastings algorithm using a beta-gamma kernel was proposed by Hosseini (2019).

By operation $(g, x) \mapsto gx$ with $G = (\mathbb{R}_+, \times)$, $E$ is a left $G$-module. We have $\mu_g = \mathcal{G}(k, g)$, and the Markov kernel $Q_g$ is the same as $Q$ replacing $c \sim \mathcal{G}(k(1 - \rho), 1)$ by $c \sim \mathcal{G}(k(1 - \rho), g)$. The Haar measure on $G$ is $\nu(dg) = g^{-1}dg$, and hence $\mu_*(dx) = x^{-1}dx$ and $K(x, dg) = \mathcal{G}(k, x)$.

**Proposition 2.11.** The Haar-mixture reversible kernel $Q_*$ is $\mu_*$-reversible.

**Proof.** Let $A, B \in \mathcal{E}$. Since $Q_g$ is $\mu_g$-reversible,

$$\int_{x \in A} \mu_*(dx)Q_*(x, B) = \int_{g \in G} \int_{x \in A} \mu_*(dx)K(x, dg)Q_g(x, B)$$

$$= \int_{g \in G} \int_{x \in A} \mu_g(dx)Q_g(x, B)\nu(dg)$$

$$= \int_{g \in G} \int_{x \in B} \mu_g(dx)Q_g(x, A)\nu(dg)$$

$$= \int_{x \in B} \mu_*(dx)Q_*(x, A).$$

A Metropolis–Hastings kernel $P_*$ of $(Q_*, \Pi, \alpha)$ is implemented as the following algorithm, where $\pi(x) = (d\Pi/d\mu_*)(x)$. In the algorithm, $U[0, 1]$ is a uniform distribution.

### 2.4 Sufficiency

Let $(G, \times)$ be a unimodular locally compact topological group; that is, the left Haar measure and the right Haar measure coincide up to a multiplicative constant. For example, all abelian groups are unimodular. Also, let $(G, \leq)$ be an ordered group, $(E, +)$ be an abelian left $G$-module, and $\Delta : E \to G$ satisfy $\Delta gx = g\Delta x$ for $g \in G$ and $x \in E$. For a $\sigma$-finite measure $\Pi$ on $E$ and a statistic $\Delta : E \to G$, we define the image measure of $\Delta$ under $\Pi$ by

$$\hat{\Pi}(A) = \int_{\{\Delta x \in A\}} \Pi(dx).$$
Algorithm 1 Metropolis–Hastings kernel with Haar-mixture reversible kernel

Input $x \in E$
Simulate $g \sim K(x, dg)$
Simulate $y \sim Q_g(x, dy)$
Simulate $u \sim \mathcal{U}[0, 1]$
if $u \leq \min\{1, \pi(y)/\pi(x)\}$ then
    set $x \leftarrow y$
end if
Output $x$

Let $\hat{\mu}_*$ be the image measure of $\Delta$ under $\mu_*$. Then it is a left Haar measure, since
\[
\hat{\mu}_*(gA) = \mu_*(\{y \in E : \Delta y \in gA\})
\]
\[
= \mu_*(\{y \in E : \Delta (g^{-1} y) \in A\})
\]
\[
= \mu_*(\{y \in E : \Delta y \in A\})
\]
\[
= \hat{\mu}_*(A)
\]
by the left-invariance of $\mu_*$. Since $G$ is unimodular, the left Haar measure $\hat{\mu}_*$ and right Haar measure $\nu$ coincide up to a multiplicative constant. From this fact, we can assume
\[
\hat{\mu}_* = \nu
\]
without loss of generality.

Definition 2.12. Let $\mu$ be a $\sigma$-finite measure. We call a statistic $\Delta$ sufficient for a $\mu$-invariant Markov kernel $Q$ if there is a Markov kernel $\hat{Q}$ and a measurable function $h_1$ on $G$ such that
\[
Q(x, \{y \in E : \Delta y \in A\}) = \hat{Q}(\Delta x, A)
\]
and
\[
\frac{d\mu}{d\mu_*}(x) = h_1(\Delta x)
\]
$\mu_*$-almost surely.

By the left-invariance of $\mu_*$,
\[
\frac{d\mu_a}{d\mu_*}(x) = h_1(g \Delta x). \tag{2.4}
\]
Let $\hat{\mu}$ be the image measure of $\Delta$ under $\mu$. If $\Delta$ is sufficient, then
\[
\frac{d\hat{\mu}}{d\nu}(a) = h_1(a).
\]
Furthermore, if $Q$ is $\mu$-reversible, then $\hat{Q}$ is $\hat{\mu}$-reversible.

Example 2.13 (A product of Markov kernels on a half-line). Suppose that each Markov kernel $Q_i$ on $\mathbb{R}_+$ is reversible with respect to a probability measure for each $i = 1, \ldots, d$. The product kernel $Q(x, dy) = Q_1(x_1, dy_1) \cdots Q_d(x_d, dy_d)$ is defined on $G = E = \mathbb{R}_+^d$. From the operation
\[
(g, x) \mapsto (g_1 x_1, \ldots, g_d x_d),
\]
$E$ is a $G$-module, where $g = (g_1, \ldots, g_d), x = (x_1, \ldots, x_d)$. Consider the ordering $\preceq_i$. Then $\Delta x = x$ is sufficient for $Q$ with $\hat{Q} = Q$ and $h_1 = d\hat{\mu}/d\nu$. If $Q(x, \cdot)$ is absolutely continuous with respect to the Lebesgue measure for each $x$, then $\Delta x$ and $\Delta' x = \sum_{i=1}^d x_i$ are equivalent.
Example 2.14 (Autoregressive kernel). Let $\rho \in (0, 1]$ and $M$ be a $d \times d$ positive definite symmetric matrix, and let $x_0 \in \mathbb{R}^d$. Further, let $N_d(x, M)$ be the normal distribution with mean $x \in \mathbb{R}^d$ and covariance matrix $M$. It is known that autoregressive kernel $Q$ on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$ defined by

$$Q(x, \cdot) = N_d(x_0 + (1 - \rho)^{1/2} (x - x_0), \rho M)$$

is $\mu_d = N_d(x_0, M)$-reversible. The autoregressive kernel corresponds to the update

$$y = x_0 + (1 - \rho)^{1/2} (x - x_0) + \rho^{1/2} M^{1/2} w,$$

where $w$ follows the standard normal distribution. Let $E = (\mathbb{R}^d, +)$ and $G = (\mathbb{R}_+, \times)$, and set $(g, x) \mapsto x_0 + g^{1/2} (x - x_0)$. Then the Haar measure is $\nu(dg) = g^{-1} dg$. A simple calculation yields $\mu_g = N_d(x_0, g^{-1} M)$ and $Q_g(x, \cdot) = N_d(x_0 + (1 - \rho)^{1/2} (x - x_0), g^{-1} \rho M)$. Also, $\mu_{\ast}(dx) x(\Delta x)^{-d/2} dx$ and $K(x, dg) = G(d/2, \Delta x/2)$ where $\Delta x = (x - x_0)^{\top} M^{-1} (x - x_0)$.

We show that $\Delta x$ is sufficient. For $\xi = (1 - \rho)^{1/2} \rho^{-1/2} M^{-1/2} (x - x_0)$,

$$\Delta y = \rho \| \xi + w \|^2,$$

where $\| \cdot \|$ is the Euclidean norm. Therefore, $\rho^{-1} \Delta y$ conditioned on $x$ follows the non-central chi-squared distribution with $d$ degrees of freedom and non-central parameter $\| \xi \|^2 = (1 - \rho) \rho^{-1} \Delta x$. Hence, the law of $\Delta y$ depends on $x$ only through $\Delta x$ and hence there exists a Markov kernel $\hat{\Gamma}$. Also, a simple calculation yields $h_1(g) = g^{d/2} \exp(-g/2)$. Therefore, $\Delta$ is sufficient.

Proposition 2.15. Suppose $\Delta$ is sufficient for a $\mu$-reversible kernel $Q$. Also, suppose a probability measure $\hat{\mu}(da) \hat{Q}(a, db)$ on $G \times G$ is absolutely continuous with respect to $\nu^\otimes 2$. Then $Q_{\ast}$ has the $(\Delta, \Gamma)$-random-walk property for a probability measure $\Gamma$. In particular, it is $\Delta$-unbiased.

Proof. Let $h(a, b)$ be a Radon–Nikodým derivative:

$$h(a, b) \nu(da) \nu(db) = \hat{\mu}(da) \hat{Q}(a, db).$$

By the $\hat{\mu}$-reversibility of $\hat{Q}$, $h(a, b) = h(b, a)$ almost surely. From the sufficiency,

$$h_1(a) = \int_{b \in G} h(a, b) \nu(db), \quad \hat{Q}(a, db) = \frac{h(a, b)}{h_1(a)} \nu(db)$$

$\nu$-almost surely. Together with (2.4), we have

$$Q_{\ast}(a, \{y : \Delta y \in A\}) = \int_{a \in G} K(x, da) Q(ax, \{y : \Delta y \in aA\})$$

$$= \int_{a \in G} \frac{d\mu_a(x)}{d\hat{\mu}_a(x)} \hat{Q}(a \Delta x, aA)$$

$$= \int_{a \in G} h_1(a \Delta x) \nu(da) \int_{b \in aA} h(a \Delta x, b) \nu(db) \nu(da)$$

$$= \int_{a \in G} \int_{b \in A} h(a \Delta x, ab) \nu(db) \nu(da)$$

$$= \int_{a \in G} \int_{b \in A} h(a, a(\Delta x)^{-1} b) \nu(db) \nu(da)$$

where the last equality follows from the right-invariance of $\nu$. Let

$$\hat{h}(a) = \int_{g \in G} h(g, ga) \nu(dg).$$
From $h(a, b) = h(b, a)$,

$$\hat{h}(a^{-1}) = \int_{g \in G} h(g, ga^{-1}) \nu(dg) = \int_{g \in G} h(ga, g) \nu(dg) = \hat{h}(a).$$

By using $\hat{h}$, we can write

$$Q_*(x, \{y; \Delta y \in A\}) = \int_{b \in A} \hat{h}((\Delta x)^{-1} b) \nu(db) = \int_{b \in (\Delta x)^{-1} A} \hat{h}(b) \nu(db).$$

The above is guaranteed to have the $(\Delta, \Gamma)$-random-walk property by introducing $\Gamma(A) = \int_{a \in A} \hat{h}(a) \nu(da)$. Hence, it is $\Delta$-unbiased by Proposition 2.8.

The $\Delta$-guided Metropolis–Hastings kernel using $Q_*$ is given as the following algorithm, where we let $\pi(x) = d\Pi/d\mu_*(x)$.

**Algorithm 2 $\Delta$-guided Metropolis–Hastings kernel**

Input $(x, z) \in E \times \{-, +\}$
Set $y = x$
while $(\Delta y - \Delta x) \times z \leq 0$ do
    Simulate $g \sim K(x, dg)$
    Simulate $y \sim Q_g(x, dy)$
end while
Simulate $u \sim U[0, 1]$
if $u \leq \min\{1, \pi(y)/\pi(x)\}$ then
    set $x \leftarrow y$
else
    else set $z \leftarrow -z$
end if
Output $(x, z)$

3 Simulation

3.1 Multiplicative $G$-module

In this simulation, we consider the autoregressive kernel $Q$ defined in Example 2.14. The Metropolis–Hastings kernel of the proposed kernel $Q$ was studied in, for example, Neal (1999), Beskos et al. (2008), Cotter et al. (2013), and we will refer to this as the preconditioned Crank–Nicolson kernel. The Metropolis–Hastings kernel using the Haar-mixture kernel, which we will refer to as the mixed preconditioned Crank–Nicolson kernel, was developed in Kamatani (2017, 2018). We compare these Markov kernels with the guided version, named the guided mixed preconditioned Crank–Nicolson kernel.

We apply them to a Gaussian process classification problem with a German credit data set from the University of California, Irvine repository (Dua and Graff (2017)). A real-valued function $f$ follows the Gaussian process with the squared exponential covariance function

$$\text{cov}(f(\xi_n), f(\xi_m)) = M_{n,m} = \exp\left(-\frac{\|\xi_n - \xi_m\|^2}{\sigma^2}\right).$$
Table 1: Markov kernels in Table 2

| Kernel      | Description                                      |
|-------------|--------------------------------------------------|
| RWM         | Random-walk Metropolis                           |
| HMC         | Hamiltonian Monte Carlo                           |
| PCN         | Preconditioned Crank–Nicolson                    |
| MPCN        | Mixed preconditioned Crank–Nicolson              |
| GMPCN       | Guided mixed preconditioned Crank–Nicolson       |

Table 2: Effective sample sizes of log-likelihood per second in Gaussian process classification model for the five Markov kernels listed in Table 1

| N   | RWM | HMC | PCN | MPCN | GMPCN |
|-----|-----|-----|-----|------|-------|
| 200 | 11.4| 24.7| 99.77| 219.18| 397.53|
| 400 | 0.79| 3.56| 8.72 | 14.53| 34.47 |
| 600 | 0.27| 0.64| 1.91 | 4.69 | 7.43  |
| 800 | 0.11| 0.29| 0.81 | 1.71 | 3.40  |
| 1000| 0.06| 0.05| 0.39 | 0.82 | 1.38  |

with $\xi_1,\ldots,\xi_N \in \mathbb{R}^{24}$, where $\| \cdot \|$ is the Euclidean norm. Let $M = (M_{n,m})_{n,m=1,\ldots,N}$ be an $N \times N$ matrix and set $\sigma^2 = 10$ throughout. We consider posterior inference of $f = \{f(\xi_n)\}_{n=1}^N$ with output

$$y_n \sim B(\Phi(f(\xi_n))), \quad (n = 1,\ldots,N),$$

where $B(\theta)$ is the Bernoulli distribution with parameter $\theta$, and $\Phi$ is the cumulative distribution function of the standard normal distribution.

We consider the effective sample size of the log-likelihood (per second) as the measure of efficiency. We will observe the behaviours of algorithms through different sample sizes $N \in \{200, 400, 600, 800, 1000\}$ out of a $10^3$ data set.

We apply Markov chain Monte Carlo methods for $10^6$ iterations by a two-step procedure. In the first $10^5$ iterations, the Markov chain Monte Carlo methods are applied with $x_0 = (0,\ldots,0)$. Then we run the remaining iterations with $x_0$ as the empirical average of the sequence in the burn-in stage. The preconditioned Crank–Nicolson kernel was expected to have nice scaling properties in this case, thanks to the reference Gaussian measure (Cotter et al. (2013), Hairer et al. (2014)). However, the mixed preconditioned Crank–Nicolson kernel was two times better, and the guided mixed preconditioned Crank–Nicolson kernel was four times better than the preconditioned Crank–Nicolson kernel. We also compared them to the Hamiltonian Monte Carlo kernel by using Stan (Carpenter et al. (2017)) and the random-walk Metropolis kernel. The Hamiltonian Monte Carlo kernel was not work well in this case. This is not entirely surprising due to the high cost of the derivative evaluation. The random-walk Metropolis kernel was even worse (Table 2). The tuning parameters of the Hamiltonian Monte Carlo kernel were chosen internally by Stan. The tuning parameters for the random-walk kernel were selected so that the average acceptance probability becomes around $23\%$. The tuning parameters were selected so that the acceptance probabilities are around $35\%$ for the guided Metropolis–Hastings kernel and $30\%$ for the other two kernels.

There is a trade-off between variability and acceptance probability. If the proposed value is more variable, then it is more likely to be rejected. Thanks to non-reversibility, the guided Metropolis–Hastings kernel has greater variability than the other kernels. Therefore, we can set a slightly larger acceptance probability for the guided Metropolis–Hastings kernel.

To illustrate the importance of $x_0$, we additionally run a numerical experiment on a 50-dimensional multivariate central $t$-distribution with degrees of freedom $\nu = 3$ and identity covariance matrix (p1
of Kotz and Nadarajah (2004)). The first element of $x_0$ is $\xi \geq 0$ and all the other elements are set to be zero. When $\xi$ is large, then the direction is less important for increasing or decreasing the likelihood. We run the algorithms on the target distribution for $10^5$ iterations. The experiment showed that the benefit of non-reversibility diminishes as the importance of the direction shrinks (Table 3).

| Table 3: Effective sample sizes of log-likelihood per second target on a 50-dimensional student distribution |
| $\xi$ | $\xi = 10^{-3}$ | $\xi = 10^{-2}$ | $\xi = 10^{-1}$ | $\xi = 1$ | $\xi = 10$ |
|------|----------------|----------------|----------------|------|---------|
| MpCN | 378-19         | 96-23          | 94-74          | 93-52| 95-33   |
| GMpCN| 4245-43        | 116-29         | 114-78         | 115-2| 117-20  |

3.2 Additive $G$-module

Next we consider the guided Metropolis–Hastings kernel using a product of the Chi-squared kernels in Example 1.1 for $L = 1$, and a product of the beta-gamma kernels in Example 2.10. In this simulation, we illustrate the difference of behaviour between the guided Metropolis–Hastings kernel and other kernels by showing trajectory plots in two dimensions.

For the product of Chi-squared kernel, we use the operation $(g, x) \rightarrow (gx_1, \ldots, gx_d)$ with $G = \mathbb{R}_+$ and $E = \mathbb{R}_+^d$. By the same argument as in Example 2.13, $\Delta x = x_1 + \cdots + x_d$ is sufficient. In this case, $K(x, dq) = \mathcal{G}(d/2, \Delta x/2)$, where $\Delta x = x_1 + \cdots + x_d$, and $\mu_\tau(dx) = (\Delta x)^{-d/2}(x_1 \cdots x_d)^{-1/2}dx$.

For the beta-gamma kernel, we use the $G$-module structure introduced in Example 2.13. By Example 1.1, $K(x, dq) = \mathcal{G}(k, x_1) \cdots \mathcal{G}(k, x_d)$ and $\mu_\tau(dx) = (x_1 \cdots x_d)^{-1}dx_1 \cdots dx_d$. Since $\Delta x$ and $\Delta' x = \sum_{i=1}^d x_i$ are equivalent, a $\Delta$-guided Metropolis–Hastings kernel for the beta-gamma proposal kernel is also a $\Delta'$-guided Metropolis–Hastings kernel.

We consider a two-dimensional distribution

$$
\frac{1}{3\pi} \frac{x_1^{1/2} x_2^{1/2}}{x_0^{1/2}} \exp \left( -\frac{x_1 + 1}{x_2} \right) dx_1 dx_2 \quad (x_1, x_2 > 0).
$$

We generated two-dimensional trajectory plots to illustrate the difference of behaviour between the Metropolis–Hastings kernel with the Haar-mixture reversible kernel and its guided version. The tuning parameters are selected so that the average acceptance probabilities are around 25%-30% in 50000 iterations. Figure 1 shows the trace plots of the last 150 iterations for the kernels. We can clearly see the greater variation in the guided kernels. Thanks to the incident variable, the guided kernel maintains its direction if the proposed value is accepted. The direction conservation property greatly contributed to increasing variability.

4 Discussion

The theory and application of non-reversible Markov kernels have been under active development recently, but there still exists a gap between the two. In order to close this gap, we have described

| Table 4: Description of Markov kernels in Figure 1 |
|------|----------------|
| MH   | Metropolis–Hastings |
| MHH  | Metropolis–Hastings with Haar-mixture reversible kernel |
| GMH  | Guided Metropolis–Hastings |

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Figure 1: Trace plots of the Metropolis–Hastings kernels. The guided kernels (the right figures) are more variable compared to their non-guided counterparts where the solid line corresponds to the negative direction and the dashed line corresponds to the positive direction. Both the $x_1$ and $x_2$ axes are log-scaled.

How to construct a non-reversible Metropolis–Hastings kernel on a general state space. We believe that the method we propose can make non-reversible kernels more attractive.

As a by-product, we have constructed the Metropolis–Hastings kernel with the proposed Haar-mixture reversible kernel. The Haar-mixture kernel imposes a new state globally by using the random walk on a group, whereas other recent Markov chain Monte Carlo methods use local topological information derived from target densities. We believe that this sheds new light on the proposed global topological approach. A combination of the global and local approaches is an area of further research.

In this paper, we have not discussed geometric ergodicity, although ergodicity is clear under appropriate regularity conditions. A popular approach for proving geometric ergodicity is based on the establishment of a Foster-Lyapunov-type drift condition, which requires kernel-specific arguments. On the other hand, our motivation is to build a general framework for the non-reversible Metropolis–Hastings kernels. Therefore, we did not focus on geometric ergodicity. A more in-depth study should be carried out in that direction.

Finally, we would like to remark that the guided Metropolis–Hastings kernel is not limited to $\mathbb{R}^d$ or $\mathbb{R}^d_+$. It is possible to construct the kernel on the $p \times q$-matrix space and the symmetric $q \times q$ positive definite matrix space, where $p, q$ are any positive integers. The applicability to other spaces is an interesting research area.

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