TWO CONVERGENCE PROPERTIES OF HYBRID SAMPLERS

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Theoretical work on Markov chain Monte Carlo (MCMC) algorithms has so far mainly concentrated on the properties of simple algorithms, such as the Gibbs sampler, or the full-dimensional Hastings-Metropolis algorithm. In practice, these simple algorithms are used as building blocks for more sophisticated methods, which we shall refer to as *hybrid samplers*. It is often hoped that good convergence properties (e.g., geometric ergodicity, etc.) of the building blocks will imply similar properties of the hybrid chains. However, little is rigorously known.

In this paper, we concentrate on two special cases of hybrid samplers. In the first case, we provide a quantitative result for the rate of convergence of the resulting hybrid chain. In the second case, concerning the combination of various Metropolis algorithms, we establish geometric ergodicity.

1. Introduction. Theoretical work on Markov chain Monte Carlo (MCMC) algorithms has so far mainly concentrated on the properties of simple algorithms such as the Gibbs sampler or the full-dimensional Hastings-Metropolis algorithm. This is understandable since even these simple algorithms are difficult to analyse and are still not fully understood. In practice, these simple algorithms are used as building blocks for more sophisticated methods, which we shall refer to as *hybrid samplers*. It is often hoped that good convergence properties of the building blocks will translate to properties of the hybrid chains; however, to date, very little work has been done to try and make these arguments rigorous. This article attempts to build on the results of Roberts and Rosenthal (1997), which considered geometric ergodicity properties of hybrid chains in terms of their constituent component algorithms.

In this paper, we concentrate on two special cases, where we can make more practical geometric ergodicity statements. In the first case, we are actually able to give a quantitative result for the rate of convergence of the resulting hybrid algorithm, although this is at the expense of imposing a very strong uniform type of geometric ergodicity on the constituent component algorithms. In the second case, we consider hybrid chains arising from combining various Metropolis algorithms, and adapt results of Roberts and Tweedie (1996) to establish geometric ergodicity.

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2. Preliminaries. Recall that, given a probability distribution $\pi(\cdot)$ on the state space $\mathscr{X} = \mathscr{X}_1 \times \mathscr{X}_2 \times \cdots \times \mathscr{X}_k$, the usual deterministic-scan Gibbs sampler (DUGS) is the Markov kernel $P = Q_1 Q_2 \cdots Q_k$, where Q_i is the Markov kernel which replaces the *i*th coordinate by a draw from $\pi(dx_i | \{x_j\}_{j \neq i})$, leaving x_j fixed for $j \neq i$. The random-scan Gibbs sampler (RSGS), given by $P = (1/k) \sum_i Q_i$, is sometimes used instead. These are standard Markov chain Monte Carlo techniques [see, e.g., Gelfand and Smith (1990); Smith and Roberts (1993); Tierney (1994)].

Often the full conditionals $\pi(dx_i | \{x_j\}_{j \neq i})$ may be easily sampled, so that DUGS or RSGS may be efficiently run on a computer. However, sometimes this is not feasible. Instead, one can define new operators P_i which are easily implemented, such that P_i^n converges to Q_i as $n \to \infty$. This is the method of "variable-at-a-time Metropolis–Hastings" or "Metropolis within Gibbs" [cf. Tierney (1994), Section 2.4; Chan and Geyer (1994), Theorem 1; Green (1994); Metropolis, Rosenbluth, Rosenbluth, Teller and Teller (1953)]. Such samplers prompt the following definition [taken from Roberts and Rosenthal (1997)].

DEFINITION. Let $C = (P_1, P_2, \ldots, P_k)$ be a collection of Markov kernels on a state space \mathscr{X} . The random-scan hybrid sampler for C is the sampler defined by

$$P_{\rm RS} = \frac{1}{k} (P_1 + \dots + P_k).$$

In addition to the mentioned variable-at-a-time Metropolis–Hastings algorithms, such hybrid samplers often arise when larger MCMC algorithms are "constructed" out of smaller ones. For example, if the P_i are themselves RSGS samplers, then the random-scan hybrid sampler would correspond to building a large Gibbs sampler out of smaller ones. Similarly, if the P_i are themselves Metropolis–Hastings algorithms, then the hybrid sampler can again be viewed as a Metropolis–Hastings algorithm, but with (in general) a singular proposal distribution [cf. Tierney (1995)]; this is considered further in Section 4.

Theoretical properties of such hybrid samplers were considered in Roberts and Rosenthal (1997). In particular, it was shown (Theorem 6) that if, for a particular model, RSGS is geometrically ergodic in an appropriate sense [say, in $L^2(\pi)$] and if $(P_i)^n \to Q_i$ as $n \to \infty$ [again, say, in $L^2(\pi)$], then the resulting random-scan hybrid sampler would again be geometrically ergodic.

However, such a result leads to further questions. First, is it possible to provide any *quantitative bounds* for these hybrid samplers? Second, can geometric ergodicity be established for, say, Metropolis-Hastings algorithms [which are ergodic but do *not* converge in $L^2(\pi)$]?

The first of these questions is addressed in the next section, and the second is addressed in the final section of this paper. **3. Strong uniform ergodicity and quantitative bounds.** An important and difficult problem in the theory of MCMC algorithms is to provide quantitative bounds on their distance to stationarity after a finite number of steps. Such bounds can then be used to determine how long to run the algorithm in practice, to achieve sufficient accuracy of results. While there have been some successes with this approach [see, e.g., Meyn and Tweedie (1994); Rosenthal (1995)], the question of quantitative bounds in general remains problematic.

In this section, we provide quantitative bounds on convergence rates for hybrid samplers, under a strong hypothesis about uniform convergence of the constituent Markov chains. We recall that a Markov chain is *uniformly ergodic* if there is $N \in \mathbf{N}$ and $\rho < 1$ such that $\|P^N(x, \cdot) - \pi(\cdot)\|_{\text{var}} \leq \rho$ for all $x \in \mathscr{X}$, or equivalently [cf. Meyn and Tweedie (1993), Theorem 16.0.2], if $\sup_{x \in \mathscr{X}} \|P^n(x, \cdot) - \pi(\cdot)\|_{\text{var}} \to 0$ as $n \to \infty$.

DEFINITION. A Markov chain $P(\cdot, \cdot)$ on a state space \mathscr{X} , with stationary distribution $\pi(\cdot)$, is (N, ε) -strongly uniformly ergodic for some $N \in \mathbf{N}$ and $\varepsilon > 0$ if

$$P^N(x,\cdot) \ge \varepsilon \pi(\cdot), \qquad x \in \mathscr{X}.$$

For such a chain, it follows that for $n \ge 0$,

$$P^{N+n}(x,\cdot) = \int P^N(x,dy) P^n(y,\cdot) \ge \int \varepsilon \pi(dy) P^n(y,\cdot) = \varepsilon \pi(\cdot).$$

In particular, *P* is also (k, ε) -strongly uniformly ergodic for any $k \ge N$.

It also follows immediately [see, e.g., Meyn and Tweedie (1993), Theorem 16.0.2] that $||P^{tN}(x, \cdot) - \pi(\cdot)||_{\text{var}} \leq (1 - \varepsilon)^t$ for t = 1, 2, ..., for any $x \in \mathscr{X}$; thus, strong uniform ergodicity implies uniform ergodicity. The converse to this implication is considered in the following proposition.

PROPOSITION 1. In general, a uniformly ergodic Markov chain need not be strongly uniformly ergodic. However, if a Markov chain is both uniformly ergodic and reversible, then it is strongly uniformly ergodic.

PROOF. For a counterexample, let \mathscr{X} be the set of all nonnegative integers, and set $P(n,0) = P(n, n + 1) = \frac{1}{2}$ for all $n \in \mathscr{X}$. Then this Markov chain is easily seen to be uniformly ergodic, but not strongly uniformly ergodic.

Suppose now that the Markov chain is reversible. By uniform ergodicity, we have that $P^n(x, \cdot) \ge \varepsilon \nu(\cdot)$ for all $x \in \mathscr{X}$, for some $n \in \mathbf{N}$, $\varepsilon > 0$ and probability measure ν on \mathscr{X} [cf. Meyn and Tweedie (1993), Theorem 16.0.2]. Then, by reversibility,

$$\pi(dx)P^n(x,dy) = \pi(dy)P^n(y,dx) \ge \pi(dy)\varepsilon\nu(dx), \qquad x,y\in\mathscr{X},$$

so that $P^n(x, dy) \ge \varepsilon (d\nu/d\pi)(x)\pi(dy)$. Choose $A \subseteq \mathscr{X}$ and $\delta > 0$ such that $(d\nu/d\pi)(x) > \delta$ for all $x \in A$, and $\pi(A) > 0$ [so that $\nu(A) > 0$]. Then for any $z \in \mathscr{X}$, setting $K = \varepsilon^2 \delta \nu(A) > 0$, we have

$$P^{2n}(z, dy) \ge P^n(z, A) \inf_{x \in A} P^n(x, dy) \ge \varepsilon \nu(A) \varepsilon \delta \pi(dy) = K \pi(dy),$$

as required. \Box

REMARK. It is easily seen that being strongly uniformly ergodic is equivalent to the existence of a strong stationary time [cf. Aldous and Diaconis (1987)] which is independent of the process itself.

We now use strong uniform ergodicity to establish quantitative bounds on certain hybrid samplers. We adopt the notation

$$egin{aligned} &x_{-i}=(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_k),\ &\mathscr{X}_{-i}=\mathscr{X}_1 imes\cdots imes\mathscr{X}_{i-1} imes\mathscr{X}_{i+1} imes\cdots imes\mathscr{X}_k \end{aligned}$$

and

$$x_{-i}^* = \{x_1\} \times \cdots \times \{x_{i-1}\} \times \mathscr{X}_i \times \{x_{i+1}\} \times \cdots \times \{x_k\}.$$

THEOREM 2. Let $\pi(\cdot)$ be a probability distribution on a state space $\mathscr{X} = \mathscr{X}_1 \times \cdots \times \mathscr{X}_k$. For $1 \leq i \leq k$, let $N_i \in \mathbb{N}$ and $\varepsilon_i > 0$ be given and let P_i be a Markov kernel on \mathscr{X} which fixes coordinates other than i. Assume that for each $x_{-i} \in \mathscr{X}_{-i}$, $P_i|_{x_{-i}^*}$ has stationary distribution $\pi(\cdot|x_{-i})$ and is (N_i, ε_i) -strongly uniformly ergodic. Assume further that RSGS, with stationary distribution $\pi(\cdot)$, is (N', ε') -strongly uniformly ergodic. Then the random-scan hybrid sampler $P_{\mathrm{RS}} = (1/k)(P_1 + \cdots + P_k)$ is (N_*, ε_*) -strongly uniformly ergodic, where

$$N_* = N' \max_{1 \le i \le k} \{N_i\}, \qquad \varepsilon_* = \varepsilon' \min_{1 \le i \le k} \{\varepsilon_i^{N'}\} k^{-N'(\max_{1 \le i \le k} \{N_i\} - 1)}.$$

REMARKS. We emphasise that this theorem requires the associated RSGS to be strongly uniformly ergodic; this may not be easy to verify in practice. We also note that, as seen from the proof, this result is rather crude for large values of N_i and N'; it is most useful when $N_1 = \cdots = N_k = N' = 1$.

PROOF. As usual, let Q_i be the Markov kernel which replaces the *i*th coordinate by a draw from $\pi(dx_i | x_{-i})$, leaving x_{-i} fixed.

It follows from the hypotheses that

$$P_i^n(x, \cdot) \ge \varepsilon_i Q_i(x, \cdot), \qquad n \ge N_i, \qquad i = 1, 2, \dots, k,$$

and

$$\left[rac{1}{k}ig(Q_1(x,\cdot)+\cdots+Q_k(x,\cdot)ig)
ight]^{N'}\geq arepsilon'\pi(\cdot).$$

Then

$$\begin{split} (P_{\mathrm{RS}})^{N'\max\{N_i\}}(x,\cdot) &= \left[\frac{1}{k} \big(P_1(x,\cdot) + \dots + P_k(x,\cdot)\big)\right]^{N'\max\{N_i\}} \\ &\geq \big(k^{-\max\{N_i\}} \big[P_1^{\max\{N_i\}}(x,\cdot) + \dots + P_k^{\max\{N_i\}}(x,\cdot)\big]\big)^{N'} \\ &\geq \Big(k^{-(\max\{N_i\}-1)}\min\{\varepsilon_i\}\frac{1}{k} \big[Q_1(x,\cdot) + \dots + Q_k(x,\cdot)\big]\Big)^{N'} \\ &\geq k^{-N'(\max\{N_i\}-1)}\min\{\varepsilon_i^{N'}\}\varepsilon'\pi(\cdot), \end{split}$$

giving the result. \Box

It follows immediately that

$$\|(P_{\rm RS})^{tN_*}(x,\cdot) - \pi(\cdot)\|_{\rm var} \le (1-\varepsilon_*)^t, \quad t=1,2,\ldots.$$

In particular, if $N' = N_1 = \cdots = N_k = 1$, then $N_* = 1$ and $\varepsilon_* = \varepsilon' \min_{1 \le i \le k} \{\varepsilon_i\}$, so that $\|(P_{\mathrm{RS}})^t(x, \cdot) - \pi(\cdot)\|_{\mathrm{var}} \le (1 - \varepsilon' \min\{\varepsilon_i\})^t$.

4. Hybrid Metropolis chains. In this section, we consider hybrid samplers whose constituent chains P_i each arise from a symmetric random-walk Metropolis algorithm [see Metroplis et al. (1953); Hastings (1970); Smith and Roberts (1993)] on the *i*th coordinate. These hybrid samplers may themselves be regarded as Metropolis algorithms, but with singular proposal distributions [cf. Tierney (1995)]. We shall prove that, under appropriate conditions, the hybrid samplers will be geometrically ergodic. Our proof uses the theory of drift and minorization conditions for general Markov chains, as in Nummelin (1984) or Meyn and Tweedie (1993), and follows an argument similar to Roberts and Tweedie (1996). Specifically, we shall eventually show that all bounded sets are small for $P_{\rm RS}$ and that for an appropriate function V (which will need to depend on the dimension k), we have $\limsup_{|\mathbf{x}|\to\infty} P_{\rm RS}V(\mathbf{x})/V(\mathbf{x}) < 1$. [Recall the definition $Pf(\mathbf{x}) = \int f(\mathbf{y})P(\mathbf{x}, d\mathbf{y})$ and that a set C is small for P if there is $n \in \mathbf{N}$, $\varepsilon > 0$ and a probability measure $\nu(\cdot)$, such that $P^n(\mathbf{x}, \cdot) \geq \varepsilon \nu(\cdot)$ for all $\mathbf{x} \in C$.]

Let π be a positive C^1 density (with respect to k-dimensional Lebesgue measure) for a probability distribution on the state space \mathbf{R}^k . For $1 \le i \le k$, let P_i be a symmetric random-walk Metropolis algorithm [with respect to $\pi(\cdot)$] on the *i*th coordinate. Thus, started from the k-vector \mathbf{x} , the proposal in the *i*th direction is given by $\mathbf{x} + Z_i \mathbf{e}_i$, where \mathbf{e}_i denotes the *i*th coordinate vector and where Z_i is drawn from a symmetric *increment density* $q_i(y)$ with respect to one-dimensional Lebesque measure; this proposal is then accepted with probability min $(1, \pi(\mathbf{x} + Z_i \mathbf{e}_i) / \pi(\mathbf{x}))$. We shall assume for simplicity that for each *i*, there exist positive constants ε_i and δ_i such that

(1)
$$q_i(y) \ge \varepsilon_i \text{ for } |y| < \delta_i$$

Finally, we let $P_{\rm RS}$ be as in Section 2.

Given $\mathbf{x} \in \mathbf{R}^k$, let $A_i(\mathbf{x}) = \{\mathbf{z}; \mathbf{z} = y\mathbf{e}_i \text{ and } \pi(\mathbf{x} + \mathbf{z}) \ge \pi(\mathbf{x})\}$ and let $R_i(\mathbf{x}) = \{\mathbf{z}; \mathbf{z} = y\mathbf{e}_i \text{ and } \pi(\mathbf{x} + \mathbf{z}) < \pi(\mathbf{x})\}$. In other words, $A_i(\mathbf{x})$ represents the set of points which if proposed would always be accepted, whereas $R_i(\mathbf{x})$ represents those which are rejected with positive probability. We will also need the *reflected set*, $-A_i(\mathbf{x}) = \{\mathbf{x}; -\mathbf{x} \in A_i(\mathbf{x})\}$.

We introduce the following conditions on π . We will assume that π is bounded, that for sufficiently small d > 0 we have

(2)
$$\int_{\mathbf{R}^k} \pi^{1-d}(\mathbf{x}) \, d\mathbf{x} < \infty$$

and that we have the "asymptotically exponentially decreasing tails" condition

(3)
$$\liminf_{|\mathbf{x}|\to\infty} |\nabla \log \pi(\mathbf{x})| > 0.$$

For each **x**, let $\kappa(\mathbf{x})$ denote the maximum curvature of all geodesic curves through the surface {**y**; $\pi(\mathbf{y}) = \pi(\mathbf{x})$ } at the point **x** [see, e.g., Boothby (1986) for the relevant definitions]. We assume that $\kappa(\mathbf{x})$ is well defined, at least for sufficiently large $|\mathbf{x}|$. We further assume that

(4)
$$\lim_{|\mathbf{x}|\to\infty}\kappa(\mathbf{x})=0,$$

that

(5)
$$\limsup_{|\mathbf{x}| \to \infty} |\langle \nabla \log |\nabla \log \pi(\mathbf{x}) |\rangle| < \infty$$

and that

(6)
$$\limsup_{|\mathbf{x}|\to\infty} \int_{R_i(\mathbf{x})} \left(\frac{\pi(\mathbf{x})^d}{\pi(\mathbf{x}-y\mathbf{e}_i)^d} - \frac{\pi(\mathbf{x}+y\mathbf{e}_i)^d}{\pi(\mathbf{x})^d} \right) \le 0$$

for all *i*, where $\{\mathbf{e}_i\}$ denotes the orthogonal coordinate set (along which the P_i 's sample).

We introduce the drift function $V(\mathbf{x}) = \pi(\mathbf{x})^{-d}$. It turns out that we will need to choose a value of d sufficiently small not only to satisfy (2), but also to satisfy a condition on the next calculation.

PROPOSITION 3. For all P_i ,

$$P_i V(\mathbf{x}) \le r(d) V(\mathbf{x}),$$

where $r(d) = 1 + (1 - d)^{(1-d)/d}d$, for all $x \in \mathscr{X}$. Hence, for all $\varepsilon > 0$, there is d with $0 < d < \varepsilon$, such that $1 < r(d) < 1 + \varepsilon$.

PROOF. Considering separately the cases where the proposal is to $R_i(\mathbf{x})$ and is rejected (so the value of V is unchanged), where the proposal is to $R_i(\mathbf{x})$ and is accepted and where the proposal is to $A_i(\mathbf{x})$ (and is necessarily

accepted), we have that

$$\begin{aligned} \frac{P_i V(\mathbf{x})}{V(\mathbf{x})} &= \int_{R_i(\mathbf{x})} q_i(y) \left(1 - \frac{\pi(\mathbf{x} + y\mathbf{e}_i)}{\pi(\mathbf{x})} \right) dy \\ &+ \int_{R_i(\mathbf{x})} q_i(y) \frac{\pi(\mathbf{x} + y\mathbf{e}_i)^{-d}}{\pi(\mathbf{x})^{-d}} \left(\frac{\pi(\mathbf{x} + y\mathbf{e}_i)}{\pi(\mathbf{x})} \right) dy \\ &+ \int_{A_i(\mathbf{x})} q_i(y) \frac{\pi(\mathbf{x} + y\mathbf{e}_i)^{-d}}{\pi(\mathbf{x})^{-d}} dy \\ &= \int_{\mathbf{R}} q_i(y) I(\mathbf{x} + y\mathbf{e}_i) dy, \end{aligned}$$

where

$$I(\mathbf{z}) = \begin{cases} 1 - \pi(\mathbf{z})/\pi(\mathbf{x}) + (\pi(\mathbf{z})/\pi(\mathbf{x}))^{1-d}, & \mathbf{z} \in R_i(\mathbf{x}), \\ (\pi(\mathbf{x})/\pi(\mathbf{z}))^d, & \mathbf{z} \in A_i(\mathbf{x}). \end{cases}$$

We claim that $I(\mathbf{z}) \leq r(d)$ for all $\mathbf{z} \in R_i(\mathbf{x}) \cup A_i(\mathbf{x})$. Indeed, $I(\mathbf{z}) \leq 1$ on $A_i(\mathbf{x})$ by definition. Furthermore, setting $w = \pi(\mathbf{z})/\pi(\mathbf{x})$, we have that for $z \in R_i(\mathbf{x})$, $I(\mathbf{z}) = 1 - w + w^{1-d}$ with $0 \leq w \leq 1$. This is maximised at $w = (1 - d)^{1/d}$ with maximising value r(d) above. The inequality follows.

The second statement is immediate since $\lim_{d \downarrow 0} r(d) = 1$. \Box

LEMMA 4. All bounded subsets of \mathbf{R}^{k} are small for P_{RS} .

PROOF. By (1), it is easy to see that $P_{RS}^{k}(x, \cdot)$ has a nontrivial continuous component with respect to *k*-dimensional Lebesgue measure. Call this continuous component $s(\mathbf{x}, \cdot)$, say. Note that by (1), for suitable constants ε and δ , we have

$$s(\mathbf{x}, \mathbf{x} + \mathbf{y}) \ge \varepsilon$$
, whenever $|y_i| \le \delta$ for $1 \le i \le k$.

Now, since π is positive and continuous, it is bounded away from zero on compact intervals. It follows that the set $[-\delta, \delta]^k$ is small. By taking convolutions, it follows that for any $N \in \mathbf{N}$, there is $\varepsilon' > 0$ such that the continuous component $s_N(\mathbf{x}, \cdot)$ of $P_{\mathrm{RS}}^{kN}(\mathbf{x}, \cdot)$ satisfies

$$s_N(\mathbf{x}, \mathbf{x} + \mathbf{y}) \ge \varepsilon'$$
, whenever $|y_i| \le N\delta/2$ for $1 \le i \le k$.

Hence, the set $[-N\delta/2, N\delta/2]^k$ is small. The result follows since any bounded set *C* is contained in $[-N\delta/2, N\delta/2]^k$ for some sufficiently large *N*. \Box

THEOREM 5. Suppose conditions (2)–(6) are satisfied. Then the randomscan hybrid chain $P_{\rm RS}$ is geometrically ergodic.

The following lemma is needed for the proof of Theorem 5. We shall write $\mathbf{n}(\mathbf{x})$ for the (outward) normal to the contour manifold through \mathbf{x} ; that is,

$$\mathbf{n}(\mathbf{x}) = \frac{-\nabla \log \pi(\mathbf{x})}{|\nabla \log \pi(x)|}.$$

LEMMA 6. Assume (4) holds and let $\{\mathbf{x}_j\} \to \infty$ be a sequence in \mathbf{R}^k . Then for all $y \in \mathbf{R}$,

(7)
$$\lim_{j\to\infty} |\mathbf{n}(\mathbf{x}_j + y\mathbf{e}_i) - \mathbf{n}(\mathbf{x}_j)| = 0.$$

Moreover, suppose that

$$\liminf_{i\to\infty} \mathbf{n}(\mathbf{x}_j) \cdot \mathbf{e}_i \equiv c_1 > 0$$

and letting $c_2 = \liminf_{j \to \infty} |\nabla \log \pi(\mathbf{x}_j)|$, then for all $y \in \mathbf{R}$,

(8)
$$\liminf_{j\to\infty}\frac{\partial}{\partial y}\log\pi(\mathbf{x}_j+y\mathbf{e}_i)\geq c_1c_2.$$

It follows that for y < 0, we have that

(9)
$$\limsup_{j\to\infty}\frac{\pi(\mathbf{x}_j+\mathbf{y}\mathbf{e}_i)}{\pi(\mathbf{x}_j)}\leq e^{\mathbf{y}c_1c_2},$$

and for $y \ge 0$,

(10)
$$\liminf_{j\to\infty}\frac{\pi(\mathbf{x}_j+y\mathbf{e}_i)}{\pi(\mathbf{x}_j)}\geq e^{yc_1c_2}.$$

Finally, if $c_2 > 0$, then

(11)
$$\lim_{j \to \infty} R_i(\mathbf{x}_j) = (-\infty, 0)$$

in the sense that $\mathbf{1}_{R_i(\mathbf{x}_i)} \to \mathbf{1}_{(-\infty,0)}$ pointwise.

Identical results exist for the case where $\limsup_{j\to\infty} \mathbf{n}(\mathbf{x}_j) \cdot \mathbf{e}_i < 0$. These results are easily written down by replacing \mathbf{e}_i by $-\mathbf{e}_i$.

Lemma 6 provides most of what is needed for the proof of Theorem 5. The only complications arise where c_1c_2 can take the value 0.

PROOF OF LEMMA 6. Statement (7) follows directly from the curvature condition, since it implies that the contours of the density at two locations \mathbf{x} and \mathbf{z} for \mathbf{x} and \mathbf{z} large and for $|\mathbf{x} - \mathbf{z}|$ small are approximately parallel to each other (otherwise they would intersect). Statement (8) now follows from the equation

$$\frac{\partial}{\partial y} \log \pi(\mathbf{x} + y\mathbf{e}_i) = |\nabla \log \pi(\mathbf{x} + y\mathbf{e}_i)| \mathbf{n}(\mathbf{x}_j + y\mathbf{e}_i) \cdot \mathbf{e}_i.$$

Statements (9), (10) and (11) then follow easily. \Box

PROOF OF THEOREM 5. Because of Lemma 4 and by (2), which ensures that $V \in L^1(\pi)$ for sufficiently small d, it suffices [see, e.g., Nummelin (1984), Proposition 5.21; Meyn and Tweedie (1993), Theorem 15.0.1, Roberts and Tweedie (1996)] to demonstrate that

$$\limsup_{|\mathbf{x}| o \infty} rac{P_{ ext{RS}} V(\mathbf{x})}{V(\mathbf{x})} < 1.$$

So, for contradiction, suppose that we have a sequence of points $\{\mathbf{x}_j\}$, with $|\mathbf{x}_j| \to \infty$, such that

$$\liminf_{i \to \infty} \frac{P_{\rm RS} V(\mathbf{x}_j)}{V(\mathbf{x}_j)} \ge 1.$$

By taking a subsequence if necessary, we can (and do) assume that $\mathbf{n}(\mathbf{x}_j)$ converges to a limiting direction \mathbf{f} . There must be at least one coordinate direction \mathbf{e}_i with $\mathbf{f} \cdot \mathbf{e}_i \neq 0$. By renumbering the coordinates as necessary and replacing \mathbf{e}_i by $-\mathbf{e}_i$ if necessary, we can assume that $1 \le n \le k$ is such that $\mathbf{e}_i \cdot \mathbf{f} > 0$ for $1 \le i \le n$, but that \mathbf{f} is orthogonal to \mathbf{e}_i for $n + 1 \le i \le k$.

We take d sufficiently small so that r(d) < (2k - 1)/(2k - 2). We compute that for large enough $|\mathbf{x}|$ we have

(12)

$$\frac{P_i V(\mathbf{x})}{V(\mathbf{x})} = \int_{R_i(\mathbf{x})} \left(1 - \frac{\pi(\mathbf{x} + y\mathbf{e}_i)}{\pi(\mathbf{x})} + \frac{\pi(\mathbf{x} + y\mathbf{e}_i)^{1-d}}{\pi(\mathbf{x})^{1-d}} \right) q_i(y) \, dy$$

$$+ \int_{A_i(\mathbf{x})} \frac{\pi(\mathbf{x})^d}{\pi(\mathbf{x} + y\mathbf{e}_i)^d} q_i(y) \, dy$$

$$= T_1(\mathbf{x}_j) + T_2(\mathbf{x}_j)$$

say, where

$$T_{1}(\mathbf{x}_{j}) = \int_{R_{i}(\mathbf{x})} \left[2 - \left(1 - \frac{\pi(\mathbf{x}_{j} + y\mathbf{e}_{i})^{1-d}}{\pi(\mathbf{x}_{j})^{1-d}} \right) \left(1 - \frac{\pi(\mathbf{x}_{j} + y\mathbf{e}_{i})^{d}}{\pi(\mathbf{x}_{j})^{d}} \right) \right] q_{i}(y) \, dy$$

and

$$T_2(\mathbf{x}_j) = \int_{A_i(\mathbf{x})} \frac{\pi(\mathbf{x}_j)^d}{\pi(\mathbf{x}_j + y\mathbf{e}_i)^d} q_i(y) \, dy - \int_{R_i(\mathbf{x})} \frac{\pi(\mathbf{x}_j + y\mathbf{e}_i)^d}{\pi(\mathbf{x}_j)^d} q_i(y) \, dy.$$

Now

$$\limsup_{j \to \infty} T_2(\mathbf{x}_j) = \limsup_{j \to \infty} \left(\int_{-\infty}^0 \frac{\pi(\mathbf{x}_j)^d}{\pi(\mathbf{x}_j - y\mathbf{e}_i)^d} q_i(y) \, dy - \int_{-\infty}^0 \frac{\pi(\mathbf{x}_j + y\mathbf{e}_i)^d}{\pi(\mathbf{x}_j)^d} q_i(y) \, dy \right) \le 0.$$

Here the equality follows from (11) and the dominated convergence theorem (since the integrand is bounded), and the inequality follows from (6). Let $c_1 = \liminf_{j \to \infty} \mathbf{n}(\mathbf{x}_j) \cdot \mathbf{e}_i$. By (3), $c_2 = \liminf_{j \to \infty} |\nabla \log \pi(\mathbf{x}_j)| > 0$. Therefore, from (10) and (11), at least for $1 \le i \le n$,

$$\begin{split} \liminf_{j \to \infty} T_1(\mathbf{x}_j) &\leq 2 \int_{-\infty}^0 q_i(y) \, dy - \int_{-\infty}^0 (1 - e^{dc_1 c_2 y}) (1 - e^{(1 - d)c_1 c_2 y}) q_i(y) \, dy \\ &\leq 1, \end{split}$$

since $\int_{-\infty}^{0} q_i(y) \, dy = 1/2$ by symmetry. Therefore, for $1 \le i \le n$, (13) $\limsup_{i} P_i V(\mathbf{x}_j) / V(\mathbf{x}_j) < 1, \quad 1 \le i \le n$.

To finish, consider the sequence $\{a_j\}$, where $a_j = |\nabla \log \pi(\mathbf{x}_j)|$. By (3), $\liminf_j a_j > 0 = 0$. Therefore (again by subsequencing if necessary), we can assume that $a_j \to a_{\infty}$ for some $a_{\infty} \in (0, \infty]$. We need to consider separately the cases where a_{∞} is finite or infinite.

If $a_{\infty} < \infty$, then by (5), we have for i > n that $\lim_{j \to \infty} (\pi(\mathbf{x}_j + y\mathbf{e}_i)/\pi(\mathbf{x}_j)) = 1$ for all $y \in \mathbf{R}$ (since $e_i \cdot f = 0$), so that $\lim_{j \to \infty} P_i V(\mathbf{x}_j)/V(\mathbf{x}_j) = 1$. Therefore, by (13), $\limsup_{j \to \infty} P_{\mathrm{RS}} V(\mathbf{x}_j)/V(\mathbf{x}_j) < 1$ for a contradiction.

If $a_{\infty} = \infty$, then for $i \leq n$, all proposed jumps into $R_i(\mathbf{x}_j)$ are asymptotically rejected [by (9)] and all jumps to $A_i(\mathbf{x}_j)$ are asymptotically accepted [by (10)]. Specifically, for $i \leq n$, $\lim_{j \to \infty} (\pi(\mathbf{x}_j + y\mathbf{e}_i)/\pi(\mathbf{x}_j)) = 0$ for y < 0 and $\lim_{j \to \infty} (\pi(\mathbf{x}_j + y\mathbf{e}_i)/\pi(\mathbf{x}_j)) = \infty$ for y > 0. It follows that the integrand in (12) converges to $\mathbf{1}_{(-\infty,0)}(y)$, and since the integrands in (12) are uniformly bounded [by r(d)], we have by the dominated convergence theorem that

$$\limsup_{j \to \infty} \frac{P_i V(\mathbf{x}_j)}{V(\mathbf{x}_j)} = \int_{-\infty}^0 q_i(y) \, dy = \frac{1}{2}.$$

It follows from Proposition 3 that

$$\begin{split} \limsup_{j \to \infty} \frac{P_{\text{RS}} V(\mathbf{x}_j)}{V(\mathbf{x}_j)} &= \limsup_{j \to \infty} \frac{1}{k} \sum_{i=1}^k \frac{P_i V(\mathbf{x}_j)}{V(\mathbf{x}_j)} \\ &\leq \frac{n}{2k} + \frac{r(d)(k-n)}{k} \leq \frac{1}{2k} + \frac{r(d)(k-1)}{k} \\ &< \frac{1}{2k} + \frac{(k-1)(2k-1)}{k(2k-2)} = 1, \end{split}$$

for a contradiction in this case. \Box

REMARK. The nature of the proof of Theorem 5 suggests that explicit bounds on the total variation distance from stationarity [cf. Meyn and Tweedie (1994); Rosenthal (1995)] may be obtainable in this case, though we do not pursue that here.

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REFERENCES

- ALDOUS, D. and DIACONIS, P. (1987). Strong stopping times and finite random walks. Adv. in Appl. Math. 8 69-97.
- BOOTHBY, W. M. (1986). An Introduction to Differentiable Manifolds and Riemannian Geometry. Academic Press, Orlando, FL.
- CHAN, K. S. and GEYE, C. J. (1994). Discussion of "Markov chains for exploring posterior distributions" by L. Tierney. Ann. Statist. 22 1747-1758.

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- GELFAND, A. E. and SMITH, A. F. M. (1990). Sampling based approaches to calculating marginal densities. J. Amer. Statist. Assoc. 85 398-409.
- GREEN, P. J. (1994). Reversible jump MCMC computation and Bayesian model determination. Technical report, Dept. Mathematics, Univ. Bristol.
- HASTINGS, W. K. (1970). Monte Carlo sampling methods using Markov chains and their applications. Biometrika 57 97-109.
- METROPOLIS, N., ROSENBLUTH, A., ROSENBLUTH, M., TELLER, A. and TELLER, E. (1953). Equations of state calculations by fast computing machines. J. Chem. Phys. 21 1087–1091.
- MEYN, S. P. and TWEEDIE, R. L. (1993). Markov Chains and Stochastic Stability. Springer, London.
- MEYN, S. P. and TWEEDIE, R. L. (1994). Computable bounds for convergence rates of Markov chains. Ann. Appl. Probab. 4 981-1011.
- NUMMELIN, E. (1984). General Irreducible Markov Chains and Non-Negative Operators. Cambridge Univ. Press.
- ROBERTS, G. O. and ROSENTHAL, J. S. (1997). Geometric ergodicity and hybrid Markov chains. Electronic Communications in Probability 2 13-25.
- ROBERTS, G. O. and TWEEDIE, R. L. (1996). Geometric convergence and central limit theorems for multidimensional Hastings and Metropolis algorithms. *Biometrika* 83 95–110.
- ROSENTHAL, J. S. (1995). Minorization conditions and convergence rates for Markov chain Monte Carlo. J. Amer. Statist. Assoc. 90 558–566.
- SMITH, A. F. M. and ROBERTS, G. O. (1993). Bayesian computation via the Gibbs sampler and related Markov chain Monte Carlo methods (with discussion). J. Roy. Statist. Soc. Ser. B 55 3-24.
- TIERNEY, L. (1994). Markov chains for exploring posterior distributions (with discussion). Ann. Statist. 22 1701-1762.
- TIERNEY, L. (1995). A note on Metropolis-Hastings kernels for general state spaces. Technical Report 606, School of Statistics, Univ. Minnesota.

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