On the limitations of single-step drift and minorization in Markov chain convergence analysis

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Abstract

Over the last three decades, there has been a considerable effort within the applied probability community to develop techniques for bounding the convergence rates of general state space Markov chains. Most of these results assume the existence of drift and minorization (d&m) conditions. It has often been observed that convergence rate bounds based on single-step d&m tend to be overly conservative, especially in high-dimensional situations. This article builds a framework for studying this phenomenon. It is shown that any convergence rate bound based on a set of d&m conditions cannot do better than a certain unknown optimal bound. Strategies are designed to put bounds on the optimal bound itself, and this allows one to quantify the extent to which a d&m-based convergence rate bound can be sharp. The new theory is applied to several examples, including a Gaussian autoregressive process (whose true convergence rate is known), and a Metropolis adjusted Langevin algorithm. The results strongly suggest that convergence rate bounds based on single-step d&m conditions are quite inadequate in high-dimensional settings.

1 Introduction

The performance of a Markov chain Monte Carlo (MCMC) algorithm is directly tied to the convergence rate of the underlying Markov chain. (As will be made precise below, the convergence rate

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is a number between 0 and 1, with smaller values corresponding to faster convergence.) Unfortunately, ascertaining the convergence rates of even mildly complex Markov chains can be extremely difficult. Indeed, over the last three decades, there has been a considerable effort within the applied probability community to develop techniques for (upper) bounding the convergence rates of general state space Markov chains. Most of these results assume the existence of drift and minorization (d&m) conditions for the chain under study. In essence, the minorization condition guarantees that the chain is well-behaved on a subset of its state space, and the drift condition guarantees that the chain will visit that subset frequently. By carefully combining the d&m, one can construct a quantitative upper bound on the chain’s convergence rate that is an explicit function of the parameters in the d&m conditions (see, e.g., [Meyn and Tweedie 1994; Rosenthal 1995; Roberts and Tweedie 1999; Douc et al. 2004; Baxendale 2005; Jerison 2019]). However, it is well known that d&m-based bounds are often overly conservative; that is, the upper bound is often very close to 1, even when the chain is known to (or at least appears to) converge rapidly. An example of this phenomenon is provided later in this section. Worse yet, the problem is often exacerbated by increasing dimension (Rajaratnam and Sparks 2015; Qin and Hobert 2019b). These facts raise the following question: Are d&m-based methods inadequate for constructing sharp convergence rate bounds in high-dimensional problems? This question is difficult to answer because, in situations where the methods fail, there are several vastly different potential reasons for the failure, including the possibility that the particular set of d&m conditions that were used are somehow faulty. In this article, we provide a partial answer to the question posed above by studying the optimal bound that can be produced using a set of d&m conditions. When applied to specific Markov chains, our results strongly suggest that d&m arguments based on single-step transition laws are quite inadequate in high-dimensional settings. In the remainder of this section, we provide an overview of our results.

Suppose that $(X, B)$ is a countably generated measurable space, and let $P : X \times B \rightarrow [0, 1]$ be a Markov transition kernel (Mtk). When the state space, $X$, is a commonly studied topological space (e.g., a Euclidean space), $B$ is assumed to be its Borel $\sigma$-algebra. For any positive integer $m$, let $P^m$ be the $m$-step transition kernel, so that $P^1 = P$. For any probability measure $\mu : B \rightarrow [0, 1]$ and measurable function $f : X \rightarrow \mathbb{R}$, denote $\int_X \mu(dx) P^m(x, \cdot)$ by $\mu P^m(\cdot)$, and $\int_X P^m(\cdot, dx) f(x)$ by $P^m f(\cdot)$. Also, let $L^2(\mu)$ denote the set of measurable, real-valued functions on $X$ that are square integrable with respect to $\mu(dx)$.

For the time being, assume that the Markov chain defined by $P$ has a stationary probability measure $\Pi$, so $\Pi = \Pi P$. The goal of convergence analysis is to understand how fast $\mu P^m$ converges
to Π as \( m \to \infty \) for a large class of \( \mu \)s. The difference between \( \mu P^m \) and Π is usually measured using the total variation distance, which is defined as follows. For two probability measures on \((X, \mathcal{B})\), \( \mu \) and \( \nu \), their total variation distance is

\[
d_{TV}(\mu, \nu) = \sup_{A \in \mathcal{B}} [\mu(A) - \nu(A)].
\]

The Markov chain is geometrically ergodic if, for each \( x \in X \), \( d_{TV}(\delta_x P^m, \Pi) \) decays at an exponential rate that is independent of \( x \) when \( m \to \infty \), where \( \delta_x \) is the point mass (Dirac measure) at \( x \). In other words, the chain is geometrically ergodic if there exist \( \rho < 1 \) and \( M : X \to [0, \infty) \) such that, for each \( x \in X \) and positive integer \( m \),

\[
d_{TV}(\delta_x P^m, \Pi) \leq M(x) \rho^m. \tag{1}
\]

Following the ideas in Roberts and Tweedie (2001), define

\[
\rho^*(P) = \exp \left[ \sup_{x \in X} \limsup_{m \to \infty} \frac{\log d_{TV}(\delta_x P^m, \Pi)}{m} \right].
\]

It can be shown that \( \rho^*(P) \in [0, 1] \). If (1) holds for all \( x \) and \( m \), then \( \rho^*(P) \leq \rho \). On the other hand, if \( \rho > \rho^*(P) \), then for each \( x \in X \), there exists \( M_x > 0 \) such that, for each \( m > M_x \),

\[
\frac{\log d_{TV}(\delta_x P^m, \Pi)}{m} < \log \rho.
\]

In this case, (1) holds with \( M(x) = \rho^{-M_x} + 1 \). Thus, \( \rho^*(P) \) can be regarded as the true (geometric) convergence rate of the chain, and the chain is geometrically ergodic if and only if \( \rho^*(P) < 1 \). Essentially, if \( \rho^*(P) \) is close to 0, then the chain converges rapidly, and the elements of the chain are nearly independent; if \( \rho^*(P) \) is close to 1, then the chain mixes slowly, and the elements of the chain are strongly correlated.

The quantity \( \rho^*(P) \) plays an important role in the analysis of MCMC algorithms (see, e.g., Jones and Hobert 2001; Roberts and Rosenthal 2004; Rajaratnam and Sparks 2015). However, despite its significance, it is typically quite difficult to get a handle on \( \rho^*(P) \) (outside of toy problems). As mentioned above, there are a number of different methods for converting \( d&m \) conditions for \( P \) into upper bounds on \( \rho^*(P) \), and the majority of them fall into two categories: those based on renewal theory, and those based on coupling. There are also several different forms of \( d&m \) in the literature, and they are all quite similar. We will study two particular versions of \( d&m \) - one used by Baxendale (2005) in conjunction with renewal theory, and another used by Rosenthal (1995) in conjunction with coupling. We begin with Baxendale’s (2005) \( d&m \) conditions, which take the following form:
(A1) There exist \( \lambda \in [0, 1) \), \( K \in [1, \infty) \), \( C \in \mathcal{B} \), and measurable \( V : X \to [1, \infty) \) such that

\[
P V(x) \leq \lambda V(x) 1_{X \setminus C}(x) + K 1_C(x)
\]

for each \( x \in X \).

(A2) There exist \( \varepsilon \in (0, 1] \) and a probability measure \( \nu : \mathcal{B} \to [0, 1] \) such that

\[
P(x, A) \geq \varepsilon \nu(A)
\]

for each \( x \in C \) and \( A \in \mathcal{B} \).

Here, (A1) and (A2) are called the drift condition and the minorization condition, respectively. The function \( V \) is the drift function, and \( C \) is referred to as a small set. We call (A1) and (A2) “single-step” drift and minorization because they only involve the one-step transition kernel \( P \). An explicit upper bound on \( \rho_*(P) \) can be derived using (A1) and (A2), and, typically, the bound is only a function of \( (\lambda, K, \varepsilon) \). Here’s an example.

**Theorem 1.** [Baxendale (2005)] Let \( P \) be a Markov chain on \( (X, \mathcal{B}) \). Suppose that (A1) and (A2) hold, and that the following condition is satisfied:

(A3) There exists \( \beta \in (0, 1] \) such that \( \nu(C) \geq \beta \).

Then \( P \) admits a unique stationary distribution, \( \Pi \), and \( \rho_*(P) < 1 \). Suppose further that \( P \) satisfies the following conditions:

(S1) The chain is reversible, i.e., for each \( f, g \in L^2(\Pi) \),

\[
\int_X g(x) P f(x) \Pi(dx) = \int_X f(x) P g(x) \Pi(dx).
\]

(S2) The chain is non-negative definite, i.e., for each \( f \in L^2(\Pi) \),

\[
\int_X f(x) P f(x) \Pi(dx) \geq 0.
\]

Then

\[
\rho_*(P) \leq \max \{ \lambda, (1 - \varepsilon)^{1/\alpha_*} \} 1_{\varepsilon < 1} + \lambda 1_{\varepsilon = 1},
\]

where

\[
\alpha_* = \frac{\log \left[ (K - \varepsilon)/(1 - \varepsilon) \right] + \log \lambda^{-1}}{\log \lambda^{-1}}.
\]

(When \( \varepsilon \in (0, 1) \) and \( \lambda = 0 \), \( \alpha_* \) is interpreted as 1.)
Remark 2. Baxendale (2005) also provides results for chains that are reversible, but not non-negative definite, and also for chains that are neither reversible nor non-negative definite. However, those bounds are much more complex than (2).

Remark 3. Jerison (2019) uses the theory of strong random times to extend and improve upon some of Baxendale’s (2005) results, but is unable to improve upon the convergence rate bound given in (2).

Results of this type have proven to be extremely useful for establishing the geometric ergodicity of Markov chains on continuous state spaces. That is, for establishing the qualitative result that \( \rho^*(P) < 1 \). However, upper bounds on \( \rho^*(P) \) that are constructed based on single-step drift and minorization, such as (2), have a reputation of being very conservative. In practice, it’s not unusual for a bound of this type to be very close to unity, even when the chain being studied apparently converges quite rapidly. The following example illustrates this situation.

Let \( X = \mathbb{R}^{10} \), and let \( P \) be given by
\[
P(x, dy) \propto \exp \left( -\frac{2}{3} \| y - \frac{x}{2} \|^2 \right) dy,
\]
where \( \| \cdot \| \) is the Euclidean norm. So \( P \) defines a Gaussian autoregressive chain on \( X \). The 10-dimensional standard Gaussian distribution is the unique stationary distribution of the corresponding Markov chain. The chain is reversible, non-negative definite, and it is well-known that \( \rho^*(P) = 0.5 \). Let us now pretend that we do not know the true convergence rate, and consider using Theorem 1 to form an upper bound on \( \rho^*(P) \). In order to apply the theorem, we must establish (A1)-(A3). A standard drift function to use is \( V(x) = \| x \|^2/k + 1 \), where \( k \) can be tuned. We take \( k = 100 \), since this appears to give good results. The small set \( C \) is usually chosen to be \( \{ x \in \mathbb{R}^{10} : V(x) \leq d \} \), where \( d \geq 1 \) can be optimized. In this case, (A1) holds whenever \( d > 1 + 10/k = 1.1 \). In fact,
\[
PV(x) \leq \frac{10d + 33}{40d} V(x) 1_{X \setminus C}(x) + \frac{10d + 33}{40} 1_C(x).
\]
Moreover, for each \( d > 1.1, a > 0, x \in C \) and \( A \in \mathcal{B} \),
\[
P(x, A) = \int_A \frac{1}{(3\pi/2)^5} \exp \left( -\frac{2}{3} \left\| y - \frac{x}{2} \right\|^2 \right) dy
\]
\[
\geq \int_A \frac{1}{(3\pi/2)^5} \inf_{\|x\|^2/k+1 \leq d} \exp \left( -\frac{2}{3} \left\| y - \frac{x'}{2} \right\|^2 \right) dy
\]
\[
\geq \int_A \frac{1}{(3\pi/2)^5} \inf_{\|x\|^2/k+1 \leq d} \exp \left\{ -\frac{2}{3} \left[ (1 + a)\|y\|^2 + \left( 1 + \frac{1}{a} \right) \left\| x' \right\|^2 \right] \right\} dy
\]
\[
\geq \int_A \frac{1}{(3\pi/2)^5} \exp \left[ -\frac{2(a+1)}{3} \|y\|^2 - \frac{100(a+1)(d-1)}{6a} \right] dy
\]
\[
= \frac{1}{(a+1)^5} \exp \left[ -\frac{100(a+1)(d-1)}{6a} \right] \nu(A),
\]
where \( \nu \) is the 10-dimensional normal distribution with mean 0 and variance \( 3I_{10}/[4(a+1)] \), with \( I_{10} \) being the \( 10 \times 10 \) identity matrix. Thus, (A2) holds. It’s obvious that (A3) holds as well. Applying Theorem 1 and optimizing over \((a, d)\), leads to the following result: \( \rho_*(P) \leq 0.99993 \). This bound is obviously extremely conservative - recall that \( \rho_*(P) = 0.5 \). This leads to the following intriguing question: (Q1) Is this terrible bound on \( \rho_*(P) \) a result of the way in which Theorem 1 was applied (i.e., a poorly chosen drift function, loose inequalities in the d&m, etc.), or is it simply impossible to use Theorem 1 to produce a sharp bound in this example? Another interesting (and more general) question is this: (Q2) Assuming that (2) is not the best possible bound that can be constructed using (A1)-(A3), how much better could we hope to do?

The two questions posed in the previous paragraph can be answered using results developed in Section 2 which is where we introduce a general framework for evaluating the effectiveness of a set of d&m conditions for bounding convergence rates. We now describe the basic ideas, and provide an overview of the results. Fix a value of the d&m parameter, \((\lambda, K, \varepsilon, \beta)\), and let \( S^{(N)}_{\lambda,K,\varepsilon,\beta} \) denote the set of all reversible, non-negative definite Mtks that satisfy (A1)-(A3) with this value of the d&m parameter. Baxendale’s (2005) result implies that, for any \( P \in S^{(N)}_{\lambda,K,\varepsilon,\beta} \), \( \rho_*(P) \) is bounded above by (2). Therefore, (2) cannot be smaller than the convergence rate of the slowest chain in \( S^{(N)}_{\lambda,K,\varepsilon,\beta} \), which we denote by \( \rho^{(N)}_{\text{opt}}(\lambda, K, \varepsilon, \beta) \). (The subscript “opt” stands for “optimal.”) While it may not be possible to calculate \( \rho^{(N)}_{\text{opt}}(\lambda, K, \varepsilon, \beta) \), it’s easy to bound it from below. Indeed, the convergence rate of any \( P \in S^{(N)}_{\lambda,K,\varepsilon,\beta} \) serves as a lower bound on \( \rho^{(N)}_{\text{opt}}(\lambda, K, \varepsilon, \beta) \). By identifying a class of particularly slow-to-converge chains that satisfy (A1)-(A3), we are able to establish that
\[
\max\{\lambda, (1-\varepsilon)^{1/\alpha}\} \varepsilon < 1 + \lambda \varepsilon = 1 \leq \rho^{(N)}_{\text{opt}}(\lambda, K, \varepsilon, \beta) \leq \max\{\lambda, (1-\varepsilon)^{1/\alpha}\} \varepsilon < 1 + \lambda \varepsilon = 1, \quad (3)
\]
where \( \alpha = [\alpha_*] \), and \([\cdot]\) returns the largest integer that does not exceed its argument. The fact that
the expressions on the right- and left-hand sides of (3) are nearly identical shows that Baxendale’s (2005) bound is actually quite sharp. Thus, we have answered (Q2).

Now suppose that $P$ is a reversible, non-negative definite, geometrically ergodic Mtk. Presumably, $P$ satisfies many different versions of (A1)-(A3), each with a different d&m parameter value. The best (i.e., smallest) upper bound on $\rho_*(P)$ that we could possibly get using (A1)-(A3), call it $\rho_{opt}^*(P)$, is the infimum of $\rho_{opt}^{(N)}(\lambda, K, \varepsilon, \beta)$ over all those different d&m parameter values. We use this idea in conjunction with a new lower bound on $\Pi(C)$ to establish the following: For any $P$ that satisfies (A1)-(A3) (not necessarily reversible or non-negative definite), we have the following:

$$\rho_{opt}^*(P) \geq \inf_{C \in B: \Pi(C) > 0} \left( 1 - \varepsilon_C \right) \left( 1 - \Pi(C) \right)^{-1} - 1,$$

where

$$\varepsilon_C = \sup \{ \varepsilon \in (0, 1] : (A2) \text{ holds for } P \text{ and } C \text{ with } \varepsilon \text{ and some probability measure } \nu \},$$

and we take $\varepsilon_C = 0$ if $(A2)$ doesn’t hold on $C$. The bound in (4) shows that $\rho_{opt}^*(P)$ is far away from unity only if there exists a set $C$ such that $\varepsilon_C$ and $\Pi(C)$ are both large. Unfortunately, $\varepsilon_C$ tends to decrease with the size of $C$, while $\Pi(C)$ tends to increase with it. In Section 2.3.1 we use (4) to show that, for the Gaussian autoregressive example, $\rho_{opt}^*(P) \geq 0.922$. Hence, it is impossible to use d&m in the form of (A1)-(A3) to get a tight bound on the convergence rate in this example, which answers (Q1).

At this point, we should make clear that, in theory, the problems with d&m that are described above can be circumvented by moving from single-step d&m to multi-step d&m. Indeed, it is well known that, if one can establish d&m conditions based on multi-step transition kernels, then the resultant convergence rate bounds can actually be quite well-behaved, even in high-dimensional settings where the single-step bounds fail completely. (See Qin and Hobert (2019b) for an example involving the Gaussian autoregressive process described above.) Unfortunately, in practical situations where the transition law is highly complex (such as in MCMC), developing d&m conditions with multi-step Mtks is usually impossible. For this reason, multi-step d&m is seldom used in practice.

We now consider Rosenthal’s (1995) d&m conditions, which take the following form:

(B1) There exist $\eta \in [0, 1), L \in [0, \infty)$, and measurable $V : X \to [0, \infty)$ such that

$$PV(x) \leq \eta V(x) + L$$

for each $x \in X$. 7
There exist \( \varepsilon \in (0, 1] \), \( d > 0 \), and a probability measure \( \nu : \mathcal{B} \to [0, 1] \) such that

\[
P(x, A) \geq \varepsilon \nu(A)
\]

for each \( x \in C \) and \( A \in \mathcal{B} \), where \( C = \{ x \in X : V(x) \leq d \} \).

The main difference between (B1)-(B3) and (A1)-(A3) is that the former puts a restriction on the structure of \( C \). Indeed, in (B2), \( C \) is assumed to be a level set of the drift function. Assume that (B1)-(B3) hold. The size of \( C \) is controlled by the parameter \( d \), which is bounded below by \( 2L/(1 - \eta) \). The lower bound on \( d \) originates from the coupling argument, and it has some interesting implications. One of these is that \( \Pi(C) > 1/2 \) (see, e.g. [Jerison, 2016]), which, as we shall see, turns out to be very important. The following result provides a recipe for converting (B1)-(B3) into a convergence rate bound.

**Theorem 4.** ([Rosenthal (1995)]) Let \( P \) be a MtM on \((X, \mathcal{B})\). Suppose that (B1)-(B3) hold. Then \( P \) admits a unique stationary distribution, \( \Pi \), and

\[
\rho_*(P) \leq (1 - \varepsilon)^{1/\alpha_{***}} 1_{\varepsilon < 1} + \tilde{\lambda} 1_{\varepsilon = 1},
\]

where

\[
\alpha_{***} = \frac{\log[\tilde{K}/(1 - \varepsilon)] + \log \tilde{\lambda}^{-1}}{\log \tilde{\lambda}^{-1}},
\]

\( \tilde{\lambda} = (1 + 2L + \eta d)/(1 + d) \) and \( \tilde{K} = 1 + 2\eta d + 2L \).

**Remark 5.** In [Rosenthal (1995)], the upper bound on \( \rho_*(P) \) depends upon an additional free parameter. The bound presented here is the result of optimizing with respect to the free parameter.

**Remark 6.** In general, coupling arguments often produce convergence bounds that are simpler than those based on renewal theory. While (5) is actually a bit more complex than (2), note that (2) is valid only when the Markov chain is reversible and non-negative definite, whereas (5) holds without this extra regularity. Moreover, the bounds that [Baxendale (2005)] developed for chains that do not satisfy the extra regularity are much more complex than (5).

**Remark 7.** [Rosenthal (1995)] also provides a version of Theorem 4 based on multi-step minorization, that is, (B1)-(B3) with \( P \) replaced by \( P^m \) for \( m \geq 1 \).
In Section 3, we use the general framework developed in Section 2 to investigate the limitations of methods based on (B1)-(B3). Our main result is an analogue of the bound in (4), which we now describe. For any geometrically ergodic $P$, let $\rho_{\text{opt}}(P)$ denote the best (i.e., smallest) upper bound on $\rho_*(P)$ that we could possibly get using (B1)-(B3). Then we have

$$\rho_{\text{opt}}(P) \geq \inf_{C \in B, \Pi(C) > 1/2} (1 - \varepsilon_C),$$

where $\varepsilon_C$ is defined just after (4). The bound in (6) suggests that $\rho_{\text{opt}}(P)$ is far away from 1 only if there exists a set $C$ such that $\Pi(C) > 1/2$ and $\varepsilon_C$ is large. The examples in Section 3.2 show that, when the state space is high-dimensional (or finite but very large), such a $C$ will often not exist, even when the associated chain mixes rapidly.

The optimality of convergence rate bounds based on d&m has been touched on in previous work (see, e.g., Meyn and Tweedie, 1994; Lund and Tweedie, 1996; Roberts and Tweedie, 2000; Baxendale, 2005; Jerison, 2016; Qin and Hobert, 2019b). For instance, Meyn and Tweedie (1994) compared their convergence rate bound with existing results for a certain class of chains, and concluded that their bound “cannot be expected to be tight.” In fact, Baxendale (2005) developed a tighter version of their bound about a decade later. However, to our knowledge, there has been no prior systematic study of the limitations of the d&m methodology in general.

The rest of this article is organized as follows. In Section 2, we introduce our general framework for studying the limitations of a set of d&m conditions for bounding convergence rates. Within this framework, we analyze the sharpness of Baxendale’s (2005) bound, and, more generally, we consider optimal bounds based on (A1)-(A3). Our results are applied to the Gaussian autoregressive example, and also to the Metropolis adjusted Langevin algorithm (MALA) in a situation where the target is high-dimensional. In Section 3, we study optimal bounds based on (B1)-(B3). The results are applied to the Gaussian autoregressive example, MALA, and several random walks on graphs. Potential strategies for overcoming the limitations of single-step d&m are discussed in Section 4. The Appendix contains several technical proofs.

2 Quantifying the Limitations of Bounds Based on (A1)-(A3)

2.1 Parameter-specific optimal bound

Consider a generic upper bound on the convergence rate that is based on (A1)-(A3). If this bound depends on (A1)-(A3) only through the d&m parameter, $(\lambda, K, \varepsilon, \beta)$, then we call it a simple upper
bound. Just to be clear, a simple upper bound cannot use the drift function, \( V(\cdot) \), the small set \( C \), nor the minorization measure \( \nu(\cdot) \). As an example, the bound in Theorem 1 is simple. Now fix a value of \( (\lambda, K, \varepsilon, \beta) \). Evidently, the smallest possible simple upper bound on the convergence rate of any Markov chain that satisfies (A1)-(A3) with this value of the d&m parameter is exactly equal to the convergence rate of the slowest Markov chain among all the chains that satisfy (A1)-(A3) with this particular value of \( (\lambda, K, \varepsilon, \beta) \). In this section, we will approximate this optimal simple upper bound by constructing a class of slowly converging Markov chains that satisfy (A1)-(A3).

For each fixed value of \( (\lambda, K, \varepsilon, \beta) \) in the set \( T_0 := [0, 1) \times [1, \infty) \times (0, 1] \times (0, 1] \), let \( S_{\lambda, K, \varepsilon, \beta} \) denote the set of Mtks that satisfy (A1)-(A3) with that d&m parameter. We do not require these chains to live on the same space. In addition, let \( S_{\lambda, K, \varepsilon, \beta}^{(R)} \) denote the subset of \( S_{\lambda, K, \varepsilon, \beta} \) consisting of reversible chains, and let \( S_{\lambda, K, \varepsilon, \beta}^{(N)} \) denote the subset of \( S_{\lambda, K, \varepsilon, \beta}^{(R)} \) consisting of non-negative definite chains. So we have \( S_{\lambda, K, \varepsilon, \beta}^{(N)} \subset S_{\lambda, K, \varepsilon, \beta}^{(R)} \subset S_{\lambda, K, \varepsilon, \beta} \). As an example, consider \( S_{0,1,1,1} \), which consists of all Mtks that define a trivial (independent) Markov chain on some countably generated state space. Hence, we have \( S_{0,1,1,1}^{(N)} = S_{0,1,1,1}^{(R)} = S_{0,1,1,1} \).

For \( (\lambda, K, \varepsilon, \beta) \in T_0 \), \( S_{\lambda, K, \varepsilon, \beta} \) is non-empty, since \( S_{0,1,1,1} \subset S_{\lambda, K, \varepsilon, \beta} \). The parameter-specific optimal bound corresponding to d&m parameter \( (\lambda, K, \varepsilon, \beta) \) is defined as follows:

\[
\rho_{\text{opt}}(\lambda, K, \varepsilon, \beta) = \sup_{P \in S_{\lambda, K, \varepsilon, \beta}} \rho_*(P).
\]

Consider the significance of \( \rho_{\text{opt}}(\lambda, K, \varepsilon, \beta) \). If \( P \) satisfies (A1)-(A3) with d&m parameter \( (\lambda, K, \varepsilon, \beta) \), then no simple upper bound on \( \rho_*(P) \) can be less than \( \rho_{\text{opt}}(\lambda, K, \varepsilon, \beta) \). Hence, if there are Markov
chains in $S_{\lambda,K,\epsilon,\beta}$ that converge substantially slower than $P$, then no simple upper bound can provide a tight bound on $\rho_\star(P)$. Of course, $P$ may satisfy (A1)-(A3) with many different values of $(\lambda,K,\epsilon,\beta)$. We will confront this complication in the next subsection.

As in Baxendale (2005), we also wish to consider situations where $P$ satisfies additional regularity beyond (A1)-(A3), such as reversibility and non-negative definiteness. To this end, define

$$\rho_{\text{opt}}^{(R)}(\lambda,K,\epsilon,\beta) = \sup_{P \in S_{\lambda,K,\epsilon,\beta}} \rho_\star(P) \quad \text{and} \quad \rho_{\text{opt}}^{(N)}(\lambda,K,\epsilon,\beta) = \sup_{P \in S_{\lambda,K,\epsilon,\beta}} \rho_\star(P).$$

Of course, $\rho_{\text{opt}}^{(N)}(\lambda,K,\epsilon,\beta)$ represents the smallest possible simple upper bound based on (A1)-(A3) for chains that are both reversible and non-negative definite, and $\rho_{\text{opt}}^{(R)}(\lambda,K,\epsilon,\beta)$ has an analogous interpretation. It is clear that

$$\rho_{\text{opt}}^{(N)}(\lambda,K,\epsilon,\beta) \leq \rho_{\text{opt}}^{(R)}(\lambda,K,\epsilon,\beta) \leq \rho_{\text{opt}}(\lambda,K,\epsilon,\beta).$$

Furthermore, all three of the parameter-specific optimal bounds that we have introduced are increasing in $\lambda$ and $K$, and decreasing in $\epsilon$ and $\beta$.

While it is usually impossible to calculate parameter-specific optimal bounds exactly, it’s easy to find lower bounds. For example, fix $(\lambda,K,\epsilon,\beta) \in T_0$, and suppose that $P_{\lambda,K,\epsilon,\beta} \in S_{\lambda,K,\epsilon,\beta}$. Then

$$\rho_{\text{opt}}(\lambda,K,\epsilon,\beta) \geq \rho_\star(P_{\lambda,K,\epsilon,\beta}).$$

Now, if for each $(\lambda,K,\epsilon,\beta) \in T_0$, we can find a particularly slowly converging chain in $S_{\lambda,K,\epsilon,\beta}$, then we can construct a good lower bound on $\rho_{\text{opt}}$. Indeed, this is precisely how the following result is proven.

**Theorem 8.** For each $(\lambda,K,\epsilon,\beta) \in T_0$, we have

$$\rho_{\text{opt}}^{(N)}(\lambda,K,\epsilon,\beta) \geq \max\{\lambda, (1-\epsilon)^{1/\alpha}\}1_{\epsilon<1} + \lambda 1_{\epsilon=1},$$

where

$$\alpha = \lfloor \alpha_\star \rfloor = \left\lfloor \frac{\log[(K-\epsilon)/(1-\epsilon)] + \log \lambda^{-1}}{\log \lambda^{-1}} \right\rfloor.$$

(When $\epsilon \in (0,1)$ and $\lambda = 0$, $\alpha_\star$ is interpreted as 1.)

**Remark 9.** The reader may have noticed that we have not mentioned any of the “usual regularity conditions” like $\psi$-irreducibility or aperiodicity. This is because these conditions are implied by geometric ergodicity, which is guaranteed under (A1)-(A3).
Proof. It is straightforward to verify that
\[
\max\{\lambda, (1 - \varepsilon)^{1/\alpha}\}1_{\varepsilon < 1} + \lambda 1_{\varepsilon = 1} = \max\{(1 - \varepsilon)^{1/\alpha}1_{\varepsilon < 1}, \lambda\},
\]
so it suffices to show that
\[
\rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta) \geq \max\{(1 - \varepsilon)^{1/\alpha}1_{\varepsilon < 1}, \lambda\}.
\]
We first prove that
\[
\rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta) \geq (1 - \varepsilon)^{1/\alpha}1_{\varepsilon < 1}.
\]
Indeed, for each value of \((\lambda, K, \varepsilon, \beta) \in T_0\) such that \(\varepsilon < 1\), we identify a \(P_{\lambda, K, \varepsilon, \beta} \in S_{\lambda, K, \varepsilon, \beta}^{(N)}\) such that
\[
\rho_{\star}(P_{\lambda, K, \varepsilon, \beta}) \geq (1 - \varepsilon)^{1/\alpha}.
\]
Fix \(\varepsilon < 1\), let \((\lambda, K, \beta) \in [0, 1) \times [1, \infty) \times (0, 1]\) be arbitrary, and note that \(\alpha \geq 1\). Let \(P_{\lambda, K, \varepsilon, \beta}\) be the Mtk of a Markov chain that lives on \(X = \{0, 1, \ldots, \alpha\}\) and that adheres to the following rules:

- If \(X_m = 0\), then \(X_{m+1} = 0\).
- If \(X_m = 1\), then with probability \(\varepsilon\), \(X_{m+1} = 0\), and with probability \(1 - \varepsilon\), \(X_{m+1} = \alpha\).
- If \(X_m \geq 2\), then \(X_{m+1} = X_m - 1\).

A Markov transition diagram for this chain is shown in Figure 1.

![Markov transition diagram](image)

Figure 1: Markov transition diagram for the Markov chain \(\{X_m\}_{m=0}^{\infty}\) when \(\alpha = 3\).

The chain admits a unique stationary distribution, which is precisely the point mass at 0, and it’s straightforward to verify that the chain is reversible and non-negative definite. (It is also aperiodic and \(\psi\)-irreducible, although it’s not irreducible in the classical sense that any two states communicate with each other.)

We now verify that \(P_{\lambda, K, \varepsilon, \beta}\) does satisfy (A1), (A2), and (A3) with parameters \((\lambda, K, \varepsilon, \beta)\), i.e., \(P_{\lambda, K, \varepsilon, \beta} \in S_{\lambda, K, \varepsilon, \beta}^{(N)}\). To this end, let \(C = \{0, 1\}\), and define \(V : X \to [1, \infty)\) as follows.
• Let $V(0) = 1$, and let $V(\alpha) = (K - \varepsilon)/(1 - \varepsilon)$.

• If $\alpha \geq 2$, let $V(x) = \lambda^{-x+1}$ for $x = 1, 2, \ldots, \alpha - 1$.

It’s clear that (A2) and (A3) hold with $\nu$ being the point mass at 0. If $\alpha = 1$, then (A1) obviously holds as well. Assume that $\alpha \geq 2$. Then $PV(0) = 1$, $PV(1) = K$, and thus, $PV(x) \leq K$ for each $x \in C$. For $x = 2, 3, \ldots, \alpha - 1$ (if $\alpha \geq 3$), $PV(x) = V(x - 1) = \lambda V(x)$. Finally, noting that

$$\alpha - 2 = \left\lfloor \frac{\log((K - \varepsilon)/(1 - \varepsilon)) - \log \lambda^{-1}}{\log \lambda^{-1}} \right\rfloor \leq \frac{\log((K - \varepsilon)/(1 - \varepsilon)) - \log \lambda^{-1}}{\log \lambda^{-1}},$$

we have

$$\frac{PV(\alpha)}{V(\alpha)} = \frac{\lambda^{-\alpha+2}}{(K - \varepsilon)/(1 - \varepsilon)} \leq \lambda.$$

Thus, (A1) is satisfied.

We now show that (12) holds. When $\alpha = 1$, for an arbitrary $m$, $d_{TV}(\delta_0 P^m_{\lambda,K,\varepsilon,\beta}, \delta_0) = 0$, and $d_{TV}(\delta_1 P^m_{\lambda,K,\varepsilon,\beta}, \delta_0) = (1 - \varepsilon)^m$. Thus, (12) holds. For the remainder of this proof, assume that $\alpha \geq 2$. It’s easy to see that, for each positive integer $m$ and $x \in X$.

$$d_{TV}(\delta_x P^m_{\lambda,K,\varepsilon,\beta}, \delta_0) = \mathbb{P}(X_m \neq 0 | X_0 = x).$$

Suppose that $X_0 \neq 0$. Each time the chain enters $\{1\}$, with probability $\varepsilon$, it arrives at 0 in the next iteration, and stays there forever; with probability $1 - \varepsilon$, it goes to $\alpha$, and then takes exactly $\alpha - 1$ steps to get back. Therefore, for any positive integer $k$, the probability that the chain does not arrive at 0 within $k\alpha$ iterations is $(1 - \varepsilon)^k$. It follows that (12) must hold, and (11) is satisfied.

We now show that

$$\rho_{opt}^{(N)}(\lambda, K, \varepsilon, \beta) \geq \lambda,$$

thereby completing the proof. Let $(\lambda, \varepsilon, K, \beta) \in T_0$ be arbitrary. If $\lambda = 0$, then (13) trivially holds. Suppose that $\lambda > 0$, and let $\delta \in (0, \lambda)$. Let $\tilde{P}_{\lambda,K,\varepsilon,\beta}$ be the Mtk of a Markov chain that lives on $X = \{0, 1\}$ and that adheres to the following rules:

- If $\tilde{X}_m = 0$, then $\tilde{X}_{m+1} = 0$.

- If $\tilde{X}_m = 1$, then with probability $\lambda - \delta$, $\tilde{X}_{m+1} = 1$, and with probability $1 - \lambda + \delta$, $\tilde{X}_{m+1} = 0$.

As before, the unique invariant distribution of this chain is the point mass at 0, and it’s easy to show that the chain is reversible and non-negative definite. Let $C = \{0\}$, and define $V : X \to [1, \infty)$
as follows: \( V(0) = 1, V(1) = (1 - \lambda + \delta)/\delta. \) It’s easy to see that (A1), (A2), and (A3) all hold for \( \tilde{P}_{\lambda,K,\varepsilon,\beta}. \) Finally, \( \rho_*(\tilde{P}_{\lambda,K,\varepsilon,\beta}) = \lambda - \delta, \) which implies that
\[
\rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta) \geq \lambda - \delta.
\]
Since \( \delta \in (0, \lambda) \) is arbitrary, (13) holds, and the proof is complete.

**Remark 10.** Combining Theorems 4 and 8 yields the following
\[
\max\{\lambda, (1 - \varepsilon)^{1/\alpha}\}1_{\varepsilon<1} + \lambda 1_{\varepsilon=1} \leq \rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta) \leq \max\{\lambda, (1 - \varepsilon)^{1/\alpha_*}\}1_{\varepsilon<1} + \lambda 1_{\varepsilon=1},
\]
where \( \alpha = \lfloor \alpha_* \rfloor. \) Note that the expressions on the right and left-hand sides are nearly identical. Consequently, for reversible and non-negative definite chains, (2) is close to optimal as a simple upper bound, and (10) is close to tight as a lower bound on \( \rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta). \)

While it is certainly of interest to develop good lower bounds on the parameter-specific optimal bounds, such bounds do not provide us with much information about the effectiveness of drift and minorization for a given Markov chain. Indeed, a single geometrically ergodic Markov chain would presumably satisfy (A1)-(A3) for many different values of \( (\lambda, K, \varepsilon, \beta). \) In the next subsection, we deal with this extra layer of complexity.

### 2.2 Chain-specific optimal bound

Consider a Mtk \( P \) on some state space \((X, B)\). In this subsection, we consider the best possible simple upper bound on \( \rho_*(P) \) that can be obtained based on (A1)-(A3) with the \( \text{d&m} \) parameters in these conditions optimized. In general, there isn’t much hope of calculating a chain-specific optimal bound exactly. In what follows, we describe a framework to bound it from below.

Define \( T(P) \subset T_0 \) as follows: \( (\lambda, K, \varepsilon, \beta) \in T(P) \) if \( P \) satisfies (A1)-(A3) with this value of the \( \text{d&m} \) parameter. If \( P \) is neither reversible nor non-negative definite, then we define the chain-specific optimal upper bound on \( \rho_*(P) \) as
\[
\rho_{\text{opt}}^*(P) = \inf_{(\lambda, K, \varepsilon, \beta) \in T(P)} \rho_{\text{opt}}(\lambda, K, \varepsilon, \beta).
\]
If \( P \) is reversible, but not non-negative definite, then we use
\[
\rho_{\text{opt}}^*(P) = \inf_{(\lambda, K, \varepsilon, \beta) \in T(P)} \rho_{\text{opt}}^R(\lambda, K, \varepsilon, \beta).
\]
Finally, if \( P \) is reversible and non-negative definite, then we take
\[
\rho_{\text{opt}}^*(P) = \inf_{(\lambda, K, \varepsilon, \beta) \in T(P)} \rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta).
\]
In all three cases, if \( T(P) = \emptyset \), then \( \rho^*_\text{opt}(P) \) is set to be unity. While our definition of the chain-specific optimal upper bound is a bit unconventional (because the definition of \( \rho^*_\text{opt}(\cdot) \) depends on the argument), the meaning is clear: \( \rho^*_\text{opt}(P) \) represents the best possible simple upper bound on \( \rho_*(P) \) that can be constructed using (A1)-(A3) (and reversibility/non-negative definiteness if applicable). Throughout the remainder of this subsection, all statements about simple upper bounds based on (A1)-(A3) remain true whether these bounds were constructed using any available additional regularity (reversibility/non-negative definiteness) or not.

Let \( \hat{\rho}(P) \) be any (nontrivial) simple upper bound on \( \rho_*(P) \) based on (A1)-(A3). Then
\[
0 \leq \rho_*(P) \leq \rho^*_\text{opt}(P) \leq \hat{\rho}(P) \leq 1.
\]

The effectiveness of drift and minorization as a method for constructing an upper bound on \( \rho_*(P) \) can be quantified by the gap between \( \rho_*(P) \) and \( \rho^*_\text{opt}(P) \). A large gap means that there does not exist a realization of (A1)-(A3) that yields a sharp simple upper bound on the chain’s true convergence rate. In particular, if \( \rho^*_\text{opt}(P) \approx 1 \), then it’s impossible to use simple bounds based on (A1)-(A3) to show that the chain mixes rapidly, even if \( \rho_*(P) \) is very small.

Recall that \( \rho^{(N)}_{\text{opt}}(\lambda, K, \varepsilon, \beta) \leq \rho^R_{\text{opt}}(\lambda, K, \varepsilon, \beta) \leq \rho_{\text{opt}}(\lambda, K, \varepsilon, \beta) \). In the previous section, we developed reasonably sharp lower bounds on \( \rho^{(N)}_{\text{opt}}(\lambda, K, \varepsilon, \beta) \). Thus, if we could identify \( T(P) \), then it would, in principle, be straightforward to bound \( \rho^*_\text{opt}(P) \) from below. Unfortunately, identifying \( T(P) \) requires finding all of the values of \( (\lambda, K) \) for which (A1) holds, which is impossible. Indeed, in practice, the only drift conditions that can be established are those associated with simple drift functions that lend themselves to the analysis of the Markov chain corresponding to \( P \). Put simply, for a given \( P \), there is a massive difference between the set of drift conditions that hold in theory, and the set of drift conditions that can actually be established in practice. In what follows, we circumvent this difficulty by constructing a lower bound on \( \rho^{(N)}_{\text{opt}}(\lambda, K, \varepsilon, \beta) \) that does not depend on \( (\lambda, K) \). The construction pivots on a lower bound for the size of the small set. A proof of the following result is provided in Appendix A.

**Theorem 11.** Suppose that \( P \) defines a \( \psi \)-irreducible, aperiodic Markov chain that satisfies (A1) and (A2) with parameters \( (\lambda, K, \varepsilon) \in [0, 1) \times [1, \infty) \times (0, 1] \) and small set \( C \). Then \( P \) admits a unique stationary distribution \( \Pi \), and
\[
\Pi(C) \geq \frac{\log \lambda^{-1}}{\log K + \log \lambda^{-1}}.
\]

The right-hand side is interpreted as 1 if \( \lambda = 0 \).
Combining Theorems 8 and 11 yields the following result.

**Corollary 12.** Let $P$ be a Mtk that satisfies (A1)–(A3) with $d\mathcal{E}m$ parameter $(\lambda, K, \varepsilon, \beta) \in T_0$ and small set $C \in \mathcal{B}$. Then $P$ admits a unique stationary distribution $\Pi$ such that $\Pi(C) > 0$, and

$$\rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta) \geq (1 - \varepsilon)^{1/\Pi(C)^{-1}}.$$  

**Proof.** (A1) to (A3) imply geometric ergodicity, which, in turn, implies $\psi$-irreducibility and aperiodicity, as well as the existence of a unique $\Pi$. By Theorem 11, $\Pi(C) > 0$. Therefore, $(1 - \varepsilon)^{1/\Pi(C)^{-1}} = 0$ when $\varepsilon = 1$. It suffices to consider the case that $\varepsilon < 1$. Fix $\varepsilon < 1$. Thus, $K \geq 1$, $(K - \varepsilon)/(1 - \varepsilon) \geq K$.

Hence,

$$\alpha = \left\lfloor \frac{\log[(K - \varepsilon)/(1 - \varepsilon)] + \log \lambda^{-1}}{\log \lambda^{-1}} \right\rfloor \geq \left\lfloor \frac{\log K + \log \lambda^{-1}}{\log \lambda^{-1}} \right\rfloor.$$  

By Theorem 11, $1/\alpha \leq \left\lfloor 1/\Pi(C) \right\rfloor^{-1}$. The result then follows from Theorem 8. \hfill \Box

For a Mtk $P$ and $C \in \mathcal{B}$, define

$$\varepsilon_C = \sup \{\varepsilon \in (0, 1] : (A2) \text{ holds for } P \text{ and } C \text{ with } \varepsilon \text{ and some probability measure } \nu\},$$  

where the right-hand side is interpreted as 0 if (A2) doesn’t hold on $C$. Here is the main result of this section.

**Theorem 13.** Let $P$ be a Mtk such that $T(P) \neq \emptyset$, and let $\Pi$ denote the stationary distribution. Then

$$\rho_{\star}^{(N)}(P) \geq \inf_{C \in \mathcal{B} : \Pi(C) > 0} \left( (1 - \varepsilon_C)^{1/\Pi(C)^{-1}} \right).$$  

**Proof.** For each $(\lambda, K, \varepsilon, \beta) \in T(P)$, there exists $C' \in \mathcal{B}$ such that (A1) to (A3) hold with parameters $(\lambda, K, \varepsilon, \beta)$ and small set $C'$. By Corollary 12, $\Pi(C') > 0$, and

$$\rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta) \geq (1 - \varepsilon)^{1/\Pi(C')^{-1}} \geq \inf_{C \in \mathcal{B} : \Pi(C) > 0} \left( (1 - \varepsilon_C)^{1/\Pi(C)^{-1}} \right).$$  

Then, since $\rho_{\star}^{(N)}(P) \geq \inf_{(\lambda, K, \varepsilon, \beta) \in T(P)} \rho_{\text{opt}}^{(N)}(\lambda, K, \varepsilon, \beta)$, the result follows. \hfill \Box

Any simple upper bound on $\rho_{\star}(P)$ based on (A1)–(A3) cannot be smaller than $\rho_{\text{opt}}^{(N)}(P)$. Of course, we’d like $\rho_{\text{opt}}^{(N)}(P)$ to be as far away from 1 as possible. Theorem 13 shows that $\rho_{\text{opt}}^{(N)}(P)$ is far away from unity only if one can find a set $C$ such that $\varepsilon_C$ and $\Pi(C)$ are both large. Unfortunately, $\varepsilon_C$ tends to decrease with the size of $C$, while $\Pi(C)$ tends to increase with it. As we shall see in the next subsection, when dimension is high and $\Pi$ tends to “spread out,” the required “Goldilocks” $C$ may not exist, even when $\rho_{\star}(P)$ is not close to 1.
2.3 Examples

2.3.1 Gaussian autoregressive chain

Let us now consider a generalization of the Gaussian autoregressive example from the Introduction. Let $X = \mathbb{R}^n$, where $n$ is a positive integer, and define $P_n$ by

$$P_n(x, dy) \propto \exp \left( -\frac{2}{3} \| y - \frac{x}{2} \|^2 \right) dy, \quad x \in \mathbb{R}^n.$$ 

The corresponding Markov chain is reversible, non-negative definite, and has a unique stationary distribution $\Pi_n$, which is the $n$-dimensional standard Gaussian distribution. The chain is geometrically ergodic, and it’s well-known that, regardless of $n$, $\rho_n(P_n) = 0$. In the Introduction, we established (A1)-(A3) for $P_{10}$ using a quadratic drift function, and then applied Theorem 1, which yielded an upper bound of 0.99993 for $\rho_n(P_{10})$. We will use the results we have developed to demonstrate that the problem here is not a poorly chosen drift function, loose d&m inequalities, etc.; it is, in fact, the inadequacy of the d&m method itself.

For a given positive integer $n$, let $C_n \subset \mathbb{R}^n$ be measurable, and let $D_n$ be the diameter of $C_n$, i.e., $\sup\{\| x - y \| : x, y \in C_n \}$. Let $B_{D_n/2}$ be the ball of diameter $D_n$ that is centered at the origin, and let $f_n(\cdot)$ be the probability density function of a $\chi^2_n$ random variable, i.e., $f_n(x) \propto x^{(n-2)/2} e^{-x/2} 1_{(0,\infty)}(x)$. Then

$$\Pi_n(C_n) \leq \int_{B_{D_n/2}} \Pi_n(dx) = \frac{1}{\alpha_n(D_n)};$$

where

$$\alpha_n(D) = \left( \int_0^{D^2/4} f_n(x) \, dx \right)^{-1} > 1$$

for $D > 0$.

Let $p_n(x, y)$ be the density function of $P_n(x, dy)$, i.e., $P_n(x, dy)/dy$. Suppose that (A2) holds for $P_n$ on $C_n$ with some $\varepsilon_n > 0$ and probability measure $\nu_n$, i.e., for each $x \in C_n$ and measurable $A \subset \mathbb{R}^n$,

$$P_n(x, A) \geq \varepsilon_n \nu_n(A) . \quad (15)$$

Then $\nu_n(\cdot)$ is absolutely continuous with respect to $P_n(x, \cdot)$ for each $x \in C_n$. This implies that $\nu_n$ admits a measurable density. It follows from (15) that, for each $x \in C_n$ and almost every $y \in \mathbb{R}^n$,

$$p_n(x, y) \geq \varepsilon_n \nu_n(dy)/dy .$$
Hence, for each $x, x' \in C_n$,
\[
\int_{\mathbb{R}^n} \min \{p_n(x, y), p_n(x', y)\} \, dy \geq \int_{\mathbb{R}^n} \varepsilon_n \nu_n(dy).
\]
Therefore,
\[
\varepsilon C_n \leq \inf_{x, x' \in C_n} \int_{\mathbb{R}^n} \min \{p_n(x, y), p_n(x', y)\} \, dy.
\]
It can be shown that
\[
\inf_{x, x' \in C_n} \int_{\mathbb{R}^n} \min \{p_n(x, y), p_n(x', y)\} \, dy = 2\Phi \left( -\frac{D_n}{2\sqrt{3}} \right),
\]
where $\Phi(\cdot)$ is the (cumulative) distribution function of the one-dimensional standard Gaussian distribution. Therefore, Theorem 13 yields the following:
\[
\rho_{\text{opt}}^*(P_n) \geq \inf_{D > 0} \left[ 1 - 2\Phi \left( -\frac{D}{2\sqrt{3}} \right) \right]^{1/\alpha_n(D)} =: \rho_n^*.
\]
No simple upper bound on $\rho_*(P_n)$ based on (A1)-(A3) can be less than $\rho_n^*$ (even if it exploits the reversibility and non-negative definiteness of $P_n$). For comparison with the analysis in the Introduction, we note that $\rho_{10}^* \approx 0.922$, which is much larger than the true convergence rate, $\rho_*(P_{10}) = 0.5$. Thus, a simple bound based on (A1)-(A3) cannot produce a tight bound on $\rho_*(P_{10})$.

Unfortunately, things only get worse as $n \to \infty$. A proof of the following result can be found in Appendix B.

**Proposition 14.** $\rho_{\text{opt}}^*(P_n) \to 1$ as $n \to \infty$.

Proposition 14 shows that (A1)-(A3) are completely inadequate for obtaining sharp upper bounds on $\rho_*(P_n)$ when $n$ is large. No matter what drift function and small set are used, and regardless of how the (simple) convergence bound is formed, this inadequacy persists.

### 2.3.2 Metropolis adjusted Langevin algorithm

Again, let $X = \mathbb{R}^n$ for some positive integer $n$. Let $\pi_n : X \to [0, \infty)$ be a differentiable probability density function, and let $f_n(x) = -\log \pi_n(x)$, $x \in X$. Denote the corresponding probability measure by $\Pi_n$. The Metropolis adjusted Langevin algorithm (MALA) is an MCMC algorithm that can be used to draw random vectors that are approximately distributed as $\Pi_n$. It is carried out by simulating a Markov chain $\{X_m\}_{m=0}^\infty$ with the following two-step transition rule.

1. **Proposal Step.** Given $X_m = x \in X$, draw $y \in X$ from the normal distribution $N_n(x - h_n \nabla f_n(x), 2h_n I_n)$, where $h_n > 0$ is the step size.
2. **Metropolis Step.** Let

\[ a_n(x, y) = \min \left\{ 1, \frac{\pi_n(y) \exp[-\|x - y + h_n \nabla f_n(y)\|^2/(4h_n)]}{\pi_n(x) \exp[-\|y - x + h_n \nabla f_n(x)\|^2/(4h_n)]} \right\}. \]

With probability \( a_n(x, y) \), accept the proposal, and set \( X_{m+1} = y \); with probability \( 1 - a_n(x, y) \), reject the proposal, and set \( X_{m+1} = x \).

\( \{X_m\} \) is reversible with respect to \( \Pi_n \), but it’s unknown if the chain is non-negative definite. Its transition kernel is given by

\[
P_n(x, A) = \int_{\mathbb{R}^n} (4\pi h_n)^{-n/2} \exp \left( -\frac{1}{4h_n} \|y - x + h_n \nabla f_n(x)\|^2 \right) \{a_n(x, y)1_A(y) + [1 - a_n(x, y)]1_A(x)\} dy.
\]

We will investigate whether one can find a sharp upper bound on \( \rho_n(P_n) \) via a drift and minorization argument based on (A1) to (A3), particularly for large \( n \).

The magnitude of the step size \( h_n \) plays an important role in the convergence of MALA. Roberts and Rosenthal (1998) argued that, if \( \pi_n \) corresponds to independent and identically distributed random components, and the chain starts from stationarity, then one should set \( h_n \) to be of order \( n^{-1/3} \). However, when the chain does not start from \( \Pi_n \), a step size of order \( n^{-1/2} \) is more appropriate (Christensen et al., 2005). Step-sizes of similar order are also recommended in more recent studies (see, e.g., Dwivedi et al., 2018).

While no concrete results have been established regarding the behavior of \( \rho_n(P_n) \) as \( n \to \infty \), recent results suggest that when \( h_n \) is chosen appropriately, \( \rho_n(P_n) \) does not tend to 1 rapidly as \( n \to \infty \) (see, e.g., Dwivedi et al., 2018). That is, it appears to be the case that MALA converges reasonably fast in high-dimensional settings. Indeed, without the Metropolis step, the algorithm is just an Euler discretization of the Langevin diffusion, which is a stochastic process defined by the stochastic differential equation

\[
dL_{n,t} = -\nabla f(L_{n,t}) \, dt + \sqrt{2} \, dW_{n,t},
\]

where \( \{W_{n,t}\} \) is the standard Brownian motion on \( X = \mathbb{R}^n \). Suppose that \( f_n \) is strongly convex with parameter \( \ell > 0 \), i.e., for each \( x, y \in X \),

\[
f_n(x) - f_n(y) - \nabla f_n(y)^T (x - y) \geq \frac{\ell}{2} \|x - y\|^2.
\]

Then under regularity conditions, the total variation distance between the distribution of \( L_{n,t} \) and \( \Pi_n \) is bounded above by a function of \( t \) which decays at a geometric rate of \( e^{-\ell/2} \) (see, e.g., Dalalyan, 2019).
It seems reasonable to believe that, when \( h_n \) is small and the Metropolis step rarely results in a rejection, \( \rho_*(P_n)^{1/h_n} \) is comparable to \( e^{-\ell/2} \). When \( \ell \) is independent of \( n \), and \( h_n \) is of order \( n^{-\gamma} \) for some constant \( \gamma > 0 \), this would suggest that \( \limsup_{n \to \infty} \rho_*(P_n)^{n^\gamma} \in [0,1) \). If this is true, then

\[
\liminf_{n \to \infty} n^\gamma[1 - \rho_*(P_n)] > 0.
\]

That is, as \( n \to \infty \), \( \rho_*(P_n) \) goes to 1 at a polynomial (or slower) rate. This is, of course, just conjecture. One possible approach to proving this assertion is to establish, for each \( n \), a set of single-step drift and minorization conditions, such as (A1) to (A3), and then to use these conditions to construct a quantitative upper bound on \( \rho_*(P_n) \). The assertion is proved if this upper bound converges to 1 at a polynomial rate as \( n \to \infty \). In what follows, we show that this argument is unlikely to work.

For simplicity, we consider the case where \( \pi_n \) satisfies the following conditions.

(H1) \( \pi_n \) corresponds to independent identically distributed random variables. That is, there exists a probability density function \( g : \mathbb{R} \to [0, \infty) \) independent of \( n \) such that, for each \( n \geq 1 \) and \( x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n \), \( \pi_n(x) = \prod_{i=1}^{n} g(x_i) \). Moreover, \( \sup_{x \in \mathbb{R}} g(x) < \infty \).

(H2) There exists a constant \( M \) such that, for each \( x_1, y_1 \in \mathbb{R} \),

\[
\left| -\frac{d \log g(x_1)}{dx_1} + \frac{d \log g(y_1)}{dy_1} \right| \leq M |x_1 - y_1|.
\]

(H1) and (H2) imply that \( f_n \) is \( M \)-smooth, i.e., for each \( x, y \in X \),

\[
\| \nabla f_n(x) - \nabla f_n(y) \| \leq M \| x - y \|.
\]

The following result is proved in Appendix C.

**Proposition 15.** Suppose that (H1) and (H2) are satisfied, and that \( h_n < n^{-\gamma} \) for some \( \gamma > 0 \). Then, for any \( \gamma' > 0 \),

\[
\lim_{n \to \infty} n^{\gamma'}[1 - \rho^*_\text{opt}(P_n)] = 0.
\]

Proposition 15 shows that, under (H1) and (H2), it is not possible to construct a simple bound based on (A1)-(A3) (and perhaps reversibility) that tends to 1 at a polynomial rate.

### 3 Quantifying the Limitations of Bounds Based on (B1)-(B3)

In this section, we develop analogues of the results in Section 2 for convergence rate bounds based on (B1)-(B3).
3.1 Optimal bounds

We will mimic what was done in Subsection 2.1 with (B1)-(B3) in place of (A1)-(A3). In this context, a “simple” upper bound based on (B1)-(B3) is one that depends on the \( \eta, L, \varepsilon, d \) parameter, but not on \( V \) or \( \nu \). For fixed \( \eta, L, \varepsilon, d \in \tilde{T}_0 := [0, 1) \times [0, \infty) \times (0, 1] \times [0, \infty] \), define \( S_{\eta, L, \varepsilon, d} \) to be the collection of Mtk\s that satisfy (B1)-(B3) with d&m parameter \( \eta, L, \varepsilon, d \). Let

\[
\rho_{\text{opt}}(\eta, L, \varepsilon, d) = \sup_{P \in S_{\eta, L, \varepsilon, d}} \rho_*(P) .
\]

This is the smallest simple upper bound that can be constructed based on (B1)-(B3) with the given d&m parameter value. Also, let \( S_{\eta, L, \varepsilon, d}^{(R)}, S_{\eta, L, \varepsilon, d}^{(N)} \), \( \rho_{\text{opt}}^{(R)}(\eta, L, \varepsilon, d) \), and \( \rho_{\text{opt}}^{(N)}(\eta, L, \varepsilon, d) \) be defined in the obvious way. Of course, as before, the parameter-specific optimal bounds are ordered as follows:

\[
\rho_{\text{opt}}^{(N)}(\eta, L, \varepsilon, d) \leq \rho_{\text{opt}}^{(R)}(\eta, L, \varepsilon, d) \leq \rho_{\text{opt}}(\eta, L, \varepsilon, d) .
\]

Here is the analogue of Theorem 8.

**Proposition 16.** For each \( \eta, L, \varepsilon, d \in \tilde{T}_0 \), we have

\[
\rho_{\text{opt}}^{(N)}(\eta, L, \varepsilon, d) \geq 1 - \varepsilon .
\]

**Proof.** Let \( \eta, L, \varepsilon, d \) be fixed, and let \( P_{\eta, L, \varepsilon, d} \) be the Mtk of a Markov chain that lives on \( \{0, 1\} \) and that adheres to the following rules:

- If \( X_m = 0 \), then \( X_{m+1} = 0 \).
- If \( X_m = 1 \), then \( X_{m+1} = 0 \) with probability \( \varepsilon \), and \( X_{m+1} = 1 \) otherwise.

It’s clear that this chain is reversible and non-negative definite. Let \( V(0) = V(1) = 0 \). Then (B1)-(B3) all hold (with \( C = X \)). It follows that \( P_{\eta, L, \varepsilon, d} \in S_{\eta, L, \varepsilon, d} \), and

\[
\rho_{\text{opt}}^{(N)}(\eta, L, \varepsilon, d) \geq \rho_*(P_{\eta, L, \varepsilon, d}) = 1 - \varepsilon .
\]

The lower bound on \( \rho_{\text{opt}}^{(N)} \) given in Proposition 16 is obviously very crude. Nevertheless, as we shall see, it’s enough to produce several interesting results. We now turn our attention to chain-specific optimal bounds.
For a Markov process \( (X, \mathcal{B}) \), define \( \tilde{T}(P) \subset \tilde{T}_0 \) as follows: \( (\eta, L, \varepsilon, d) \in \tilde{T}(P) \) if \( P \) satisfies (H1)-(H3) with this value of the \( \text{d&m} \) parameter. If \( P \) is neither reversible nor non-negative definite, then we define the chain-specific optimal upper bound on \( \rho^*(P) \) as

\[
\rho^\dagger_{\text{opt}}(P) = \inf_{(\eta, L, \varepsilon, d) \in \tilde{T}(P)} \rho_{\text{opt}}(\eta, L, \varepsilon, d).
\]

If \( P \) is reversible, but not non-negative definite, then we use

\[
\rho^\dagger_{\text{opt}}(P) = \inf_{(\eta, L, \varepsilon, d) \in \tilde{T}(P)} \rho_{\text{opt}}(R)(\eta, L, \varepsilon, d).
\]

Finally, if \( P \) is reversible and non-negative definite, then we take

\[
\rho^\dagger_{\text{opt}}(P) = \inf_{(\eta, L, \varepsilon, d) \in \tilde{T}(P)} \rho_{\text{opt}}(N)(\eta, L, \varepsilon, d).
\]

In all three cases, if \( \tilde{T}(P) = \emptyset \), then \( \rho^\dagger_{\text{opt}}(P) \) is defined to be 1.

To get a handle on \( \tilde{T}(P) \), we study the size of the small set \( C \). The following result can be found in Chapter 2 of \cite{Jerison2016}.

**Proposition 17.** \cite{Jerison2016} Suppose that (H1) - (H3) hold. Then \( \Pi(C) > 1/2 \).

**Proof.** Since \( \Pi \) is stationary, it follows from (H1) that

\[
\Pi V := \int_X V(x) \Pi(\text{d}x) \leq \eta \Pi V + L,
\]

which implies that \( \Pi V \leq L/(1 - \eta) \) \cite{Hairer2006} Proposition 4.24. On the other hand, since \( V(x) > d \) for \( x \in X \setminus C \), \( \Pi V \geq d(1 - \Pi(C)) \). Combining the upper and lower bounds on \( \Pi V \) yields

\[
1 - \Pi(C) \leq \frac{L}{d(1 - \eta)}.
\]

Hence, by (H3), \( \Pi(C) > 1/2 \). \qed

**Remark 18.** As argued in \cite{Jerison2016}, the bound \( \Pi(C) > 1/2 \) holds much more generally. Indeed, in coupling arguments, drift conditions like (H1) are usually used in conjunction with regularity conditions like (H3) to establish bivariate drift conditions of the following form.

(C1) There exist \( \lambda' < 1 \), \( K' \in [1, \infty) \), \( C' \in \mathcal{B} \), and measurable function \( V_1 : X \to [1/2, \infty) \) such that

\[
P V_1(x) + P V_1(y) \leq \lambda'[V_1(x) + V_1(y)]1_{(X \times X) \setminus (C' \times C')} + K'1_{C' \times C'}(x, y)
\]

for each \( x, y \in X \).
This type of bivariate drift condition is then used to bound the time it takes for two coupled copies of the Markov chain defined by $P$ to enter the set $C'$ simultaneously. For instance, to prove Theorem 4, Rosenthal (1995) derived (C1) for $V_1(x) = V(x) + 1/2$ and $C' = C$. (C1) is also crucial for deriving $d\varepsilon m$-based bounds in Roberts and Tweedie (1999) and Roberts and Rosenthal (2004). It turns out that, whenever (C1) holds, one must have $\Pi(C') > 1/2$. This is essentially established in Jerison (2016). We provide a more general result in Appendix D.

Remark 19. The bound $\Pi(C) > 1/2$ is also closely related to the aperiodicity of the Markov chain defined by $P$ (see, e.g., Roberts and Rosenthal, 2004). Indeed, one can easily show that, when $\Pi(C) > 1/2$ and the minorization condition (B2) holds, the chain must be aperiodic.

Proposition 17 shows that, under (B1) - (B3), the size of $C$ cannot be too small. This typically leads to a restriction on the minorization parameter $\varepsilon$, which in turn puts a bound on $\rho^\dagger_{\text{opt}}(P)$. The next result, which is the analogue of Theorem 13, is an immediate consequence of Proposition 16 in conjunction with Proposition 17.

**Theorem 20.** Let $P$ be a Mtk such that $\tilde{T}(P) \neq \emptyset$, and let $\Pi$ denote the stationary distribution. Then

$$\rho^\dagger_{\text{opt}}(P) \geq \inf_{C \in B, \Pi(C') > 1/2} \left(1 - \varepsilon_C\right),$$

where $\varepsilon_C$ is defined by (14) in Subsection 2.2.

Theorem 20 suggests that $\rho^\dagger_{\text{opt}}(P)$ is far away from 1 only if there exists a set $C$ such that $\Pi(C) > 1/2$ and $\varepsilon_C$ is large. As we shall see in the next subsection, when the state space is high-dimensional (or finite but large), such a $C$ will often not exist, even when the associated chain mixes rapidly.

### 3.2 Examples

#### 3.2.1 Gaussian autoregressive chain

Here we take one final look at the Gaussian autoregressive chain, which has Mtk given by

$$P_n(x, dy) \propto \exp\left(-\frac{2}{3} \left\| y - \frac{x}{2} \right\|^2 \right) dy, \quad x \in \mathbb{R}^n.$$ 

It is shown in Qin and Hobert (2019b) that the convergence rate bound in Theorem 4, which is based on (H1)-(H3), converges to 1 as $n \to \infty$. The following result, which is the analogue of Proposition 14, shows that, in fact, the optimal bound also converges to 1.
Proposition 21. $\rho^\dagger_{\text{opt}}(P_n) \to 1$ as $n \to \infty$.

Proof. For a given positive integer $n$, let $C_n \subset \mathbb{R}^n$ be measurable, and let $D_n$ be its diameter. Suppose that $\Pi_n(C_n) > 1/2$. Then $D_n^2/4$ must be larger than the median of the $\chi^2_n$ distribution, which we denote by $m_n$. Let $p_n(x,y)$ be the density function of $P_n(x,dy)$. Then as shown in Section 2.3.1

$$
\varepsilon_{C_n} \leq \inf_{x,x' \in C_n} \int_{\mathbb{R}^n} \min\{p_n(x,y), p_n(x',y)\} dy.
$$

One can verify that

$$
\inf_{x,x' \in C_n} \int_{\mathbb{R}^n} \min\{p_n(x,y), p_n(x',y)\} dy = 2\Phi\left(\frac{-D_n}{2\sqrt{3}}\right) \leq 2\Phi\left(-\sqrt{\frac{m_n}{3}}\right),
$$

where $\Phi(\cdot)$ is, again, the distribution function of the one-dimensional standard Gaussian distribution. By Theorem 20

$$
\rho^\dagger_{\text{opt}}(P_n) \geq 1 - 2\Phi\left(-\sqrt{\frac{m_n}{3}}\right).
$$

Since $m_n \to \infty$ as $n \to \infty$, the result follows immediately. \qed

3.2.2 Metropolis adjusted Langevin algorithm

Consider again the MALA algorithm described in Section 2.3.2, and, as before, denote its Mtk and step size by $P_n$ and $h_n$, respectively. The following analogue of Proposition 15, whose proof is given in Appendix E, shows that any simple upper bound on $\rho_\star(P_n)$ based on (B1)-(B3) converges to 1 at a faster than polynomial rate.

Proposition 22. Suppose that (H1) and (H2) are satisfied, and that $h_n < n^{-\gamma}$ for some $\gamma > 0$. Then for any $\gamma' > 0$,

$$
\lim_{n \to \infty} n^{\gamma'} [1 - \rho^\dagger_{\text{opt}}(P_n)] = 0.
$$

3.2.3 Markov chains on graphs

Let $G = (X,E)$ be an undirected simple graph, and consider a Markov chain moving on $X$. Denote its transition kernel by $P$, and its stationary distribution (which is assumed to uniquely exist) by $\Pi$. For $x, y \in X$, $P(x, \{y\}) > 0$ only if $x$ and $y$ are connected by an edge. (Note that, under this assumption, $P(x, \{x\}) = 0$ for each $x \in X$.) The chain is called a random walk if at each step it moves uniformly at random to a new vertex (with which it shares an edge). Let

$$
m_0 = \inf_{C \subset X, \Pi(C) > 1/2} \#(C),
$$

24
where \( \#(C) \) is the cardinality of \( C \subseteq X \), and let

\[
m_0 = \frac{n + 1}{2},
\]

\[
m_1 = \sup_{x \in X} d(x),
\]

where \( d(x) \) is the degree of \( x \). Then, in order for the minorization condition \((E2)\) to hold on a set \( C \), there must exist a vertex \( x_C \in X \) that’s connected to every vertex in \( C \). Therefore, when \( m_0 > m_1 \), it is impossible for \((E1)\), \((E2)\) and \((E3)\) to all hold simultaneously, so \( \rho_{\text{opt}}(P) = 1 \).

In the remainder of this subsection, we examine four different Markov chains on graphs, the first three of which are random walks. A simple example of each type of graph is provided in Figure 2. The convergence properties of these random walks are well understood (see Diaconis and Stroock, 1991). Here we simply focus on the question of whether one can construct sharp bounds on the (known) convergence rates by establishing \((B1)\) to \((B3)\).

**Random walk on \( \mathbb{Z}/n\mathbb{Z} \).** Let \( n \geq 3 \) be an odd number, and let \( X = \mathbb{Z}/n\mathbb{Z} = \{\overline{0}, \overline{1}, \ldots, \overline{n-1}\} \), the set of integers mod \( n \). Arrange the elements of \( X \) in a loop, so that two vertices are connected if and only if they differ by \( \overline{1} \). For each \( \overline{x} \in X \), \( P(\overline{x}, \{\overline{y}\}) = 1/2 \) for \( \overline{y} = \overline{x} - \overline{1} \) and \( \overline{y} = \overline{x} + \overline{1} \). It’s easy to verify that the stationary distribution is uniform, \( m_0 = (n+1)/2 \), and \( m_1 = 2 \). It follows that \((E2)\) and \((E3)\) cannot hold simultaneously whenever \( n \geq 5 \). On the other hand, the true convergence rate \( \rho_*(P) \) is always strictly less than 1, and \( 1 - \rho_*(P) \) is of order \( n^{-2} \) when \( n \) is large.

**Random walk on \((\mathbb{Z}/2\mathbb{Z})^n\).** Let \( X = (\mathbb{Z}/2\mathbb{Z})^n \) be the set of binary \( n \)-tuples, where \( n \geq 2 \) is a positive integer. Two vertices in \( X \) are neighbors if all their components coincide except for one. Thus, the degree of each vertex is \( n \), and \( m_1 = n \). For each \( x \in X \) and its neighbor \( y \), \( P(x, \{y\}) = 1/n \). Again, the stationary distribution is uniform, and it’s easy to see that \( m_0 = 2^{n-1} + 1 \). Hence, it’s impossible for \((E2)\) and \((E3)\) to hold simultaneously. In truth, \( \rho_*(P) = 1 - 2/n \).
Random walk on binary tree. Consider the full binary tree of depth $n$, where $n \geq 1$. The degree of any vertex is either 1, 2, or 3. For each $x \in X$ and its neighbor $y$, $P(x, \{y\}) = 1/d(x)$. It can be shown that, for each $x \in X$, $\Pi(\{x\}) = d(x)/[2(2^{n+1} - 2)]$. Therefore, $m_0 > (2^{n+1} - 2)/3$, and $m_1 = 3$. It follows that (B1) and (B2) cannot hold simultaneously when $n \geq 3$. In truth, $\rho^* \leq 1$, and $1 - \rho^* \leq O(2^{-n})$ for large $n$.

Lazy random walk on a “star”. Consider a graph with a central vertex, $x_0$, and $n$ outside vertices, $x_1, x_2, \ldots, x_n$. Each outside vertex is connected to $x_0$ but not to other vertices. For this example, we allow the chain to be lazy, i.e., we no longer assume that $P(x, \{x\}) = 0$ for each $x \in X$. To be specific, assume that

$$P(x_0, \{x_i\}) = \theta_{1_i=0} + \frac{1 - \theta}{n}1_{i \neq 0},$$

and that, for $i \neq 0$,

$$P(x_i, \{x_j\}) = \theta_{1_{j=i}} + (1 - \theta)1_{j=0},$$

where $\theta \in (0, 1)$ is a constant. In this case, $\rho^*(P) = \max\{\theta, 1 - 2\theta\}$, which is independent of $n$.

It can be verified that $\Pi(\{x_0\}) = 1/2$, and $\Pi(\{x_i\}) = 1/(2n)$ for $i \neq 0$. Therefore, $\Pi(C) > 1/2$ if and only if $\{x_0\}$ is a proper subset of $C$. It’s not difficult to verify that when $C = \{x_0, x_i\}$ for some $i \neq 0$,

$$\varepsilon_C = \min\{\theta, (1 - \theta)/n\} + \min\{1 - \theta, \theta\}.$$

If $C$ contains additional elements, $\varepsilon_C$ is, of course, smaller. By Theorem 20,

$$\rho^*_opt(P) \geq \max\{\theta, 1 - \theta\} - \min\{\theta, (1 - \theta)/n\}. $$

This does not rule out the possibility of obtaining a sharp upper bound on $\rho^*(P)$ based on (B1) to (B3). Indeed, letting $V(x_i) = 0$ for $i = 0, 1, \ldots, n$, one can show that (B1) holds with $\eta = 0$, $L = 0$, while (B2) and (B3) hold with $d > 0$ and $\varepsilon = \min\{\theta, 1 - \theta\}$. Plugging these parameters into Theorem 4 and letting $d \to \infty$ yields a coupling-based upper bound on the true convergence rate $\rho^*(P)$, that is,

$$1 - \varepsilon = \max\{\theta, 1 - \theta\}.$$

Note that this bound is tight whenever $\theta \geq 1/2$.

4 Discussion

We have demonstrated that methods based on single-step d&k can have serious limitations in the construction of convergence rate bounds for Markov chains. On the other hand, it is certainly not
the case that these methods are incapable of producing sharp bounds, see, e.g., Yang and Rosenthal (2019); Qin and Hobert (2019a); Ekvall and Jones (2019). It’s also worth noting that we’ve only examined the most basic version of drift and minorization. Indeed, it is well-known that multi-step drift and minorization can lead to sharp convergence rate bounds even in situations where single-step methods fail completely. Unfortunately, it is almost always impossible to get a handle on (much less a closed form for) the multi-step Mtk associated with practically relevant Monte Carlo Markov chains. As such, sharp multi-step drift and minorization inequalities are typically out of reach. For a more detailed discussion on this issue, see, e.g., Section 2 of Qin and Hobert (2019b).

More generally, one can construct coupling schemes that take into account the multi-step dynamics of a Markov chain, and these can lead to sharp convergence rate bounds. One such technique is one-shot coupling (Roberts and Rosenthal, 2002), which can be understood as constructing convergence bounds with respect to some Wasserstein distance, and then transforming these to total variation bounds (Madras and Sezer, 2010). These types of techniques are promising because convergence rate bounds with respect to Wasserstein distances are often more robust to increasing dimension, see, e.g., Hairer et al. (2014); Bou-Rabee et al. (2018); Durmus and Moulines (2019); Qin and Hobert (2019b). Finally, the idea of drift and minorization can also be employed to convergence analysis with respect to Wasserstein distances, and this idea has led to a series of useful results (see, e.g., Hairer et al., 2011; Butkovsky, 2014; Douc et al., 2018).

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Appendix

A Proof of Theorem 11

Proof. (A1) implies that

\[ PV(x) \leq \lambda V(x) + K1_C(x). \]

Along with the other assumptions, this drift condition implies that the chain is geometrically ergodic (Meyn and Tweedie, 2009 Theorem 15.0.1). Thus, \( P \) admits a unique stationary distribution \( \Pi \).

If \( \lambda = 0 \), then \( PV(x) \leq 0 \) for each \( x \notin C \). Since \( V \geq 1 \), this implies that \( C = X \), and \( \Pi(C) = 1 \).

In the remainder of the proof, we assume that \( \lambda \in (0, 1) \).
Note that $C \neq \emptyset$. Otherwise, (A1) implies that $P^m V(x) \leq \lambda^m V(x)$ for each positive integer $m$ and $x \in X$. This implies that $P^m V(x) < 1$ for sufficiently large $m$, which is not possible since $V \geq 1$.

Let $\{X_m\}_{m=0}^{\infty}$ be a chain evolving according to $P$ such that $X_0 \in C$ is fixed, and let $\{F_m\}$ be its natural filtration. For $m \geq 1$, let $N_m = \sum_{i=0}^{m-1} 1_C(X_i)$, and set $N_0 = 0$. We now use a standard argument to bound $\mathbb{P}(N_m \geq i)$ for a positive integer $i$ (see, e.g., Roberts and Rosenthal 2004). For any positive integer $j$, let

$$Z_j = (\lambda^{-1} K)^{-N_j} \lambda^{-j} V(X_j).$$

If $X_{j-1} \notin C$, then $N_j = N_{j-1}$, and

$$\mathbb{E}(Z_j | F_{j-1}) = (\lambda^{-1} K)^{-N_{j-1}} \lambda^{-j} \mathbb{E}[V(X_j)|X_{j-1}] \leq (\lambda^{-1} K)^{-N_{j-1}} \lambda^{-j} \lambda V(X_{j-1}) = Z_{j-1}.$$

If $X_{j-1} \in C$, then $N_j = N_{j-1} + 1$, and

$$\mathbb{E}(Z_j | F_{j-1}) = (\lambda^{-1} K)^{-N_{j-1}} \lambda^{-j} \mathbb{E}[V(X_j)|X_{j-1}] \leq (\lambda^{-1} K)^{-N_{j-1}} \lambda^{-j} \lambda \leq Z_{j-1}.$$

It follows that

$$\mathbb{E}Z_m \leq \mathbb{E}Z_1 \leq (\lambda^{-1} K)^{-1}.$$

By Markov’s inequality,

$$\mathbb{P}(N_m < i) \leq \mathbb{E}(\lambda^{-1} K)^{i-1-N_m} \leq (\lambda^{-1} K)^i \lambda^m \mathbb{E}Z_m \leq (\lambda^{-1} K)^{i-1} \lambda^m.$$

For a positive integer $m$, let $i_m = \lceil m \log \lambda^{-1}/(\log \lambda^{-1} + \log K) \rceil$. Then $(\lambda^{-1} K)^{i_m} \leq \lambda^{-m}$. It follows that

$$\mathbb{E}N_m \geq \sum_{i=1}^{i_m} \mathbb{P}(N_m \geq i) \geq i_m - \lambda^m (\lambda^{-1} K)^{i_m} \geq i_m - \frac{1 - \lambda^m}{\lambda^{-1} K - 1}. \tag{18}$$

The strong law of large numbers holds for any ergodic chain (Tierney 1994). Therefore, $N_m/m \to \Pi(C)$ as $m \to \infty$, almost surely. Since $N_m/m$ is bounded, by the dominated convergence theorem,

$$\mathbb{E}N_m/m \to \Pi(C) \text{ as } m \to \infty.$$ Then (18) implies that

$$\Pi(C) \geq \frac{\log \lambda^{-1}}{\log K + \log \lambda^{-1}}.$$

\[\square\]

**B Proof of Proposition 14**

*Proof.* By (16),

$$\rho_n^* = \inf_{D > 0} \left[ 1 - 2\Phi \left( \frac{D}{2\sqrt{3}} \right) \right]^{1/|\alpha_n(D)|} \leq \rho_{opt}(P_n) \leq 1,$$

28
where
\[ \alpha_n(D) = \left( \int_0^{D^2/4} f_n(x) \, dx \right)^{-1}, \]
and \( f_n \) is the density function of the \( \chi_n^2 \) distribution. It suffices to show that \( \rho_n^a \to 1 \) as \( n \to \infty \).

Let \( \delta > 0 \) be arbitrary. There exists \( M_\delta > 0 \) such that
\[ 1 - 2\Phi \left( -\frac{D}{2\sqrt{3}} \right) \geq 1 - \delta \]
whenever \( D \geq M_\delta \). Since \( \alpha_n(D) \) is bounded below by 1,
\[ \left[ 1 - 2\Phi \left( -\frac{D}{2\sqrt{3}} \right) \right]^{1/\lfloor \alpha_n(D) \rfloor} \geq 1 - \delta \quad \forall D \geq M_\delta. \] (19)

Now, let \( 0 < D < M_\delta \). By the mean value theorem,
\[ 1 - 2\Phi \left( -\frac{D}{2\sqrt{3}} \right) \geq A_\delta D, \]
where
\[ A_\delta = \frac{1}{\sqrt{6\pi}} \exp \left( -\frac{M_\delta^2}{24} \right). \]

The mode of \( f_n(\cdot) \) is known to be \( n - 2 \) for \( n \geq 2 \). For \( n \geq M_\delta^2/4 + 2 \),
\[ \frac{1}{\alpha_n(D)} = \int_0^{D^2/4} f_n(x) \, dx \leq \frac{f_n(M_\delta^2/4)}{4} D^2. \]

It follows that, when \( n \geq M_\delta^2/4 + 2 \),
\[ \frac{1}{\lfloor \alpha_n(D) \rfloor} \leq \left[ \frac{4}{f_n(M_\delta^2/4) D^2} \right]^{-1}. \]

Recall that, for each \( x > 0 \),
\[ f_n(x) = \frac{1}{2^{n/2} \Gamma(n/2)} x^{n/2-1} e^{-x/2}. \]

It’s easy to verify that, as \( n \to \infty \), \( f_n(x) \to 0 \). It follows that there exists \( N_\delta > M_\delta^2/4 + 2 \) such that, for each \( n \geq N_\delta \),
\[ \left[ \frac{4}{f_n(M_\delta^2/4) D^2} \right]^{-1} \leq \left( \frac{4}{f_n(M_\delta^2/4) D^2} - 1 \right)^{-1} \leq \frac{f_n(M_\delta^2/4) D^2}{4 - f_n(M_\delta^2/4) M_\delta^2} \leq B_\delta D^2, \]
where
\[ B_\delta = -2eA_\delta^2 \log(1 - \delta). \]

Thus, for \( n \geq N_\delta \) (and \( D \in (0, M_\delta) \)),
\[ \left[ 1 - 2\Phi \left( -\frac{D}{2\sqrt{3}} \right) \right]^{1/\lfloor \alpha_n(D) \rfloor} \geq (A_\delta D)^{B_\delta D^2}. \]
It can be shown that
\[ \inf_{x > 0} (A_\delta x)^{B_\delta x^2} = 1 - \delta. \]
Combining this fact with \([19]\) shows that
\[ \inf_{D > 0} \left[ 1 - 2\Phi \left( -\frac{D}{\sqrt{2}h} \right) \right] \frac{1}{G_n(D)} \geq 1 - \delta \]
whenever \( n \geq N_\delta \). This completes the proof. \(\square\)

C Proof of Proposition \([15]\)

Proof. The proof is an application of Theorem \([13]\). For a positive integer \( n \), let \( C_n \) be a measurable subset of \( \mathbb{R}^n \) such that \( \Pi_n(C_n) > 0 \). Since \( \Pi_n \) admits a density function, the diameter of \( C_n \), which we denote by \( D_n \), must be non-vanishing. It’s clear that \( \Pi_n(C_n) \leq (GD_n)^n \), where \( G = \sup_{x \in \mathbb{R}} g(x) < \infty \), and \( g : \mathbb{R} \to [0, \infty) \) is defined in Condition \((H1)\).

Next, we bound \( \varepsilon_{C_n} \). To this end, first note that the transition kernel of a MALA chain can be written as
\[ P_n(x, dy) = a_n(x, y)q_n(x, y) dy + \int_X \left[ 1 - a_n(x, z) \right] q_n(x, z) dz \delta_x(dy), \quad x \in X, \]
where \( q_n(x, \cdot) \) is the probability density function of the \( N_n(x - h_n \nabla f_n(x), 2h_n I_n) \) distribution, and \( a_n(\cdot, \cdot) \leq 1 \) is defined as in \([17]\). Suppose that \((A2)\) holds on \( C_n \) with \( \varepsilon_n > 0 \) and probability measure \( \nu_n \). Let \( x, x' \in C_n \) be such that \( x \neq x' \). Then
\[ a_n(x, y)q_n(x, y) dy + \int_X \left[ 1 - a_n(x, z) \right] q_n(x, z) dz \delta_x(dy) \geq \varepsilon_n \nu_n(dy), \]
and
\[ a_n(x', y)q_n(x', y) dy + \int_X \left[ 1 - a_n(x', z) \right] q_n(x', z) dz \delta_{x'}(dy) \geq \varepsilon_n \nu_n(dy). \]
It’s easy to see that \( \nu_n(\{x\}) = \nu_n(\{x'\}) = 0 \), and thus, almost surely,
\[ q_n(x, y) \geq \varepsilon_n \nu_n(dy)/dy \quad \text{and} \quad q_n(x', y) \geq \varepsilon_n \nu_n(dy)/dy. \]

It follows that
\[ \varepsilon_n \leq \int_X \min\{q_n(x, y), q_n(x', y)\} dy = 2\Phi \left( -\frac{\|x - h_n \nabla f_n(x) - x' + h_n \nabla f_n(x')\|}{2\sqrt{2}h_n} \right). \]
Recall that, under \((H1)\) and \((H2)\), \( f_n \) is \( M \)-smooth. Thus, whenever \( h_n M < 1 \),
\[ \|x - h_n \nabla f_n(x) - x' + h_n \nabla f_n(x')\| \geq (1 - h_n M)\|x - x'\|. \]
Letting $x$ and $x'$ vary in $C_n$ shows that
\[
\varepsilon_{C_n} \leq 2\Phi\left( \frac{(1 - h_n M) D_n}{2\sqrt{2h_n}} \right).
\]

By Theorem 13 and the assumption that $h_n < n^{-\gamma}$, for $n$ large enough, $1 - h_n M > 1/\sqrt{2}$, and
\[
\rho^\ast_{opt}(P_n) \geq \inf_{D > 0} \left[ 1 - 2\Phi\left( \frac{(1 - h_n M) D}{2\sqrt{2h_n}} \right) \right]^{(GD)^{-n}]^{-1}\wedge 1}
\geq \inf_{D > 0} \left[ 1 - 2\Phi\left( -Dn^{\gamma/2}/4 \right) \right]^{(GD)^{-n}]^{-1}\wedge 1},
\]
where $a \wedge b$ means $\min\{a, b\}$. When $D > 1/(2G)$,
\[
\left[ 1 - 2\Phi\left( -Dn^{\gamma/2}/4 \right) \right]^{(GD)^{-n}]^{-1}\wedge 1} \geq 1 - 2\Phi(-n^{\gamma/2}/(8G)).
\]  \hfill (20)

When $D \leq 1/(2G)$, $[(GD)^{-n}] \geq (2^{n-1} - 1)(GD)^{-1}$. This implies that, whenever $D \leq 1/(2G)$ and $n > 1$,
\[
\left[ 1 - 2\Phi\left( -Dn^{\gamma/2}/4 \right) \right]^{(GD)^{-n}]^{-1}\wedge 1} \geq \left[ 1 - 2\Phi\left( -Dn^{\gamma/2}/4 \right) \right]^{GD/(2^{n-1}-1)}
\geq \left\{ \inf_{x > 0} \left[ 1 - 2\Phi(-x/4) \right]^{Gx} \right\}^{1/(2^{n-1}n^{\gamma/2} - n^{\gamma}/2)} \geq \left\{ \inf_{x > 0} \left[ 1 - 2\Phi(-x/4) \right] \right\}^{Gx} \geq \left\{ \inf_{x > 0} \left[ 1 - 2\Phi(-x/4) \right] \right\}^{Gx} \geq \left\{ \inf_{x > 0} \left[ 1 - 2\Phi(-x/4) \right] \right\}^{Gx}.
\]  \hfill (22)

To proceed, we study the asymptotic behavior of the right-hand sides of (21) and (22). One can verify that, for any $\gamma' > 0$, as $n \to \infty$, $n^{\gamma'} \Phi(-n^{\gamma/2}/(8G)) \to 0$. Moreover,
\[
c = \inf_{x > 0} \left[ 1 - 2\Phi(-x/4) \right]^{Gx} > 0,
\]
which implies that, for any $\gamma' > 0$,
\[
\lim_{n \to \infty} n^{\gamma'} \left[ 1 - e^{1/(2^{n-1}n^{\gamma/2} - n^{\gamma}/2)} \right] = 0.
\]

The proof is completed by combining (20), (21), and (22).

\section*{D Proof of an Assertion in Remark 18}

For a set $\tilde{C} \in \mathcal{B} \times \mathcal{B}$, let
\[
\tilde{C}_1 = \{ x \in X : (x, y) \in \tilde{C} \}, \quad \tilde{C}_2 = \{ y \in X : (x, y) \in \tilde{C} \}
\]
be its projections. The following is a generalization of Jerison's (2016) Proposition 2.16.
Proposition 23. Let $P$ be a transition kernel that admits a stationary distribution $\Pi$. Suppose that there exist $\lambda' < 1$, $K' \in (0, \infty)$, $\tilde{C} \in \mathcal{B} \times \mathcal{B}$, and measurable functions $V_1 : X \to [0, \infty)$ and $V_2 : X \to [0, \infty)$ such that $\inf_{x,y \in X} [V_1(x) + V_1(y)] > 0$, where $\hat{C}_i \in \mathcal{B}$ for $i = 1, 2$, and

$$PV_1(x) + PV_2(y) \leq \lambda'[V_1(x) + V_2(y)]1_{(X \times X) \setminus \tilde{C}}(x, y) + K'1_{\tilde{C}}(x, y)$$

for each $x, y \in X$. Then $\Pi(\tilde{C}_1) + \Pi(\tilde{C}_2) > 1$.

Proof. Let $\tilde{\Pi}$ be a probability measure on $(X \times X, \mathcal{B} \times \mathcal{B})$ such that, for each $A \in \mathcal{B}$,

$$\tilde{\Pi}(A \times X) = \tilde{\Pi}(X \times A) = \Pi(A). \quad (23)$$

In other words, $\tilde{\Pi}$ is the joint distribution of some random element $(X, Y)$ such that, marginally, $X$ and $Y$ are distributed as $\Pi$. By assumption, for each $x, y \in X$,

$$PV_1(x) + PV_2(y) \leq \lambda'V_1(x) + \lambda'V_2(y) + K'1_{\tilde{C}}(x, y).$$

Taking expectations on both sides with respect to $\tilde{\Pi}(dx, dy)$ yields

$$\Pi V_1 + \Pi V_2 \leq \lambda' \Pi V_1 + \lambda' \Pi V_2 + K'\tilde{\Pi}(\tilde{C}),$$

where $\Pi V_i = \int_X V_i(x)\Pi(dx)$. By Proposition 4.24 in [Hairer (2006)], $\Pi V_1 + \Pi V_2 < \infty$. It follows that

$$K'\tilde{\Pi}(\tilde{C}) \geq (1 - \lambda')(\Pi V_1 + \Pi V_2) \geq (1 - \lambda') \inf_{x,y \in X} [V_1(x) + V_1(y)] > 0.$$

Since $K' < \infty$, $\tilde{\Pi}(\tilde{C}) > 0$.

It’s now straightforward to prove the result by contradiction. Suppose that $\Pi(\tilde{C}_1) + \Pi(\tilde{C}_2) \leq 1$, and note that $\tilde{C} \subset \tilde{C}_1 \times \tilde{C}_2$. We only need to construct a joint distribution $\tilde{\Pi}$ such that \eqref{eq:prop23} holds and $\tilde{\Pi}(\tilde{C}_1 \times \tilde{C}_2) = 0$. If $\Pi(\tilde{C}_1) = 1$ or $\Pi(\tilde{C}_2) = 1$, then we only need to set $\tilde{\Pi}(dx, dy) = \Pi(dx)\Pi(dy)$. Suppose that $\Pi(\tilde{C}_1)$ and $\Pi(\tilde{C}_2)$ are both strictly less than 1. Define $\tilde{\Pi}$ as follows:

$$\tilde{\Pi}(dx, dy) = \left\{ \frac{1_{\tilde{C}_1 \times (X \setminus \tilde{C}_2)}(x, y)}{1 - \Pi(\tilde{C}_2)} + \frac{1_{(X \setminus \tilde{C}_1) \times \tilde{C}_2}(x, y)}{1 - \Pi(\tilde{C}_1)} + \frac{[1 - \Pi(\tilde{C}_1) - \Pi(\tilde{C}_2)]1_{(X \setminus \tilde{C}_1) \times (X \setminus \tilde{C}_2)}(x, y)}{[1 - \Pi(\tilde{C}_1)][1 - \Pi(\tilde{C}_2)]} \right\} \Pi(dx)\Pi(dy).$$

It’s easy to verify that $\tilde{\Pi}$ is a probability measure that satisfies \eqref{eq:prop23} and that $\tilde{\Pi}(\tilde{C}_1 \times \tilde{C}_2) = 0$. This completes the proof. \hfill $\Box$

The bivariate drift condition in Proposition 23 is very common among works that utilize d&m and coupling. Usually, $V_1$ and $V_2$ are taken to be the same univariate drift function, and $\tilde{C}$ is either the Cartesian product of a small set with itself, or a level set of the additive bivariate drift function $V_1(x) + V_2(y)$. In particular, taking $V_1 = V_2$ and $\tilde{C} = C' \times C'$ yields (C) in Remark 18.
E Proof of Proposition 22

Proof. The proof is an application of Theorem 20. Let $n$ be fixed. Let $C_n \subset \mathbb{R}^n$ be measurable, and denote its diameter by $D_n$. Note that $\Pi_n(C_n) \leq (GD_n)^n$, where $G = \sup_{x \in \mathbb{R}} g(x) < \infty$. When $\Pi_n(C_n) > 1/2$,

$$D_n \geq \frac{1}{2^{1/n}G} \geq \frac{1}{2G}.$$  

(24)

Recall that $M > 0$ is a constant defined in Condition (H2). In the proof of Proposition 15 it is shown that, whenever $h_n M < 1$,

$$\varepsilon_{C_n} \leq 2\Phi\left(-\frac{(1 - h_n M)D_n}{2\sqrt{2}h_n}\right).$$

If $\Pi_n(C_n) > 1/2$ and thus, (24) holds, then

$$1 - \varepsilon_{C_n} \geq 1 - 2\Phi\left(-\frac{1 - h_n M}{4\sqrt{2}h_n G}\right).$$

Recall that $h_n < n^{-\gamma}$. By Theorem 20 for sufficiently large $n$, $h_n M \leq 1/\sqrt{2}$, and

$$\rho^*_\text{opt}(P_n) \geq 1 - 2\Phi\left(-\frac{1 - h_n M}{4\sqrt{2}h_n G}\right) \geq 1 - 2\Phi\left(-\frac{n^{\gamma/2}}{8G}\right).$$

The asymptotic behavior of $\Phi(x)$ as $x \to -\infty$ yields the desired result.

\[\square\]

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