Optimal Scaling of MCMC Beyond Metropolis

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Abstract

The problem of optimally scaling the proposal distribution in a Markov chain Monte Carlo algorithm is critical to the quality of the generated samples. Much work has gone into obtaining such results for various Metropolis-Hastings (MH) algorithms. Recently, acceptance probabilities other than MH are being employed in problems with intractable target distributions. There is little resource available on tuning the Gaussian proposal distributions for this situation. We obtain optimal scaling results for a general class of acceptance functions, which includes Barker’s and Lazy-MH. In particular, optimal values
for the Barker’s algorithm are derived and found to be significantly different from that obtained for the MH algorithm. Our theoretical conclusions are supported by numerical simulations indicating that when the optimal proposal variance is unknown, tuning to the optimal acceptance probability remains an effective strategy.

1 Introduction

Over the past few decades, Markov chain Monte Carlo (MCMC) methods have become an abundantly popular computational tool, enabling practitioners to conveniently sample from complicated target distributions (see Brooks et al., 2011; Meyn and Tweedie, 2012; Robert and Casella, 2013). This popularity can be attributed to easy-to-implement accept-reject based MCMC algorithms for target densities available only up to a proportionality constant. Here, draws from a proposal kernel are accepted with a certain acceptance probability. The choice of the acceptance probability and the proposal kernel can yield varying performances of the MCMC samplers.

Unarguably, the most popular acceptance probability is Metropolis-Hastings (MH) of Metropolis et al. (1953); Hastings (1970) due to its acknowledged optimality (Peskun, 1973; Billera and Diaconis, 2001). Efficient implementation of the MH algorithm requires tuning within the chosen family of proposal kernels. For the MH acceptance function, various optimal scaling results have been obtained under assumptions on the proposal and the target distribution. This includes the works of Roberts et al. (1997); Roberts and Rosenthal (1998, 2001); Neal and Roberts (2006); Bédard (2008); Sherlock and Roberts (2009); Zanella et al. (2017); Yang et al. (2020), among others. Despite the popularity of the MH acceptance function, other acceptance probabilities remain practically and theoretically relevant. Recently, the Barker’s acceptance rule
and the Lazy-MH (see Latuszyński and Roberts, 2013) have found use in Bernoulli factory based MCMC algorithms for intractable posteriors (Herbei and Berliner, 2014; Gonçalves et al., 2017; Smith, 2018; Vats et al., 2021).

Barker’s acceptance function has also proven to be optimal with respect to search efficiency (Menezes and Kabamba, 2014) and it guarantees variance improvements for waste-recycled Monte Carlo estimators (Delmas and Jourdain, 2009). Further, a class of acceptance probabilities from Bédard (2008) has been of independent theoretical interest. We also introduce a new family of generalized Barker’s acceptance probabilities and present a Bernoulli factory for use in problems with intractable posteriors.

To the best of our knowledge, there are no theoretical and practical guidelines concerning optimal scaling outside of MH and its variants (although see Sherlock et al., 2021 for a discussion on delayed acceptance MH and Sherlock et al., 2015; Doucet et al., 2015; Schmon et al., 2021 for analyses pertaining to pseudo-marginal MCMC).

We obtain optimal scaling results for a large class of acceptance functions; Barker’s, Lazy-MH, and MH are members of this class.

We restrict our attention to the framework of Roberts et al. (1997) with a random walk Gaussian proposal kernel and a $d$-dimensional decomposable target distribution. Similar to MH, our general class of acceptance functions require the proposal variance to be scaled by $1/d$. We find that, typically, for lower acceptance functions, the optimal proposal variance is larger than the optimal proposal variance for MH, implying the need for larger jumps. For the Barker’s acceptance rule, the asymptotically optimal acceptance rate (AOAR) is approximately 0.158, in comparison to the 0.234 rate for MH (Roberts et al., 1997). Similar AOARs are presented for other acceptances.

In Section 2 we describe our class of acceptance probabilities with the main results
presented in Section 3. Asymptotically optimal acceptance rate for Barker’s and other functions are obtained in Section 3.1. In Section 4 we present numerical results under settings that both do and do not comply with our assumptions. A trailing discussion on the scaling factor for different acceptance functions and generalizations of our results is provided in the last section. All proofs are in the appendices.

2 Class of acceptance functions

Let \( \pi \) be the target distribution, with corresponding Lebesgue density \( \pi \) and support \( \mathcal{X} \) so that an MCMC algorithm aims to generate a \( \pi \)-ergodic Markov chain, \( \{X_n\} \). Let \( Q \) be a Markov kernel with an associated Lebesgue density \( q(x, \cdot) \) for each \( x \in \mathcal{X} \). We assume throughout that \( q \) is symmetric. Further, let the acceptance probability function be \( \alpha(x, y) : \mathcal{X} \times \mathcal{X} \to [0, 1] \). Starting from an \( X_0 \in \mathcal{X} \), at the \( n \)th step, a typical accept-reject MCMC algorithm proposes \( y \sim q(X_{n-1}, \cdot) \). The proposed value is accepted with probability \( \alpha(X_{n-1}, y) \), otherwise it is rejected, implying that \( X_n = X_{n-1} \). The acceptance function \( \alpha \) is responsible for guaranteeing \( \pi \)-reversibility and thus \( \pi \)-invariance of the Markov chain.

Let \( a \land b \) denote \( \min(a, b) \), and, \( s(x, y) = \pi(y)/\pi(x) \). We define \( \mathcal{A} \), the class of acceptance functions for which our optimal scaling results will hold, as follows:

**Definition 1.** Each \( \alpha \in \mathcal{A} \) is a map \( \alpha(x, y) : \mathcal{X} \times \mathcal{X} \to [0, 1] \) and for every \( \alpha \in \mathcal{A} \), there exists a balancing function, \( g_\alpha : [0, \infty) \to [0, 1] \), such that,

\[
\alpha(x, y) = g_\alpha(s(x, y)), \quad x, y \in \mathcal{X}, \tag{1}
\]

\[
g_\alpha(z) = zg_\alpha\left(\frac{1}{z}\right), \quad 0 \leq z < \infty, \tag{2}
\]

\[
g_\alpha(e^z), z \in \mathbb{R} \text{ is Lipschitz continuous.} \tag{3}
\]
Properties (1) and (2) are standard and easy to verify, with (1) ensuring intractable constants in $\pi$ cancel away and (2) ensuring $\pi$-reversibility. Property (3) is not required for $\alpha$ to be a valid acceptance function, however, we need it for our optimal scaling results (to establish Lemma 4) and holds true for all common acceptance probabilities. Moreover, each $\alpha \in A$ can be identified by the corresponding $g_\alpha$ and we will use $\alpha$ and $g_\alpha$ interchangeably.

If $g_{MH}$ denotes the balancing function for MH acceptance function ($\alpha_{MH}$), then,

$$g_{MH}(z) = 1 \land z, \quad z \geq 0.$$  \tag{4}

It is easy to see that $\alpha_{MH} \in A$. The Lazy-MH ($\alpha_L$) acceptance of Latuszyński and Roberts (2013); Herbei and Berliner (2014) also belongs to $A$. For a fixed $\epsilon \in [0, 1]$, it is defined using,

$$g_L(z) = (1 - \epsilon)(1 \land z), \quad z \geq 0.$$  \tag{5}

The Barker’s acceptance function is $\alpha_B(x, y) = g_B(s(x, y))$ for all $x, y \in X$ where,

$$g_B(z) = \frac{z}{1 + z}, \quad z \geq 0.$$  \tag{6}

Then, (2) follows immediately. For differentiable functions, property (3), i.e. Lipschitz continuity of $g_\alpha(e^z)$ can be verified by bounding the first derivative. In particular, we have $|g_\alpha'(e^z)| \leq 1$ for all $z \in \mathbb{R}$ and hence, $\alpha_B \in A$. Due to Peskun (1973), it is well known that in the context of Monte Carlo variability of ergodic averages, MH is superior to Barker’s. Even so, the Barker’s acceptance function has had a recent resurgence aided by its use in Bernoulli factory MCMC algorithms for Bayesian intractable posteriors where MH algorithms are not implementable.
We present a generalization of (6); for $r \geq 1$ define
\[ g^R_r(z) = \begin{cases} 
  z(z^r - 1)^r, & z \neq 1 \\
  z^{-1}, & z = 1.
\end{cases} 
\]

For $r \in \mathbb{N}$, the above can be rewritten as:
\[ g^R_r(z) = \frac{z + \cdots + z^r}{1 + z + \cdots + z^r}, \quad z \geq 0, \quad r \in \mathbb{N}. \tag{7} \]

If $\alpha^R_r$ is the associated acceptance function, then, $\alpha^R_r \in \mathcal{A}$ for all $r \geq 1$. Moreover, $g^R_1 \equiv g_B$ and $g^R_r \uparrow g_{M\overline{H}}$ as $r \to \infty$. For $r \in \mathbb{N}$, we present a natural Bernoulli factory in the spirit of Gonçalves et al. (2017b) that generates events of probability $\alpha^R_r$ without explicitly evaluating it; see Appendix D. An alternative approach would be to follow the general sampling algorithm of Morina et al. (2021) for rational functions.

Let $\Phi(\cdot)$ be the standard normal distribution function. For a theoretical exposition, Bédard (2008) defines the following acceptance probability for some $h > 0$:
\[ g^H_h(z) = \Phi\left(\frac{\log z - h/2}{\sqrt{h}}\right) + z \cdot \Phi\left(-\frac{\log z - h/2}{\sqrt{h}}\right), \quad z \geq 0. \tag{8} \]

For each $h > 0$, $\alpha^H_h \in \mathcal{A}$ and observe that as $h \to 0$, $g^H_h \to g_{M\overline{H}}$ and as $h \to \infty$, $g^H_h \to 0$, i.e. the chain never moves. Similar examples can be constructed by considering other well behaved distribution functions in place of $\Phi$. Lastly, it is easy to see that $\mathcal{A}$ is convex. Thus, it also includes situations when each update of the algorithm randomly chooses an acceptance probability. Moreover, as evidenced in (5), $\mathcal{A}$ is also closed under scalar multiplication as long as the resulting function lies in $[0, 1]$. 

6
3 Main theorem

Let \( f \) be a 1-dimensional density function and consider a sequence of target distributions \( \{ \pi_d \} \) such that for each \( d \), the joint density is

\[
\pi_d(x^d) = \prod_{i=1}^{d} f(x^d_i), \quad x^d = (x^d_1, \ldots, x^d_d)^T \in \mathbb{R}^d.
\]

**Assumption 1.** Density \( f \) is positive and in \( C^2 \)–the class of all real-valued functions with continuous second order derivatives. Further, \( f'/f \) is Lipschitz and the following moment conditions hold,

\[
\mathbb{E}_f \left[ \left( \frac{f'(X)}{f(X)} \right)^8 \right] < \infty, \quad \mathbb{E}_f \left[ \left( \frac{f''(X)}{f(X)} \right)^4 \right] < \infty. \tag{9}
\]

Consider the sequence of Gaussian proposal kernels \( \{ Q_d(x^d, \cdot) \} \) with associated density sequence \( \{ q_d \} \), so that \( Q_d(x^d, \cdot) = N(x^d, \sigma^2_d I_d) \) where for some constant \( l \in \mathbb{R}^+ \),

\[
\sigma^2_d = l^2/(d-1).
\]

The proposal \( Q_d \) is used to generate a \( d \)--dimensional Markov chain, \( X^d = \{ X^d_n, n \geq 0 \} \), following the accept-reject mechanism with acceptance function \( \alpha \). Under these conditions and with \( \alpha = \alpha_{\text{MH}}, \) Roberts et al. (1997) established weak convergence to an appropriate Langevin diffusion for the sequence of 1-dimensional stochastic processes, constructed from the first component of these Markov chains. Since the coordinates are independent and identically distributed, this limit informs the limiting behaviour of the full Markov chain in high-dimensions. In what follows, we extend their results to the class of acceptance functions, \( \mathcal{A} \), as defined in Definition.

Let \( \{ Z^d, d > 1 \} \) be a sequence of processes constructed by speeding up the Markov
chains by a factor of $d$ as follows,

$$Z^d_t = X^d_{[dt]} = (X^d_{[dt],1}, X^d_{[dt],2}, \ldots, X^d_{[dt],d})^T; \quad t > 0.$$  

Suppose $\{\eta_d : \mathbb{R}^d \to \mathbb{R}\}$ is a sequence of projection maps such that $\eta_d(x^d) = x^d_1$. Define a new sequence of 1-dimensional processes $\{U^d, d > 1\}$ as follows,

$$U^d_t := \eta_d \circ Z^d_t = X^d_{[dt],1}; \quad t > 0.$$ 

Under stationarity, we show that $\{U^d, d > 1\}$ weakly converges (in the Skorokhod topology, see Ethier and Kurtz, 1986) to a Markovian limit $U$. We denote weak convergence of processes in the Skorokhod topology by “⇒” and standard Brownian motion at time $t$ by $B_t$. The proofs are in the appendices.

**Theorem 1.** Let $\{X^d, d \geq 1\}$ be the sequence of $\pi_d$-invariant Markov chains constructed using acceptance function $\alpha$ and proposal $Q_d$ such that $X^d_0 \sim \pi_d$. Further, suppose $\alpha \in \mathcal{A}$ and $\pi_d$ satisfies Assumption [2]. Then, $U^d \Rightarrow U$, where $U$ is a diffusion process that satisfies the Langevin stochastic differential equation,

$$dU_t = (h_\alpha(l))^{1/2} dB_t + h_\alpha(l) \frac{f'(U_t)}{2f(U_t)} dt,$$

with $h_\alpha(l) = l^2 M_\alpha(l)$, where,

$$M_\alpha(l) = \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 I}} \exp \left\{ -\frac{(b + l^2 I/2)^2}{2l^2 I} \right\} \, db,$$  

and,

$$I = \mathbb{E}_f \left[ \left( \frac{f'(X)}{f(X)} \right)^2 \right].$$
Remark 1. Since $\alpha_{\text{MH}} \in A$, our result aligns with Roberts et al. (1997) since

$$M_{\text{MH}}(l) = \int_{\mathbb{R}} g_{\text{MH}}(e^b) \frac{1}{\sqrt{2\pi l^2 I}} \exp \left\{ -\frac{(b + l^2 I/2)^2}{2l^2 I} \right\} \, db = 2\Phi \left( -\frac{l\sqrt{I}}{2} \right).$$

Remark 2. For symmetric proposals, Definition 1 requires $\alpha$ to be a function of only the ratio of the target densities at the two contested points. Thus, the result is not applicable to acceptances in Mira (2001); Banterle et al. (2019); Vats et al. (2021).

In Theorem 1, $h_\alpha(l)$ is the speed measure of the limiting diffusion process and so the optimal choice of $l$ is $l^*$ such that

$$l^* = \arg \max_l h_\alpha(l).$$

Denote the average acceptance probability by

$$\alpha_d(l) := \mathbb{E}_{\pi_d, Q_d} \left[ \alpha(X^d, Y^d) \right] = \int \int \pi(x^d) \alpha(x^d, y^d) q_d(x^d, y^d) \, dx^d \, dy^d,$$

and the asymptotic acceptance probability as $\alpha(l) := \lim_{d \to \infty} \alpha_d(l)$. The dependence on $l$ is through the variance of proposal kernel. We then have the following corollary.

Corollary 1. Under the setting of Theorem 1, we obtain $\alpha(l) = M_\alpha(l)$ and the asymptotically optimal acceptance probability is $M_\alpha(l^*)$.

Corollary 1 is of considerable practical relevance since for different acceptance functions it yields the optimal target acceptance probability to tune to.
3.1 Optimal results for some acceptance functions

In Section 2, we discussed some important members of the class \( \mathcal{A} \). Corollary 1 can then be used to obtain the AOAR for them by maximizing the speed measure of the limiting diffusion process. For Barker’s algorithm, from Theorem 1 and (6), the speed measure \( h_B(l) \) of the corresponding limiting process is

\[
M_B(l) = \int_{\mathbb{R}} \frac{1}{1 + e^{-b}} \frac{1}{\sqrt{2\pi l^2 I}} \exp \left\{ -\frac{(b + \frac{l^2 I}{2})^2}{2l^2 I} \right\} \, db.
\]

Maximizing \( h_B(l) \), the optimal value, \( l^* \), is approximately (see Appendix C),

\[
l^* = \frac{2.46}{\sqrt{I}}.
\]

By Corollary 1 using this \( l^* \) yields an asymptotic acceptance rate of approximately 0.158. Hence, when the optimal variance is not analytically tractable in high dimensions, one may consider tuning their algorithm so as to achieve an acceptance probability of approximately 0.158. Additionally, the right plot in Figure 1 verifies that the relative efficiency of Barker’s versus MH, as measured by the ratio of their respective speed measures for a fixed \( l \), remains above 0.5 (see Theorem 4 in Latuszyński and Roberts, 2013); this relative efficiency increases as \( l \) increases. Ad-
ditionally, the ratio of the speed measures of Barker’s versus MH at their respective optimal scalings is 0.72. This quantifies the loss in efficiency in running the best version of Barker’s compared to the best version of MH algorithm. We can also study the respective speed measures as a function of the acceptance rate; this is given in the left plot in Figure 1. We find that as the asymptotic acceptance rate increases, the speed measure for Barker’s decreases more rapidly than MH. This suggests that there is much to gain by appropriately tuning the Barker’s algorithm.

\[ \text{Figure 2: Optimal acceptance rate against number of dimensions.} \]

For lower dimensions, the optimal acceptance rate is higher than the AOAR. Figure 2 shows optimal values for MH and Barker’s algorithms on isotropic Gaussian targets in dimensions 1 to 10; proposal kernel being the same as in the setting of Theorem 1. This plot is produced using the criterion of minimizing first order auto-correlations in each component \cite{Gelman1996, Roberts1998}. For \( \alpha_{\text{MH}} \) and \( \alpha_{\text{B}} \), the optimal acceptance rate in one dimension is 0.43 and 0.27 respectively. For Lazy-MH with \( \epsilon \in [0, 1] \), Corollary \cite{Lee2011} implies that the AOAR of the algorithm is \((1 - \epsilon)0.234\) with the same optimal \( l^* \) as MH. For the acceptance functions, \( \alpha_h^H \) in \cite{Lee2011},

\[ M_h(l) = 2\Phi \left( -\frac{\sqrt{h + l^2I}}{2} \right). \]
With $h = 0$, we obtain the result of [Roberts et al. (1997)] for MH. Further, the left plot of Figure 3 highlights that as $h \to 0$, the AOAR increases to 0.234 and the algorithm worsens as $h$ increases. Moreover, for $h \approx 1.913$, the AOAR is roughly 0.158, i.e. equivalent to the Barker’s acceptance function.

![Figure 3: Optimal acceptance rates for $\alpha_H^h$ against $h$ (left) and $\alpha_R^r$ against $r$ (right).]

Lastly, the AOARs for $\alpha_R^r$ in (7) are available. For $r = 1, \ldots, 10$, the results have been plotted in the right plot of Figure 3. As anticipated, the AOAR approaches 0.234 as $r$ increases. Notice that $\alpha_2^R$ yields an AOAR of 0.197, which is a considerable increase from $\alpha_B^R = \alpha_1^R$. Table 1 below summarizes the results of this section.\footnote{Codes for all plots and tables are available at https://github.com/Sanket-Ag/BarkerScaling}

| $M_q(l^*)$ | $\alpha_{MH}$ | $\alpha_1^H$ | $\alpha_{1.913}^H$ | $\alpha_5^H$ | $\alpha_{10}^R$ | $\alpha_5^R$ | $\alpha_2^R$ | $\alpha_B^R$ |
|----------|---------------|--------------|--------------------|--------------|----------------|--------------|--------------|---------------|
| 0.234    | 0.189         | 0.158        | 0.129              | 0.229        | 0.223          | 0.197        | 0.158        |
| $|l^*\sqrt{T}|$ | 2.38          | 2.43          | 2.46               | 2.49         | 2.39           | 2.39         | 2.42         | 2.46          |

Table 1: Optimal proposal variance and asymptotic acceptance rates.

4 Numerical results

We study the estimation quality for different expectations as a function of the proposal variance (acceptance rate) for the generalized Barker’s acceptance function,
\(\alpha^R\). We focus on \(r = 1\) (Barker’s algorithm) and \(r = 2\). Suppose \(f : \mathbb{R}^d \to \mathbb{R}\) is the function whose expectation with respect to \(\pi_d\) is of interest. Let \(\{f(X_n)\}\) be the mapped process. Similar to Roberts and Rosenthal (2001), we assess choice of proposal variance by the convergence time:

\[
\text{convergence time} := -\frac{k}{\log(\rho_k)}
\]

where \(\rho_k\) is the lag-\(k\) autocorrelation in \(\{f(X_n)\}\). In each of the following simulations, convergence time is estimated by averaging over \(10^3\) replications of Markov chains, each of length \(10^6\) with \(k = 1\). We chose a range of values of \(l\) where \(l\) is such that \(\sigma_d^2 = l^2/d\) in a Gaussian proposal kernel \(Q_d(x^d, \cdot) = N(x^d, \sigma_d^2 I_d)\).

Consider first the case of an isotropic target, \(\pi_d = N_d(0, I_d)\) with isotropic Gaussian proposals; the conditions of Theorem 1 are satisfied. The estimated convergence time for \(f(x) = x_1\) and \(f(x) = \bar{x}\) where \(\bar{x}\) is the mean of all components, \(x_1, \ldots, x_d\), is plotted in Figure 4 (top row). Here, \(d = 50\). For both functions of interest, the optimal performance i.e. the minimum convergence time, corresponds to an acceptance rate of approximately 0.158 for \(\alpha^B\) and 0.197 for \(\alpha^R_2\); the slight overestimation is due to the finite dimensional setting.

Next, we consider \(\pi_d = N_d(0, \Sigma_d)\) where \(\Sigma_d\) is a \(d \times d\) matrix with 1 on its diagonal and all other elements are equal to some non-zero \(\rho\). Here, the assumptions in Theorem 1 are not satisfied. For such a target and for \(\alpha_{\text{MH}}\), Roberts and Rosenthal (2001) showed that the rate of convergence of the algorithm is governed by the eigenvalues of \(\Sigma_d\). In particular, the eigenvalues of \(\Sigma_d\) are \(dp + 1 - \rho\) and \(1 - \rho\) with associated eigenvectors \(\bar{x}\) and \(x_i - \bar{x} (i = 1, \ldots, d)\), respectively. Then, it was shown that the algorithm converges quickly for functions orthogonal to \(\bar{x}\), but much more slowly for \(\bar{x}\). Despite the differing rates of convergence, the optimal acceptance rate, corresponding to the minimum convergence time, remains the same. We find this to
Figure 4: Convergence times for $\alpha_B$ against acceptance rate in the isotropic setting (top row) and the correlated target setting (bottom row).

be also true for $\alpha_B$ and $\alpha^R_2$ as illustrated in Figure 4 (bottom row) where we present convergence times for $x_1 - \bar{x}$ and $\bar{x}$. Once again, $d = 50$. The large difference between convergence times for both is quite evident from the $y$-axis of the two plots. The minimum again lies in a region around the asymptotic optimal. We note that due to the slow convergence rate of $\bar{x}$, the process demonstrates slow mixing, yielding more variable estimates of the convergence time. For both simulation settings, we see the expected improvement in the convergence time for $\alpha^R_2$ compared to $\alpha_B$.

4.1 A Bayesian logistic regression example

We consider fitting a Bayesian logistic regression model to the famous Titanic dataset which contains information on crew and passengers aboard the 1912 RMS Titanic ship. Let $y$ denote the response vector (whether they survived or not) and $X$ denote the $n \times d$ model matrix; here $d = 10$. We assume a multivariate zero-mean Gaussian
prior on $\beta$ with covariance $100I_{10}$. The resulting target density is

$$
\pi(\beta \mid y) \propto \exp \left\{ \frac{-\beta^T \beta}{2} \prod_{i=1}^{n} \frac{\exp(-x_i^T \beta)^{1-y_i}}{1 + \exp(-x_i^T \beta)} \right\}.
$$

For the Titanic dataset, the resulting posterior has a complicated covariance structure with many components exhibiting an absolute mutual correlation of beyond .50. The posterior is also ill-conditioned with the condition number of the estimated target covariance matrix being $\approx 10^5$. As seen in the bottom row of Figure 4, in such situations an isotropic proposal kernel might perform poorly for most functions. We instead consider a Gaussian proposal scheme where the proposal covariance matrix is taken to be proportional to the target covariance matrix. This is a common strategy for dealing with targets with correlated components and forms the basis for many adaptive MCMC kernels (Roberts and Rosenthal, 2009). We implement the Barker’s algorithm to sample from the posterior. Let $\Sigma_d$ denote the covariance matrix associated with the posterior distribution of $\beta$, then the proposal kernel $Q_d(x^d, \cdot) = N(x^d, \sigma_d^2 \Sigma_d)$. Since $\Sigma_d$ is unavailable, we estimate it from a pilot MCMC run of size $10^7$. We then consider various values of $\sigma_d^2 = l^2/d$.

The performance of the algorithm for different functions of interest is plotted in Figure 5. Since this is a 10-dimensional problem, the optimal acceptance rate from Figure 2 is approximately 0.18. The convergence times for both, $\beta_1 - \bar{\beta}$ and $\bar{\beta}$, are similar. Further, both are minimized at approximately the same acceptance rate of 0.18. It is natural here to be interested in estimating the posterior mean vector. Thus, we also study the properties of vector $\beta$ with efficiency measured via the multivariate effective sample size (ESS) (Vats et al., 2019). The ESS returns the equivalent number of iid samples from $\pi$ that would yield the same variability in estimating the posterior mean as the given set of MCMC samples. In Figure 5, we see that the optimal acceptance rate corresponding to the highest ESS values is
achieved around 0.18.

Figure 5: Convergence times for $\alpha_B$ (left and middle) and multivariate ESS for the posterior mean vector (right) against acceptance rate.

5 Conclusions

We obtain optimal scaling and acceptance rates for a large class of acceptance functions. In doing so, we found that the scaling factor of $1/d$ for the proposal variance holds for all acceptance functions, indicating that the acceptance functions are not likely to affect the rate of convergence, just the constants associated with that rate. Thus, practitioners need not hesitate in switching to other acceptance functions when the MH acceptance probability is not tractable, as long as Corollary 1 is used to tune their algorithm accordingly. There is also an inverse relationship between optimal variance and AOAR (see Table 1) implying that when dealing with sub-optimal acceptance functions, the algorithm seeks larger jumps. The computational cost of the Bernoulli factory we present for $\alpha^R_r$ in Appendix D increases with $r$. Given the large jump in the optimal acceptance probability from $r = 1$ to $r = 2$, the development of more efficient Bernoulli factories is an important problem for future work.

The assumption of starting from stationarity is a restrictive one. For MH with Gaussian proposals, the scaling factor of $1/d$ is still optimal when the algorithm is in the transient phase [Christensen et al. 2005, Jourdain et al. 2014, Kuntz et al.].
The optimal acceptance probability may vary depending on the starting distribution. We envision similar results are viable for the general class of acceptance functions, and this is important future work. Our results are limited to only Gaussian proposals and trivially decomposable target densities. Other proposal distributions may make use of the gradient of the target e.g. Metropolis-adjusted Langevin algorithm (Roberts and Tweedie, 1996) and Hamiltonian Monte Carlo (Duane et al., 1987). In problems where $\alpha_{\text{MH}}$ cannot be used, the gradient of the target density is likely unavailable, thus limiting our attention to a Gaussian proposal is reasonable. On the other hand, generalizations to other target distributions is important. For MH algorithms, Bédard (2008); Sherlock and Roberts (2009) relax the independence assumption, while Roberts and Rosenthal (2001) relax the identically distributed assumption. Additionally, Yang et al. (2020) present a proof of weak convergence for MH for more general targets, and Schmon and Gagnon (2021) provide optimal scaling results for general Bayesian targets using large-sample asymptotics. In these situations, extensions to other acceptance probabilities are similarly possible. Additionally, we encourage future work in optimal scaling to leverage our proof technique to demonstrate results for the wider class of acceptance probabilities.

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A Proof of Theorem 1

The proof is structurally similar to the seminal work of Roberts et al. (1997), in that we will show that the generator of the sped-up process, $Z^d$, converges to the generator of an appropriate Langevin diffusion. Define the discrete-time generator of $Z^d$ as,

$$G_d V(x^d) = d \cdot \mathbb{E}_{Y^d} \left[ (V(Y^d) - V(x^d)) \alpha(x^d, Y^d) \right], \quad (11)$$

for all those $V$ for which the limit exists. Since, interest is in the first component of $Z^d$, we consider only those $V$ which are functions of the first component only. Now, define the generator of the limiting Langevin diffusion process with speed measure $h_\alpha(l)$ as,

$$GV(x) = h_\alpha(l) \left[ \frac{1}{2} V''(x) + \frac{1}{2} \frac{d}{dx} (\log f)(x) V'(x) \right]. \quad (12)$$

The unique challenge in our result is identifying the speed measure $h_\alpha(l)$ for a general acceptance function $\alpha \in \mathcal{A}$. Proposition 1 is a key result that helps us obtain a form of $h_\alpha(l)$ without resorting to approximations.

To prove Theorem 1 we will show that there are events $F_d \subseteq \mathbb{R}^d$ such that for all $t$,

$$\mathbb{P}[Z^d_s \in F_d, \ 0 \leq s \leq t] \to 1 \text{ as } d \to \infty \quad \text{and}$$

$$\lim_{d \to \infty} \sup_{x^d \in F_d} |G_d V(x^d) - GV(x^d_1)| = 0,$$

for a suitably large class of real-valued functions $V$. Moreover, due to conditions of Lipschitz continuity on $f'/f$, a core for the generator $G$ has domain $C^\infty_c$, the class of infinitely differentiable functions with compact support (Ethier and Kurtz 1986, Theorem 2.1, Chapter 8). Thus, we can limit our attention to only those $V \in C^\infty_c$ that are a function of the first component.

Consider now the setup of Theorem 1. Let $w = \log f$ and $\alpha \in \mathcal{A}$ with the balancing
function \( g_\alpha \). Let \( w' \) and \( w'' \) be the first and second derivatives of \( w \) respectively. Define the sequence of sets \( \{ F_d \subseteq \mathbb{R}^d, d > 1 \} \) by,

\[
F_d = \{ |R_d(x_2, \ldots, x_d) - I| < d^{-1/8} \} \cap \{ |S_d(x_2, \ldots, x_d) - I| < d^{-1/8} \}
\]

where,

\[
R_d(x_2, \ldots, x_d) = \frac{1}{d-1} \sum_{i=2}^{d} [\log(f(x_i))]^2 = \frac{1}{d-1} \sum_{i=2}^{d} [w'(x_i)]^2
\]

and

\[
S_d(x_2, \ldots, x_d) = -\frac{1}{d-1} \sum_{i=2}^{d} [\log(f(x_i))]'' = -\frac{1}{d-1} \sum_{i=2}^{d} [w''(x_i)].
\]

The following results from Roberts et al. (1997) will be needed.

**Lemma 1** (Roberts et al. (1997)). Let Assumption 1 hold. If \( X_0^d \sim \pi_d \) for all \( d \), then, for a fixed \( t \), \( \mathbb{P}[Z_s^d \in F_d, 0 \leq s \leq t] \to 1 \) as \( d \to \infty \).

**Lemma 2** (Roberts et al. (1997)). Let Assumption 2 hold. Also, let

\[
W_d(x_1, \ldots, x_d) = \sum_{i=2}^{d} \left( \frac{1}{2} w''(x_i)(Y_i - x_i)^2 + \frac{l^2}{2(d-1)} w'(x_i)^2 \right),
\]

where \( Y_i \sim N(x_i, \sigma_d^2) \), \( i = 2, \ldots, d \). Then, \( \sup_{x^d \in F_d} \mathbb{E} |W_d(x^d)| \to 0 \).

**Lemma 3** (Roberts et al. (1997)). For \( Y \sim N(x, \sigma_d^2) \) and \( V \in C_c^\infty \),

\[
\limsup_{d \to \infty} \sup_{x \in \mathbb{R}} d \mathbb{E}[|V(Y) - V(x)|] < \infty.
\]

For the following proposition, we will utilize the property (2) imposed on \( A \). This proposition is the key to obtaining our main result in such generality.

**Proposition 1.** Let \( X \sim N(-\theta/2, \theta) \) for some \( \theta > 0 \). Let \( \alpha \in A \) with the corresponding balancing function \( g_\alpha \). Then \( \mathbb{E} [Xg_\alpha(e^X)] = 0. \)
Proof. We have,

\[ |E[Xg_\alpha(e^X)]| \leq E[|Xg_\alpha(e^X)|] \leq E[|X|] < \infty; \]

the second inequality follows from the assumption that \( g_\alpha \) lies in \([0,1]\). Hence, the expectation exists and is equal to the integral,

\[ \int_{\mathbb{R}} xg_\alpha(e^x) \frac{1}{\sqrt{2\pi\theta}} \exp \left\{ \frac{-(x+\theta/2)^2}{2\theta} \right\} \, dx =: \int_{\mathbb{R}} h(x)\,dx. \]

Observe that, using (2),

\[ h(-x) = -xg_\alpha(e^{-x}) \frac{1}{\sqrt{2\pi\theta}} \exp \left\{ \frac{-(x+\theta/2)^2}{2\theta} \right\} \]

\[ = -xg_\alpha(e^{-x}) \frac{1}{\sqrt{2\pi\theta}} \exp \left\{ \frac{-1}{2\theta} \left( x^2 + \frac{\theta^2}{4} - x\theta \right) \right\} \]

\[ = -xe^{-x}g_\alpha(e^x) \frac{1}{\sqrt{2\pi\theta}} \exp \left\{ \frac{-1}{2\theta} \left( x^2 + \frac{\theta^2}{4} - x\theta \right) \right\} \]

\[ = -xg_\alpha(e^x) \frac{1}{\sqrt{2\pi\theta}} \exp \left\{ \frac{-1}{2\theta} \left( x^2 + \frac{\theta^2}{4} + x\theta \right) \right\} \]

\[ = -xg_\alpha(e^x) \frac{1}{\sqrt{2\pi\theta}} \exp \left\{ \frac{-(x+\theta/2)^2}{2\theta} \right\} \]

\[ = -h(x). \]

Hence, the result follows. \( \square \)

Lemma 4. Suppose \( V \in C^\infty_c \) is restricted to only the first component of \( \mathbb{Z}^d \). Then,

\[ \sup_{x^d \in F_d} |G_dV(x^d) - GV(x^d)| \to 0 \text{ as } d \to \infty. \]

Proof. In the expression for \( G_dV(x^d) \) given in (11), we can decompose the proposal
\( Y^d \) into \((Y_1^d, Y^{d-})\) and thus rewrite the expectation as follows,

\[
G_dV(x^d) = dE_{Y_1^d} \left[ (V(Y_1^d) - V(x_1^d)) \mathbb{E}_{Y^d} \left[ \alpha(x^d, Y^d) \mid Y_1^d \right] \right]. \tag{13}
\]

Let \( E_{d,\alpha} \) denote the inner expectation in (13) and define \( E_{d,\alpha}^{\text{lim}} \) as,

\[
E_{d,\alpha}^{\text{lim}} = E_{Y^d} \left[ g_{\alpha} \left( \exp \left\{ \log \frac{f(Y_1^d)}{f(x_1^d)} + \sum_{i=2}^d \left( w'(x_i^d)(Y_i^d - x_i^d) - \frac{l^2 w'(x_i^d)^2}{2(d-1)} \right) \right\} \right] \bigg| Y_1^d \right]. \tag{14}
\]

Also, a Taylor series expansion of \( w \) about \( x_i^d \) for \( i = 2, \ldots, d \) gives,

\[
E_{d,\alpha} = E_{Y^d} \left[ g_{\alpha} \left( \exp \left\{ \log \frac{f(Y_i^d)}{f(x_i^d)} + \sum_{i=2}^d \left( w'(x_i^d)(Y_i^d - x_i^d) + \frac{1}{2} w''(x_i^d)(Y_i^d - x_i^d)^2 + \frac{1}{6} w'''(Z_i)(Y_i^d - x_i^d)^3 \right) \right\} \right] \bigg| Y_i^d \right]
\]

for \( Z_i \) lying between \( x_i^d \) and \( Y_i^d \). Hence, the triangle inequality and Lipschitz continuity of \( g(e^z) \) gives, for some Lipschitz constant \( K < \infty \),

\[
|E_{d,\alpha} - E_{d,\alpha}^{\text{lim}}| \leq K E_{Y^d} \left[ \sum_{i=2}^d \frac{1}{2} w''(x_i^d)(Y_i^d - x_i^d)^2 + \frac{1}{6} w'''(Z_i)(Y_i^d - x_i^d)^3 + \frac{l^2 w'(x_i^d)^2}{2(d-1)} \right] \leq K E_{Y^d} \left[ |W_d(x^d)| \right] + K \sup_{z \in \mathbb{R}} |w'''(z)| \frac{l^3}{(d-1)^{1/2}}, \tag{15}
\]

where \( W_d(x^d) \) is as defined in Lemma 2. From Lemma 2, Lemma 3 and (15),

\[
\sup_{x^d \in F_d} \left| G_dV(x^d) - dE_{Y_1^d} \left[ (V(Y_1^d) - V(x_1^d)) E_{d,\alpha}^{\text{lim}} \right] \right| \to 0 \text{ as } d \to \infty. \tag{16}
\]

Now let \( \epsilon(y) = \log f(y) - \log f(x_1^d) \). Also from (14), it is clear that given \( x^d \), \( E_{d,\alpha}^{\text{lim}} \) is a function of \( Y_1^d \) alone, to wit,

\[
(M_{d,\alpha} \circ \epsilon)(Y_1^d) := E_{d,\alpha}^{\text{lim}} = E \left[ g_{\alpha}(e^{B_d}) \right], \tag{17}
\]
where \( B_d \sim N(\mu_d, \Sigma_d) \) with \( \mu_d = \epsilon(Y_1^d - l^2 R_d/2) \) and \( \Sigma_d = l^2 R_d \). Thus by (15), it is enough to consider the asymptotic behaviour of,

\[
d\mathbb{E}_{Y_1^d} \left[ (V(Y_1^d) - V(x_1^d)) M_{d,\alpha}(\epsilon(Y_1^d)) \right].
\]

Let \( N_{d,\alpha} = M_{d,\alpha} \circ \epsilon \) and apply Taylor series expansion on the inner term to obtain,

\[
(V(Y_1^d) - V(x_1^d)) M_{d,\alpha}(\epsilon(Y_1^d))
= \left( V'(x_1^d)(Y_1^d - x_1^d) + \frac{1}{2} V''(x_1^d)(Y_1^d - x_1^d)^2 + \frac{1}{6} V'''(K_d)(Y_1^d - x_1^d)^3 \right)
\times \left( N_{d,\alpha}(x_1^d) + N'_{d,\alpha}(x_1^d)(Y_1^d - x_1^d) + \frac{1}{2} N''_{d,\alpha}(L_d)(Y_1^d - x_1^d)^2 \right)
\]

where \( K_d, L_d \in [Y_1^d, x_1^d] \) or \([x_1^d, Y_1^d]\) and,

\[
N_{d,\alpha}(x_1^d) = M_{d,\alpha}(\epsilon(x_1^d)) = M_{d,\alpha} \left( \log \frac{f(x_1^d)}{f(x_1^d)} \right) = M_{d,\alpha}(0)
\]

(18)

\[
N'_{d,\alpha}(x_1^d) = M'_{d,\alpha}(\epsilon(x_1^d)) \epsilon'(x_1^d) = M'_{d,\alpha}(0) \epsilon'(x_1^d).
\]

Now, for all \( d \),

\[
M_{d,\alpha}(\epsilon) = \mathbb{E} \left[ g_\alpha(e^{B_d}) \right] = \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \exp \left\{ \frac{-(b - \epsilon + l^2 R_d/2)^2}{2l^2 R_d} \right\} db.
\]

So, \( M_{d,\alpha}(0) = \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \exp \left\{ \frac{-(b + l^2 R_d/2)^2}{2l^2 R_d} \right\} db.\)

Also, \( M'_{d,\alpha}(\epsilon) = \frac{d}{d\epsilon} \left( \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \exp \left\{ \frac{-(b - \epsilon + l^2 R_d/2)^2}{2l^2 R_d} \right\} db. \right). \)

Derivatives and integral are exchanged due to the dominated convergence theorem. So,

\[
M'_{d,\alpha}(\epsilon) = \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \left( \frac{2(b - \epsilon + l^2 R_d/2)}{2l^2 R_d} \right) \exp \left\{ \frac{-(b - \epsilon + l^2 R_d/2)^2}{2l^2 R_d} \right\} db.
\]
So, $M'_{d,\alpha}(0) = \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \left( \frac{(b + l^2 R_d/2)}{l^2 R_d} \right) \exp \left\{ \frac{-(b + l^2 R_d/2)^2}{2 l^2 R_d} \right\} \, db$

$$= \frac{1}{l^2 R_d} \int_{\mathbb{R}} b g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \exp \left\{ \frac{-(b + l^2 R_d/2)^2}{2 l^2 R_d} \right\} \, db$$

$$+ \frac{1}{2} \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \exp \left\{ \frac{-(b + l^2 R_d/2)^2}{2 l^2 R_d} \right\} \, db$$

$$= \frac{1}{2} M_{d,\alpha}(0),$$

where the first term vanishes due to Proposition 1. Hence, for all $d$,

$$2M'_{d,\alpha}(0) = M_{d,\alpha}(0) = \int_{\mathbb{R}} g_\alpha(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \exp \left\{ \frac{-(b + l^2 R_d/2)^2}{2 l^2 R_d} \right\} \, db. \quad (19)$$

Now, we plug the expressions obtained above into the Taylor series expansion of $(V(Y^d_1) - V(x^d_1)) M_{d,\alpha}(e(Y^d_1))$. The rest of the proof, with the help of Assumption 1, follows similarly as in Lemma 2.6, Roberts et al. (1997).

Proof of Theorem 1. From Lemma 4, we have uniform convergence of generators on the sequence of sets with limiting probability 1. And so by Corollary 8.7, Chapter 4 of Ethier and Kurtz (1986), we have the required result of weak convergence (the condition that $C^\infty_c$ separates points was verified by Roberts et al. 1997).

Proof of Corollary. Let $E^{d,\alpha}$ be the inner expectation in (13) and $E^{d,\alpha}_{lim}$ be from (14). Then,

$$\mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y^d_1} \left[ E^{d,\alpha} - E^{d,\alpha}_{lim} \, \bigg| \, x^d \right] \right] \to 0 \quad \text{as } d \to \infty.$$

Proof. Consider,

$$\left| \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y^d_1} \left[ E^{d,\alpha} - E^{d,\alpha}_{lim} \, \bigg| \, x^d \right] \right] \right| \leq \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y^d_1} \left[ E^{d,\alpha} - E^{d,\alpha}_{lim} \, \bigg| \, x^d \in F_d \right] \right] P(x^d \in F_d)$$
\[
\begin{align*}
&+ \left| \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y_1} \left[ E_{d,\alpha}^d - E_{lim}^{d,\alpha} \, \big| \, x^d \in F^C_d \right] \right] \right| P(x^d \in F^C_d) \right|.
\end{align*}
\]

Second term goes to 0 since the expectation is bounded and by construction \( P(x^d \in F^C_d) \to 0 \) as \( d \to \infty \). Also, following [Roberts et al. (1997)],

\[
\sup_{x^d \in F_d} |E_{d,\alpha}^d - E_{lim}^{d,\alpha}| \to 0 \text{ as } d \to \infty.
\]

Then,

\[
\left| \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y_1} \left[ E_{d,\alpha}^d - E_{lim}^{d,\alpha} \, \big| \, x^d \in F_d \right] \right] \right| P(x^d \in F_d) \right| \\
\leq \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y_1} \left[ \sup_{x^d \in F_d} |E_{d,\alpha}^d - E_{lim}^{d,\alpha}| \, \big| \, x^d \in F_d \right] \right] \to 0.
\]

\[
\square
\]

**Proof of Corollary 1.** Consider equation (17). Using Taylor series approximation of second order around \( x_1 \),

\[
\mathbb{E}_{Y_1}[E_{lim}^{d,\alpha}] = \mathbb{E}[N_{d,\alpha}(Y_1^d)] = N_{d,\alpha}(x_1^d) + \frac{1}{2} N''_{d,\alpha}(W_{d,1}) \frac{l^2}{d-1}.
\]

where \( W_{d,1} \in [x_1^d, Y_1^d] \) or \([Y_1^d, x_1^d]\). Since \( N'' \) is bounded (Roberts et al., 1997),

\[
\alpha(l) = \lim_{d \to \infty} \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y_1^d} \left[ \mathbb{E}_{Y_1^d} \left[ \alpha(X^d, Y^d) \, \big| \, Y_1^d, x^d \right] \, \big| \, X^d \right] \right]
\]

\[
= \lim_{d \to \infty} \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y_1^d} \left[ E_{lim}^{d,\alpha} + E_{lim}^{d,\alpha} - E_{lim}^{d,\alpha} \, \big| \, x^d \right] \right]
\]

As all expectations exist, we can split the inner expectation and use Lemma 5 so that

\[
\alpha(l) = \lim_{d \to \infty} \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y_1^d} \left[ E_{lim}^{d,\alpha} \, \big| \, x^d \right] \right] + \lim_{d \to \infty} \mathbb{E}_{\pi_d} \left[ \mathbb{E}_{Y_1^d} \left[ E_{lim}^{d,\alpha} - E_{lim}^{d,\alpha} \, \big| \, x^d \right] \right]
\]

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\[
\begin{align*}
&= \lim_{d \to \infty} \mathbb{E}_{\pi, d} \left[ M_{d, \alpha}(0) + \frac{1}{2} N''_{d, \alpha}(W_{d, 1}) \frac{l^2}{d - 1} \right] \\
&= \lim_{d \to \infty} \mathbb{E}_{\pi, d} \left[ \int_{\mathbb{R}} g_{\alpha}(e^b) \frac{1}{\sqrt{2\pi l^2 R_d}} \exp \left\{ -\frac{(b + l^2 R_d/2)^2}{2l^2 R_d} \right\} db \right] \\
&= \int_{\mathbb{R}} g_{\alpha}(e^b) \frac{1}{\sqrt{2\pi l^2 I}} \exp \left\{ -\frac{(b + l^2 I/2)^2}{2l^2 I} \right\} db = M_{\alpha}(l).
\end{align*}
\]

The last equality is by the law of large numbers and continuous mapping theorem. \(\square\)

C Optimizing speed for Barker’s acceptance

We need to maximise \(h_B(l) = l^2 M_B(l)\). Let \(I\) be fixed arbitrarily.

\[
h_B(l) = \frac{1}{I} \cdot l^2 I \cdot \int_{\mathbb{R}} \frac{1}{1 + e^{-b}} \frac{1}{\sqrt{2\pi l^2 I}} \exp \left\{ -\frac{(b + l^2 I/2)^2}{2l^2 I} \right\} db.
\]

For a fixed \(I\), we can reparametrize the function by taking \(\theta = l^2 I\) and so maximizing \(h_B(l)\) over positive \(l\) will be equivalent to maximizing \(h_B^1(\theta)\) over positive \(\theta\) where,

\[
h_B^1(\theta) = \int_{\mathbb{R}} \frac{\theta}{1 + e^{-b}} \frac{1}{\sqrt{2\pi \theta}} \exp \left\{ -\frac{(b + \theta/2)^2}{2\theta} \right\} db.
\]

We make the substitution \(z = (b + \theta/2)/\sqrt{\theta}\) in the integrand to obtain

\[
h_B^1(\theta) = \int_{\mathbb{R}} \frac{\theta}{1 + \exp\{-z\sqrt{\theta} + \theta/2\}} \frac{1}{\sqrt{2\pi}} e^{-z^2/2} dz = \mathbb{E} \left[ \frac{\theta}{1 + \exp\{-Z\sqrt{\theta} + \theta/2\}} \right],
\]

where the expectation is taken with respect to \(Z \sim N(0, 1)\). This expectation however is not available in closed form. However standard numerical integration routines yield the optimal value of \(\theta\) to be 6.028. This implies that the optimal value of \(l\), say \(l^*\), is approximately equal to,

\[ l^* \approx \frac{2.46}{\sqrt{I}} \text{ (up to 2 decimal places)} \]
Using this $l^*$ yields an asymptotically optimal acceptance rate of approximately 0.158.

D Bernoulli factory

To sample events of probability $\alpha_B$, the two-coin algorithm, an efficient Bernoulli factory, was presented in Gonçalves et al. (2017b). Generalizing this to a die-coin algorithm, we present a Bernoulli factory for $\alpha_r^R$ for $r = 2$; extensions to other $r$ can be done similarly. Let $\pi(x) = c_x p_x$ with $p_x \in [0, 1]$ and $c_x > 0$. Then,

$$\alpha_2^R(x, y) = \frac{\pi(y)^2 + \pi(x)\pi(y)}{\pi(y)^2 + \pi(x)^2} = \frac{c_y p_y^2 + c_x c_y p_y}{c_y^2 p_y^2 + c_x p_x c_y p_y + c_x^2 p_x^2}.$$

**Algorithm 1** Die-coin algorithm for $\alpha_2^R(x, y)$

1: Draw $D \sim \text{Categorical}\left(\frac{c_y^2}{c_x^2 + c_x c_y + c_y^2}, \frac{c_x c_y}{c_y^2 + c_x c_y + c_x^2}, \frac{c_x^2}{c_y^2 + c_x c_y + c_x^2}\right)$
2: if $D = 1$ then
3: Draw $C_1 \sim \text{Bern}(p_y^2)$
4: if $C_1 = 1$ then output 1 else go back to Step 1
5: if $D = 2$ then
6: Draw $C_1 \sim \text{Bern}(p_x p_y)$
7: if $C_1 = 1$ then output 1 else go back to Step 1
8: if $D = 3$ then
9: Draw $C_1 \sim \text{Bern}(p_x^2)$
10: if $C_1 = 1$ then output 0 else go back to Step 1

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