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STABILITY OF ADVERSARIAL MARKOV CHAINS, WITH AN APPLICATION TO ADAPTIVE MCMC ALGORITHMS

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We consider whether ergodic Markov chains with bounded step size remain bounded in probability when their transitions are modified by an adversary on a bounded subset. We provide counterexamples to show that the answer is no in general, and prove theorems to show that the answer is yes under various additional assumptions. We then use our results to prove convergence of various adaptive Markov chain Monte Carlo algorithms.

1. Introduction. This paper considers whether bounded modifications of stable Markov chains remain stable. Specifically, we let P be a fixed time-homogeneous ergodic Markov chain kernel with bounded step size, and let $\{X_n\}$ be a stochastic process which follows the transition probabilities P except on a bounded subset K where an "adversary" can make arbitrary bounded jumps. Under what conditions must such a process $\{X_n\}$ be bounded in probability?

One might think that such boundedness would follow easily, at least under mild regularity and continuity assumptions, that is, that modifying a stable continuous Markov chain inside a bounded set K couldn't possibly lead to unstable behavior out in the tails. In fact the situation is rather more subtle, as we explore herein. We will provide counterexamples to show that boundedness may fail even for well-behaved continuous chains. We will then show that under various additional conditions, including bounds on transition probabilities and/or small set assumptions and/or geometric ergodicity, such boundedness does hold.

The specific question considered here appears to be new, though it is somewhat reminiscent of previous bounds on non-Markovian stochastic processes such as those related to *adversarial queuing theory* [6, 13, 21]. We present our formal setup in Section 2, our main results in Section 3 and some counterexamples in Section 4. Our results are then proven in Sections 5 through 10.

In Section 11, we turn our attention to adaptive Markov chain Monte Carlo (MCMC) algorithms. MCMC proceeds by running a Markov chain long enough to approximately converge to its stationary distribution and thus provide useful

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samples. Adaptive MCMC algorithms attempt to improve on MCMC by modifying the Markov chain transitions as they run, but this destroys the Markov property and makes convergence to stationarity notoriously difficult to prove. We use our main results herein to establish general conditions for convergence of certain adaptive MCMC algorithms (Theorem 21). We then apply this result to a simple but useful adaptive MCMC algorithm (Proposition 22), and also to a detailed statistical application involving a probit model for lupus patient data (Section 12). For details and references about adaptive MCMC algorithms, see Section 11.

2. Formal setup and assumptions. Let $\mathcal{X}$ be a nonempty general (i.e., possibly uncountable) state space, on which is defined a metric η, which gives rise to a corresponding Borel σ-algebra $\mathcal{F}$. Assume that $\mathcal{X}$ contains some specified "origin" point $\mathbf{0} \in \mathcal{X}$. (In our examples and applications, $\mathcal{X}$ will usually be a subset of $\mathbf{R}^d$ with the usual Euclidean metric.) Let P be the transition probability kernel for a fixed time-homogeneous Markov chain on $\mathcal{X}$. Assume that P is Harris ergodic with stationary probability distribution π, so that

$$\lim_{n\to\infty} \bigl\| P^n(x,\cdot) - \pi \bigr\| := \lim_{n\to\infty} \sup_{A\in\mathcal{F}} \bigl| P^n(x,A) - \pi(A) \bigr| = 0, \qquad x \in \mathcal{X}. \tag{1}$$

We assume, to relate the Markov chain to the geometry of $\mathcal{X}$, that there is a constant $D < \infty$ such that P never moves more than a distance D, that is, such that

$$P\bigl(x, \{y \in \mathcal{X} : \eta(x,y) \le D\}\bigr) = 1, \qquad x \in \mathcal{X}. \tag{2}$$

Let $K \in \mathcal{F}$ be a fixed *bounded* nonempty subset of $\mathcal{X}$, and for $r > 0$ let K_r be the set of all states within a distance r of K (so each K_r is also bounded).

In terms of these ingredients, we define our "adversarial Markov chain" process $\{X_n\}$ as follows. It begins with $X_0 = x_0$ for some specific initial state x_0; for simplicity (see the proof of Lemma 8) we assume that $x_0 \in K$. Whenever the process is outside of K, it moves according to the Markov transition probabilities P, that is,

$$\mathbf{P}(X_{n+1} \in A | X_0, X_1, \ldots, X_n) = P(X_n, A), \qquad n \ge 0, A \in \mathcal{F}, X_n \notin K. \tag{3}$$

When the process is inside of K, it can move *arbitrarily*, according to an adversary's wishes, perhaps depending on the time n and/or the chain's history in a nonanticipatory manner (i.e., adapted to $\{X_n\}$; see also Example 3 below), subject only to measurability [i.e., $\mathbf{P}(X_{n+1} \in A | X_0, X_1, \ldots, X_n)$ must be well defined for all $n \ge 0$ and $A \in \mathcal{F}$], and to the restriction that it can't move more than a distance D at each iteration—or more specifically that from K, it can only move to points within K_D. In summary, $\{X_n\}$ is a stochastic process which is "mostly" a Markov chain following the transition probabilities P, except that it is modified by an adversary when it is within the bounded subset K.

We are interested in conditions guaranteeing that this process $\{X_n\}$ will be bounded in probability, that is, will be tight, that is, will satisfy that

$$\lim_{L\to\infty} \sup_{n\in\mathbf{N}} \mathbf{P}\bigl(\eta(X_n, \mathbf{0}) > L | X_0 = x_0\bigr) = 0. \tag{4}$$

3. Main results. We now consider various conditions under which (4) will or will not hold. For application of our results to the verification of adaptive MCMC algorithms, see Section 11 below.

3.1. *First results*. We first note that such boundedness is guaranteed in the *absence* of an adversary:

PROPOSITION 1. *In the setup of Section 2, suppose* $\{X_n\}$ *always follows the transitions* P (*including when it is within* K, *i.e., there is no adversary*). *Then* (4) *holds*.

Indeed, Proposition 1 follows immediately since if P is Harris ergodic as in (1), then it converges in distribution, so it must be tight and hence satisfy (4). [In fact, even if P is just assumed to be ϕ-irreducible with period $d \geq 1$ and stationary probability distribution π, then this argument can be applied separately to each of the sequences $\{X_{dn+j}\}_{n=0}^{\infty}$ for $j = 0, 1, \ldots, d-1$ to again conclude (4).]

Boundedness also holds for a lattice like $\mathbf{Z}^d$, or more generally if the state space $\mathcal{X}$ is topologically discrete (i.e., countable and such that each state x is topologically isolated and hence open in $\mathcal{X}$). In this case, bounded subsets like K_{2D} must be *finite*, and the result holds without any further assumptions:

PROPOSITION 2. *In the setup of Section 2, suppose* P *is an irreducible positive-recurrent Markov chain with stationary probability distribution* π *on a countable state space* $\mathcal{X}$ *such that* K_{2D} *is finite. Then* (4) *holds*.

Proposition 2 is proved in Section 5 below.

However, (4) does not hold in general, not even under a strong continuity assumption:

PROPOSITION 3. *There exist adversarial Markov chain examples following the setup of Section 2, on state spaces which are countable subsets of* $\mathbf{R}^2$, *which fail to satisfy* (4), *even under the strong continuity condition that* $\mathcal{X}$ *is closed and*

$$\forall x \in \mathcal{X}, \forall \epsilon > 0, \exists \delta > 0 \quad s.t. \quad \|P(y, \cdot) - P(x, \cdot)\| < \epsilon \quad \text{whenever } \eta(x, y) < \delta. \tag{5}$$

Proposition 3 is proved in Section 4 below, using two different counterexamples.

Proposition 3 says that the adversarial process $\{X_n\}$ may not be bounded in probability, even if we assume a strong continuity condition on P. Hence, additional assumptions are required, as we consider next.

REMARK 1. The counterexamples in Proposition 3 are discrete Markov chains in the sense that their state spaces are countable. However, their state spaces $\mathcal{X}$ are not *topologically* discrete, since they contain accumulation points, and in particular sets like K_{2D} are not finite there, so there is no contradiction with Proposition 2.

3.2. *A result using expected hitting times.* We now consider two new assumptions. The first provides an upper bound on the Markov chain transitions out of K_D:

(A1) There is $M < \infty$, and a probability measure μ_* concentrated on $K_{2D} \setminus K_D$, such that $P(x, dz) \le M\mu_*(dz)$ for all $x \in K_D \setminus K$ and $z \in K_{2D} \setminus K_D$.

Note that in (A1) we always have $z \neq x$, which is helpful when considering, for example, Metropolis algorithms which have positive probability of not moving. Choices of μ_* in (A1) might include Uniform$(K_{2D} \setminus K_D)$, or $\pi|_{K_{2D}\setminus K_D}$. The second assumption bounds an expected hitting time:

(A2) The expected time for a Markov chain following the transitions P to reach the subset K_D, when started from the distribution μ_* in (A1), is finite.

In terms of these two assumptions, we have:

THEOREM 4. *In the setup of Section 2, if* (A1) *and* (A2) *hold for the same* μ_*, *then* (4) *holds*; *that is*, $\{X_n\}$ *is bounded in probability.*

Theorem 4 is proved in Section 5 below.

3.3. *A result assuming a small set condition.* Condition (A2), that the hitting time of K_D has finite expectation, may be difficult to verify directly. As an alternative, we consider a different assumption:

(A3) The set $K_{2D} \setminus K_D$ is small for P; that is, there is some probability measure ν_* on $\mathcal{X}$, and some $\epsilon > 0$, and some $n_0 \in \mathbf{N}$, such that $P^{n_0}(x, A) \ge \epsilon\nu_*(A)$ for all states $x \in K_{2D} \setminus K_D$ and all subsets $A \in \mathcal{F}$.

We then have:

THEOREM 5. *In the setup of Section 2, if* (A1) *and* (A3) *hold where either* (a) $\nu_* = \mu_*$, *or* (b) P *is reversible and* $\mu_* = \pi|_{K_{2D}\setminus K_D}$, *then* (4) *holds*; *that is*, $\{X_n\}$ *is bounded in probability.*

Theorem 5 is proved in Section 7 below.

Assumption (A3) is often straightforward to verify. For example:

PROPOSITION 6. *Suppose $\mathcal{X}$ is an open subset of $\mathbf{R}^d$ which contains a bounded rectangle J which contains $K_{2D} \setminus K_D$. Suppose there are $\delta > 0$ and $\epsilon > 0$ such that*

$$P(x, dy) \geq \epsilon \,\mathrm{Leb}(dy) \qquad \text{whenever } x, y \in J \text{ with } |y - x| < \delta, \tag{6}$$

where Leb *is Lebesgue measure on $\mathbf{R}^d$. Then* (A3) *holds with $\nu_* = \mathrm{Uniform}(K_{2D} \setminus K_D)$.*

Proposition 6 is proved in Section 8 below.

3.4. *A result assuming geometric ergodicity.* Assumption (A3) can be verified for various Markov chains, as we will see below. However, its verification will sometimes be difficult. An alternative approach is to consider *geometric ergodicity*, as follows (see, e.g., [17] for context):

(A4) The Markov chain transition kernel P is geometrically ergodic; that is, there is $\rho < 1$ and a π-a.e. finite measurable function $\xi : \mathcal{X} \to [1, \infty]$ such that $\|P^n(x, \cdot) - \pi\| \leq \xi(x)\rho^n$ for $n \in \mathbf{N}$ and $x \in \mathcal{X}$.

We also require a slightly different version of (A1):

(A5) There is $M < \infty$ such that $P(x, dz) \leq M\pi(dz)$ for all $x \in K_D$ and $z \in K_{2D}$.

[Of course, (A5) holds trivially for $z \notin K_{2D}$, since then $P(x, dz) = 0$.] We then have:

THEOREM 7. *In the setup of Section 2, if* (A4) *and* (A5) *hold, then* (4) *holds; that is, $\{X_n\}$ is bounded in probability.*

Theorem 7 is proved in Section 10 below.

4. Counterexamples to prove Proposition 3. We next present two counterexamples to illustrate that with the setup and assumptions of Section 2, the bounded in probability property (4) might fail. Each example has a state space $\mathcal{X}$ which is a countable subset of $\mathbf{R}^2$ with the usual Euclidean metric $\eta(x, y) := |y - x|$. In Example 1, $\mathcal{X}$ is not closed, and (5) does not hold; this is remedied in Example 2.

EXAMPLE 1. Let $\mathcal{X} = \{(\frac{1}{i}, j) : i \in \mathbf{N}, j = 0, 1, \ldots\}$ be the state space. That is, $\mathcal{X} = \bigcup_{i \in \mathbf{N}} \mathcal{X}_i$ where each $\mathcal{X}_i \equiv \{(\frac{1}{i}, j)\}_{j=0,1,\ldots}$ is a different "column." Let $\pi(\frac{1}{i}, j) = 2^{-i}(\frac{1}{i})(1 - \frac{1}{i})^j$, so that π restricted to each $\mathcal{X}_i$ is a geometric distribution with mean i. Let $K = \{(\frac{1}{i}, 0)\}$ consist of the bottom element of each column; see Figure 1.

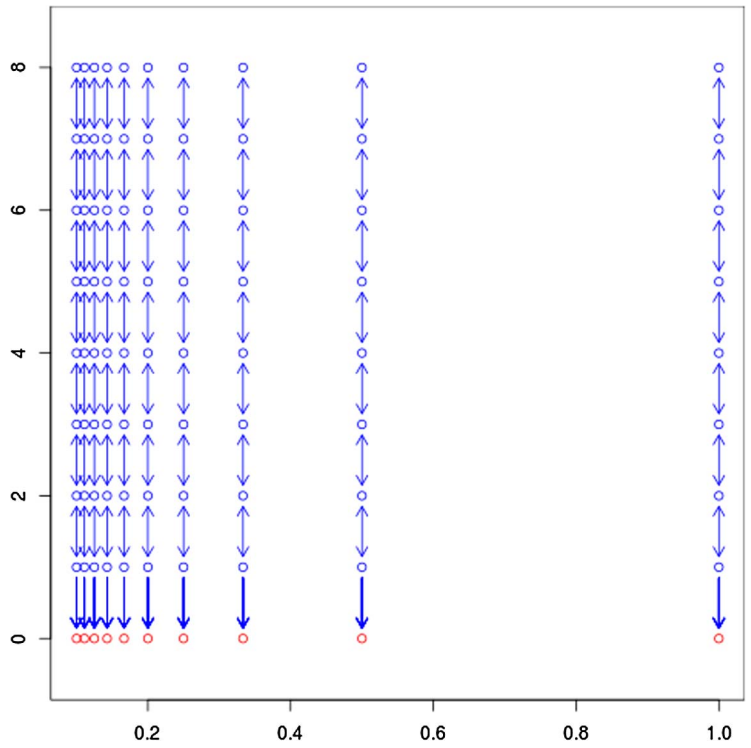

FIG. 1. *Part of the state space in Example 1.*

Let the Markov chain P proceed, outside of K, by doing a simple ± 1 Metropolis algorithm up and down its current column $\mathcal{X}_i$ to be reversible with respect to π. That is, for $j \geq 1$, $P((\frac{1}{i}, j), (\frac{1}{i}, j-1)) = \frac{1}{2}$ and $P((\frac{1}{i}, j), (\frac{1}{i}, j+1)) = \frac{1}{2}(1 - \frac{1}{i})$, and the leftovers $P((\frac{1}{i}, j), (\frac{1}{i}, j)) = 1 - P((\frac{1}{i}, j), (\frac{1}{i}, j-1)) - P((\frac{1}{i}, j), (\frac{1}{i}, j+1))$. Intuitively, the larger the column number i, the higher is the conditional mean of π on $\mathcal{X}_i$, so the higher the chain will tend to move within $\mathcal{X}_i$, and the longer it will take to return to K.

Inside of K, choose any appropriate transitions to make the chain irreducible and reversible with respect to π; for example, choose $P((\frac{1}{i}, 0), (\frac{1}{i}, 1)) = \frac{1}{2}(1 - \frac{1}{i})$ and $P((\frac{1}{i}, 0), (\frac{1}{i-1}, 0)) = 1/4$ (for $i > 1$ only, otherwise 0), and $P((\frac{1}{i}, 0), (\frac{1}{i+1}, 0)) = i/8(i+1)$, and the leftovers $P((\frac{1}{i}, 0), (\frac{1}{i}, 0)) = 1 - P((\frac{1}{i}, 0), (\frac{1}{i+1}, 0)) - P((\frac{1}{i}, 0), (\frac{1}{i-1}, 0)) - P((\frac{1}{i}, 0), (\frac{1}{i}, 1))$.

Let the adversary proceed within K as follows. If $X_n \in K$, then $X_{n+1} = (\frac{1}{n}, 1)$. That is, the chain moves from K to higher and higher column numbers as time goes on.

With these specifications, K is bounded, and the process $\{X_n\}$ never moves more than a distance $D = 1$, so the setup of Section 2 is satisfied. However,

the process $\{X_n\}$ will, over time, move closer and closer to 0 in the x-direction, and will then tend to climb higher and higher in the y-direction. More formally, write $X_{n,1}$ and $X_{n,2}$ for the x-coordinate and y-coordinate of X_n. Then given any $L < \infty$, choose $m \in \mathbf{N}$ such that the median of a mean-m Geometric random variable, $\lceil -1/\log_2(1 - \frac{1}{m}) \rceil$, is at least L. Then let $\tau = \inf\{n : X_{n,1} \le \frac{1}{m}\}$. Then after time τ, the y-coordinate of X_n will be stochastically larger than a usual ± 1 Metropolis algorithm for a Geometric distribution with mean m. Hence, $\liminf_{n\to\infty} \mathbf{P}(X_{n,2} \ge L)$ will be at least as large as the probability that a mean-m Geometric random variable will be $\ge L$. This probability is at least $\frac{1}{2}$. It follows that $\{X_{n,2}\}$, and hence also $\{X_n\}$, are not bounded in probability, that is, that (4) does not hold.

(Alternatively, the adversary could proceed within K by moving from $(\frac{1}{i}, 0)$ to either $(\frac{1}{i}, 1)$ with probability $\frac{1}{2}(1 - \frac{1}{i})$, or to $(\frac{1}{i+1}, 0)$ with probability $(1 + \frac{1}{i})/4$, or to $(\frac{1}{i-1}, 0)$ with probability $(1 + \frac{1}{i})/4$ [for $i > 1$ only, otherwise 0], or remain at $(\frac{1}{i}, 0)$ with the leftover probability. This would make the process $\{X_n\}$ be time-homogeneous Markov and reversible with respect to the infinite measure $\overline{\pi}$ defined by $\overline{\pi}(\frac{1}{i}, j) = (\frac{1}{i})(1 - \frac{1}{i})^j$. Then $\{X_n\}$ will therefore be null recurrent. Hence, again, (4) will not hold.)

Now, in the above example, the state space $\mathcal{X}$ is not closed. One could easily "extend" the example to include $\{(0, j) : j \in \mathbf{N}\}$ and thus make $\mathcal{X}$ closed. However, this cannot be done in a continuous way; that is, there is no way to satisfy (5) in this example. This might lead one to suspect that a continuity condition such as (5) suffices to guarantee (4). However, that is not the case, as the following example shows:

EXAMPLE 2. Our state space $\mathcal{X}$ will be another countable subset of $\mathbf{R}^2$, defined as follows. Let $O = (0, 0)$ be the origin. Let $S_0 = \{(i, 0) : i \in \mathbf{N}\}$. Let $\{\beta_k\}_{k=1}^{\infty}$ be an increasing sequence of integers with $\beta_k > k$ to be specified later. For $k \in \mathbf{N}$, let S_k consist of the k points $(i, \frac{i}{k})$ for $i = 1, 2, \ldots, k$, together with $\beta_k - 1$ additional points equally spaced on the line segment from $(k, 1)$ to the y-axis point $(0, \beta_k)$. Finally, let $\mathcal{Y} = \{(0, i) : i \in \mathbf{N}\}$ be the positive integer y-axis. Then $\mathcal{X} = O \cup \mathcal{Y} \cup \bigcup_{k=0}^{\infty} S_k$; see Figure 2.

Define transitions P on $\mathcal{X}$ as follows. On S_0, we have $P((i, 0), (i - 1, 0)) = 1$; that is, it always moves toward the origin. Similarly, on $\mathcal{Y}$, we have $P((0, i), (0, i - 1)) = 1$; that is, it again always moves toward the origin. On the first $k - 1$ points of S_k, we have $P((i, \frac{i}{k}), (i + 1, \frac{i+1}{k})) = \frac{i}{k}$, and $P((i, \frac{i}{k}), (i - 1, 0)) = 1 - \frac{i}{k}$; that is, it either continues upwards on S_k, or moves toward the origin on S_0. On the remaining points of S_k, with probability 1 it moves one additional point along S_k's path toward $(0, \beta_k)$. The chain's step sizes are thus all bounded above by, for example, $D = \sqrt{2}$.

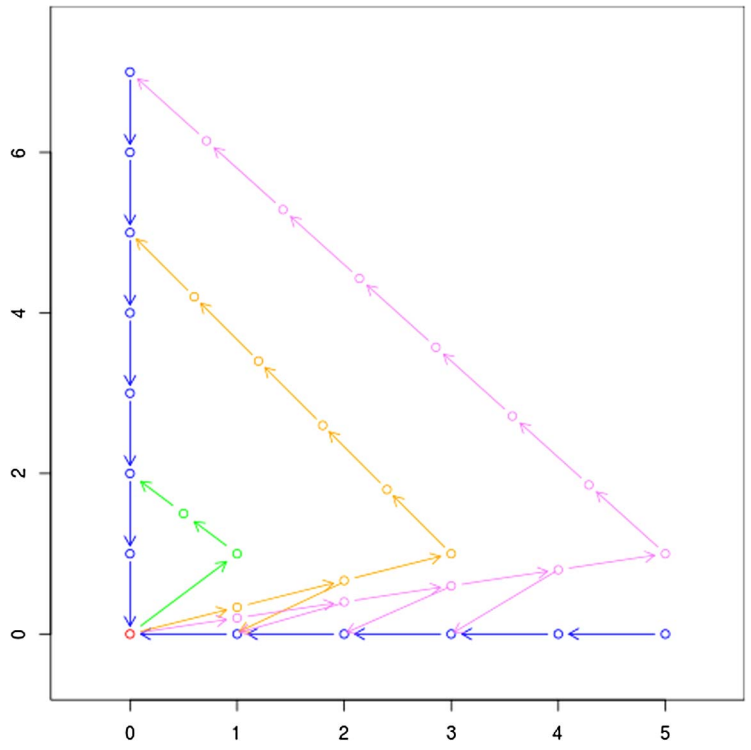

FIG. 2. *Part of the state space in Example 2, including O (origin), and $\mathcal{Y}$ (y-axis), and S_0 (x-axis), and S_1 with $\beta_1 = 2$ [through $(1,1)$], and S_3 with $\beta_3 = 5$ [through $(3,1)$], and S_5 with $\beta_5 = 7$ [through $(5,1)$].*

Note that these transition probabilities are continuous in a very strong sense: if $x_n \to x$ (which can only happen for $x \in S_0$ or for a.a. constant sequences), then $P(x_n, y) \to P(x, y)$ for all $y \in \mathcal{X}$, and in particular $\|P(x_n, \cdot) - P(x, \cdot)\| \to 0$. So, (5) is satisfied.

Note also that if this chain is started at $(1, \frac{1}{k})$, then it has probability $\prod_{i=1}^{k}(\frac{i}{k}) > 0$ of continuing along S_k all the way to $(k, 1)$, in which case it will take a total of $k + 2\beta_k$ iterations to return to O. Otherwise, for $1 \le j \le k-1$, it takes $2j-1$ iterations with probability $(\prod_{i=1}^{j-1} \frac{i}{k})(1 - \frac{j}{k})$. Thus, if $r_k = \mathbf{E}(\tau_O | X_0 = (1, \frac{1}{k}))$ is the expected return time to O from $(1, \frac{1}{k})$, then

$$r_k = (k + 2\beta_k)\left(\prod_{i=1}^{k} \frac{i}{k}\right) + \sum_{j=1}^{k-1}(2j-1)\left(\prod_{i=1}^{j-1} \frac{i}{k}\right)\left(1 - \frac{j}{k}\right).$$

In particular, by letting β_k grow sufficiently quickly, we can make r_k grow as quickly as desired.

Finally, we specify that from O, for $k \in \mathbf{N}$ the Markov chain moves to $(1, \frac{1}{k})$ with probability a_k, for some positive numbers a_k summing to 1 to be specified later.

Meanwhile, the adversary's compact set is given by the single state $K = \{O\}$. From O, the adversary proceeds simply by moving to each $(1, \frac{1}{k})$ with probability b_k, where the b_k are nonnegative and sum to 1, and will be specified later. (Thus, the adversary's actions are chosen to still be time-homogeneous Markov.)

To complete the construction, we choose $\{\beta_k\}$ and $\{a_k\}$ and $\{b_k\}$ so that $\sum_k a_k r_k < \infty$ but $\sum_k b_k r_k = \infty$. For example, we can do this by first choosing β_k so that $r_k k^{-k} \to 1$, and then letting $a_k \propto (2k)^{-k}$ and $b_k \propto (k/2)^{-k}$.

It then follows that for the Markov chain P (governed by the $\{a_k\}$) the expected return time to O from O is finite, and hence the chain has a unique stationary probability measure π. On the other hand, for the adversarial process $\{X_n\}$ (governed by the $\{b_k\}$) the expected return time to O from O is infinite. Hence, the adversarial process is null recurrent, so it will move to larger and larger S_k as time progresses. In particular, the adversarial process will *not* be bounded in probability, even though the transition probabilities P are continuous.

REMARK 2. Example 2 is only defined on a countable state space $\mathcal{X}$, but if desired it could be "extended" to a counterexample on all of $\mathbf{R}^2$. For instance, we could let $\delta = 10^{-6}$, and replace $\pi(\cdot)$ by the convolution $\pi(\cdot) * N(O, \delta^2)$ with a tiny normal distribution, and replace $P(x, \cdot)$ by the convolution $P(x, \cdot) * N(O, \delta^2)$ for each $x \in \mathcal{X}$, and then continuously interpolate new transition probabilities $P(x, \cdot)$ at all $x \in \mathbf{R}^2 \setminus \mathcal{X}$ such that $P(x, \cdot)$ is a probability measure for each $x \in \mathbf{R}^2$, and the mapping $x \mapsto P(x, A)$ is continuous over $x \in \mathbf{R}^2$ for each fixed $A \in \mathcal{F}$. This could be done in such a way that (5) would still be satisfied, but (4) would still fail, thus providing a counter-example even on the continuous state space $\mathbf{R}^2$.

Finally, in a rather different direction, we consider what happens if the process is allowed to be anticipatory, that is, to make moves based on future randomness, with (3) replaced by the weaker condition that $\mathbf{P}(X_{n+1} \in A | X_n = x) = P(x, A)$ but without conditioning on the previous history $X_0, \ldots, X_{n-1}$. It turns out that, under this subtle change, our theorems no longer hold:

EXAMPLE 3. Let $\mathcal{X} = [0, \infty) \subseteq \mathbf{R}$. Define Markov chain transitions P as follows. For $x \le 1$, $P(x, \cdot) = \text{Uniform}[0, 2]$. For $1 < x \le 3$, $P(x, \cdot) = \text{Uniform}[x - 1, x + 1]$. For $3 < x \le 4$, $P(x, \cdot) = \text{Uniform}[4, 5]$. For $x > 4$, $P(x, \cdot) = \frac{1}{2}\delta_{x+1}(\cdot) + \frac{1}{2}\text{Uniform}[x - 2, x - 1]$, where δ_{x+1} is a point-mass at $x + 1$. Then P is ϕ-irreducible, with negative drift for $x > 4$, so P must be positive recurrent with some stationary probability distribution π to which it converges as in (1). Also, P never moves more than a distance $D = 2$ as in (2).

We next define the adversarial process $\{X_n\}$. Let $K = [0, 2]$, so $K_D = [0, 4]$ and $K_{2D} = [0, 6]$. Let $\{B_i\}_{i=0}^{\infty}$ be i.i.d. with $\mathbf{P}(B_i = 0) = \mathbf{P}(B_i = 1) = 1/2$, and let $\{U_i\}_{i=0}^{\infty}$ be i.i.d. $\sim \text{Uniform}[0, 1]$, and let $a_* = 4 + \sum_{i=1}^{\infty} B_i 2^{-i}$. For any $r \in \mathcal{X}$, let

$r[i]$ be the coefficient of 2^i in the nonterminating binary expansion of r, so that $r = \sum_{i \in \mathbf{Z}} r[i] 2^i$. Conditionally on X_n, we construct X_{n+1} by: (a) if $X_n \le 1$, then $X_{n+1} = 2U_n$; (b) if $1 < X_n \le 3$, then $X_{n+1} = X_n - 1 + 2U_n$; (c) if $3 < X_n \le 4$, then $X_{n+1} = a_*$; (d) if $X_n > 4$, then $X_{n+1} = I_n(X_n + 1) + (1 - I_n)(X_n - 1 - U_n)$, where $I_n = \mathbf{1}_{X_n[-n]=B_n}$ is the indicator function of whether the coefficient of 2^{-n} in the binary expansion of X_n is equal to B_n.

Then it is easily checked that $\{X_n\}$ follows the one-step transitions P for all $x \in \mathcal{X}$ (including $x \in K$), in the sense that $\mathbf{P}(X_{n+1} \in A | X_n = x) = P(x, A)$ for all A (but without also conditioning on $X_0, \ldots, X_{n-1}$). Furthermore, (A1) holds with $M = 1$ and $\mu_* = \text{Uniform}[4, 5]$. Also, (A2) holds for the same μ_* due to P's negative drift for $x > 4$.

On the other hand, by construction a_* has the property that $a_*[-n] = B_n$ for all $n \in \mathbf{N}$. Hence, once the chain hits the interval $(3, 4]$, then it will move to a_*, and from there it will always add 1 with probability 1. Therefore, $X_n \to \infty$ with probability 1, so $\{X_n\}$ is not bounded in probability, so (4) does not hold. This process thus provides a counterexample to Theorem 4 if we assume only that $\mathbf{P}(X_{n+1} \in A | X_n = x) = P(x, A)$, without also conditioning on the previous history $X_0, \ldots, X_{n-1}$ as in (3).

5. Proof of Theorem 4 and Proposition 2. We begin by letting $\{Y_n\}$ be a "cemetery process" which begins in the distribution μ_* at time 0, and then follows the fixed transition kernel P, and then *dies* as soon as it hits K_D. Assumption (A2) then says that this cemetery process $\{Y_n\}$ has finite expected lifetime. For $L > \ell_0 := \sup\{\eta(x, \mathbf{0}) : x \in K_D\}$, let $B_L = \{x \in \mathcal{X} : \eta(x, \mathbf{0}) \ge L\}$, and let N_L denote the cemetery process's total occupation time of B_L (i.e., the number of iterations that $\{Y_n\}$ spends in B_L before it dies). We then have:

LEMMA 8. *Let $\{X_n\}$ be the adversarial process as defined previously. Then assuming* (A1), *for any $n \in \mathbf{N}$, and any $L > \ell_0$, and any $x \in K$, we have*

$$\mathbf{P}(X_n \in B_L | X_0 = x) \le M \mathbf{E}(N_L),$$

where N_L is the occupation time of B_L for the cemetery process $\{Y_n\}$ defined above.

PROOF. Let σ be the last return time of $\{X_n\}$ to K_D by time n (which must exist since $X_0 \in K_D$), and let μ_k be the (complicated) law of X_k when starting from $X_0 = x_0$. Then letting $I = K_D \setminus K$ ("inside") and $O = K_{2D} \setminus K_D$ ("outside"), we have

$$\begin{aligned}
&\mathbf{P}(X_n \in B_L | X_0 = x_0) \\
&\quad = \sum_{k=0}^{n-1} \mathbf{P}(X_n \in B_L, \sigma = k | X_0 = x_0) \\
&\quad = \sum_{k=0}^{n-1} \int_{y \in I} \int_{z \in O} \mathbf{P}(X_k \in dy, X_{k+1} \in dz, X_n \in B_L, \sigma = k | X_0 = x_0)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{k=0}^{n-1} \int_{y\in I} \int_{z\in O} \mu_k(dy) P(y, dz) \\
&\qquad\qquad \times \mathbf{P}(X_n \in B_L, \sigma = k | X_0 = x_0, X_k = y, X_{k+1} = z) \\
&\le \sum_{k=0}^{n-1} \int_{y\in I} \int_{z\in O} \mu_k(dy) M\mu_*(dz) \\
&\qquad\qquad \times \mathbf{P}(X_n \in B_L, \sigma = k | X_0 = x_0, X_k = y, X_{k+1} = z) \\
&\le \sum_{k=0}^{n-1} \int_{y\in I} \int_{z\in O} \mu_k(dy) M\mu_*(dz) \mathbf{P}(Y_{n-k-1} \in B_L | Y_0 = z)
\end{aligned}
$$

(by letting $Y_n = X_{n+k+1}$, and noting that if $\sigma = k$, then the process did not return to K_D by time n, so it behaved like the cemetery process between times $n-k-1$ and n)

$$
\begin{aligned}
&\le M \sum_{k=0}^{n-1} \int_{z\in O} \mathbf{P}(Y_{n-k-1} \in B_L | Y_0 = z) \mu_*(dz) \\
&\le M \sum_{j=0}^{\infty} \int_{z\in O} \mathbf{P}(Y_j \in B_L | Y_0 = z) \mu_*(dz).
\end{aligned}
$$

But this last sum is precisely the expected total number of iterations that the cemetery process $\{Y_n\}$ spends in B_L when started from the distribution μ_*. □

PROOF OF THEOREM 4. For each $A \in \mathcal{F}$, let $\nu(A)$ be the above cemetery process's expected occupation measure, that is, the expected number of iterations that the cemetery process $\{Y_n\}$ spends in the subset A. Then the total measure $\nu(\mathcal{X})$ equals the expected lifetime of the cemetery process, and is thus finite by (A2). Hence, by the usual continuity of measures,

$$
\lim_{L\to\infty} \nu(B_L) = \nu\left(\bigcap_L B_L\right) = \nu(\varnothing) = 0.
$$

This shows that $\mathbf{E}(N_L) \to 0$ as $L \to \infty$. Hence, by Lemma 8,

$$
\lim_{L\to\infty} \sup_{n\in\mathbf{N}} \mathbf{P}(X_n \in B_L | X_0 = x_0) \le M \lim_{L\to\infty} \mathbf{E}(N_L) = 0,
$$

so $\{X_n\}$ is bounded in probability. □

We now turn our attention to discrete chains as in Proposition 2. We begin with a lemma. [Here and throughout, $\mathbf{E}_x(\cdots)$ means expected value conditional on the process starting at the initial state $x \in \mathcal{X}$.]

LEMMA 9. *For an irreducible Markov chain on a discrete state space with stationary probability distribution π, for any two states x and y, we have $\mathbf{E}_x(\tau_y) < \infty$; that is, the chain will move from x to y in finite expected time.*

PROOF. If this were not the case, then it would be possible from y to travel to x and then take infinite expected time to return to y. This would imply that $\mathbf{E}_y(\tau_y) = \infty$, contradicting the fact that we must have $\mathbf{E}_y(\tau_y) = 1/\pi(y) < \infty$ by positive recurrence. □

PROOF OF PROPOSITION 2. Since $\mathcal{X}$ is countable and P is irreducible, $\pi(x) > 0$ for all $x \in \mathcal{X}$. Let $O = K_{2D} \setminus K_D$, and assume that $\pi(O) > 0$ [otherwise increase D to make this so, which can be done unless $\pi(K_D) = 1$ in which case the statement is trivial].

Since K_{2D} is finite, assumption (A1) with $\mu_* = \pi|_{K_{2D}\setminus K_D}$ follows immediately with, for example, $M = (\max_{x,z\in K_{2D}} P(x,z))/(\min_{z\in K_{2D}} \pi(z)) < \infty$.

Next, note that $\mathbf{E}_x(\tau_{K_D}) < \infty$ for each individual $x \in O$; indeed, this follows by applying Lemma 9 with any one specific $y \in K_D$ (which must exist since we assume K is nonempty). But then $\mathbf{E}_{\mu_*}(\tau_{K_D}) = \sum_{x\in O} \mu_*(x)\mathbf{E}_x(\tau_{K_D})$, which must also be finite since O is finite. Hence, (A2) also holds. The result thus follows from Theorem 4. □

6. Two additional probability lemmas. In this section, we prove two probability results which we will use in the following section.

We first consider expected hitting times. Lemma 9 above shows that *discrete* ergodic Markov chains always have $\mathbf{E}_x(\tau_y) < \infty$. On a general state space, one might think by analogy that for any positive-recurrent ϕ-irreducible Markov chain with stationary distribution π, if $\pi(A) > 0$ and $\pi(B) > 0$, then we must have $\mathbf{E}_{\pi|A}(\tau_B) < \infty$, where τ_B is the hitting time of B. However, this is false. For example, consider a birth-death chain on the positive integers having stationary distribution $\pi(j) \propto j^{-2}$. Then if $B = \{1\}$ and $A = \{J, J+1, J+2, \dots\}$ for any $J > 1$, then $\mathbf{E}_{\pi|A}(\tau_B) \geq \sum_{j=J}^{\infty} \pi(j)(j-1) \propto \sum_{j=J}^{\infty} j^{-2}(j-1) = \infty$.

On the other hand, this result *is* true in the case $A = B$. Indeed, we have:

LEMMA 10. *Consider a Markov chain with stationary probability distribution π, and let $A \in \mathcal{F}$ with $\pi(A) > 0$. Then*:

(i) $\mathbf{E}_{\pi|A}(\tau_A) = 1/\pi(A) < \infty$, *where τ_A is the first return time to A.*

(ii) *For all $k \in \mathbf{N}$, $\mathbf{E}_{\pi|A}(\tau_A^{(k)}) = k/\pi(A) < \infty$, where $\tau_A^{(k)}$ is the kth return time to A.*

PROOF. Part (i) is essentially the formula of Kac [14]. Indeed, using Theorem 10.0.1 of [17] with $B = \mathcal{X}$, we obtain

$$1 = \pi(\mathcal{X}) = \int_{x\in A} \pi(dx)\mathbf{E}_x\left[\sum_{n=1}^{\tau_A} \mathbf{1}_{X_n\in\mathcal{X}}\right] = \int_{x\in A} \pi(dx)\mathbf{E}_x[\tau_A] = \pi(A)\mathbf{E}_{\pi|A}[\tau_A],$$

giving the result.

For part (ii), we expand the original Markov chain to a new Markov chain on $\mathcal{X} \times \{0, 1, \ldots, k-1\}$, where the first variable is the original chain, and the second variable is the count (mod k) of the number of times the chain has returned to A. That is, each time the original chain visits A, the second variable increases by 1 (mod k). Then the expanded chain has stationary distribution $\pi \times \text{Uniform}\{0, 1, \ldots, k-1\}$. Hence, by part (i), if we begin in $(\pi|A) \times \delta_0$, then the expected return time of the expanded chain to $A \times \{0\}$ equals $1/[\pi(A) \times (1/k)] = k/\pi(A)$. But the first return time of the expanded chain to $A \times \{0\}$ corresponds precisely to the kth return time of the original chain to A. $\square$

We also require the following generalization of Wald's equation.

LEMMA 11. *Let $\{W_n\}$ be a sequence of nonnegative random variables each with finite mean $m < \infty$, and let $\{I_n\}$ be a sequence of indicator variables each with $\mathbf{P}(I_n = 1) = p > 0$. Assume that the sequence of pairs $\{(W_n, I_n)\}$ is i.i.d. [i.e., the sequence $\{Z_n\}$ is i.i.d. where $Z_n = (W_n, I_n)$]. Let $\tau = \inf\{n : I_n = 1\}$, and let $S = \sum_{i=1}^{\tau} W_i$. Then $\mathbf{E}(S) = \frac{m}{p} < \infty$.*

PROOF. We can write $S = \sum_{i=1}^{\infty} W_i \mathbf{1}_{\tau \geq i}$. Now, the event $\{\tau \geq i\}$ is equivalent to the event that $I_1 = I_2 = \cdots = I_{i-1} = 0$. Hence it is contained in $\sigma(Z_1, \ldots, Z_{i-1})$ and is thus independent of W_i by assumption. Also, τ is distributed as Geometric(p) and hence has mean $1/p$. We then compute that

$$\mathbf{E}(S) = \mathbf{E}\left(\sum_{i=1}^{\infty} W_i \mathbf{1}_{\tau \geq i}\right) = \sum_{i=1}^{\infty} \mathbf{E}(W_i \mathbf{1}_{\tau \geq i})$$

$$= \sum_{i=1}^{\infty} \mathbf{E}(W_i)\mathbf{E}(\mathbf{1}_{\tau \geq i}) = \sum_{i=1}^{\infty} m\mathbf{P}(\tau \geq i) = m\mathbf{E}(\tau) = m/p,$$

as claimed. $\square$

7. Proof of Theorem 5. The key to the proof is the following fact about Markov chain hitting times.

LEMMA 12. *Consider a ϕ-irreducible Markov chain on a state space $(\mathcal{X}, \mathcal{F})$ with transition kernel P and stationary probability distribution π. Let $B, C \in \mathcal{F}$ with $\pi(B) > 0$ and $\pi(C) > 0$, and let μ be any probability measure on $(\mathcal{X}, \mathcal{F})$. Suppose C is a small set for P with minorizing measure μ; that is, there is $\epsilon > 0$ and $n_0 \in \mathbf{N}$ such that $P^{n_0}(x, A) \geq \epsilon\mu(A)$ for all states $x \in C$ and all subsets $A \in \mathcal{F}$. Let τ_B be the first hitting time of B. Then $\mathbf{E}_\mu(\tau_B) < \infty$.*

PROOF. It suffices to consider the case where $n_0 = 1$, since if not we can replace P by P^{n_0} and note that the hitting time of B by P is at most n_0 times the hitting time of B by P^{n_0}.

We use the Nummelin splitting technique [17, 19]. Specifically, we expand the state space to $\mathcal{X} \times \{0, 1\}$, where the second variable is an indicator of whether or not we are currently regenerating according to μ.

Let $\alpha = \mathcal{X} \times \{1\}$. Then α is a Markov chain atom (i.e., the chain has identical transition probabilities from every state in α), and it has stationary measure $\pi(\alpha) = \epsilon\pi(C) > 0$. So, by Lemma 10(i) above, if the expanded chain is started in α (corresponding to the original chain starting in μ), then it will return to α in finite expected time $1/\pi(\alpha) < \infty$.

We now let W_n be the number of iterations between the $(n-1)$st and nth returns to α, and let $I_n = 1$ if this nth tour visits B, otherwise $I_n = 0$. Then $\mathbf{P}[I_n = 1] > 0$ by the ϕ-irreducibility of P. Hence, $\{(W_n, I_n)\}$ satisfies the conditions of Lemma 11.

Therefore, by Lemma 11, the expected number of iterations until we complete a tour which includes a visit to B is finite. Hence, the expected hitting time of B is finite. □

COROLLARY 13. (A3) *with* $\nu_* = \mu_*$ *implies* (A2).

PROOF. This follows immediately by applying Lemma 12 with $C = K_{2D} \setminus K_D$, and $B = K_D$, and $\mu = \mu_* = \nu_*$. □

PROOF OF THEOREM 5. Under assumption (a) that $\nu_* = \mu_*$, result (4) follows by combining Corollary 13 with Theorem 4. Under assumption (b) that P is reversible and $\mu_* = \pi_{K_{2D} \setminus K_D}$, it follows from the Appendix (Section 12.5 below) that (A3) also holds with $\nu_* = \pi|_{K_{2D} \setminus K_D} = \mu_*$. Hence assumption (a) still applies, so (4) again follows. □

REMARK 3. One might wonder if it suffices in Theorem 5 to assume (A1) with *any* distribution μ_*, and (A3) with *any* distribution ν_*, without requiring that either $\nu_* = \mu_*$ or $\mu_* = \pi|_{K_{2D} \setminus K_D}$. Under these assumptions, it would still follow from Lemma 10(ii) that the return times to K_{2D} all have finite expectation. And it would still be true that *if* we regenerate from ν_* in finite expected time, then we will eventually hit K_D in finite expected time. The problem is that the expected time to *first* regenerate from ν_* might be infinite. Indeed, conditionally upon visiting K_{2D} but repeatedly *failing* to regenerate, the chain could perhaps move to worse and worse states from which it would then take longer and longer to return to K_{2D}. (It is tempting to apply Lemma 11 here where W_n is the time between consecutive visits to K_{2D} and $I_n = 1$ if we regenerate otherwise 0, but unfortunately in this case $\{(W_n, I_n)\}$ are not i.i.d., and conditionally on nonregeneration the values of $\mathbf{E}[W_n | I_1 = \cdots = I_n = 0]$ could grow unboundedly.)

8. Proof of Proposition 6. Let $A \subseteq \mathbf{R}^d$ be the ball centered at the origin of radius 1, and let $B \subseteq \mathbf{R}^d$ be the ball centered at the point $(3/2, 0, 0, \ldots, 0)$ of radius 1. Then $A \cap B$ has nonempty interior, so $v_d := \mathrm{Leb}(A \cap B) > 0$. In terms of this, we have:

LEMMA 14. *Let $A, B \subseteq \mathbf{R}^d$ be two balls with radii $r \le R$, such that their centers are a distance $w \le 3r/2 + (R - r)$ apart. Then* $\mathrm{Leb}(A \cap B) \ge r^d v_d$.

PROOF. If $r = R = 1$, then this is just the definition of v_d. If one of the balls is stretched by a factor $R > 1$ while moving its center a distance $R - r$ further away, then the new ball contains the old ball, so $\mathrm{Leb}(A \cap B)$ can only increase. Finally, if each of w and r and R are multiplied by the same constant $a > 0$, then the entire geometry is scaled by a factor of a, so $\mathrm{Leb}(A \cap B)$ is multiplied by a^d. Combining these facts, the result follows. □

LEMMA 15. *Let P be a Markov chain on an open subset $\mathcal{X} \subseteq \mathbf{R}^d$. Let J be a rectangular subset of $\mathcal{X}$, of the form $J = (a_1, b_1) \times \cdots \times (a_d, b_d) \subseteq \mathcal{X}$, where $a_i < b_i$ are extended real numbers (i.e., we might have $a_i = -\infty$ and/or $b_i = \infty$ for some of the i). Suppose there are $\delta > 0$ and $\epsilon > 0$ satisfying the condition (6) that $P(x, dy) \ge \epsilon \,\mathrm{Leb}(dy)$ whenever $x, y \in J$ with $|y - x| < \delta$. Then for each $n \in \mathbf{N}$, there is $\beta_n > 0$ such that $P^n(x, dy) \ge \beta_n \,\mathrm{Leb}(dy)$ whenever $x, y \in J$ with $|y - x| < \delta(n + 1)/2$.*

PROOF. We first consider the case where $a_i = -\infty$ and $b_i = \infty$ for all i. The result for $n = 1$ follows by assumption. Suppose the result is true for some $n \ge 1$. Let $|y - x| < \delta(n + 1)/2$, let A be the ball centered at x of radius $\delta(n + 1)/2$ and let B be the ball centered at y of radius δ. Then applying Lemma 14 with $r = \delta$ and $R = \delta(n + 1)/2$ and $w = \delta(n + 2)/2$, we see that $\mathrm{Leb}(A \cap B) \ge \delta^d v_d$. The result now follows from the calculation

$$\begin{aligned} P^{n+1}(x, dy) &= \int_{z \in \mathcal{X}} P^n(x, dz) P(z, y) \ge \int_{z \in A \cap B} P^n(x, dz) P(z, y) \\ &\ge \int_{z \in A \cap B} \beta_n \,\mathrm{Leb}(dz) \epsilon \,\mathrm{Leb}(dy) \ge \mathrm{Leb}(A \cap B) \beta_n \epsilon \,\mathrm{Leb}(dy) \\ &\ge \delta^d v_d \beta_n \epsilon \,\mathrm{Leb}(dy) =: \beta_{n+1} \,\mathrm{Leb}(dy). \end{aligned}$$

For the general case, by shrinking δ as necessary, we can assume that $\delta < \frac{1}{2} \min_i (b_i - a_i)$. Then in the above calculation we can only use those parts of $A \cap B$ which are still inside J. But here J must contain at least half of $A \cap B$ in each coordinate, that is, at least $1/2^d$ of $A \cap B$ overall. Hence, $\mathrm{Leb}(A \cap B \cap J) \ge (1/2^d) \,\mathrm{Leb}(A \cap B)$. So, the above calculation still goes through, except now with β_{n+1} multiplied by an extra factor of $1/2^d$. □

PROOF OF PROPOSITION 6. Let $z = \mathrm{Diam}(J) < \infty$. Find $n_0 \in \mathbf{N}$ such that $\delta(n_0+1)/2 > z$. Then it follows from Lemma 15 that there is $\epsilon_{n_0} > 0$ such that $P^{n_0}(x, dy) \geq \epsilon_{n_0} \mathrm{Leb}(dy)$ for all $x, y \in J \supseteq K_{2D} \setminus K_D$. Hence, (A3) holds for this n_0 with $\nu_* = \mathrm{Uniform}(K_{2D} \setminus K_D)$ and $\epsilon = \epsilon_{n_0} \mathrm{Leb}(K_{2D} \setminus K_D)$. $\square$

9. Some facts about geometric ergodicity. To prove Theorem 7, we need to understand the implications of the geometric ergodicity assumption (A4). The following proposition shows that we can always find a geometric drift function of a certain form. To state it, let $PV(x) = \int_{y \in \mathcal{X}} V(y) P(x, dy)$ be the action of the Markov kernel P on a function V, and let $\tau_C = \inf\{n \geq 1 : X_n \in C\}$ be the first hitting time of C by a Markov chain $\{X_n\}$ following the transitions P. Also, say that V is a *geometric drift function* if

$$PV(x) \leq \lambda V(x) + b\mathbf{1}_C(x) \tag{7}$$

for some small set $C \in \mathcal{F}$ and some real numbers $\lambda < 1$ and $b < \infty$.

PROPOSITION 16. *If P is geometrically ergodic as in* (A4), *then there is a small set $C \subseteq \mathcal{X}$ with $\pi(C) > 0$, and a real number $\kappa > 1$, such that the function $V : \mathcal{X} \to \mathbf{R}$ defined by $V(x) = \mathbf{E}_x(\kappa^{\tau_C})$ is π-a.e. finite, and $r := \sup_{x \in C} V(x) < \infty$, and the geometric drift equation* (7) *holds with this C for some $b < \infty$ and with $\lambda = \kappa^{-1} < 1$. Furthermore, there is $\rho < 1$ and $c < \infty$ such that $\|P^n(x, \cdot) - \pi\| \leq cV(x)\rho^n$ for all $n \in \mathbf{N}$ and $x \in \mathcal{X}$.*

PROOF. Let $A_M = \{x \in \mathcal{X} : \xi(x) \leq M\}$. Since $\pi\{x \in \mathcal{X} : \xi(x) < \infty\} = 1$, we can find $M < \infty$ with $\pi(A_M) > 0$. The existence of *some* small set $C \subseteq A_M$ with $\pi(C) > 0$ follows from, for example, [20] (where they are called *C-sets*) or [19] or Theorem 5.2.2 of [17]. The fact that $C \subseteq A_M$ then implies condition (15.1) of [17] for this C [with $P^\infty(C) = \pi(C)$ and $M_C = M$ and $\rho_C = \rho$]. The existence of a (possibly different) small set C and $\kappa > 1$ with $\pi(C) > 0$ and $r := \sup_{x \in C} \mathbf{E}_x(\kappa^{\tau_C}) < \infty$. then follows from Theorem 15.0.1(ii) of [17].

Let $V(x) = \mathbf{E}_x(\kappa^{\tau_C})$. We compute directly that if $\{W_n\}$ follows P, then for $x \notin C$,

$$\begin{aligned} V(x) &= \mathbf{E}\big(\kappa^{\tau_C} | W_0 = x\big) = \mathbf{E}\big[\mathbf{E}\big(\kappa^{\tau_C} | W_1\big) | W_0 = x\big] \\ &= \int_{y \in \mathcal{X}} \mathbf{E}\big(\kappa^{\tau_C} | W_1 = y\big) P(x, dy) = \int_{y \in \mathcal{X}} \mathbf{E}\big(\kappa^{\tau_C + 1} | W_0 = y\big) P(x, dy) \\ &= \int_{y \in \mathcal{X}} \kappa \mathbf{E}\big(\kappa^{\tau_C} | W_0 = y\big) P(x, dy) = \kappa \int_{y \in \mathcal{X}} V(y) P(x, dy) = \kappa PV(x), \end{aligned}$$

which shows that $PV(x) = \kappa^{-1} V(x)$ for $x \notin C$.

To prove the geometric drift condition, it remains only to prove that $b := \sup_{x \in C} PV(x)$ is finite. For this we use some additional results from [17]. We

first compute that in the special case $f \equiv 1$, we have that

$$\sup_{x\in C} \mathbf{E}_x\left(\sum_{k=0}^{\tau_C-1} f(W_k)\kappa^k\right) = \sup_{x\in C} \mathbf{E}_x\left(\sum_{k=0}^{\tau_C-1} \kappa^k\right) = \sup_{x\in C} \mathbf{E}_x\left(\frac{\kappa^{\tau_C}-1}{\kappa-1}\right)$$
$$= \frac{\sup_{x\in C} \mathbf{E}_x(\kappa^{\tau_C})-1}{\kappa-1} = \frac{r-1}{\kappa-1} < \infty.$$

This means that C is an "f-Kendall set" for $f \equiv 1$, as defined on page 368 of [17]. Hence, by Theorem 15.2.4 of [17], the function $G(x) := G_C^{(\kappa)}(x, f)$ which equals 1 inside C and equals

$$\mathbf{E}_x\left(\sum_{k=0}^{\tau_C} f(W_k)\kappa^k\right) = \mathbf{E}_x\left(\sum_{k=0}^{\tau_C} \kappa^k\right) = \frac{\mathbf{E}_x(\kappa^{\tau_C+1})-1}{\kappa-1} = \frac{\kappa V(x)-1}{\kappa-1} \tag{8}$$

outside of C, satisfies its own geometric drift condition, say $PG(x) \le \lambda_G G(x) + b_G \mathbf{1}_C(x)$ where $\lambda_G < 1$ and $b_G < \infty$. In particular, since $G(x) = 1$ for $x \in C$, this means that $\sup_{x\in C} PG(x) \le \lambda_G + b_G < \infty$. Now, by (8), for $x \notin C$ we have $V(x) = \frac{1}{\kappa}[1 + (\kappa-1)G(x)] \le 1 + G(x)$. Since $V(x) \le r$ for $x \in C$, it follows that for all $x \in \mathcal{X}$, we have $V(x) \le r + G(x)$. Therefore, $PV(x) \le r + PG(x)$. This shows, finally, that

$$b := \sup_{x\in C} PV(x) \le r + \sup_{x\in C} PG(x) \le r + \lambda_G + b_G < \infty.$$

The above two facts together show that $PV(x) \le \kappa^{-1}V(x) + b\mathbf{1}_C(x)$ with $b < \infty$.

The bound on $\|P^n(x,\cdot) - \pi\|$ then follows from Theorem 16.0.1 of [17]. □

We next establish some bounds based on geometric-drift-type inequalities.

LEMMA 17. *Let $\{Z_n\}$ be any stochastic process. Suppose there are $0 < \lambda < 1$ and $b < \infty$ such that for all $n \in \mathbf{N}$, we have $\mathbf{E}(Z_n|Z_0, \ldots, Z_{n-1}) \le \lambda Z_{n-1} + b$. Then for all $n \in \mathbf{N}$,*

$$\mathbf{E}(Z_n|Z_0) \le \lambda^n Z_0 + \frac{b}{1-\lambda} \le Z_0 + \frac{b}{1-\lambda}.$$

PROOF. We claim that for all $n \ge 0$,

$$\mathbf{E}(Z_n|Z_0) \le \lambda^n Z_0 + (1 + \lambda + \cdots + \lambda^{n-1})b. \tag{9}$$

Indeed, for $n = 0$ this is trivial, and for $n = 1$ this is equivalent to the hypothesis of the lemma. Suppose now that (9) holds for some value of n. Then

$$\mathbf{E}(Z_{n+1}|Z_0) = \mathbf{E}\big(\mathbf{E}(Z_{n+1}|Z_0, \ldots, Z_n)|Z_0\big) \le \mathbf{E}(\lambda Z_n + b|Z_0)$$
$$\le \lambda\big(\lambda^n Z_0 + (1 + \lambda + \cdots + \lambda^{n-1})b\big) + b$$
$$= \lambda^{n+1} Z_0 + (1 + \lambda + \cdots + \lambda^{n-1} + \lambda^n)b,$$

so (9) holds for $n + 1$. Hence, by induction, (9) holds for all $n \ge 0$.

The result now follows since $1 + \lambda + \cdots + \lambda^{n-1} = \frac{1-\lambda^n}{1-\lambda} \le \frac{1}{1-\lambda}$. □

PROPOSITION 18. *If P is geometrically ergodic with stationary probability distribution π and π-a.e. finite geometric drift function V satisfying $PV(x) \le \lambda V(x) + b$ where $0 \le \lambda < 1$ and $0 \le b < \infty$, then $\mathbf{E}_\pi(V) \le b/(1-\lambda) < \infty$.*

PROOF. Choose any $x \in \mathcal{X}$ with $V(x) < \infty$ (which holds for π-a.e. $x \in \mathcal{X}$). Then applying Lemma 17 to $Z_n = P^n V(x)$ gives $P^n V(x) \le V(x) + \frac{b}{1-\lambda}$, and in particular $P^n V(x) \not\to \infty$. But Theorem 14.3.3 of [17] with $f = V$ states that if $\pi(V) = \infty$, then $P^n V(x) \to \infty$ for all $x \in \mathcal{X}$. Hence, by contraposition, we must have $\pi(V) < \infty$.

Finally, we have by stationarity that $\pi(V) = \pi(PV)$. So, taking expectations with respect to π of both sides of the inequality $PV \le \lambda V + b$ and using that $\pi(V) < \infty$, we obtain that $\pi(V) \le \lambda\pi(V) + b$, whence $\pi(V) \le b/(1-\lambda)$. □

REMARK 4. If P is *uniformly ergodic*, meaning that (A4) holds for a *constant* function $V < \infty$, then it follows from Theorem 16.0.2(vi) of [17] that $U := \sup_{x\in\mathcal{X}} \mathbf{E}_x(\tau_{K_D}) < \infty$, which implies that $\mathbf{E}_{\mu_*}(\tau_{K_D}) \le U < \infty$, so (A2) must hold.

10. Proof of Theorem 7. The key to the proof is a uniform bound on certain powers of P:

LEMMA 19. *Assuming* (A4) *and* (A5), *with V as in Proposition 16*, $\sup_{x\in K_D} \sup_{n\ge 0} P^n V(x) < \infty$.

PROOF. For $x \in K_D$, $PV(x) = \mathbf{E}_{y\sim P(x,\cdot)} V(y) \le M\mathbf{E}_{y\sim\pi} V(y) = M\pi(V) < \infty$ by (A5) and Proposition 18. Then applying Lemma 17 to $Z_n = P^n V(x)$ gives $P^n V(x) \le M\pi(V) + \frac{b}{1-\lambda}$. In particular, $\sup_{x\in K_D} \sup_{n\ge 1} P^n V(x) < \infty$.

Furthermore, for $x \in K_D$, $V(x) = \mathbf{E}_x(\kappa^{\tau_C}) = \kappa\mathbf{E}_{P(x,\cdot)}(\kappa^{\tau_C}) \le \kappa M\mathbf{E}_\pi(\kappa^{\tau_C}) = \kappa M\pi(V) < \infty$ by Proposition 18, so the above "sup" can be extended to include $n = 0$ too. □

REMARK 5. For Metropolis algorithms on continuous state spaces, usually $P(x,\{x\}) > 0$ for most $x \in \mathcal{X}$, so (A5) usually won't hold [though (A1) often will; see Section 11]. On the other hand, if $P(x,\cdot) = r(x)\delta_x(\cdot) + (1-r(x))R(x,\cdot)$ where δ_x is a point-mass at x and $0 \le r(x) \le 1$ and R satisfies (A5), then it is easily seen that if $\kappa r(x) \le B < 1$ for all $x \in K_D$, then Lemma 19 still holds with $\sup_{x\in K_D} V(x) \le \kappa M\pi(V)/(1-B) < \infty$, and the rest of the proof of Theorem 7 then goes through without change.

PROPOSITION 20. *Assuming* (A4) *and* (A5), *the random sequence* $\{V(X_n)\}$ *is bounded in probability.*

PROOF. Lemma 19 with $n = 0$ says that $U := \sup_{x \in K_D} V(x) < \infty$. Since the adversary can only adjust the values of $\{X_n\}$ within K_D, it follows that the adversary can only change the "next value of $V(X_n)$" by at most U, so $\{X_n\}$ will still satisfy a drift condition similar to (7), for the same C and λ but with b replaced by $b + U < \infty$. (Of course, C might not be a small set for the adversarial process.) More precisely, it follows from (7) that the adversarial process $\{X_n\}$ satisfies that $\mathbf{E}[V(X_n)|X_0, X_1, \ldots, X_{n-1}] \le \lambda V(X_{n-1}) + b + U$. Hence, applying Lemma 17 to $Z_n = V(X_n)$ says that $\{\mathbf{E}_{x_0}[V(X_n)]\}$ is bounded in probability, that is, that $\zeta := \sup_{x \in K_D} \sup_{n \ge 0} \mathbf{E}[V(X_n)|X_0 = x_0] < \infty$. It then follows by Markov's inequality that $\mathbf{P}_{x_0}[V(X_n) \ge R] \le \zeta/R$ for all n and all $R > 0$. Hence, $\{V(X_n)\}$ is bounded in probability. □

REMARK 6. Proposition 20 immediately implies a bound on the *ϵ-convergence times* [24] defined by $M_\epsilon(x) = \inf\{n \ge 1 : \|P^n(x, \cdot) - \pi(\cdot)\| \le \epsilon\}$. Indeed, by Proposition 16 we have $\|P^n(x, \cdot) - \pi\| \le cV(x)\rho^n$, whence $M_\epsilon(x) \le \lceil \log(cV(x)/\epsilon)/\log(1/\rho) \rceil$. Since $\{V(X_n)\}$ is bounded in probability by Proposition 20, it follows that $\{M_\epsilon(X_n)\}$ is bounded in probability too; see also the containment condition (15) below.

PROOF OF THEOREM 7. The bounded-jumps condition (2) implies that the small set C must be bounded (in fact, of diameter $\le 2Dn_0$). Let $r = \sup\{|x| : x \in C\} < \infty$. Then if $|x| > r$, it takes at least $(|x| - r)/D$ steps to return to C from x. Hence, $V(x) \ge \kappa^{(|x|-r)/D}$. Therefore, $|x| \le r + D \log(V(x))/\log(\kappa)$, so $|X_n| \le r + D \log(V(X_n))/\log(\kappa)$. But $\{V(X_n)\}$ is bounded in probability by Proposition 20. Hence, so is $\{X_n\}$. □

11. Application to adaptive MCMC algorithms. *Markov chain Monte Carlo (MCMC) algorithms* proceed by running a Markov chain $\{X_n\}$ with stationary probability distribution π, in the hopes that $\{X_n\}$ converges in total variation distance to π, that is, that

$$\lim_{n \to \infty} \sup_{A \in \mathcal{F}} \left| \mathbf{P}(X_n \in A) - \pi(A) \right| = 0, \qquad x \in \mathcal{X}, A \in \mathcal{F}. \tag{10}$$

If so then for large n, the value of X_n is approximately a "sample" from π. Such algorithms are hugely popular in, for example, Bayesian statistical inference; for an overview see, for example, [7].

Adaptive MCMC algorithms [11] attempt to speed up the convergence (10) and thus make MCMC more efficient by modifying the Markov chain transitions during the run (i.e., "on the fly") in a search for a more optimal chain; for a brief introduction, see, for example, [26]. Such algorithms often appear to work very well in practice (e.g., [4, 8, 10, 25]). However, they are no longer Markov chains (since the adaptions typically depend on the process's entire history), making it extremely difficult to establish mathematically that the convergence (10) will even be

preserved (much less improved). As a result, many papers either make the artificial assumption that the state space $\mathcal{X}$ is compact (e.g., [4, 8, 11]), or prove the convergence (10) using complicated mathematical arguments requiring strong and/or uncheckable assumptions (e.g., [1–3, 10, 15, 24, 28]), or do not prove (10) at all and simply hope for the best. It is difficult to find simple, easily checked conditions which provably guarantee the convergence (10) for adaptive MCMC algorithms.

One step in this direction is in [24], where it is proved that convergence (10) is implied by two conditions. The first condition is *diminishing adaptation*, which says that the process adapts less and less as time goes on; see (14) below. The second condition is *containment*, which says that the process's convergence times are bounded in probability; see (15) below. The first of these two conditions is usually easy to satisfy directly by wisely designing the algorithm, so it is not of great concern. However, the second condition is notoriously difficult to verify (see, e.g., [5]) and thus a severe limitation (though an essential condition; cf. [16]). On the other hand, the containment condition (15) is reminiscent of the boundedness in probability property (4), which is implied by our various theorems above. This suggests that our theorems might be useful in establishing the containment condition (15) for certain adaptive MCMC algorithms, as we now explore.

11.1. *The adaptive MCMC setup.* We define an adaptive MCMC algorithm within the context of Section 2 as follows. Let $\mathcal{X}$ be an open subset of $\mathbf{R}^d$ for some $d \in \mathbf{N}$, on which π is some probability distribution. Assume that for some compact index set $\mathcal{Y}$, there is a collection $\{P_\gamma\}_{\gamma\in\mathcal{Y}}$ of Markov kernels on $\mathcal{X}$, each of which leaves π stationary and in fact is Harris-ergodic to π as in (1). The adversary proceeds by choosing, at each iteration n, an index $\Gamma_n \in \mathcal{Y}$ (possibly depending on n and/or the process's entire history, though not on the future). The process $\{X_n\}$ then moves at time n according to the transition kernel P_{Γ_n}, that is,

$$\mathbf{P}(X_{n+1} \in A | X_n = x, \Gamma_n = \gamma, X_0, \ldots, X_{n-1}, \Gamma_0, \ldots, \Gamma_{n-1}) = P_\gamma(x, A).$$

To reflect the bounded jump condition (2), we assume there is $D < \infty$ with

$$P_\gamma\big(x, \{y \in \mathcal{X} : |y - x| \le D\}\big) = 1, \qquad x \in \mathcal{X}, \gamma \in \mathcal{Y}. \tag{11}$$

To reflect that the adversary can only adapt inside K, we assume that the P_γ kernels are all equal outside of K, that is, that

$$P_\gamma(x, A) = P(x, A), \qquad A \in \mathcal{F}, x \in \mathcal{X} \setminus K, \tag{12}$$

for some fixed Markov chain kernel $P(x, dy)$ also satisfying (1). We further assume that

$$\exists M < \infty \quad \text{s.t.} \quad P(x, dy) \le M \,\mathrm{Leb}(dy), \qquad x \in K_D \setminus K, z \in K_{2D} \setminus K_D. \tag{13}$$

We also assume the ϵ–δ condition (6) that $P(x, dy) \ge \epsilon \,\mathrm{Leb}(dy)$ whenever $x, y \in J$ with $|y - x| < \delta$, for some bounded rectangle J with $K_{2D} \setminus K_D \subseteq J \subseteq \mathcal{X}$.

We shall particularly focus on the case where each P_γ is a Metropolis–Hastings algorithm. This means that P_γ proceeds, given X_n, by first choosing a proposal state $Y_{n+1} \sim Q_\gamma(X_n, \cdot)$ for some proposal kernel $Q_\gamma(x, \cdot)$ having a density $q_\gamma(x, y)$ with respect to Leb. Then, with probability $\alpha_\gamma(X_n, Y_{n+1}) := \min[1, \frac{\pi(Y_{n+1})q_\gamma(Y_{n+1}, X_n)}{\pi(X_n)q_\gamma(X_n, Y_{n+1})}]$ it *accepts* this proposal by setting $X_{n+1} = Y_{n+1}$. Otherwise, with probability $1 - \alpha_\gamma(X_n, Y_{n+1})$, it *rejects* this proposal by setting $X_{n+1} = X_n$. That is,

$$P_\gamma(x, A) = r(x)\delta_x(A) + \int_{y\in A} Q_\gamma(x, dy)\alpha_\gamma(x, y),$$

where $\delta_x(\cdot)$ is a point-mass at x, and $r(x) = 1 - \int_{y\in\mathcal{X}} Q_\gamma(x, dy)\alpha_\gamma(x, y)$ is the overall probability of rejecting. Note that (11), (12) and (13) are each automatically satisfied for P_γ and P if the corresponding equations are satisfied for corresponding Q_γ and Q.

11.2. *An adaptive MCMC theorem.* Our theorem shall follow up on the result from [24] that convergence (10) is implied by the twin properties of diminishing adaptation and containment. *Diminishing adaptation* says that the process adapts less and less as time goes on, or more formally that

$$\lim_{n\to\infty} \sup_{x\in\mathcal{X}} \sup_{A\in\mathcal{F}} \left| P_{\Gamma_{n+1}}(x, A) - P_{\Gamma_n}(x, A) \right| = 0 \qquad \text{in probability.} \tag{14}$$

Containment says that the process's convergence times are bounded in probability, or more formally that

$$\left\{ M_\epsilon(X_n, \Gamma_n) \right\}_{n=1}^{\infty} \qquad \text{is bounded in probability,} \tag{15}$$

where $M_\epsilon(x, \gamma) = \inf\{n \geq 1 : \| P_\gamma^n(x, \cdot) - \pi(\cdot) \| \leq \epsilon\}$ is the *ϵ-convergence time*. The containment condition (unlike diminishing adaptation) is notoriously difficult to establish in practice (see, e.g., [5]), but the theorems herein can help. To state a clean theorem, we assume continuous densities, as follows:

(A6) π has a continuous positive density function (with respect to Leb), and the transition probabilities $P_\gamma(x, dy)$ either (i) have densities which are continuous functions of x and y and γ, or (ii) are Metropolis–Hastings algorithms whose proposal kernel densities $q_\gamma(x, dy)$ are continuous functions of x, y and γ.

In terms of the above setup, we have:

THEOREM 21. *Consider an adaptive MCMC algorithm as in Section* 11.1, *on an open subset $\mathcal{X}$ of $\mathbf{R}^d$, such that the kernels P_γ (or the proposal kernels Q_γ in the case of adaptive Metropolis–Hastings) have bounded jumps as in* (11), *and no adaption outside of K as in* (12), *with the fixed kernel P (or a corresponding fixed proposal kernel Q) bounded above as in* (13). *We further assume the ϵ–δ condition* (6) *for P, and the continuous densities condition* (A6). *Then the algorithm satisfies the containment condition* (15). *Hence, assuming diminishing adaptation* (14), *the algorithm converges in distribution to π as in* (10).

Theorem 21 is proved in Section 11.3 below. Clearly, similar reasoning also applies with alternative assumptions and to other versions of adaptive MCMC including, for example, adaptive Metropolis-within-Gibbs algorithms (with P replaced by P^d for random-scan); cf. [15].

Theorem 21 requires many conditions, but they are all easy to ensure in practice, as illustrated by the following type of adaptive MCMC algorithm:

The bounded adaption Metropolis (BAM) algorithm. Let $\mathcal{X} = \mathbf{R}^d$, let $K \subseteq \mathcal{X}$ be bounded, let π be a continuous positive density on $\mathcal{X}$ and let $D > 0$. Let $\mathcal{Y}$ be a compact collection of d-dimensional positive–definite matrices, and let $\Sigma_* \in \mathcal{Y}$ be fixed. Define a process $\{X_n\}$ as follows: $X_0 = x_0$ for some fixed $x_0 \in K$. Then for $n = 0, 1, 2, \ldots$, given X_n, we generate a proposal Y_{n+1} by: (a) if $X_n \notin K$, then $Y_{n+1} \sim N(X_n, \Sigma_*)$; (b) if $X_n \in K$ with $\operatorname{dist}(X_n, K^c) > 1$, then $Y_{n+1} \sim N(X_n, \Sigma_{n+1})$, where the matrix $\Sigma_{n+1} \in \mathcal{Y}$ is selected in some fashion, perhaps depending on X_n and on the chain's entire history; (c) if $X_n \in K$ but $\operatorname{dist}(X_n, K^c) = u$ with $0 \le u \le 1$, then $Y_{n+1} \sim (1-u)N(X_n, \Sigma_*) + uN(X_n, \Sigma_{n+1})$. Once Y_{n+1} is chosen, then if $|Y_{n+1} - X_n| > D$, the proposal is rejected so $X_{n+1} = X_n$. Otherwise, if $|Y_{n+1} - X_n| \le D$, then with probability $\min[1, \frac{\pi(Y_{n+1})}{\pi(X_n)}]$ the proposal is accepted so $X_{n+1} = Y_{n+1}$, or with the remaining probability the proposal is rejected so $X_{n+1} = X_n$.

REMARK 7. In the above BAM algorithm, $q_\gamma(Y_{n+1}, X_n) = q_\gamma(X_n, Y_{n+1})$, so those factors cancel in the formula for the acceptance probability.

REMARK 8. One good choice for the proposal covariance matrix Σ_{n+1} in part (b) of the BAM algorithm is $(2.38)^2 V_n/d$, where V_n is the empirical covariance matrix of $X_0, \ldots, X_n$ from the process's previous history (except restricted to some compact set $\mathcal{Y}$), since that choice approximates the optimal proposal covariance; see the discussion in Section 2 of [25].

PROPOSITION 22. *The above BAM algorithm satisfies containment* (15). *Hence, if the selection of the* Σ_n *satisfies diminishing adaptation* (14), *then convergence* (10) *holds.*

PROOF. The BAM algorithm satisfies all of the conditions of Theorem 21. Indeed, bounded jumps (11) and no adaption outside of K (12) are both immediate. Here the fixed kernel Q is bounded above (13) by the constant $M = (2\pi)^{-d/2}|\Sigma_*|^{-1/2}$, and the ϵ–δ condition (6) holds by the formula for Q together with the continuity of the density π (which guarantees that it is bounded above and below on any compact rectangle J containing the compact set K_{2D}). Furthermore the continuous densities condition (A6) holds by construction. Hence, the result follows from Theorem 21. □

11.3. *Proof of Theorem 21.* We begin with a result linking the boundedness property (4) for $\{X_n\}$ with the containment condition (15) for $\{M_\epsilon(X_n, \Gamma_n)\}$, as follows:

PROPOSITION 23. *Consider an adaptive MCMC algorithm as in Section 11.1. Suppose (4) holds, and for each $n \in \mathbf{N}$ the mapping $(x, \gamma) \mapsto \Delta(x, \gamma, n) := \|P_\gamma^n(x, \cdot) - \pi(\cdot)\|$ is continuous. Then the containment condition (15) holds.*

PROOF. Since each P_γ is Harris ergodic, $\lim_{n\to\infty} \Delta(x, \gamma, n) = 0$ for each fixed $x \in \mathcal{X}$ and $\gamma \in \mathcal{Y}$. Also, since π is a stationary distribution for P_γ, the mapping $n \mapsto \Delta(x, \gamma, n)$ is nonincreasing; see, for example, Proposition 3(c) of [23]. If the mapping $(x, \gamma) \mapsto \Delta(x, \gamma, n)$ is continuous, then it follows by Dini's theorem (e.g., [27], page 150) that for any compact subset $C \subseteq \mathcal{X}$, since $\mathcal{Y}$ is compact,

$$\lim_{n\to\infty} \sup_{x\in C} \sup_{\gamma\in\mathcal{Y}} \Delta(x, \gamma, n) = 0.$$

Hence, given C and $\epsilon > 0$, there is $n \in \mathbf{N}$ with $\sup_{x\in C} \sup_{\gamma\in\mathcal{Y}} \Delta(x, \gamma, n) < \epsilon$. It follows that $\sup_{x\in C} \sup_{\gamma\in\mathcal{Y}} M_\epsilon(x, \gamma) < \infty$ for any fixed $\epsilon > 0$.

Now, if $\{X_n\}$ is bounded in probability as in (4), then for any $\delta > 0$, we can find a large enough compact subset C such that $P(X_n \notin C) \le \delta$ for all n. Then given $\epsilon > 0$, and if $L := \sup_{x\in C} \sup_{\gamma\in\mathcal{Y}} M_\epsilon(x, \gamma)$, then $L < \infty$, and $P(M_\epsilon(X_n, \Gamma_n) > L) \le \delta$ for all n as well. Since δ was arbitrary, it follows that $\{M_\epsilon(X_n, \Gamma_n)\}_{n=0}^\infty$ is bounded in probability. □

We then need a lemma guaranteeing continuity of $\Delta(x, \gamma, n)$:

LEMMA 24. *Under the continuous density assumptions* (A6), *for each $n \in \mathbf{N}$, the mapping $(x, \gamma) \mapsto \Delta(x, \gamma, n)$ is continuous.*

PROOF. Assuming (A6)(ii), this fact is contained in the proof of Corollary 11 of [24]. The corresponding result assuming (A6)(i) is similar but easier. □

PROOF OF THEOREM 21. The bounded jumps condition (11), together with no adaption outside of K (12), ensure that the algorithm $\{X_n\}$ fits within the setup of Section 2. Since the densities of $P(x, dy)$ are bounded above by (13), it follows that (A1) holds with $\mu_* = \text{Uniform}(K_{2D} \setminus K_D)$. Also, using the ϵ–δ condition (6), it follows from Proposition 6 that (A3) holds for $\nu_* = \mu_*$. Hence, by Theorem 5(a), $\{X_n\}$ is bounded in probability; that is, (4) holds. In addition, using the continuity assumption (A6), it follows from Lemma 24 that $\Delta(x, \gamma, n)$ is a continuous function. Containment (15) thus follows from Proposition 23. The final assertion about convergence (10) then follows from [24]. □

12. A detailed statistical MCMC example: RCA. Relying on the theoretical advances in this paper, we shall now demonstrate the effectiveness of a general adaptive strategy which we call *regime change algorithm (RCA)* that can be implemented in a wide number of practical instances. Specifically, during the initialization period the chain is run using a transition kernel that can provide some information about the target. We do not assume that this initial kernel is optimal in any way, just that it would be a reasonable initial choice for an MCMC algorithm. After the initialization period, inside a chosen compact set, the initial kernel is slowly replaced by an adaptive kernel that is shown to exhibit better mixing. In a statistical example below, we shall see that this regime change dramatically increases the algorithm efficiency, since the adaptive kernel is increasingly more suitable for sampling the target inside the compact. Our regime change idea is in the same general vein as the two-stage adaptation proposed by Giordani and Kohn [10]. However, their theoretical justification follows a rather different approach from ours.

12.1. *Model and data.* We shall consider a Bayesian probit regression model applied to a well-known collection of lupus patient data originally supplied by Haas [12] and later simplified in [29]. The data, shown in Table 1, contain disease status for 55 patients of which 18 have been diagnosed with latent membranous lupus, together with two clinical covariates, IgA and ΔIgG (which is equal to $IgG3 - IgG4$ in the lupus context), which are computed from their levels of immunoglobulin of type A and of type G, respectively. We consider a probit regression (PR) model; that is, for each patient $1 \le i \le 55$, and we model the disease

TABLE 1

The number of latent membranous lupus nephritis cases (*numerator*), *and the total number of cases* (*denominator*), *for each combination of the values of the two covariates*, *for the* 55 *lupus patients in the data set described in Section* 12.1

	IgA				
ΔIgG	**0**	**0.5**	**1**	**1.5**	**2**
−3.0	0/1	–	–	–	–
−2.5	0/3	–	–	–	–
−2.0	0/7	–	–	–	0/1
−1.5	0/6	0/1	–	–	–
−1.0	0/6	0/1	0/1	–	0/1
−0.5	0/4	–	–	1/1	–
0	0/3	–	0/1	1/1	–
0.5	3/4	–	1/1	1/1	1/1
1.0	1/1	–	1/1	1/1	4/4
1.5	1/1	–	–	2/2	–

indicator variables as independent

$$Y_i \sim \text{Bernoulli}\big(\Phi(x_i^T \beta)\big),$$

where $\Phi(\cdot)$ is the CDF of $N(0,1)$, $x_i = (1, \Delta IgG_i, IgA_i)$ is the vector of covariates, and β is a 3×1 vector of parameters which is assigned a flat prior $p(\beta) \propto 1$. The posterior is thus

$$\begin{aligned}\pi_{\text{PR}}(\vec{\beta}|\vec{Y}, \vec{IgA}, \vec{\Delta IgG}) &\propto \prod_{i=1}^{55}\big[\Phi(\beta_0 + \Delta IgG_i\beta_1 + IgA_i\beta_2)^{Y_i} \\ &\quad \times \big(1 - \Phi(\beta_0 \Delta IgG_i\beta_1 + IgA_i\beta_2)\big)^{(1-Y_i)}\big].\end{aligned}$$

We wish to design effective algorithms to sample from this posterior distribution π_{PR}.

12.2. *The best previous algorithm*: *PX-DA*. The current state-of-the-art most efficient algorithm to sample from the above posterior distribution π_{PR} is the *parameter expanded data augmentation (PX-DA)* algorithm developed by van Dyk and Meng [29]. The PX-DA transition kernel for updating $\beta^{(t)}$ is defined by the following steps:

- Draw
$$\phi_i^{(t+1)} \sim \begin{cases} N_+\big(x_i^T \beta^{(t)}, 1\big), & \text{if } Y_i = 1, \\ N_-\big(x_i^T \beta^{(t)}, 1\big), & \text{if } Y_i = 0, \end{cases}$$
where $N_+(\mu, \sigma^2)$ and $N_-(\mu, \sigma^2)$ are normal distributions with mean μ and variance σ^2 that are truncated to $(0, \infty)$ and $(-\infty, 0)$, respectively. Set $\phi^{(t+1)} = (\phi_1^{(t+1)}, \ldots, \phi_n^{(t+1)})$.
- Let $\tilde{\beta}^{t+1} = (X^T X)^{-1} X^T \phi^{(t+1)}$, and define $R^{(t+1)} = \sum_{i=1}^n (\phi_i^{(t+1)} - x_i^T \tilde{\beta}^{(t+1)})^2$.
- Sample $Z \sim N(0,1)$, $W \sim \chi_n^2$ and set $\beta^{(t+1)} = \sqrt{\frac{W}{R^{(t+1)}}}\tilde{\beta}^{(t+1)} + \text{Chol}[(X^T \times X)^{-1}]Z$.

12.3. *A new algorithm*: *RCA*. The regime change algorithm (RCA) is initialized by running the PX-DA chain for M iterations. Based on the samples obtained, we determine a compact subset K and a distance bound D which remain fixed for the rest of the simulation. The algorithm then proceeds by constructing a Gaussian approximation of the target inside K that continuously evolves as the samples are collected, thus allowing for better and better proposal values.

To proceed, for $n \geq M$ we define

$$\mu_n := \frac{\langle X_0 \rangle + \langle X_1 \rangle + \cdots + \langle X_{n-1} \rangle}{n},$$

and

$$\Sigma_n := \mathrm{Cov}\big(\langle X_0\rangle, \langle X_1\rangle, \ldots, \langle X_{n-1}\rangle\big) + \epsilon I_d,$$

where Cov is the empirical covariance function, and $\langle r\rangle$ is the shrunken version of $r \in \mathbf{R}^d$ with each coordinate shrunk into the interval $[-L, L]$, that is, $\langle r\rangle_i = \max[-L, \min(L, r_i)]$. We then define K to be the ball centered at μ_M, of radius $\max_{1\le i\le d}(\Sigma_M)_{ii}^{1/2}$ (i.e., the largest sample standard deviation on the diagonal of Σ_M), and we let D be any suitably large distance bound (e.g., $D = 20$).

We then consider the independence Metropolis (IM) transition kernel P_{μ_n,Σ_n}, with proposal distribution given (independently of the current state of the process) by the Gaussian distribution $N(\mu_n, \Sigma_n)$, except truncated (in a continuous manner; see Remark 9 below) to remain in the compact K and to never move more than a distance D. We also let $P_{PX}(x, y)$ be the PX-DA algorithm described above, also truncated in a continuous manner to remain in the compact K and to never move more than a distance D.

In terms of these definitions, the update for the RCA follows these steps:

(1) If $X_n \in K^c$, then $X_{n+1} \sim P_{PX}(X_n, \cdot)$.
(2) If $X_n \in K$ and $d(X_n, K^c) > 1$, then

$$X_{n+1} \sim \lambda_{n+1} P_{\mu_n,\Sigma_n}(X_n, \cdot) + (1 - \lambda_{n+1}) P_{PX}(X_n, \cdot),$$

with $\lambda_n = \min[\max(\theta_n, 0.2), 0.8]$, where θ_n is the empirical acceptance rate of all of the IM proposals made so far between time $M + 1$ and time $n - 1$ (or we simply set $\lambda_n = 1/2$ if there have been no such proposals).

(3) If $X_n \in K$ and $d(X_n, K^c) = u$ with $0 \le u \le 1$, then

$$X_{n+1} \sim u\big[\lambda_{n+1} P_{\mu_n,\Sigma_n}(X_n, \cdot) + (1 - \lambda_{n+1}) P_{PX}(X_n, \cdot)\big] + (1 - u) P_{PX}(X_n, \cdot),$$

with λ_n as above.

That is, letting $\gamma_n = (\mu_n, \Sigma_n, \lambda_n)$ be the complete adaptive parameter, we can say that when $d(X_n, K^c) > 1$, the chain moves according to the adaptive kernel

$$P_{K,\gamma_n}(X_n, \cdot) = \lambda_{n+1} P_{\mu_n,\Sigma_n}(X_n, \cdot) + (1 - \lambda_{n+1}) P_{PX}(X_n, \cdot),$$

and when $X_n \in K^c$ the chain follows the transition $P_{PX}(X_n, \cdot)$, with a linear interpolation near the boundary of K to satisfy the continuous densities condition (A6).

REMARK 9. In our description of RCA above, we required certain Gaussian distributions to be restricted to certain subsets. If this is done naively, then it will result in a discontinuous density, which may violate (A6). However, this issue can be easily avoided if we make the density continuous by smoothing the edge via a linear interpolation. For example, to restrict a univariate normal density with mean μ and variance σ^2 to the range (a, b) for $a < b$, one can choose small $\upsilon > 0$ and define

$$f_\upsilon(x|\mu, \sigma, a, b) = \frac{(2\pi\sigma^2)^{-1/2} \exp[-(x - \mu)^2/(2\sigma^2)]}{\Phi(b - \upsilon) - \Phi(a + \upsilon)},$$

and then use the density function proportional to

$$g(x|\mu,\sigma,a,b,\upsilon)=\begin{cases} f_\upsilon(x|\mu,\sigma,a,b), & \text{if } a+\upsilon\le x\le b-\upsilon,\\ f_\upsilon(b-\upsilon|\mu,\sigma,a,b)(b-x)/\upsilon, & \text{if } b-\upsilon<x<b,\\ f_\upsilon(a+\upsilon|\mu,\sigma,a,b)(x-a)/\upsilon, & \text{if } a<x<a+\upsilon,\\ 0, & \text{otherwise.}\end{cases}$$

The general multivariate case can be handled by similarly truncating each of the independent univariate Gaussian variables used to construct the multivariate Gaussian. In this way, it can be assured that even truncated Gaussians still have continuous densities.

12.4. *Verification of the theoretical assumptions.* To justify the use of our new RCA algorithm, we wish to prove asymptotic convergence as in (10). Proving such convergence of adaptive MCMC algorithms is usually very difficult, but we shall manage this by applying Theorem 21. To do this, we need to verify the assumptions of Theorem 21 including those which are implicit in the setup of Section 11.1. Fortunately, this is not too difficult.

For the RCA algorithm, the "bounded jumps" condition (11) and the "fixed kernel outside of K" condition (12) are both satisfied by construction.

Furthermore, the "fixed kernel bounded above by a multiple of Lebesgue" condition (13), and the "ϵ–δ bounded below by a multiple of Lebesgue" condition (6), both concern the transition probabilities outside of K, and hence they both follow since our fixed transition probabilities are absolutely continuous with respect to Lebesgue measure with densities that are uniformly bounded away from 0 and ∞ on compact subsets.

In addition, the continuous densities condition (A6) is satisfied since all transition kernels involved in the construction of the chain are Metropolis–Hastings (MH) kernels with proposal densities that are continuous functions of the adaption parameters and of x and y; cf. Remark 9.

Finally, we note that RCA also satisfies the diminishing adaptation condition (14), since the difference between the values of each of the adaptation parameters at iterations n and $n+1$ is always $O(n^{-1})$.

Hence RCA satisfies all of the assumptions of Theorem 21 and Section 11.1, and also satisfies Diminishing Adaptation (14), so we conclude:

COROLLARY 25. *The RCA algorithm described above converges asymptotically to π as in* (10).

12.5. *A simulation study.* To test our new RCA algorithm in practice, we ran[1] both it and the PX-DA algorithm, each for 5000 iterations starting with X_0 equal to the maximum likelihood estimate (MLE).

[1]The R computer program we used is available at: www.probability.ca/lupus

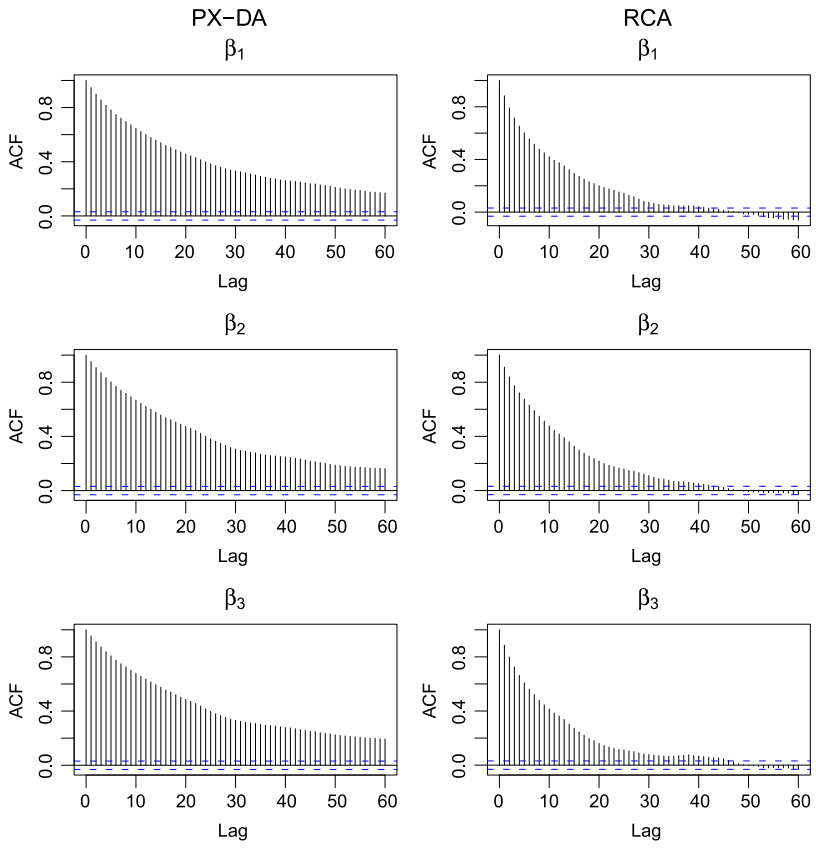

FIG. 3. *Autocorrelation (ACF) plots for the probit regression model simulation study of Section 12.5, comparing the PX-DA (left column) and RCA (right column) algorithms, for each of the three parameters β_0 (top), β_1 (middle) and β_2 (bottom), showing significantly smaller autocorrelations (and hence better performance) for RCA than for PX-DA.*

We found that the RCA algorithm did indeed perform significantly more efficiently than PX-DA did. As one measure of this, we plotted the autocorrelation function (ACF) plots of both algorithms for each of the three parameters (Figure 3). This plot indicates that the autocorrelations for RCA are significantly smaller than those for PX-DA, thus indicating faster mixing and thus a more efficient algorithm. Indeed, the sums of the nonnegligible positive-lag autocorrelations for the three parameters were respectively 41.20, 40.87 and 43.87 for PX-DA, but just 10.56, 11.88 and 10.00 for RCA, and again showing much greater efficiency of RCA.

Another way to think about this is in terms of effective sample size (ESS). This is a measure of how many true independent samples our algorithm is equivalent to, in terms of variance of the resulting estimator. The ESS is well known (see, e.g., [9], page 2) to be inversely proportional to $1 + 2S$ where S is the autocorrelation

sum as above. By this measure, in our simulations the ESS for RCA is larger than for PX-DA, for the three parameters respectively, by factors of 3.77, 3.34 and 4.23. This indicates quite significant improvements in efficiency of RCA over PX-DA for this example.

We conclude that having the possibility to sample from the IM kernel reduces the autocorrelation within the samples produced by the algorithm and thus significantly increases the effective sample size. This indicates that the RCA algorithm (as justified in Corollary 25, by applying Theorem 21) is indeed a superior algorithm for this problem.

APPENDIX: REPLACING THE MINORIZING MEASURE BY π

Recall that assumption (A3) requires that the set $K_{2D} \setminus K_D$ be small for P, with some minorizing measure ν_*. It turns out that if assumption (A3) holds for any ν_*, and if P is reversible, then assumption (A3) also holds for the specific choice $\nu_* = \pi|_{K_{2D}\setminus K_D}$, that is, where $\nu_*(A) = \pi(A \cap (K_{2D} \setminus K_D))/\pi(K_{2D} \setminus K_D)$, with the step size n_0 replaced by $2n_0$. Under the additional assumption of uniform ergodicity, this fact is Proposition 1 of [22]. For arbitrary reversible chains, this fact follows from Lemma 5.9 of the Polish doctoral thesis [18], which for completeness we now reproduce:

LEMMA 26 (Lemma 5.9 of [18]). *Let P be a Markov chain transition kernel on $(\mathcal{X}, \mathcal{F})$, with invariant probability measure π. Let $C \in \mathcal{F}$ such that $\pi(C) > 0$. Assume that C is a small set for P; that is, for some $n_0 \in \mathbf{N}$ and $\beta > 0$ and probability measure ν,*

$$P^{n_0}(x, A) \geq \beta \mathbf{1}_C(x)\nu(A), \qquad A \in \mathcal{F}. \tag{16}$$

Then

$$P^{n_0}\big(P^*\big)^{n_0}(x, A) \geq \tfrac{1}{4}\beta^2 \mathbf{1}_C(x)\pi(A \cap C), \qquad A \in \mathcal{F}, \tag{17}$$

where P^* is the $L^2(\pi)$ adjoint of P. In particular, if P is reversible with respect to π, so that $P^* = P$, then

$$P^{2n_0}(x, A) \geq \tfrac{1}{4}\beta^2 \mathbf{1}_C(x)\pi(A \cap C), \qquad A \in \mathcal{F}.$$

Hence if $K_{2D} \setminus K_D$ is an n_0-small set with minorizing measure ν, and P is reversible with respect to π, then $K_{2D} \setminus K_D$ is a $(2n_0)$-small set with minorizing measure $\pi|_{K_{2D}\setminus K_D}$.

PROOF OF LEMMA 26. By replacing P by P^{n_0} and P^* by $(P^*)^{n_0}$, it suffices to assume that $n_0 = 1$. Now, the Radon–Nikodym derivative $\frac{d\nu}{d\pi}$ of ν with respect to π satisfies that $\int_{\mathcal{X}} \frac{d\nu}{d\pi}(x)\pi(dx) = \nu(\mathcal{X}) = 1$. Hence, for every $\varepsilon \in [0, 1]$, the set

$$D(\varepsilon) := \left\{x \in \mathcal{X} : \frac{d\nu}{d\pi}(x) \geq \varepsilon\right\} \tag{18}$$

has $\pi(D(\varepsilon)) > 0$. We then compute that

$$\nu\big(D(\varepsilon)^c\big) = \int_{D(\varepsilon)^c} \frac{d\nu}{d\pi}(x)\pi(dx) \le \varepsilon \int_{\mathcal{X}} \pi(dx) = \varepsilon$$

and hence

$$\nu\big(D(\varepsilon)\big) \ge 1 - \varepsilon. \tag{19}$$

Recall also that the adjoint P^* satisfies

$$\pi(dx)P(x, dy) = \pi(dy)P^*(y, dx). \tag{20}$$

Now let $x \in C$, and $A \in \mathcal{F}$ with $A \cap C \neq \varnothing$. Using first (16) and then (18),

$$\begin{aligned} PP^*(x, A) &= \int_{z\in\mathcal{X}} P^*(z, A)P(x, dz) \ge \beta \int_{z\in\mathcal{X}} P^*(z, A \cap C)\nu(dz) \\ &\ge \beta \int_{z\in D(\varepsilon)} \int_{y\in A\cap C} P^*(z, dy)\varepsilon\pi(dz). \end{aligned}$$

To continue, use (20), then (16) again and finally (19) to obtain

$$\begin{aligned} PP^*(x, A) &\ge \beta\varepsilon \int_{z\in D(\varepsilon)} \int_{y\in A\cap C} \pi(dy)P(y, dz) \\ &\ge \beta^2\varepsilon\nu\big(D(\varepsilon)\big)\pi(A \cap C) \ge \beta^2\varepsilon(1 - \varepsilon)\pi(A \cap C). \end{aligned}$$

Setting $\varepsilon = 1/2$ yields (17). □

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