Optimal design of the Barker proposal and other locally-balanced Metropolis–Hastings algorithms

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Abstract

We study the class of first-order locally-balanced Metropolis–Hastings algorithms introduced in [9]. To choose a specific algorithm within the class the user must select a balancing function \( g : \mathbb{R} \rightarrow \mathbb{R} \) satisfying \( g(t) = tg(1/t) \), and a noise distribution for the proposal increment. Popular choices within the class are the Metropolis-adjusted Langevin algorithm and the recently introduced Barker proposal. We first establish a universal limiting optimal acceptance rate of 57% and scaling of \( n^{-1/3} \) as the dimension \( n \) tends to infinity among all members of the class under mild smoothness assumptions on \( g \) and when the target distribution for the algorithm is of the product form. In particular we obtain an explicit expression for the asymptotic efficiency of an arbitrary algorithm in the class, as measured by expected squared jumping distance. We then consider how to optimise this expression under various constraints. We derive an optimal choice of noise distribution for the Barker proposal, optimal choice of balancing function under a Gaussian noise distribution, and optimal choice of first-order locally-balanced algorithm among the entire class, which turns out to depend on the specific target distribution. Numerical simulations confirm our theoretical findings and in particular show that a bi-modal choice of noise distribution in the Barker proposal gives rise to a practical algorithm that is consistently more efficient than the original Gaussian version.

1 Introduction

Markov chain Monte Carlo algorithms are the workhorse of many contemporary statistical analyses, and an essential part of the modern data science toolkit. Despite many advances, however, reliable inference using Markov chain Monte Carlo can still be a cumbersome task. It is common for practitioners to dedicate much effort to making careful algorithm design choices and adjusting algorithmic tuning parameters to ensure that performance is adequate for a given problem. Failure to do this can be catastrophic; examples for which a well-designed algorithm performs adequately but a less carefully-chosen alternative does not are ubiquitous (e.g. [19]).

Suitable guidelines on the intelligent design and implementation of Markov chain Monte Carlo methods are therefore important. They are not always easy to offer, however, the best choice of method can depend on the user and the problem at hand. In some contexts, a simpler algorithm with less need for adjustment and for which potential problems are easy to diagnose may be preferable. In others contexts, one may be comfortable with more complex methods, which can perform adequately on a larger class of problems if enough fine tuning is done.

For Metropolis–Hastings algorithms, perhaps the most celebrated guidelines concern the choice of optimal acceptance rate [15]. Rigorous theoretical justification for certain values tend to be restricted to the case in which dimension tends to infinity and the distribution from which samples are desired has a particular structure (such as a product form), but empirically the same values are known to be appropriate in many

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other settings \cite{15}. The apparent lack of dependence of these optimal choices on the target distribution allows particularly simple recommendations to be offered to the user for a given algorithm.

Adaptive Markov chain Monte Carlo methods have also facilitated efficient implementation \cite{11,16}. Users can implement adaptive algorithms in which algorithmic tuning parameters are automatically adjusted towards guideline values, using ideas from stochastic optimisation and controlled Markov chains. When combined with appropriate theory, adaptive algorithms can therefore allow users to implement their chosen method on a given problem without the need for cumbersome hand-tuning. Such innovations have made it possible to develop popular tailored software packages for users of Markov chain Monte Carlo \cite{18,3}.

Not all adaptive algorithms are created equally, however. Empirically it has long been observed that certain approaches are more sensitive to tuning than others \cite{11}. In recent work \cite{9} provided some theoretical justification for this phenomenon, in particular showing that for popular gradient-based approaches such as the Metropolis-adjusted Langevin algorithm and Hamiltonian Monte Carlo spectral gaps decay exponentially quickly to zero as the tuning parameters are perturbed from their optimal values. By contrast, spectral gaps for the simpler random walk Metropolis decay at a polynomial rate, indicating that the algorithm is much more robust to tuning. This has a compounding effect if the tuning parameters are learned adaptively, as adaptive algorithms typically learn based on past samples from the Markov chain, and if these past samples are very poor as a result of the initial tuning parameters being sub-optimal it can mean that the learning occurs very slowly. The moral of the story is that algorithms can still perform poorly in practice even if an optimally-tuned version would in theory perform well.

These findings present a conundrum, as gradient-based algorithms are considered the state-of-the-art in Markov chain Monte Carlo to sample from continuous and smooth distributions when properly tuned. To explore the phenomenon in more detail \cite{9} introduce a general class of gradient-based algorithms, termed first order locally-balanced Metropolis–Hastings, of which the Metropolis-adjusted Langevin algorithm is a special case. Constructing a member of the class requires a Markov kernel, which can be thought of as the initial noise distribution for the transition, together with a balancing function, which must satisfy certain properties (see Section 2). The authors consider different choices from within the class, and in particular construct a method called the Barker proposal. This algorithm has spectral gaps that are robust to tuning as in the random walk Metropolis. The authors also establish sufficient conditions for geometric ergodicity and some preliminary results on scaling with dimension, suggesting that relaxation times are $O(n^{1/3})$, where $n$ is the dimension of the state. Empirical results in the paper show that the Barker algorithm pairs extremely well with adaptive learning of tuning parameters, and enables reliable sampling on complex examples in which other gradient-based methods may not, despite being remarkably simple to implement. More discussion and a pedagogical derivation of the Barker algorithm is provided in \cite{7}.

Several unexplored questions remain regarding locally-balanced Metropolis–Hastings algorithms. The initial noise distribution in the Barker algorithm is simply chosen to be Gaussian in \cite{9}, but no justification besides convenience is given for this choice. It could be that a different choice leads to a more effective algorithm. Similarly, general guidelines on the optimal acceptance rate for the Barker algorithm are not established. More generally, little discussion is provided on other first-order locally-balanced Metropolis–Hastings. It is natural to wonder whether all members of the class will exhibit $O(n^{1/3})$ relaxation times, if the Metropolis–adjusted Langevin is the most efficient choice when optimally tuned, and indeed whether such a direct quantitative comparison of methods is possible in general. These questions are of both theoretical and practical interest, as they have direct implications for the optimal design of algorithms.

In this paper we make several new contributions. First we present universal results on the optimal choice of acceptance rate and scaling with dimension of any algorithm within the class of first order locally-balanced Markov processes (under mild regularity conditions). In particular in Section 3 we show that the 57% guideline acceptance rate for the Metropolis-adjusted Langevin algorithm also holds for the Barker proposal and several other methods, as does the $O(n^{1/3})$ scaling with dimension as measured by expected squared jump distance. Despite having the same optimal acceptance rate and scaling with dimensionality, however, all such schemes have a different asymptotic efficiency, which we explicitly characterize, enabling for principled and generic optimization of the algorithmic design. We first consider optimal design of the Barker proposal, in particular with respect to the noise distribution, which is chosen to be Gaussian in \cite{9}. We find, both theoretically and empirically, that it is in fact beneficial to choose a bi-modal noise distribution for each coordinate, and offer some discussion and practical user guidelines in Section 4.1. We then consider the case in which the noise distribution is fixed and an optimal balancing function is chosen in Section 4.2 and the
general scenario in which both the noise distribution and balancing function are optimized over in Section 4.3. Both cases yield surprising results, such as optimality being reached by having positive probability of keeping some coordinates fixed at each iteration. We conduct numerical experiments to verify the theory in Section 5, and provide a discussion in Section 6. Our theoretical results build on the recently introduced optimal scaling framework of [21, 24]. One powerful aspect of this approach is the ability to analyze fairly generic schemes without requiring overly case-specific calculations (e.g. those related to proposal distributions with Gaussian noise, linear drift, etc.), while still obtaining explicit expressions for the asymptotic performances that can directly be compared among algorithms. This allows characterization of the quantitative interplay between fine-scale properties of the target and proposal distributions (such as moments of the noise, aggressiveness of the balancing function and derivatives of the target) in the resulting asymptotic efficiency, thus enabling precise methodological guidance.

2 Locally-balanced Markov processes

2.1 General framework

Consider a Markov transition kernel \( Q \) defined on a Borel space \((\mathcal{X}, \mathcal{F})\). We restrict attention to \( \mathcal{X} \subset \mathbb{R}^n \) for some finite \( n \). We say \( Q \) satisfies the detailed balance equations with respect to a probability measure \( \pi \) if

\[
\int f(x)h(y)\pi(dx)Q(y, dx) = \int f(x)h(y)\pi(dy)Q(y, dx)
\]

for any \( f, h \in L^2(\pi) \). When \( Q \) does not satisfy (1), a new kernel can be constructed using the concept of a balancing function. Let \( g : [0, \infty) \to [0, \infty) \) be such that \( g(0) = 0 \) and for \( t > 0 \)

\[
g(t) = tg(1/t),
\]

and note that by Proposition 1 in [20] there exists a symmetric set \( \mathcal{R} \times \mathcal{R} \subset \mathcal{X} \times \mathcal{X} \) such that the Radon–Nikodym derivative

\[
t(x, y) = \frac{\pi(dy)Q(y, dx)}{\pi(dx)Q(x, dy)}
\]

is well-defined and such that \( 0 < t(x, y) < \infty \) if \( x, y \in \mathcal{R} \) and \( t(x, y) = 0 \) otherwise. Then the kernel

\[
\tilde{P}(x, dy) = g \left\{ \frac{\pi(dy)Q(y, dx)}{\pi(dx)Q(x, dy)} \right\} Q(x, dy)
\]

satisfies (1). However, the kernel \( \tilde{P} \) is not necessarily Markov. One way of enforcing that (4) integrates to one is to restrict attention to \( g \leq 1 \), ensuring that \( \tilde{P}(x, \mathcal{X}) \leq 1 \), and then combine with \( r(x, dy) = \{1 - \tilde{P}(x, \mathcal{X})\} \delta_x(dy) \), where \( \delta_x(A) = 1 \) if \( x \in A \) and 0 otherwise. The resulting kernel \( \mathcal{P}(x, dy) + r(x, dy) \) is Metropolis–Hastings (e.g. [20]).

An alternative strategy introduced in [23, 12, 9] is to instead allow any \( g \) for which \( Z(x) = \tilde{P}(x, \mathcal{X}) \) is finite, and then set

\[
\mathcal{P}(x, dy) = \frac{\tilde{P}(x, dy)}{Z(x)}.
\]

Note that \( \mathcal{P} \) does not satisfy (1) in general, in fact \( \mathcal{P} \) is invariant with respect to the measure \( Z(x)\pi(dx) \). A \( \pi \)-invariant Markov jump process can be constructed, however, by introducing a holding time \( Z(x) \) at each state \( x \), and then choosing the next state according to \( \mathcal{P} \). This construction is called a locally-balanced Markov process (see [12, 4] for more detail).

2.2 First order locally-balanced processes

The function \( Z(x) \) will not be tractable in general, meaning further work is needed to design a sampling algorithm based on a locally-balanced Markov process. One approach is to restrict attention to symmetric \( Q \), and \( \pi \) absolutely continuous with respect to the Lebesgue measure on \( \mathbb{R}^n \) with differentiable Lebesgue density
Let Proposition 1. 

The concept of a log-Metropolis–Hastings random variable will be crucial for our analysis of optimal scaling. We recall some key results here, for more detail see Section 3 of [21].

### 3 A universality result on the optimal acceptance rate and scaling with dimension

#### 3.1 Preliminaries

The concept of a log-Metropolis–Hastings random variable will be crucial for our analysis of optimal scaling. We recall some key results here, for more detail see Section 3 of [21].
Definition 1. For a probability measure $\pi$, Markov kernel $Q$ on $(X, \mathcal{F})$ and $\mathcal{R}$ as in Section 2.1, let $X \sim \pi$ and $Y \sim Q(X, \cdot)$. The associated log-Metropolis-Hastings-ratio random variable is

$$\rho(X,Y) = \begin{cases} \log \left( \frac{\pi(dy)Q(y, dx)}{\pi(dx)Q(x, dy)} \right) & \text{if } (X,Y) \in \mathcal{R} \times \mathcal{R}, \\ 0 & \text{otherwise.} \end{cases}$$

Let $\pi : \mathbb{R} \to [0, \infty)$ be a probability density on $\mathbb{R}$ and for any fixed $\sigma > 0$ let $Q_\sigma : \mathbb{R} \times \mathbb{R} \to [0,1]$ be a Markov kernel. We introduce the product measure $\pi_n(dx) = \prod_{i=1}^n \pi(x_i) dx_i$ on $\mathbb{R}^n$ and the product kernel $Q_n(x, dy) = \prod_{i=1}^n Q_\sigma(x_i, dy_i)$, where $(\sigma_n)_{n \in \mathbb{N}}$ is a sequence of positive real numbers. The associated log-Metropolis–Hastings random variable is

$$\rho(X_n,Y_n) = \sum_{i=1}^n \rho_n(X_{n,i}, Y_{n,i}),$$

where $X_n = (X_{n,1}, \ldots, X_{n,n}) \sim \pi_n$, $Y_n \sim Q_n(X_n, \cdot)$, and $\rho_n$ is the log-Metropolis–Hastings random variable associated with $f$ and $Q_\sigma$. The following is established in [21].

**Theorem 1.** Assume that there exists a positive sequence $(a_n)_{n \in \mathbb{N}}$ with $\lim_{n \to \infty} a_n = 0$ such that

$$\lim_{n \to \infty} \mathbb{E}[(\rho_n^2 1_{\rho_n < -a_n})/\mathbb{E}[\rho_n^2]] = 0,$$

where $1$ denotes the indicator function. If in addition $(\sigma_n)_{n \in \mathbb{N}}$ is chosen such that $\lim_{n \to \infty} n\mathbb{E}[\rho_n^2] = \sigma^2$ for some constant $\sigma > 0$, then as $n \to \infty$

$$\sum_{i=1}^n \rho_n(X_{n,i}, Y_{n,i}) \Rightarrow \mathcal{N}\left(-\frac{1}{2} \sigma^2, \sigma^2\right). \quad (7)$$

**Remark 1.** The expectation $n\mathbb{E}[-\rho_n]$ denotes the Kullback–Leibler divergence between the forward and reverse Markov transition kernels, $\pi(dx)Q(x, dy)$ and $\pi(dy)Q(y, dx)$. In fact, it is further shown in [21] that under the above assumptions $\lim_{n \to \infty} \mathbb{E}[\rho_n]/\mathbb{E}[\rho_n^2] = -1/2$, meaning that both the mean and variance on the right-hand side of (7) can be interpreted in terms of the Kullback–Leibler divergence in the limiting case $n \to \infty$.

Guaranteeing the first condition, i.e. understanding how fast $\mathbb{E}[\rho_n^2]$ decays, is key for identifying the optimal scaling of a Metropolis-Hastings algorithm. The other condition is technical and related to the uniform integrability of $n\rho_n^2$ and to the conditions required in the Lindeberg’s version of Central Limit Theorem (see Theorem 4.15 of [8]). It suffices for example, to show that $\rho_n$ has higher moments that vanish faster than $1/n$.

### 3.2 The asymptotic acceptance rate for locally-balanced proposals

We will establish that the above central limit theorem holds for first order locally-balanced Metropolis–Hastings under Assumption 1 below, and then consider optimal acceptance rates and dimension dependence in terms of the expected squared jump distance in each coordinate. We restrict attention to the class of target distributions $\pi_n(x) = \prod_{i=1}^n \exp\{\phi(x_i)\}$, for some $\phi : \mathbb{R} \to \mathbb{R}$, and impose regularity conditions on $\phi$ below. Let $b(x) = \log\{g(e^x)\}$, and without loss of generality set $g(1) = 1$.

**Assumption 1.** There exist constants $H \in (0,1), \gamma > 0, \beta \geq 0, \epsilon > 0$ such that

(i) $\phi \in C^{3+H}(\mathbb{R})$ and for $f = \phi''', \phi'' \phi', \phi'^3, \phi'' \phi'|^{1+\beta}$ the integrability condition $\int_{\mathbb{R}} f(x)^{2+\epsilon}(1+|\phi'(x)|^\beta)\pi(x)dx < \infty$ as well as the mixed growth-Hölder condition

$$|f(x + \delta) - f(x)| \leq K(x) \max(|\delta|^H, |\delta|^\gamma)$$

are satisfied. Function $K$ is such that $\int_{\mathbb{R}} K(x)^2 (1 + |\phi'(x)|^\beta)\pi(x)dx < \infty$. 

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(ii) \( b \in C^2(\mathbb{R}) \) and \( b', b'', b''' \) are all bounded above.

(iii) \( \int z^2 \mu(dz) = 1, \int |z|^5 \mu(dz) < \infty \) for \( \xi = \max(6 + 3c, 2 + 2H, 2 + 2\gamma) \), and for all \( a \in \mathbb{R} \) and some positive \( \mu > 0 \)

\[
\int_{\mathbb{R}} e^{b(a^2)} |z|^5 \mu(dz) \leq C_\mu (1 + |a|^2) \int_{\mathbb{R}} e^{b(a^2)} \mu(dz) < \infty.
\]

Part (i) of the above refers to the target distribution, part (ii) to the balancing function and part (iii) to the interplay between them. Part (i) is straightforwardly satisfied for many statistical models of interest, for example likelihoods from exponential families and suitably smooth priors. Part (ii) is satisfied by all cases explicitly studied in the paper, such as \( g(t) = \sqrt{t} \) and \( g(t) = 2t/(1 + t) \). Part (iii) highlights the need to control the growth of \( g \) and \( b \) using the tails of \( \mu \). If \( g \) is bounded, as in the Barker case, then any \( \mu \) with a moment generating function is sufficient for it to be satisfied (and for many targets actually much weaker conditions are required). When \( g(t) = \sqrt{t} \), which is not bounded above, then stronger conditions on the tails of \( \mu \) are needed, such as Gaussian tails.

Part (i) is explicitly weaker than the typical assumptions made in the optimal scaling literature (e.g. [14]). A form of part (i) as well as \( \int z^6 \mu(dz) < \infty \) and \( g \in C^4 \) are crucial to the analysis. Part (iii) imposes uniform control (with respect to \( x \)) of measures \( e^{b(\sigma_n z^\phi(x))} (Z_{\sigma_n}(x))^{-1} \mu(z)dz \) in terms of only the measure \( \mu(z)dz \). This is required so that the normalising constants \( Z_{\sigma_n} \) and their second derivatives are well defined. It may be possible to significantly relax parts (ii) or (iii), especially in specific settings, at the expense of strengthening elsewhere. The following Proposition identifies some simple cases in which part (iii) is satisfied.

**Proposition 2.** Part (iii) of Assumption 1 is satisfied in the following cases.

(i) If \( \mu \) has a density with compact support, for any \( g \).

(ii) If \( g \) is bounded, non-decreasing and \( \int |z|^5 \mu(dz) < \infty \) for \( \xi \) as in Assumption 1.

(iii) If \( g \) satisfies part (ii) of Assumption 1 and there exists \( \tilde{C}_\mu, \tilde{\beta} > 0 \) such that for all \( a \in \mathbb{R} \)

\[
\int_{\mathbb{R}} e^{a^2} |z|^5 \mu(dz) \leq \tilde{C}_\mu (1 + |a|^\tilde{\beta}) \int_{\mathbb{R}} e^{a^2} \mu(dz) < \infty.
\]

(iv) If \( g \) satisfies part (ii) of Assumption 1, \( \mu \) has a density \( \mu \in C^1(\mathbb{R}) \) such that \( \lim_{z \to \pm \infty} e^{a^2} \mu(z) = 0 \) for any \( a \in \mathbb{R} \) and there exists constants \( A, B > 0 \) for which

\[
|z|^p \mu(z) \leq A \mu(z) - B z \mu'(z).
\]

In specific examples we typically verify (i), (ii) or (iv) of Proposition 2. For instance, choices of the form \( \mu(dz) \propto e^{-|z|^p} dz \) for \( p \geq 1 \) satisfy (iv). Note that a statement analogous to (ii) but for the function \( b \) is not valid. Even if \( g \) is bounded, \( b \) is only bounded from infinity above, not below. In fact, since \( b(x) = x + b(-x) \) holds, \( b \) can never be bounded. These conditions are required to analyze Taylor series remainder terms for the normalising constant. It is apparent from Proposition 2 that less conditions on \( \mu \) must be assumed for the Barker proposal, for which \( g \) is bounded, compared to the Langevin choice \( g(t) = \sqrt{t} \).

**Theorem 2.** Under Assumption 1 it holds that \( \lim_{n \to \infty} \sigma_n^{-6} E[\rho_n^2] = \theta^2 \) for some \( \theta \in [0, \infty) \). In addition, if \( \theta > 0 \) and \( \sigma_n \) is chosen such that \( \lim_{n \to \infty} n^{1/6} \sigma_n = \ell \), then

\[
\sum_{i=1}^n \rho_n (X_{n,i}, Y_{n,i}) \Rightarrow N \left( \frac{1}{2} g_\theta^2, \ell^6 \theta^2 \right).
\]

Denoting \( g = g''(1) \), \( \mu_4 = \int_{\mathbb{R}} z^4 \mu(dz) \), \( \mu_6 = \int_{\mathbb{R}} z^6 \mu(dz) \) and \( A_\phi = E_\pi [(\phi''')^2], B_\phi = E_\pi [(\phi')^2], C_\phi = E_\pi [\phi'' \phi'^{\prime\prime}] \) the constant \( \theta^2 \) takes the form

\[
\theta^2 = \mu_6 \left\{ \frac{1}{144} A_\phi + \left( \frac{1}{4} + g \right)^2 B_\phi - \frac{1}{6} \left( \frac{1}{4} + g \right) C_\phi \right\}
\]

\[
+ \mu_4 \left\{ \frac{1}{6} \left( \frac{1}{2} + g \right) C_\phi - 2 \left( \frac{1}{4} + g \right) \left( \frac{1}{2} + g \right) B_\phi \right\} + \left( \frac{1}{2} + g \right)^2 B_\phi.
\]

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Note that the specific choice of the scaling parameter $\sigma_n \propto n^{-1/6}$ in Theorem 3 is the only rate leading to a non-trivial distributional limit for $\sum_{i=1}^n \rho_n(X_{n,i}, Y_{n,i})$, despite the fact that $\lim_{n \to \infty} \sigma_n^{-6} E[\rho_n^2] = \theta^2$ holds for any decay rate. Note also that the expression for $\theta^2$ depends on both the balancing function $g$ and the distribution $\mu$. In Section 4, we consider optimal ways to choose $g$ and $\mu$ for certain purposes. We consider some example choices below.

**Example 1.** In the Langevin case $\eta(t) = \sqrt{t}$ and $\mu$ is standard Gaussian, so that $\eta'(1) = -1/4$ and $\mu_4 = 3$, $\mu_6 = 15$. Then

$$\theta^2 = \frac{5}{48} A_{\phi} + \frac{1}{8} C_{\phi} + \frac{1}{16} B_{\phi}$$

which if $\lim_{x \to \pm \infty} e^{\eta(x)} \phi'(x) \phi''(x)^2 = 0$ can also be written (using integration by parts)

$$\theta^2 = \frac{5}{48} E[(\phi'')^2] - \frac{1}{16} E[(\phi''')^3],$$

a formula that appears in [14].

**Example 2.** For the Barker proposal $\eta(t) = 2t/(1 + t)$ and $\mu$ can be any centred and symmetric distribution such that $\int z^5 \mu(dz) < \infty$. With these choices $\eta''(1) = -1/2$ and

$$\theta^2 = \frac{\mu_6}{144} (A_{\phi} + 6C_{\phi} + 9B_{\phi}). \quad (10)$$

An important consequence of Theorem 3 and in particular of (8), is a simple expression for the asymptotic acceptance rate for a first order locally-balanced Metropolis–Hastings algorithm (see e.g. Proposition 2.4 in [13]).

**Corollary 1.** Setting $\alpha_n(X, Y) = \min\{1, \sum_{i=1}^n \rho_n(X_i, Y_i)\}$, under the conditions of Theorem 3

$$\lim_{n \to \infty} E[\alpha_n] = 2\Phi(-\ell^3\theta/2)$$

where $\Phi$ is the standard Normal cumulative distribution function.

### 3.3 Optimal acceptance rates

Given the simplified limiting expression for $\alpha_n$ in Corollary 1, we can consider optimal choices of the constant $\ell$ for a fixed $\theta$, leading to an optimal acceptance rate. We consider optimising the expected squared jump distance here, which is well-studied and has a strong justification motivated by diffusion limits in various settings [15].

Using the same notation as above denote by $(\mathcal{E}_{n, \mu}^g)_{n \in \mathbb{N}}$ the sequence of expected squared jump distances for the first (or any other) coordinate, defined as

$$\mathcal{E}_{n, \mu}^g = E[(Y_{n,1} - X_{n,1})^2 \alpha(X_n, Y_n)],$$

where $X_n \sim \pi_n$ and $Y_n$ is generated from $X_n$ using a first order locally-balanced proposal, defined in [6], with distribution $\mu$, balancing function $g$ and variance parameter $\sigma_n$. We have the following result.

**Theorem 3.** Let Assumption 4 and Theorem 3 be satisfied for $\phi$, $\mu$ and $g$ and $\theta > 0$. Let $(\sigma_n)_{n \in \mathbb{N}}$ be a positive sequence with $\lim_{n \to \infty} \sigma_n = 0$. If either $\lim_{n \to \infty} n^{1/6} \sigma_n = 0$ or $\lim_{n \to \infty} n^{1/6} \sigma_n = \infty$ then as $n \to \infty$

$$n^{1/3} \mathcal{E}_{n, \mu}^g \to 0.$$

If $\lim_{n \to \infty} n^{1/6} \sigma_n = \ell$ for some $\ell \in (0, \infty)$, then as $n \to \infty$

$$n^{1/3} \mathcal{E}_{n, \mu}^g \to h(\ell) = 2\ell^2 \Phi(-\ell^3\theta/2),$$

where $\Phi$ is the standard Normal cumulative distribution function on $\mathbb{R}$. Furthermore, there exists a unique optimal $\ell^* (= \ell^*(g, \mu))$ that maximizes $h(\ell)$, for which $2\Phi(-\ell^*^3\theta/2) \approx 0.574$. The corresponding optimal asymptotic efficiency satisfies

$$h(\ell^*) = C_h\theta^{-2/3},$$

where $C_h \approx 0.652$. 

The above shows that any first order locally-balanced Metropolis–Hastings algorithm will have the same asymptotic optimal acceptance rate of 0.57, and that algorithmic efficiency as measured by expected squared jump distance will scale as \( O(n^{-1/3}) \) for \( n \to \infty \). This includes both Barker and Langevin proposals as well as many other possibilities. Theorem 3 also suggests a route to both comparison and optimal design of first order locally-balanced Metropolis–Hastings algorithms, in the former case by comparing \( \theta^2 \) for different choices of \( \mu \) and \( g \), and in the latter by choosing \( \mu \) and \( g \) so that \( \theta^2 \) in Theorem 2 is minimized. According to the same theorem, under Assumption 1 the constant \( \theta^2 \) will depend on \( \phi \) through \( A_\phi, B_\phi \) and \( C_\phi \), on \( \mu \) only through \( \mu_2 \) and \( \mu_6 \) and on \( g \) only through \( g = g^6(1) \). We explore optimal design under different constraints in the next Section.

In the Langevin proposal case, the constant \( h(\ell) \) was shown to correspond to the speed measure of an overdamped Langevin diffusion limit in [13]. We conjecture that the same is true for locally balanced proposals in general, but do not prove explicitly diffusion limit results in this paper. Proving diffusion limit results for general locally balanced proposals is a non-trivial open problem, as it would require a conditional proof.

**Example 3.** Take the Gaussian target case \( \phi(x) = -x^2/2 \). Then \( \phi'(x) = -x, \phi''(x) = -1 \) and \( \phi'''(x) = 0 \), meaning \( A_\phi = C_\phi = 0 \) and \( B_\phi = \mathbb{E}[x^2] = 1 \). For Langevin proposals with \( g(\ell) = \sqrt{\ell} \) and \( \mu \) taken as Gaussian, the constant \( \theta^2 \) in (8) becomes \( \theta^2_L = 1/16 \), whereas for the Barker choice \( g(\ell) = 2\ell/(1+\ell) \) and the same \( \mu \) we have \( \theta^2_B = \mu_6/16 \). The ratio of asymptotic expected squared jump distances is therefore \( (\theta_B/\theta_L)^{2/3} = \mu_6^{1/3} \). Here \( \mu_6 = 15 \) meaning that Langevin proposals are asymptotically \( 15^{1/3} \approx 2.47 \) times more efficient than Barker proposals with Gaussian noise when optimally tuned. This is consistent with experiments in Section 5.2 of [2].

**Example 4.** Consider hyperbolic targets, \( \phi(x) = (\delta^2 + x^2)^{1/2} \), with \( \delta^2 = 0.1 \) as in [9]. Then \( A_\phi \approx 12.99, B_\phi \approx 0.22 \) and \( C_\phi \approx 1.68 \). The same calculations as above imply that Langevin proposals are 1.18 times more efficient than Barker proposals with Gaussian noise when optimally tuned, which is also consistent with Section 5.2 of [9].

4 Optimal choices among the class of locally-balanced algorithms

4.1 Optimal choice of noise in the Barker algorithm

In this setting we fix \( g(\ell) = 2\ell/(1+\ell) \) and minimize \( \theta^2 \) with respect to \( \mu \), for a given but arbitrary choice of \( \phi \). In this case \( \theta^2 \) is given by (10), and the only influence of \( \mu \) comes from the sixth moment \( \mu_6 \). The asymptotic expected squared jump distance can therefore be straightforwardly maximised by minimising the sixth moment of \( \mu \) subject to the constraint that \( \mu_2 = 1 \). Note that by Jensen’s inequality \( \mu_6 \geq \mu_3^2 = 1 \), and in fact the lower bound is uniquely attained by choosing \( \mu \) to be a Rademacher distribution, such that if \( W \sim \mu \) then \( W = 1 \) with probability \( 1/2 \) and \( W = -1 \) otherwise. We state this formally below.

**Proposition 3.** If \( g(\ell) = 2\ell/(1+\ell) \) then \( \theta^2 \) is minimized when \( W \sim \mu \) is chosen to take values \( +1 \) and \( -1 \) each with probability \( 1/2 \).

We can compare the relative efficiency of Barker with Rademacher versus Gaussian noise using (10) in a similar manner to Examples 3 and 4. Doing this shows that for any \( \phi \) the Rademacher version will be \( \mu_6^{1/3} \approx 2.47 \) times more efficient than the Gaussian version. It is particularly convenient that the optimal choice of \( \mu \) does not depend in any way on \( \phi \) and therefore generic methodological guidance can be provided for the algorithm. The comparison with the Langevin proposal is instead target dependent, as exemplified below.

**Example 5.** When \( \phi(x) = -x^2/2 \) as in Example 3, the Barker proposal with Rademacher noise will be exactly as efficient as the Langevin proposal. When \( \phi(x) = (\delta^2 + x^2)^{1/2} \) with \( \delta^2 = 0.1 \) as in Example 4 then the Rademacher proposal will be 2.08 times more efficient than the Langevin proposal.

We compare these theoretical results with empirical performances in Section 5. The Rademacher version of the Barker proposal is not per se a practical sampling algorithm given that the resulting algorithm will not in general produce a \( \pi \)-irreducible Markov chain. One simple alternative that we propose is therefore to
set $\mu$ to be an evenly-weighted mixture of two Normal distributions centred at $\pm \sqrt{1-\sigma^2}$, each with variance $\sigma^2 < 1$. The resulting approach, termed bi-modal Barker, will satisfy $\mu_6 = 1 + 12\sigma^2 + 18\sigma^4 - 16\sigma^6$ and be $15^{1/3}\mu_6^{-1/3}$ times more efficient than the version with Gaussian noise. For small $\sigma$ this is close to optimal whilst also being practical. For instance, for the choice $\sigma^2 = 0.1^2$, which is the one we use in simulations below, bi-modal Barker is approximately 2.37 times more efficient than the Gaussian version.

The result on the Rademacher optimality may seem surprising at first given the lack of $\pi$-irreducibility. Similar results have, however, been uncovered previously, for example it is known that the optimum expected squared jump distance for the random walk Metropolis when the target distribution is spherically symmetric is found by choosing the proposal distribution to be uniform on a hyper-sphere of fixed radius from the current point \[10\]. Given the product form of $\pi$ considered in this work, the Rademacher structure is therefore natural. For the random walk Metropolis, however, the benefits of choosing such an optimized proposal distribution vanish as the dimension increases \[10,22\], whereas in the Barker case they do not.

An intuitive explanation for this may be that bi-modal Barker proposal choice makes the MCMC method less diffusive and puts more effort on moving at least a certain distance away. This is consistent with motivation for other kinds of development of MCMC methods, for instance Hamiltonian Monte Carlo and non-reversible Piece-wise deterministic Markov processes \[5,6\].

### 4.2 Optimising over the choice of balancing function for a fixed noise distribution

In this section we switch attention to the optimal choice of $g$ for a fixed choice of $\mu$. The expression \[9\] in this case becomes a simple quadratic in $g$, which can be straightforwardly solved to find an optimum choice for a given $\phi$, as given in \[11\] below.

**Proposition 4.** Given $\phi$ and a fixed noise distribution $\mu$ with finite fourth and sixth moments $\mu_4 < \mu_6 < \infty$, the optimum choice of $g$ is

$$g^* = \frac{\mu_6 (C_\phi - 3B_\phi) + \mu_4 (9B_\phi - C_\phi) - 6B_\phi}{12B_\phi (\mu_6 - 2\mu_4 + 1)}.$$  \[11\]

Any family of balancing functions for which $g = g''(1)$ can be modified to take a desired value could therefore in principle be used to create an optimized algorithm for a particular $\mu$ and $\phi$. Consider the family

$$g_\gamma(t) = \frac{1}{2} \left( t^{1+\gamma} + t^{1-\gamma} \right),$$  \[12\]

indexed by $\gamma \geq 0$, where for $\gamma = 0$ we recover the Langevin case $g(t) = \sqrt{t}$. Any choice within the family is a balancing function, and is such that $g_\gamma(1) = 1$ and $g = g''(1) = \gamma^2 - \frac{1}{4}$. For a given $\phi$, the choice of $\gamma$ can therefore be adjusted to achieve the optimum asymptotic efficiency provided that $g^*$ in \[11\] is larger than $-1/4$.

Given the results of the previous section it would seem natural to set $\mu$ as a Rademacher distribution, however in this case it turns out that all choices of $g$ give equivalent algorithms. This follows straightforwardly from the fact that \[2\] implies $g(t)/(g(t)+g(t^{-1})) = 1/(1+t^{-1})$, which is independent of $g$. In fact Proposition \[4\] does not apply to the Rademacher case since $\mu_4 = \mu_6$. Another natural option is to fix $\mu$ to be standard Gaussian. In this case \[11\] implies that the maximum efficiency is found by choosing $g = C_\phi/(10B_\phi) - 1/5$. This scheme can be implemented using the family in \[12\], and sampling from the resulting first order locally-balanced proposal is straightforward as it consists in a mixture of two Gaussians, see the supplement for details. We do not implement this scheme in the simulations, however, in favour of the more efficient alternatives discussed in the next section.

### 4.3 Optimising over the choice of both noise distribution and balancing function

In this section we consider optimizing over both $g$ and $\mu$ jointly. The following proposition identifies the best possibly achievable asymptotic efficiency with first order locally-balanced proposals for a given target.
Proposition 5. A non-negative lower bound for $\theta^2$ that is independent of both $\mu$ and $g$ is

$$\theta^2 \geq \frac{1}{144} \left( A_\phi - \frac{C_\phi^2}{B_\phi} \right).$$

(13)

Furthermore, $\theta^2$ can be made arbitrarily close to the lower bound by choosing $\mu_4 > 1$ sufficiently close to one, setting $\mu_6 = \mu_4^2$ and choosing

$$g = \frac{\mu_4 (C_\phi - 3B_\phi) + 6B_\phi}{12B_\phi(\mu_4 - 1)}.$$  

(14)

Proof. Given $A_\phi > 0, B_\phi > 0$ and $C_\phi \in \mathbb{R}$ we must solve the constrained quadratic optimisation problem of minimising $\theta^2$ subject to $1 \leq \mu_4 \leq \sqrt{\mu_6}$. The constraints on $\mu_4$ and $\mu_6$ are necessary because $1 = \mu_2 \leq \sqrt{\mu_4}$ by Jensen’s inequality and $\mu_4 \leq \sqrt{(\mu_2\mu_6)} = \sqrt{\mu_4}$ by Cauchy’s inequality. Moreover the Hamburger moment problem tells us these constraints are sufficient: if they are fulfilled then there exists a symmetric proposal distribution on $\mathbb{R}$ that satisfies them.

Defining the new variables $m_1 = (g + 1/4)\phi'\phi'' - \phi'''/12$ and $m_2 = -(g + 1/2)\phi'\phi''$, we can rewrite $\theta^2$ as

$$\theta^2 = (\mu_6 - \mu_4^2) E[m_1^2] + E \left[ (\mu_4 m_1 + m_2)^2 \right] \geq E \left[ (\mu_4 m_1 + m_2)^2 \right].$$

(15)

where the inequality follows from $\sqrt{\mu_6} \geq \mu_4$. Expressing this lower bound in terms of $A_\phi, B_\phi$ and $C_\phi$ gives

$$\theta^2 \geq B_\phi \left\{ \left( \mu_4 g - g + \frac{\mu_4}{4} - \frac{1}{2} \right) \frac{\mu_4 C_\phi}{12 B_\phi} \right\}^2 + \frac{\mu_4^2}{144} \left( A_\phi - \frac{C_\phi^2}{B_\phi} \right),$$

which can itself be lower bounded, giving

$$\theta^2 \geq \frac{\mu_4^2}{144} \left( A_\phi - \frac{C_\phi^2}{B_\phi} \right) \geq \frac{1}{144} \left( A_\phi - \frac{C_\phi^2}{B_\phi} \right).$$

We have used three inequalities. The first, in (15), is realised if and only if $\mu_6 = \mu_4^2; \text{ the second simply}$ bounds a square below by zero and is realised if and only if $g$ is defined as in (14), which requires $\mu_4 > 1; \text{ the third relies on } \mu_4 \geq 1 \text{ and is realised if and only if } \mu_4 = 1$. Note that the last two equalities cannot be realised simultaneously. The final lower bound is always non-negative due to $B_\phi A_\phi \geq C_\phi^2$ by Cauchy’s inequality.

Denote by $\nu(a)$ for $a > 1$ a discrete symmetric distribution taking three possible values $-\sqrt{a}, 0, \sqrt{a}$, such that the probability of a non-zero value is $1/a$, and note that this is the unique symmetric distribution $\mu$ with moments satisfying $\mu_2 = 1, \mu_4 = a$ and $\mu_6 = a^2$. Letting $g$ be defined by (14), choosing $\mu = \nu(\mu_4)$ and taking $\mu_4$ arbitrarily close to one results in $\theta^2$ becoming arbitrarily close to the lower bound (13). This three point proposal results in an algorithm that achieves close to optimal asymptotic expected squared jump distance among the class of first order locally-balanced samplers provided that $g$ is chosen according to (14).

Remark 2. This three point proposal is in fact also the optimal choice of $\mu$ for any fixed choice of $g$, but the amount of mass given to point zero will vary depending on $g$. In the Barker case, for example, this point achieves no mass, resulting in the Rademacher choice for $\mu$.

It is natural to consider taking the limit $\mu_4 \rightarrow 1$ and expect optimality to be reached there. When the dimension $n$ is fixed and finite, however, this results in a Rademacher proposal, which is suboptimal. This can be seen by noting that the lower bound (13) is always smaller than $B_\phi/16 + A_\phi/144 + C_\phi/24$, the value attained by the Rademacher proposal, because

$$\frac{B_\phi}{16} + \frac{A_\phi}{144} + \frac{C_\phi}{24} = \frac{A_\phi}{144} + \left( \frac{B_\phi/16}{4} + \frac{C_\phi}{12B_\phi/16} \right)^2 - \frac{C_\phi^2}{144B_\phi} \geq \frac{1}{144} \left( A_\phi - \frac{C_\phi^2}{B_\phi} \right).$$

Inspecting the proof of Theorem 2 shows that $g$ must be increased sufficiently slowly as a function of $n$ to control the remainder terms in order for the asymptotic expression for $\theta^2$ to be a valid representation of the
expected squared jump distance. In other words, as \( \mu_4 \to 1 \) it takes increasingly large \( n \) for the asymptotic regime to be representative of the finite \( n \) setting. For a finite \( n \), it is therefore necessary to choose \( \mu_4 > 1 \). We explore this phenomenon further in the supplement. In all simulations below, we set \( \mu_4 = 2 \) unless stated otherwise.

A surprising consequence of these findings is that the three point proposal with some mass at zero outperforms a Rademacher choice that is optimum for the Barker proposal when the freedom to choose \( g \) is given. In terms of sampling, this suggests that efficiency gains can be made by allowing some components of the state to remain unchanged at each iteration of the algorithm with a probability that depends on the size of the gradient in that direction. The same family of balancing functions introduced in (12) can again be used to create this optimum sampler.

A particular case of interest is the Gaussian setting \( \phi(x) = -x^2/2 \), in which case \( \phi''(0) \) and therefore \( A_0 = C_0 = 0 \). This means that by choosing any \( \mu_4 > 1 \) and \( g \) according to (14) we can achieve zero asymptotic \( \theta^2 \). The result of this is a super-efficient sampler whose efficiency will effectively decay at a slower rate than \( n^{-1/3} \). We illustrate this surprising finding numerically in Section 5, but also stress that this property only holds when \( \phi(x) = -x^2/2 \) to the best of our knowledge.

5 Simulation Study

5.1 Efficiency with dimension on product targets

We examine the expected squared jump distance of the first component of two different product form target distributions as a function of dimension. This setting is directly captured by the theoretical results of Sections 3 and 4. The two target distributions considered are the multi-dimensional standard Gaussian distribution and the hyperbolic distribution of Example 3. In each case we compare the random walk Metropolis, the Metropolis-adjusted Langevin algorithm, Barker with Gaussian noise, Barker with Rademacher noise, Barker with bi-modal noise as described in Section 4.1 and the optimal choice over both balancing function and noise distribution described in Section 4.3, which will hereafter be called the three point proposal.

The results for the Gaussian target distribution are shown in Figure 1(a). It is clear from the plots that among the Barker algorithms the Rademacher and bi-modal choices are comparable and perform similarly to MALA, whereas the Barker algorithm with Gaussian noise has a lower expected squared jump distance by a factor of 2-2.5, in accordance with the theoretical value of 2.47. The three points proposal performs best and appears to exhibit a slightly slower than \( n^{-1/3} \) decay in expected squared jumping distance when the dimension in large. This is because in the special case of Gaussian target \( \theta^2 \) from (9) equals zero when the choices described in Section 4.3 are made.

For the hyperbolic target results are shown in Figure 1(b). The main difference compared to the Gaussian example is that now the Barker algorithms with Rademacher and bi-modal noise both outperform the Langevin algorithm, as predicted by the theory described in Section 4.1. The three points proposal is still the best performing algorithm.

5.2 Poisson random effects model

To consider a realistic example in which the target distribution is not of the product form, we compare algorithms on the Poisson random effects model described in Section 6.3 of [9]. We compare the Barker algorithm with bi-modal noise to the Barker algorithm with Gaussian noise, the Langevin algorithm and the random walk Metropolis. The main purpose of this example is to assess whether or not the above theoretical guidelines for the noise distribution in the Barker algorithm lead to good choices even when the target distribution does not have independent and identically distributed components.

The target distribution under consideration is a 51-dimensional posterior distribution, \( p(\mu, \eta_1, \ldots, \eta_{50}|y) \), arising from a Poisson random effects model defined hierarchically as \( \mu \sim N(0, 10^2) \), \( \eta_i|\mu \sim N(\mu, \sigma_\eta^2) \) and \( y_{ij}|\eta_i \sim \text{Poisson}(\exp(\eta_i)) \), independently for \( i = 1, \ldots, 50 \) and \( j = 1, \ldots, 5 \). In our experiment we generate the observed data \( y = (y_{ij})_{ij} \) from the model likelihood, i.e. sampling \( y_{ij} \sim \text{Poisson}(\exp(\eta_i^*)) \) independently, where \( \eta_1^*, \ldots, \eta_5^* \) are themselves generated independently from a \( N(\mu^*, \sigma_\eta^2) \) distribution with \( \mu^* = 5 \). Here \( \sigma_\eta \) is a fixed value and two scenarios are considered: in the first we set \( \sigma_\eta = 1 \), while in the second we set \( \sigma_\eta = 3 \). Effectively, \( \sigma_\eta \) is a parameter that governs the heterogeneity across groups \( i = 1, \ldots, 50 \) in the
hierarchy. Thus, larger values of $\sigma_\eta$ lead to a target distribution with more heterogeneity of scales across coordinates, which make the adaptation and sampling process more challenging.

In each case algorithmic tuning parameters consisting of a diagonal pre-conditioning matrix and a global scale are learned using Algorithm 4 of [1], in the same manner as described in Section 6.3 of [9]. We measure efficiency in terms of effective sample size for a given number of iterations since all algorithms under comparison, apart from Random Walk Metropolis, have a roughly equivalent cost per iteration, which is dominated by gradient computations. Figure 2 reports the median effective sample sizes across parameters for 100 independent runs of $5 \times 10^4$ iterations of each algorithm. All algorithms were randomly initialized by sampling parameter values from their prior distributions.

Both versions of the Barker algorithm appear to be more robust to different hyperparameter values than the Langevin algorithm, which sometimes performs well but sometimes poorly in the first scenario and always performs poorly in the second. This is because the Langevin algorithm is very sensitive to tuning parameter selection, and the adaptive procedure fails to converge on sensible values for these across the time scales of the simulation. The random walk Metropolis also performs poorly, which is largely explained by the dimension of the problem. The Barker algorithm with bi-modal noise is approximately two times as efficient in terms of effective sample size as the version with Gaussian noise in this setting. More precisely, the median improvement in estimated effective sample size is 2.08 in scenario 1 (10th and 90th quantiles across the 100 repetitions 2.05 and 2.11 respectively) and 2.04 in scenario 2 (10th and 90th quantiles 1.98 and 2.14 respectively). Similar numbers were obtained when looking at minimum (rather than median) effective sample sizes across parameters. These values suggest that the asymptotic theory developed in this paper,
which quantifies bi-modal Barker to be 2.37 times more efficient than Gaussian Barker, is highly predictive of
dontions observed in practice also for moderate dimensionality and targets that have neither independent
nor identically distributed coordinates. More generally, in all our simulations, we consistently observed an
improvement in efficiency when going from Gaussian to bimodal Barker with factors typically between 2 and
2.5.

5.3 A correlated example

Unlike the Random Walk or Langevin algorithms, the Barker and three points schemes rely on a choice of
coordinate system. This may raise the concern of how much performance depends on specific choices of
coordinate systems, and in particular whether the $O(n^{1/3})$ scaling behaviour proved above is sensitive to the
theoretical assumption that the target factorizes across the same coordinate axes as the proposal. Here we
explore these issues numerically, performing high dimensional scaling experiments similar to Section 5.1 but
for non-product form targets with significant correlation. In particular, we consider Gaussian distributions
with non-diagonal covariance matrix $\Sigma$ chosen in two ways. In the first case we set $\Sigma_{ii} = 1$ for $i = 1, \ldots, n$
and $\Sigma_{ij} = \rho$ for $i \neq j$, while in the second we take $\Sigma_{ij} = \rho^{|i-j|}$. In both cases we set $\rho = 0.99$ to depart
drastically from the independence case. As in Section 5.1 we compute the expected square jump distance
per coordinate. For all algorithms under consideration we use isotropic proposals, meaning we do not use
preconditioning to avoid aligning proposal and target axes, and we choose a step-size that is numerically
optimized to maximize performance as measured by expected square jump distance. The results are reported
in Figure 3. As expected, all schemes perform worse than in the product case (note the different scales on the
$y$-axes between Figure 1 and Figure 3), but the relative comparison between different schemes remains
nearly unchanged and fully coherent with the theoretical predictions obtained from Sections 3 and 4. In
particular the Langevin, Barker bi-modal and Barker Radamacher schemes perform nearly equivalently,
while Barker with Gaussian noise performs around 2-2.5 times worse. Overall, the experiment suggests that
the relative performances of the Random Walk, Langevin and Barker algorithms is not particularly sensitive
to correlation and to the specific choice of coordinate system. The three point proposal performs well also
in these correlated examples and actually performs surprisingly well when $\Sigma_{ij} = \rho^{|i-j|}$. Providing better
understanding of such unexpected behaviour will be the subject of future research. Note, however, that
the three point proposal implicitly uses knowledge about the target distribution when choosing the optimal
values of the tuning parameters $g$ and $\mu_4$, and thus it has been given a somewhat unfair and potentially
unrealistic advantage compared to the other schemes considered here. In particular, in this example $g$
was chosen according to the optimal value in (14) with $B_0 = 1$ and $C_0 = 0$ as given by product-form Gaussian
targets.

Figure 3: Expected squared jump distance against dimensionality for correlated Gaussian targets. Left:
$\Sigma_{ii} = 1$ and $\Sigma_{ij} = 0.99$ for $i \neq j$. Right: $\Sigma_{ij} = 0.99^{|i-j|}$.
6 Discussion

The main results of this paper rely on a product form structure of \( \pi \), and the corresponding optimal choice of locally-balanced algorithm also has a product form. We have shown in Section 5 that this choice is still effective when the target distribution is no longer of the product form, and therefore recommend the use of the bi-modal Barker algorithm in practice. It is surprising that using a non-local noise distribution of this kind results in such a pronounced and consistent improvement in efficiency across multiple examples. We believe that this represents a good case study of theoretical analysis motivating new practical methodology that would be otherwise hard to devise. It is also worth noting that any improvement in efficiency discussed above essentially comes for free, since all the gradient-based schemes considered in the paper have a comparable cost per iteration, which is typically dominated by gradient computations, and all schemes are equally simple to implement.

The detailed quantitative analysis and comparison of algorithms within the locally-balanced class in the high-dimensional limit is made possible by the mathematical framework developed in Section 3 of [21]. This framework identifies and uses only essential Taylor series expansions related to the limiting Kullback–Leibler divergence between a locally-balanced proposal and its time reversal. Using this we establish optimal scaling for a broad class of algorithms including Barker and Langevin with a single unified proof, along with significantly weaker assumptions on the smoothness and tails of the target distribution than those in [14]. Our results are at present restricted to limiting expected squared jump distances, rather than diffusion limits as in [13] or [14], but we believe that it is possible to uncover a limiting process under the current assumptions and such a line of enquiry is being pursued at the time of writing, continuing the axiomatic approach in [21].

One intriguing finding of this work concerns the sub-optimality of the Langevin choice \( g(t) = \sqrt{t} \) with proposal input noise \( \mu \) chosen to be Gaussian. This is by far the most historically popular choice within the first order locally-balanced class of algorithms. The results in this paper show that according to asymptotic efficiency as measured by expected squared jump distance not only is this combination of \( \mu \) and \( g \) not optimum, but in addition that the optimum choice of \( \mu \) when \( g(t) = \sqrt{t} \) is not Gaussian, and also that the optimum choice of \( g \) when using Gaussian \( \mu \) is not \( \sqrt{t} \).

A natural open question is whether the insights of Section 4.3 can be used to create a novel new algorithm based on the three point proposal scheme. We have resisted doing so here because such an algorithm would require a problem-specific choice of balancing function and some appropriate randomisation of the noise distribution to prevent reducibility issues. It may be possible, however, to design an adaptive Markov chain Monte Carlo method that is able to learn these quantities during the simulation. We look forward to designing practical methodology based on the insights of Section 4.3 in subsequent work.

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A Sampling from optimal locally-balanced kernels with Gaussian noise

We consider here fixing \( \mu \) to be standard Gaussian, as is the choice made in default versions of the Langevin and Barker algorithms. Setting \( \mu_6 = 15 \) and \( \mu_4 = 3 \) into (11) implies that the maximum efficiency is found by choosing \( g = C_\phi/(10B_\phi) - 1/5 \). Such value of \( g \) can be imposed using, e.g., the family of balancing functions defined in (12).

Sampling from a first order locally-balanced proposal using (12) and standard Gaussian \( \mu \) can then be done using Algorithm 2 applied to each coordinate. Also, any choice of balancing function within the family (12) and \( \mu \) chosen as a mixture of Gaussians results in a proposal density with analytically tractable normalising constant, meaning Metropolis–Hastings acceptance rates can be evaluated.
The random variable $Y$



Proof of Proposition 1.

C.1 Section 2

C Miscellaneous proofs

Here we compare the three point proposal with different choices of $\mu$ on the Hyperbolic target distribution considered in Section 5.1 of the paper. For any value of $\mu_4$, the optimal value of $g$ as given by Proposition 5 in the paper is used. Theory suggests that optimal asymptotic performances are given by choosing $\mu_4$ arbitrarily close to 1 but, as discussed in the paper, values of $\mu_4$ close to 1 may need very large dimensionality for the actual asymptotic regime to kick in. Figure 2 illustrates this phenomenon. For small dimensionality, the value $\mu_4 = 2$ is best (among the ones considered) but as dimensionality increases $\mu_4 = 1.5$ starts outperforming and then $\mu_4 = 1.25$. Dimension $n = 35000$ is not yet sufficient to for $\mu_4 = 1.1$ to outperform $\mu_4 = 1.25$, although theory suggests that this will eventually happen.

B Illustration of different choices of $\mu_4$ in the optimal choice of first order locally-balanced proposal

Here we compare the three point proposal with different choices of $\mu_4$ on the Hyperbolic target distribution considered in Section 5.1 of the paper. For any value of $\mu_4$, the optimal value of $g$ as given by Proposition 5 in the paper is used. Theory suggests that optimal asymptotic performances are given by choosing $\mu_4$ arbitrarily close to 1 but, as discussed in the paper, values of $\mu_4$ close to 1 may need very large dimensionality for the actual asymptotic regime to kick in. Figure 2 illustrates this phenomenon. For small dimensionality, the value $\mu_4 = 2$ is best (among the ones considered) but as dimensionality increases $\mu_4 = 1.5$ starts outperforming and then $\mu_4 = 1.25$. Dimension $n = 35000$ is not yet sufficient to for $\mu_4 = 1.1$ to outperform $\mu_4 = 1.25$, although theory suggests that this will eventually happen.

C Miscellaneous proofs

C.1 Section 2

Proof of Proposition 2

Algorithm 2 Simulate from the locally-balanced proposal using (12).

Require: $x \in \mathbb{R}$ and $\sigma > 0$

Set $p_x \leftarrow (1 + e^{-\gamma \sigma^2 \phi(x)^2})^{-1}$$

Draw $u_x \sim \text{Bernoulli}(p_x)$ and set $b_x \leftarrow 2u_x - 1$

Draw $z \sim N(0, 1)$ and set $y \leftarrow x + (1/2 + b_x \gamma) \sigma^2 \phi'(x) + \sigma z$

Output $y$

The random variable $Y$ is a mixture of two Gaussians with the same variance. Setting $\mu^+_x = x + (1/2 + \gamma)\sigma^2 \phi'(x)$ and $\mu^-_x = x + (1/2 - \gamma)\sigma^2 \phi'(x)$, the density of $\xi(y)$ of $Y$ satisfies

$$
\sigma \sqrt{2\pi} \xi(y) = \frac{p(x) e^{-\frac{(y-\mu^+_x)^2}{2\sigma^2}} + (1-p(x)) e^{-\frac{(y-\mu^-_x)^2}{2\sigma^2}}}{e^{-\frac{(y-\mu^+_x)^2}{2\sigma^2}} + e^{-\frac{(y-\mu^-_x)^2}{2\sigma^2}}}
$$

as required.

Proof of Proposition 6. Algorithm 2 produces a sample from a distribution with density proportional to $\sigma^{-1} \mu((y-x)/\sigma) g_{\gamma}(e^{\phi(x)(y-x)})$. 

Proof. First note that

$$
p(x) = \frac{e^{-\frac{1}{2}(\gamma + \frac{1}{2})^2 \sigma^2 \phi'(x)}}{e^{-\frac{1}{2}(\gamma + \frac{1}{2})^2 \sigma^2 \phi'(x)} + e^{\frac{1}{2}(\gamma - \frac{1}{2})^2 \sigma^2 \phi'(x)}},
$$

so that

$$
p(x) e^{-\frac{1}{2}(\gamma + \frac{1}{2})^2 \sigma^2 \phi'(x)} = (1 - p(x)) e^{-\frac{1}{2}(\gamma - \frac{1}{2})^2 \sigma^2 \phi'(x)}.
$$

The random variable $Y$ is a mixture of two Gaussians with the same variance. Setting $\mu^+_x = x + (1/2 + \gamma)\sigma^2 \phi'(x)$ and $\mu^-_x = x + (1/2 - \gamma)\sigma^2 \phi'(x)$, the density of $\xi(y)$ of $Y$ satisfies

$$
\sigma \sqrt{2\pi} \xi(y) = \frac{p(x) e^{-\frac{(y-\mu^+_x)^2}{2\sigma^2}} + (1-p(x)) e^{-\frac{(y-\mu^-_x)^2}{2\sigma^2}}}{e^{-\frac{(y-\mu^+_x)^2}{2\sigma^2}} + e^{-\frac{(y-\mu^-_x)^2}{2\sigma^2}}}
$$

as required.
Figure 4: Expected squared jump distance against dimensionality for various three point proposals on an hyperbolic product target distribution.

Similarly for the second part

$$h_g(-x) = e^{x/2} g_h(e^{-x}) = e^{-x/2} g_h(e^x) = h_g(x)$$

using that $g_h(e^{-x}) = e^{-x} g_h(e^x)$. Noting also that $h_g : \mathbb{R} \rightarrow [0, \infty)$ shows that $h_g \in \mathcal{H}$.

C.2 Section 3

Proof of Theorem 1. See Section 3, particularly the proof of Theorem 8, in [21].

Proof of Proposition 2.

(i) Easy to verify.

(ii) Since $\int_\mathbb{R} z^2 \mu(dz) < \infty$, we have

$$\int_\mathbb{R} e^{b(az)} |z|^\xi \mu(dz) = \int_\mathbb{R} g(e^{az}) |z|^\xi \mu(dz) \leq \|g\|_\infty \int_\mathbb{R} |z|^\xi \mu(dz).$$

On the other hand $b$ is non decreasing and $b(0) = 0$ so

$$\int_\mathbb{R} e^{b(az)} \mu(dz) \geq \int_0^\infty \mu(dz) = \frac{1}{2}.$$ 

(iii) This essentially holds because $b'$ is bounded and hence $b$ is at most linear. Clearly $\mu$ has finite polynomial moments. Next note that by fundamental theorem of calculus and $b(0) = 0$ we have

$$b(az) = \int_0^1 a z b'(azs)ds.$$
Hence
\[
\int_{\mathbb{R}} e^{b(a z)} |z|^\xi \mu(z) dz = \int_{\mathbb{R}} e^{a z} \int_{\mathbb{R}} b'(sz) ds |z|^\xi \mu(z) dz \\
\leq C \mu \left(1 + |a| \int_{0}^{1} b'(sa z) ds \right) \int_{\mathbb{R}} e^{a z} b(s a z) ds \mu(z) dz \\
\leq C \mu \max(1, ||b'||_{L^\infty}) \left(1 + |a| |b'|_{L^\infty} \frac{2}{b-a} e^{-c(b-a)} \right) \int_{\mathbb{R}} e^{b(a z)} \mu(z) dz.
\]

(iv) We will prove this implies a special instance of (iii). Due to symmetry of \(\mu\) we may assume without loss of generality that \(a > 0\). Firstly, \(\mu\) has finite moment generating function since for any \(b > a\) and \(c > 0\) we have
\[
\int_{\mathbb{R}} e^{az} \mu(z) dz \leq 2 \int_{0}^{\infty} e^{b(a z)} \mu(z) dz \leq 2 \left(\sup_{z \leq c} e^{az} \mu(z) + \frac{2}{b-a} e^{-c(b-a)} \sup_{z > c} e^{az} \mu(z) \right).
\]

Secondly, we will use inequalities \(|z|^{\lambda}_{[-1,1]}(z) \leq |z|^{\lambda+1}\) and \(e^{a} = e^{a} \int_{0}^{\infty} 2 \mu(z) dz \leq 2 \int_{\mathbb{R}} e^{az} \mu(z) dz \leq 2 \int_{\mathbb{R}} e^{az} \mu(z) dz\), which follows by Jensen’s inequality. Integration by parts implies that for any \(\lambda > p-1\) we have
\[
\int_{\mathbb{R}} e^{az} \left|z\right|^{\lambda} \mu(z) dz \leq \int_{[-1,1]} e^{az} \mu(z) dz + A \int_{[-1,1]} e^{az} \left|z\right|^{\lambda-p} \mu(z) dz - B \int_{[-1,1]} e^{az} \left|z\right|^{\lambda-p} \mu(z) dz \\
= \int_{[-1,1]} e^{az} \mu(z) dz + A \int_{[-1,1]} e^{az} \left|z\right|^{\lambda-p} \mu(z) dz \\
+ B \int_{[-1,1]} e^{az} \left((\lambda-p+1) \left|z\right|^{\lambda-p} + a \left|z\right|^{\lambda-p} \mu(z) dz + B \mu(1)(e^{a} - e^{-a}) \\
\leq (1 + 2B \mu(1)) \int_{\mathbb{R}} e^{az} \mu(z) dz + (A + B(\lambda - p + 1) + |a|B) \int_{\mathbb{R}} e^{az} \left|z\right|^{\lambda-p+1} \mu(z) dz.
\]

Thus, we have successfully reduced the power of \(z\) in the integrand by \(p-1\) at the expense of producing an \(|a|\). Noting that \(|z|^{\xi} \leq 1 + |z|^{|L_{\infty}|(p-1)}\) and recursively applying the same argument establishes the claim.

**Proof of Theorem 2.** Denote \(b(x) = \log g(e^{x})\) and note that \(b(0) = 0, b'(0) = 1/2\) and \(b''(0) = 1/4 + g''(1)\). First consider \(n\) as fixed. By definition for any \(y \in \mathbb{R}\)
\[
\rho_{n}(x, y) = \phi(y) - \phi(x) + b(\phi'(y)(x - y)) - b(\phi'(x)(y - x)) - \log(Z_{\sigma_{n}}(x)) + \log(Z_{\sigma_{n}}(y)).
\]

We will be using the fundamental theorem of calculus
\[
U(1) - U(0) = \int_{0}^{1} U'(s) ds
\]
for various functions \(U\). Denote \(w = (y - x)/\sigma_{n}\), and note that \(Z_{\sigma_{n}}(x) = \int_{\mathbb{R}} e^{b(\phi'(x)\sigma_{n} z)} \mu(dz)\) by an analogous substitution. Then note that
\[
\log \left(\frac{Z_{\sigma_{n}}(x + \sigma_{n} w)}{Z_{\sigma_{n}}(x)}\right) = \sigma_{n}^{2} w \int_{0}^{1} \phi''(x + t \sigma_{n} w) \int_{\mathbb{R}} e^{b(\phi'(x + t \sigma_{n} w) \sigma_{n} z)} b'(\phi'(x + t \sigma_{n} w) \sigma_{n} z) \mu(dz) dt \\
= \int_{\mathbb{R}} e^{b(\phi'(x + t \sigma_{n} w) \sigma_{n} z)} \mu(dz) dt
\]
using (17) with the function \(U_{1}(t) = \log(Z_{\sigma_{n}}(x + t \sigma_{n} w))\). Using (17) again with the function \(U_{2}(s) = b'(s \phi'(x + t \sigma_{n} w) \sigma_{n} z)\) and recalling that \(b'(0) = 1/2\), this can be written as
\[
\frac{\sigma_{n}^{2}}{2} w \int_{0}^{1} \phi''(x + t \sigma_{n} w) \int_{\mathbb{R}} e^{b(\phi'(x + t \sigma_{n} w) \sigma_{n} z)} \mu(dz) dt \\
+ \sigma_{n}^{3} \int_{[0,1]} \phi''(x + t \sigma_{n} w) \phi'(x + t \sigma_{n} w) \int_{\mathbb{R}} e^{b(\phi'(x + t \sigma_{n} w) \sigma_{n} z)} b''(s \phi'(x + t \sigma_{n} w) \sigma_{n} z) \mu(dz) dt ds.
\]
Using \([17]\) in the numerator of the first term with the function \(U_3(u) = e^{b(u\phi'(x + t\sigma_n w)\sigma_n z)}\) and recalling that \(b(0) = 0\) gives
\[
\frac{\sigma_n^3 w}{2} \int_{[0,1]^2} \phi''(x + t\sigma_n w)\phi'(x + t\sigma_n w)\int_{\mathbb{R}} e^{b(u\phi'(x + t\sigma_n w)\sigma_n z) b'(u\phi'(x + t\sigma_n w)\sigma_n z) z^2 \mu(du)} dt du
\]
\[+ \sigma_n^3 w \int_{[0,1]^2} \phi''(x + t\sigma_n w)\phi'(x + t\sigma_n w)\int_{\mathbb{R}} e^{b(u\phi'(x + t\sigma_n w)\sigma_n z) b''(u\phi'(x + t\sigma_n w)\sigma_n z) z^2 \mu(du)} dt du.
\]
And further simplification leads to the expression
\[
\sigma_n^3 w \int_{[0,1]^2} \phi''(x + t\sigma_n w)\phi'(x + t\sigma_n w) \times \int_{\mathbb{R}} e^{b(u\phi'(x + t\sigma_n w)\sigma_n z) (\frac{1}{2} b'(u\phi'(x + t\sigma_n w)\sigma_n z) + b''(u\phi'(x + t\sigma_n w)\sigma_n z)) z^2 \mu(du)} dt ds.
\]
\[
= \sigma_n^3 w \phi''(x)\phi'(x) \left( \frac{1}{2} b'(0) + b''(0) \right) + R_{1,n}(x, w) + R_{2,n}(x, w) + R_{3,n}(x, w)
\]
where
\[
R_{1,n}(x, w) = \sigma_n^3 w \left( \frac{1}{2} b'(0) + b''(0) \right) \int_0^1 (\phi''(x + t\sigma_n w)\phi'(x + t\sigma_n w) - \phi''(x)\phi'(x)) dt
\]
\[
R_{2,n}(x, w) = \sigma_n^3 w \left( \frac{1}{2} b'(0) + b''(0) \right) \int_0^1 \phi''(x + t\sigma_n w)\phi'(x + t\sigma_n w)\int_{\mathbb{R}} e^{b(u\phi'(x + t\sigma_n w)\sigma_n z) (z^2 - 1) \mu(du)} dt
\]
\[
R_{3,n}(x, w) = \sigma_n^3 w \int_{[0,1]^2} \phi''(x + t\sigma_n w)\phi'(x + t\sigma_n w) dt
\]
\[
\times \int_{\mathbb{R}} e^{b(u\phi'(x + t\sigma_n w)\sigma_n z) (\frac{1}{2} b'(u\phi'(x + t\sigma_n w)\sigma_n z) + b''(u\phi'(x + t\sigma_n w)\sigma_n z) - \frac{1}{2} b'(0) - b''(0)) z^2 \mu(du)} dt ds.
\]
To expand the remaining terms of \([16]\) we use the exact third order Taylor expansion
\[
b(t) = b(0) + tb'(0) + t^2 \frac{b''(0)}{2} + t^3 \frac{b'''(0)}{6} + t^3 \frac{1}{2} \int_0^1 (b'''(ut) - b''(0))(1 - u)^2 du
\]
\[
= b(0) + tb'(0) + t^2 \frac{b''(0)}{2} + t^3 \frac{1}{2} \int_0^1 b'''(ut)(1 - u)^2 du
\]
on each of the terms involving \(b\) to obtain
\[
b(-\phi'(x + \sigma_n w)\sigma_n w) - b(\phi'(x)\sigma_n w) = -\frac{\sigma_n w}{2} (\phi'(x) + \phi'(x + \sigma_n w))
\]
\[+ \sigma_n^3 w^2 \left( \frac{1}{8} + \frac{\phi''(1)}{2} \right) (\phi'(x + \sigma_n w)^2 - \phi'(x)^2)
\[+ R_{6,n}(x, w) + R_{7,n}(x, w)
\]
where
\[
R_{6,n}(x, w) = -\frac{1}{2} \sigma_n^3 w^3 \phi'(x + \sigma_n w)^3 \int_0^1 b'''(-u\phi'(x + \sigma_n w)\sigma_n w)(1 - u)^2 du,
\]
\[
R_{7,n}(x, w) = -\frac{1}{2} \sigma_n^3 w^3 \phi'(x)^3 \int_0^1 b'''(u\phi'(x)\sigma_n w)(1 - u)^2 du.
\]
Taking one half of the difference of the exact Taylor expansions

\[ \phi(x + \sigma_n w) - \phi(x) = \sigma_n w \phi'(x) + \sigma_n^2 w^2 \int_0^1 \phi''(x + u \sigma_n w)(1 - u) du, \]

\[ \phi(x) - \phi(x + \sigma_n w) = -\sigma_n w \phi'(x + \sigma_n w) + \sigma_n^2 w^2 \int_0^1 \phi''(x + (1 - u) \sigma_n w)(1 - u) du \]

and setting \( v = 1 - u \) reveals that

\[ \phi(x + \sigma_n w) - \phi(x) - \frac{\sigma_n w}{2} (\phi'(x) + \phi'(x + \sigma_n w)) = \frac{\sigma_n^2 w^2}{2} \int_0^1 \phi''(x + u \sigma_n w)(1 - 2u) du \]

\[ = \frac{\sigma_n^2 w^2}{2} \int_0^1 (\phi''(x + u \sigma_n w) - \phi''(x))(1 - 2u) du \]

\[ = \frac{\sigma_n^3 w^3}{2} \int_0^1 u(1 - 2u) \int_0^1 \phi'''(x + uv \sigma_n w) dv du \]

\[ = -\frac{\sigma_n^3 w^3}{12} \phi'''(x) + R_{4,n}(x, w), \]

where

\[ R_{4,n}(x, w) = \frac{\sigma_n^3 w^3}{2} \int_0^1 u(1 - 2u) \int_0^1 (\phi'''(x + uv \sigma_n w) - \phi'''(x)) dv du. \]

Similarly,

\[ \sigma_n^2 w^2 \left( \frac{1}{8} + \frac{g''(1)}{2} \right) (\phi'(x + \sigma_n w)^2 - \phi'(x)^2) = \sigma_n^3 w^3 \left( \frac{1}{4} + g''(1) \right) \int_0^1 \phi' \phi''(x + u \sigma_n w) du \]

\[ = \sigma_n^3 w^3 \left( \frac{1}{4} + g''(1) \right) \phi'(x) \phi''(x) + R_{5,n}(x, w), \]

where

\[ R_{5,n}(x, w) = \sigma_n^3 w^3 \left( \frac{1}{4} + g''(1) \right) \int_0^1 (\phi' \phi''(x + u \sigma_n w) - \phi' \phi''(x)) du. \]

Next, we will denote with \( \tilde{E}_n \) the expectation with respect to the measure \( Z_{\sigma_n}^{-1}(x) e^{b(\phi(x) \sigma_n w)} \pi(x) dx \mu(dw) \). We will show that \( \tilde{E}_n[R_{1,n}^2] \) decays faster than \( \sigma_n^6 \) for \( i = 1, 2, \ldots, 7 \) as \( n \to \infty \). Note that Assumption \( 1 \) iii) is the tool enabling the control of the Radon-Nikodým derivatives of various proposals (indexed by \( n \)) with respect to \( \mu \), making it possible for us to represent these expectations with respect to the measure \( \pi(x) dx \mu(dw) \). Using \( a \lesssim b \) to denote that \( a \leq cb \) for some positive finite \( c \) independent of \( n \), the bound for the first term \( R_{1,n} \) follows by Assumption \( 1 \) ii) and iii) as

\[ \tilde{E}_n[R_{1,n}^2] \lesssim \sigma_n^6 \int_{\mathbb{R}^2} \int_0^1 (\phi''(x + t \sigma_n w) \phi'(x + t \sigma_n w) - \phi''(x) \phi'(x))^2 w^2 e^{b(\phi'(x) \sigma_n w)} Z_{\sigma_n}(x) dt \mu(dw) \pi(x) dx \]

\[ \leq \sigma_n^6 \int_{\mathbb{R}^2} \int_0^1 K(x)^2 w^2 \max(|t \sigma_n w| H, |t \sigma_n w|) |t \sigma_n w|^2 e^{b(\phi'(x) \sigma_n w)} Z_{\sigma_n}(x) dt \mu(dw) \pi(x) dx \]

\[ \lesssim \sigma_n^{6+2H} \int_{\mathbb{R}} K(x)^2 \pi(x) \int_{\mathbb{R}} |w| e^{b(\phi'(x) \sigma_n w)} Z_{\sigma_n}(x) \mu(dw) dx \]

\[ \lesssim \sigma_n^{6+2H+\beta} \int_{\mathbb{R}} K(x)^2 (1 + |\phi'(x)|^\beta) \pi(x) dx. \]

To bound the second term \( \tilde{E}_n R_{2,n} \), note that \( \lim_{\sigma_n \to 0} \sigma_n^{-3} R_{2,n} = 0 \) for every \( x \) and \( w \), so we only need to provide a dominating bound for the integrand. Using Assumption \( 1 \) iii) gives that this is

\[ \lesssim \int_{\mathbb{R}^2} \int_0^1 \phi''(x + t \sigma_n w)^2 \phi'(x + t \sigma_n w)^2 (1 + \sigma_n^{2\beta} \phi'(x + t \sigma_n w)^{2\beta}) e^{b(\phi'(x) \sigma_n w)} Z_{\sigma_n}(x)^2 w^2 dt \mu(dw) \pi(x) dx. \]
To show that this is finite we use Assumption 1 [i] to control the perturbation of functions \( \phi'' \phi' \) and \( \phi'' |\phi'|^{1+\beta} \) from \( x \) to \( x+\sigma_n w \) and Assumption 1 [ii] to control the Radon-Nikodym derivative \( Z_{\sigma_n}(x)^{-1} e^{b(\phi'(x)\sigma_n w)} \) (as in the argument for the term \( \tilde{E}_n[R_{1,n}] \)):  

\[
\int_{\mathbb{R}^2} \int_0^1 \phi''(x+t\sigma_n w)^2 \phi'(x+t\sigma_n w)^2 \left( 1 + |\phi'(x+t\sigma_n w)|^\beta \right)^2 w^2 e^{b(\phi'(x)\sigma_n w)} \frac{Z_{\sigma_n}(x)}{Z_{\sigma_n}(x)} dt \mu(dw) \pi(x) dx 
\]

\[
\lesssim \int_{\mathbb{R}^2} \int_0^1 \phi''(x)^2 \phi'(x)^2 \left( 1 + |\phi'(x)|^\beta \right)^2 w^2 e^{b(\phi'(x)\sigma_n w)} \frac{Z_{\sigma_n}(x)}{Z_{\sigma_n}(x)} \mu(dw) \pi(x) dx 
\]

\[
+ \int_{\mathbb{R}^2} \int_0^1 \phi''(x+t\sigma_n w) \phi'(x+t\sigma_n w) \phi''(x) \phi'(x)^2 dt w^2 e^{b(\phi'(x)\sigma_n w)} \frac{Z_{\sigma_n}(x)}{Z_{\sigma_n}(x)} \mu(dw) \pi(x) dx 
\]

\[
+ \int_{\mathbb{R}^2} \int_0^1 \phi''(x+t\sigma_n w) \phi'(x+t\sigma_n w)^{1+\beta} - \phi''(x) \phi'(x)^{1+\beta} dt w^2 e^{b(\phi'(x)\sigma_n w)} \frac{Z_{\sigma_n}(x)}{Z_{\sigma_n}(x)} \mu(dw) \pi(x) dx 
\]

\[
\lesssim \int_{\mathbb{R}^2} \phi''(x)^2 \phi'(x)^2 \left( 1 + |\phi'(x)|^\beta \right)^3 \pi(x) dx + \sigma_n^{2H+\beta} \int_{\mathbb{R}} K(x)^2 \pi(x) \int_{\mathbb{R}} |w|^3 e^{b(\phi'(x)\sigma_n w)} \frac{Z_{\sigma_n}(x)}{Z_{\sigma_n}(x)} \mu(dw) dx 
\]

\[
\lesssim \int_{\mathbb{R}} \phi''(x)^2 \phi'(x)^2 \left( 1 + |\phi'(x)|^\beta \right)^3 \pi(x) dx + \int_{\mathbb{R}} K(x)^2 \left( 1 + |\phi'(x)|^\beta \right) \pi(x) dx 
\]

The term \( \tilde{E}[R_{3,n}] \) is handled similarly with the dominated convergence theorem as \( \sigma_n^{-3} R_3 \) converges point-wise to zero as \( \sigma_n \to 0 \). The dominating bound is very similar as for \( R_{2,n} \) once we notice that \( b' \) and \( b'' \) are both bounded by Assumption 1 [i].

By Assumption 1 [i] the terms \( R_{4,n} \) and \( R_{5,n} \) are bounded absolutely by a constant multiplier of \( K(x) \sigma_n^{3+H} \max(|w|^{3+H},|w|^{3+\gamma}) \), hence \( \lim_{\sigma_n \to 0} \sigma_n^6 \tilde{E}_n[R_{4,n}^2] = \lim_{\sigma_n \to 0} \sigma_n^6 \tilde{E}_n[R_{5,n}^2] = 0 \). The square of \( R_{7,n} \) can be seen to decay faster than \( \sigma_n^6 \) by the Dominated convergence theorem, since \( b'''(0) = 0 \) and integrability guaranteed by Assumption 1 [i]. Similarly

\[
R_{6,n} = -\frac{1}{2} \sigma_n^3 w^3 \phi'(x)^3 \int_0^1 b'''(-u\phi'(x+\sigma_n w)\sigma_n w)(1-u)^2 du 
\]

\[
- \frac{1}{2} \sigma_n^3 w^3 \left( \phi'(x+\sigma_n w)^3 - \phi'(x)^3 \right) \int_0^1 b'''(-u\phi'(x+\sigma_n w)\sigma_n w)(1-u)^2 du , 
\]

so again the square of the first part decays faster than \( \sigma_n^6 \) by the Dominated convergence theorem (as for \( R_{7,n} \)) and the second part is dominated by a constant multiplier of \( K(x) \sigma_n^{3+H} \max(|w|^{3+H},|w|^{3+\gamma}) \) due to Assumption 1 [i].

Write

\[
T(x,w) = w^3 \left( -\frac{1}{12} \phi'''(x) + \left( \frac{1}{4} + g''(1) \right) \phi'(x) \phi''(x) \right) - w \left( \frac{1}{2} + g''(1) \right) \phi'(x) \phi''(x) 
\]

and set \( R_n(x,w) = \sum_{i=1}^7 R_{i,n}(x,w) \). Clearly

\[
\tilde{E}_n[R_n^2] = \tilde{E}_n \left[ (\sigma^3 T + R_n)^2 \right] = \tilde{E}_n \left[ \sigma^6 T^2 \right] + 2 \tilde{E}_n \left[ \sigma^3 \sigma^3 TR_n \right] + \tilde{E}_n \left[ R_n^2 \right] . 
\]

Using the inequalities \( \tilde{E}_n \left[ T R_n \right]^2 \leq \tilde{E}_n[T^2] \tilde{E}_n[R_n^2] \) and \( \tilde{E}_n[R_n^2] \leq 7 \sum_{i=1}^7 \tilde{E}_n[R_{i,n}^2] \) we see that the last two terms decay faster than \( \sigma_n^{-6} \). We can now identify the limiting \( \theta^2 \) using the Dominated convergence theorem. We show that \( \lim_{n \to \infty} \sigma_n^{-6} \tilde{E}_n[R_n^2] = \lim_{n \to \infty} \tilde{E}_n[T^2] = E[T^2] = \theta^2 \) where the last expectation is with respect to \( \pi(x) dx \mu(dw) \). Indeed,

\[
\tilde{E}_n[T^2] = \int_{\mathbb{R}} T^2(x,w) e^{\sigma_n w \phi'(x)} \frac{Z_{\sigma_n}(x)}{Z_{\sigma_n}(x)} \mu(dw) \pi(x) dx . 
\]

The integrand converges point-wise to \( T^2(x,w) \) and is dominated by \( T^2(x,w)(1+|\phi'(x)|^\beta) \) which is integrable by Assumption 1 [i]. Expanding the expression for \( T \) and integrating with respect to \( \mu(dw) \pi(x) dx \) leads to the claimed form of \( \theta^2 \).
Finally, to finish the proof using Theorem 1 notice that by choosing \( \sigma_n \) such that \( n\sigma_n^6 \to \ell^6 \) we get
\[
\lim_{n \to \infty} n\mathbb{E}[\rho_n^2] = \lim_{n \to \infty} n\sigma_n^6\mathbb{E}[\rho_n^2] = \ell^6\theta^2.
\]
We also need to prove that \( \lim_{n \to \infty} \mathbb{E}_n[\rho_n^21_{\rho_n < -\sigma_n}] = 0 \). Indeed,
\[
\mathbb{E}_n[\rho_n^21_{\rho_n < -\sigma_n}] = \mathbb{E}_n[\rho_n^2] = 2\sigma_n^2\mathbb{E}_n[TR_n1_{\rho_n < -\sigma_n}] + \mathbb{E}_n[R_n^21_{\rho_n < -\sigma_n}]
\]
\[
\leq \sigma_n^6\mathbb{E}_n[T^21_{\rho_n < -\sigma_n}] + 2\sigma_n^3\sqrt{\mathbb{E}_n[T^2]\mathbb{E}_n[R_n^2]} + 2\mathbb{E}[R_n^2].
\]
We have already established that the last two terms decay faster than \( \sigma_n^{-6} \). The first term can be bounded using the Hölder and Markov inequalities by
\[
\sigma_n^6\mathbb{E}_n[T^21_{\rho_n < -\sigma_n}] \leq \mathbb{E}_n[\rho_n^2]^{1+\epsilon} \mathbb{E}_n[\rho_n < -\sigma_n]^{1-\epsilon}
\]
\[
\leq \sigma_n^6\mathbb{E}_n[T^2+\epsilon]^{1+\epsilon} \mathbb{E}_n[\rho_n^2]^{1-\epsilon} \mathbb{E}_n[\rho_n < -\sigma_n]^{1-\epsilon}
\]
\[
= \sigma_n^{6+\epsilon}\mathbb{E}_n[T^2+\epsilon]^{1+\epsilon} \mathbb{E}_n[\rho_n^2]^{1-\epsilon} \mathbb{E}_n[\rho_n < -\sigma_n]^{1-\epsilon}.
\]
Analogously as before \( \mathbb{E}_n[T^2+\epsilon] \to \mathbb{E}[T^2+\epsilon] < \infty \) by the Dominated convergence theorem and Assumption 1 i) and we have already established that \( \mathbb{E}_n[\rho_n^2] \to \theta^2 \). Together these establish that
\[
\lim_{n \to \infty} \mathbb{E}_n[\rho_n^21_{\rho_n < -\sigma_n}] = 0
\]
which completes the proof.

**Proof of Theorem 3** We fix \( g \) and \( \mu \) that satisfy Assumption 1 and suppress the notation with respect to them for the rest of the proof. First assume \( \lim_{n \to \infty} n^{1/6}\sigma_n = 0 \), which implies that
\[
\sigma_n^{-2}\mathbb{E}[(Y_{n,1} - X_{n,1})^2] = \sigma_n^{-2}\int_{\mathbb{R}}\int_{\mathbb{R}}Z_{\sigma_n}^{-1}(x)g(\phi'(x)w\sigma_n)w^2\mu(dw)\pi(x)dx \to 1
\]  
(18)  
as \( n \to \infty \). Convergence to one follows by the Dominated convergence theorem as \( \sigma_n \to 0 \). The dominating bound is provided by Assumption 1(iii). Hence, \( \mathbb{E}[(Y_{n,1} - X_{n,1})^2] \) decays as \( \sigma_n^2 \) which is by definition faster than \( n^{-1/3} \). Because the acceptance rate is bounded above by one, we must have that \( \lim_{n \to \infty} n^{1/3}\mathcal{E}_n = 0 \).

Next assume \( \lim_{n \to \infty} n^{1/6}\sigma_n = \infty \). First we will establish that
\[
\mathbb{E}\left[\left(Y_{n,1} - X_{n,1}\right)^2(1 \land e)\left(\sum_{i=1}^{n}\rho_{n,i}\right)\right] \leq 2\mathbb{E}\left[\left(Y_{n,1} - X_{n,1}\right)^2\right]\mathbb{E}\left[(1 \land e)\left(\sum_{i=2}^{n}\rho_{n,i}\right)\right].
\]
(19)  
The statement (without the two) is clear if \( \rho_{n,1} \) is negative. When it is positive then using Lemma 1 with respect to the log-Metropolis–Hastings random variable \( \rho_{n,1} \) and \( h(x,y) = (y-x)^2 \) gives
\[
\mathbb{E}\left[\left(Y_{n,1} - X_{n,1}\right)^2(1 \land e)\left(\sum_{i=1}^{n}\rho_{n,i}\right)\right]_{\rho_{n,1} \geq 0} \leq \mathbb{E}\left[\left(Y_{n,1} - X_{n,1}\right)^2e^{\rho_{n,1}} : (1 \land e)\left(\sum_{i=2}^{n}\rho_{n,i}\right)1_{[0,\infty)}(\rho_{n,1})\right]
\]
\[
= \mathbb{E}\left[\left(Y_{n,1} - X_{n,1}\right)^2(1 \land e)\left(\sum_{i=2}^{n}\rho_{n,i}\right)1_{[0,\infty)}(-\rho_{n,1})\right]
\]
\[
\leq \mathbb{E}\left[\left(Y_{n,1} - X_{n,1}\right)^2\right]\mathbb{E}\left[(1 \land e)\left(\sum_{i=2}^{n}\rho_{n,i}\right)\right].
\]
Adding terms corresponding to the sign of \( \rho_{n,1} \) implies (19).

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We still need to bound the acceptance rate. To do this we split the probability space regarding the event $A_n := \{ \sum_{i=1}^n \rho_{n,i} \leq \sum_{i=2}^n \mathbb{E}[\rho_{n,i}] / 2 \}$. On the set where this holds we have, using Theorem 1 and Theorem 2
\[
\mathbb{E} \left[ (1 \land e) \left( \sum_{i=1}^n \rho_{n,i} \right) 1_{A_n} \right] \leq \exp \left( \frac{1}{2} \sum_{i=1}^n \mathbb{E}[\rho_{n,i}] \right)
\]
\[
\leq \exp \left( -\frac{n}{4} \mathbb{E}[\rho_{n,1}^2] \left( 1 - \frac{\mathbb{E}[\rho_{n,1}] + \frac{1}{2} \mathbb{E}[\rho_{n,1}^2]}{\mathbb{E}[\rho_{n,1}^2]} \right) \right)
\]
\[
\leq \exp \left( -\frac{n}{4} \sigma_n^6 \left( \sigma_n^{-6} \mathbb{E}[\rho_{n,1}^2]) \right) \right)
\]
\[
\leq \exp \left( -\frac{\theta^2}{8} n \sigma_n^6 \right)
\]
for all large enough $n \in \mathbb{N}$. On the complement $A_n^c$ using Markov’s inequality gives
\[
\mathbb{E} \left[ (1 \land e) \left( \sum_{i=1}^n \rho_{n,i} \right) 1_{A_n^c} \right] \leq \mathbb{P}[A_n^c]
\]
\[
= \mathbb{P} \left[ \sum_{i=1}^n (\rho_{n,i} - \mathbb{E}[\rho_{n,i}]) > -\frac{1}{2} \sum_{i=1}^n \mathbb{E}[\rho_{n,i}] \right]
\]
\[
\leq \frac{4 \text{Var}[\rho_{n,1}^2]}{n \mathbb{E}[\rho_{n,1}^2]^2}
\]
\[
\leq \frac{16}{n \mathbb{E}[\rho_{n,1}^2] \left( 1 - \frac{4 \mathbb{E}[\rho_{n,1}] + \frac{1}{2} \mathbb{E}[\rho_{n,1}^2]}{\mathbb{E}[\rho_{n,1}^2]} \right)}
\]
\[
\leq \frac{32}{\theta^2 n \sigma_n^6}
\]
for all large enough $n \in \mathbb{N}$.

Together with (18) and (19) these bounds imply
\[
\mathbb{E} \left[ (Y_{n,1} - X_{n,1})^2 (1 \land e) \left( \sum_{i=1}^n \rho_{n,i} \right) \right] \leq 2 \sigma_n^2 \left( e^{-\frac{\theta^2}{8} n \sigma_n^6} + \frac{32}{\theta^2 n \sigma_n^6} \right) \leq C \frac{1}{n^{1/3}} \frac{1}{n^{2/3} \sigma_n^6}
\]
for an appropriate constant $C > 0$. Since $n \sigma_n^6 \to \infty$, this decay rate is faster than $n^{-1/3}$, meaning $\mathcal{E}_n$ also decays faster than $n^{-1/3}$.

Now assume, $\lim_{n \to \infty} n^{1/6} \sigma_{n,\ell} = \ell$. Splitting the expectation gives
\[
\mathbb{E} \left[ (Y_{n,1} - X_{n,1})^2 (1 \land e) \left( \sum_{i=1}^n \rho_{n,i} \right) \right] = \mathbb{E} \left[ (Y_{n,1} - X_{n,1})^2 \right] \left( 1 \land e \right) \left( \sum_{i=2}^n \rho_{n,i} \right)
\]
\[
+ \mathbb{E} \left[ (Y_{n,1} - X_{n,1})^2 \left( 1 \land e \right) \left( \sum_{i=1}^n \rho_{n,i} \right) - (1 \land e) \left( \sum_{i=1}^n \rho_{n,i} \right) \right].
\]
For the first term on the right-hand side we have by (18) and Theorem 2 that
\[
n^{1/3} \mathbb{E} \left[ (Y_{1}^{(n)} - X_1)^2 \right] \left( 1 \land e \right) \left( \sum_{i=2}^n \rho_{n,i} \right) \to h(\ell)
\]
as $n \to \infty$. The second term vanishes. To see this note that by Theorem 2 and the fact that the function $t \mapsto 1 \land e^t$ is 1-Lipschitz and bounded imply that the expression
\[
\left( 1 \land e \right) \left( \sum_{i=1}^n \rho_{n,i} \right) - (1 \land e) \left( \sum_{i=2}^n \rho_{n,i} \right)
\]

converges to zero in the $L^2$ sense, and therefore also in probability. On the other hand (18) and Assumption 1 iii) imply that the random variables $n^{1/3}(Y_{n,1} - X_{n,1})^2$ have an integrable dominating bound. Their product is therefore uniformly integrable and converges to zero in probability, meaning it is also true that

$$n^{1/3}\mathbb{E}\left[(Y_{n,1} - X_{n,1})^2 \left(1 + e \sum_{i=1}^n \rho_{n,i} \right) - (1 + e \sum_{i=2}^n \rho_{n,i})\right] \to 0$$

as $n \to \infty$.

Finally we will optimize over the choice of $\ell$. The function $h(\ell) = 2\ell^2\Phi(-\ell^3\theta/2)$ is smooth in $\ell$ and converges to zero both when $\ell \to 0$ and when $\ell \to \infty$. Hence, its maximum is attained at a stationary point. Setting $s = \ell^3\theta/2$ we can find the stationary points of $s \mapsto s\varphi_N(-s)/\Phi(-s)$, where $\varphi_N$ denotes the standard Gaussian probability density function. There exists a unique solution $s^*$, as the function $s \mapsto s\varphi_N(-s)/\Phi(-s)$ is strictly increasing, meaning $h(\ell)$ attains its maximal value at a specific value $\ell^*$ satisfying $s^* = (\ell^*)^3\theta/2$, corresponding to an average acceptance rate of $2\Phi(-s^*)$, which turns out to numerically equal to 57.4% to three decimal places. This is also implies that

$$h(\ell^*) = \theta^{-2/3} \cdot 2^{5/3}(s^*)^{2/3}\Phi(-s^*) \approx 0.651637 \times \theta^{-2/3},$$

which completes the proof.

\[\square\]

## D Technical results

**Lemma 1.** Let $\rho$ be a log-Metropolis–Hastings random variable associated with a probability measure $\pi$ and a Markov kernel $Q$ on $(\mathcal{X}, \mathcal{F})$. Let $f : \mathcal{X} \to \mathbb{R}$ and $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be such that $h(X,Y) = h(Y,X)$. Then the following are true:

(i) $-\rho(X,Y) = \rho(Y,X)$.

(ii) If the integrals are finite, then setting $h = h(X,Y)$ and $\rho = \rho(X,Y)$

$$\mathbb{E}[hf(\rho\rho)] = \mathbb{E}[hf(-\rho)].$$

**Proof of Lemma 1.** The proof is given Proposition 3 of [21], with the only minor difference that we carry a symmetric function $h$ through the entire derivation.

### References

[1] Christophe Andrieu and Johannes Thoms. A tutorial on adaptive mcmc. *Statistics and computing*, 18(4):343–373, 2008.

[2] Av A Barker. Monte carlo calculations of the radial distribution functions for a proton-electron plasma. *Australian Journal of Physics*, 18(2):119–134, 1965.

[3] Bob Carpenter, Andrew Gelman, Matthew D Hoffman, Daniel Lee, Ben Goodrich, Michael Betancourt, Marcus Brubaker, Jiqiang Guo, Peter Li, and Allen Riddell. Stan: A probabilistic programming language. *Journal of statistical software*, 76(1):1–32, 2017.

[4] Michael CH Choi. Metropolis–Hastings reversiblizations of non-reversible Markov chains. *Stochastic Processes and their Applications*, 130(2):1041–1073, 2020.

[5] Simon Duane, Anthony D Kennedy, Brian J Pendleton, and Duncan Roweth. Hybrid monte carlo. *Physics letters B*, 195(2):216–222, 1987.

[6] Paul Fearnhead, Joris Bierkens, Murray Pollock, and Gareth O Roberts. Piecewise deterministic markov processes for continuous-time monte carlo. *Statistical Science*, 33(3):386–412, 2018.
[7] Max Hird, Samuel Livingstone, and Giacomo Zanella. A fresh take on ‘Barker dynamics’ for MCMC. *arXiv preprint arXiv:2012.09731*, 2020.

[8] Olav Kallenberg. *Foundations of modern probability*, volume 2. Springer, 1997.

[9] Samuel Livingstone and Giacomo Zanella. The Barker proposal: combining robustness and efficiency in gradient-based MCMC. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, *in press*, 2021.

[10] Peter Neal and Gareth Roberts. Optimal scaling of random walk metropolis algorithms with non-gaussian proposals. *Methodology and Computing in Applied Probability*, 13(3):583–601, 2011.

[11] Radford M Neal. Slice sampling. *The annals of statistics*, 31(3):705–767, 2003.

[12] Samuel Power and Jacob Vorstrup Goldman. Accelerated Sampling on Discrete Spaces with Non-Reversible Markov Processes. *arXiv preprint arXiv:1912.04681*, 2019.

[13] Gareth O Roberts, Andrew Gelman, and Walter R Gilks. Weak convergence and optimal scaling of random walk Metropolis algorithms. *The annals of applied probability*, 7(1):110–120, 1997.

[14] Gareth O Roberts and Jeffrey S Rosenthal. Optimal scaling of discrete approximations to Langevin diffusions. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 60(1):255–268, 1998.

[15] Gareth O Roberts and Jeffrey S Rosenthal. Optimal scaling for various Metropolis-Hastings algorithms. *Statistical science*, 16(4):351–367, 2001.

[16] Gareth O Roberts and Jeffrey S Rosenthal. Examples of adaptive mcmc. *Journal of computational and graphical statistics*, 18(2):349–367, 2009.

[17] Gareth O Roberts and Richard L Tweedie. Exponential convergence of Langevin distributions and their discrete approximations. *Bernoulli*, pages 341–363, 1996.

[18] Jeffrey S Rosenthal. Anmcmc: An r interface for adaptive mcmc. *Computational Statistics & Data Analysis*, 51(12):5467–5470, 2007.

[19] Chris Sherlock, Paul Fearnhead, and Gareth O Roberts. The random walk metropolis: linking theory and practice through a case study. *Statistical Science*, 25(2):172–190, 2010.

[20] Luke Tierney. A note on Metropolis-Hastings kernels for general state spaces. *Annals of applied probability*, pages 1–9, 1998.

[21] Jure Vogrinc and Wilfrid S Kendall. Counterexamples for optimal scaling of Metropolis–Hastings chains with rough target densities. *The Annals of Applied Probability*, 31(2):972–1019, 2021.

[22] Ziheng Yang and Carlos E Rodríguez. Searching for efficient markov chain monte carlo proposal kernels. *Proceedings of the National Academy of Sciences*, 110(48):19307–19312, 2013.

[23] Giacomo Zanella. Informed proposals for local MCMC in discrete spaces. *Journal of the American Statistical Association*, 115(530):852–865, 2020.

[24] Giacomo Zanella, Mylene Bédard, and Wilfrid S Kendall. A Dirichlet form approach to MCMC optimal scaling. *Stochastic Processes and their Applications*, 127(12):4053–4082, 2017.