# <span id="page-0-0"></span>**CLTs and Asymptotic Variance of Time-Sampled Markov Chains**

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**Abstract** For a Markov transition kernel P and a probability distribution  $\mu$  on nonnegative integers, a time-sampled Markov chain evolves according to the transition kernel  $P_{\mu} = \sum_{k} \mu(k) P^{k}$ . In this note we obtain CLT conditions for time-sampled Markov chains and derive a spectral formula for the asymptotic variance. Using these results we compare efficiency of Barker's and Metropolis algorithms in terms of asymptotic variance.

**Keywords** Time-sampled Markov chains**·** Barker's algorithm **·** Metropolis algorithm **·** Central Limit Theorem **·** Asymptotic variance **·** Variance bounding Markov chains**·** MCMC estimation

# **AMS 2000 Subject Classifications** 60J05 **·** 60F05

# **1 Introduction**

Let *P* be an ergodic transition kernel of a Markov chain  $(X_n)_{n\geq 0}$  with limiting distribution  $\pi$  on  $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$  and let  $f : \mathcal{X} \to \mathbb{R}$  be in  $L^2(\pi)$ . A typical MCMC procedure for estimating  $I = \pi f := \int_{\mathcal{X}} f(x)\pi(dx)$  would use  $\hat{I}_n := \frac{1}{n}\sum_{i=0}^{n-1} f(X_i)$ . Under appropriate assumptions on *P* and *f* a CLT holds for  $\hat{I}_n$ , i.e.

$$
\sqrt{n}(\hat{I}_n - I) \to \mathcal{N}(0, \sigma_{f,P}^2), \tag{1}
$$

where the constant  $\sigma_{f,P}^2 < \infty$  is called asymptotic variance and depends only on *f* and *P*.

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<span id="page-1-0"></span>The following theorem from Kipnis and Varadha[n](#page-9-0) [\(1986](#page-9-0)) is a fundamental result on conditions that guarantee Eq. [1](#page-0-0) for reversible Markov chains.

**Theorem 1** (Kipnis and Varadha[n](#page-9-0) [1986](#page-9-0)) *For a reversible and ergodic Markov chain, and a function*  $f \in L^2(\pi)$ , *if* 

$$
Var(f, P) := \lim_{n \to \infty} n \text{Var}_{\pi}(\hat{I}_n) < \infty,\tag{2}
$$

*then Eq.* [1](#page-0-0) *holds with*

$$
\sigma_{f,P}^2 = Var(f, P) = \int_{[-1,1]} \frac{1+x}{1-x} E_{f,P}(dx), \tag{3}
$$

*where*  $E_{f,P}$  *is the spectral measure associated with*  $f$  *and*  $P$ *.* 

We refer to Eq. 2 as the Kipnis–Varadhan condition. Assuming that Eq. 2 holds and *P* is reversible, in Section 2 we obtain conditions for the CLT and derive a spectral formula for the asymptotic variance  $\sigma_{f, P_\mu}^2$  of a time-sampled Markov chain of the form

$$
P_{\mu} := \sum_{k=0}^{\infty} \mu(k) P^{k}, \qquad (4)
$$

where  $\mu$  is a probability distribution on the nonnegative integers. Time-sampled Markov chains are of theoretical interest in the context of petite sets (cf. Chapter 5 of Meyn and Tweedi[e](#page-9-0) [1993\)](#page-9-0), and also in the context of computational algorithms (Rosentha[l](#page-10-0) [2003a,](#page-10-0) [b\)](#page-10-0).

Next we p[r](#page-9-0)oceed to analyze efficiency of Barker's algorithm (Barker [1965\)](#page-9-0). Barker's algorithm, similarly as Metropolis, uses an irreducible transition kernel *Q* to draw proposals. A move form  $X_n = x$  to a proposal  $Y_{n+1} = y$  is then accepted with probability

$$
\alpha^{(\text{B})}(x, y) = \frac{\pi(y)q(y, x)}{\pi(y)q(y, x) + \pi(x)q(x, y)},
$$
\n(5)

where  $q(x, \cdot)$  is the transition density of  $Q(x, \cdot)$ . It is well known that with the same proposal kernel *Q*, the Metropolis acceptance ratio results in a smaller asymptotic variance then Barker's. In Section [3](#page-6-0) we show that the asymptotic variance of Barker's algorithm is not bigger then, roughly speaking, two times that of Metropolis. We also motivate our considerations by recent advances in exact MCMC for diffusion models. The theoretical results are illustrated by a simulation study in Section [4.](#page-8-0)

## **2 Time-sampled Markov Chains**

In this section we work under assumptions of Theorem 1 which imply that the asymptotic variance  $\sigma_{f,P}^2$  equals  $Var(f, P)$  defined in Eq. 2 and satisfies Eq. 3. For other Markov chain CLT conditions we refer to Jone[s](#page-9-0) [\(2004\)](#page-9-0), Roberts and Rosentha[l](#page-10-0) [\(2004](#page-10-0), [2008](#page-10-0)), Meyn and Tweedi[e](#page-9-0) [\(1993\)](#page-9-0) and Bednorz et al[.](#page-9-0) [\(2008\)](#page-9-0).

<span id="page-2-0"></span>**Theorem 2** *Let P be a reversible and ergodic transition kernel with stationary measure*  $\pi$ , and let  $f \in L^2(\pi)$ . Assume that the Kipnis–Varadhan condition [\(2\)](#page-1-0) holds for f and *P. For a probability distribution* μ *on nonnegative integers, let the time-sampled kernel P*<sup>μ</sup> *be def ined by Eq.* [4](#page-1-0)*. Then, if any of the following conditions hold*

- (i)  $\mu_{odd} := \mu({1, 3, 5, \dots}) > 0$ ,
- (ii) μ(0) < 1 *and P is geometrically ergodic,*

*the CLT holds for f and P*μ, *moreover*

$$
\sigma_{f,P_{\mu}}^2 = \int_{[-1,1]} \frac{1 + G_{\mu}(x)}{1 - G_{\mu}(x)} E_{f,P}(dx) < \infty,\tag{6}
$$

*where*  $G_{\mu}$  *is the probability generating function of*  $\mu$ *, i.e.*  $G_{\mu}(z) := \mathbb{E}_{\mu} z^{K}$ ,  $|z| \leq 1$ ,  $K \sim \mu$ , and  $E_{f,P}$  *is the spectral measure associated with f and P.* 

*Remark 1* The condition  $\mu_{\text{odd}} > 0$  in the above result is necessary, which we show below by means of a counterexample.

*Proof* The proof is based on the functional analytic approach (see e.g. Kipnis and Varadha[n](#page-9-0) [1986;](#page-9-0) Roberts and Rosentha[l](#page-10-0) [1997](#page-10-0)). Without loss of generality assume that  $\pi f = 0$ . A reversible transition kernel *P* with invariant distribution  $\pi$  is a self-adjoint operator on  $L_0^2(\pi) := \{ f \in L^2(\pi) : \pi f = 0 \}$  with spectral radius bounded by 1. By the spectral decomposition theorem for self adjoint operators, for each  $f \in L_0^2(\pi)$  there exists a finite positive measure  $E_{f,P}$  on  $[-1, 1]$ , such that

$$
\langle f, P^n f \rangle = \int_{[-1,1]} x^n E_{f,P}(dx),
$$

for all integers  $n \geq 0$ . Thus in particular

$$
\sigma_f^2 = \pi f^2 = \int_{[-1,1]} 1 E_{f,P}(dx) < \infty,\tag{7}
$$

and by Kipnis and Varadha[n](#page-9-0) [\(1986](#page-9-0)) (c.f. also Theorem 4 of Häggström and Rosentha[l](#page-9-0) [2007\)](#page-9-0) one obtains

$$
\sigma_{f,P}^2 = \int_{[-1,1]} \frac{1+x}{1-x} E_{f,P}(dx) < \infty. \tag{8}
$$

Since  $P_{\mu}^{n} = (\sum_{k} \mu(k)P^{k})^{n}$ , b[y](#page-9-0) the spectral mapping theorem (Conway [1990\)](#page-9-0), we have

$$
\langle f, P_{\mu}^{n} f \rangle = \int_{[-1,1]} x^{n} E_{f,P_{\mu}}(dx) = \int_{[-1,1]} \left( \sum_{k} \mu(k) x^{k} \right)^{n} E_{f,P}(dx)
$$

$$
= \int_{[-1,1]} \left( G_{\mu}(x) \right)^{n} E_{f,P}(dx),
$$

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and consequently, applying the same argument as Kipnis and Varadha[n](#page-9-0) [\(1986\)](#page-9-0) and Häggström and Rosentha[l](#page-9-0) [\(2007](#page-9-0)), we obtain

$$
\sigma_{f,P_{\mu}}^2 = \int_{[-1,1]} \frac{1+x}{1-x} E_{f,P_{\mu}}(dx)
$$
  
= 
$$
\int_{[-1,1]} \frac{1+G_{\mu}(x)}{1-G_{\mu}(x)} E_{f,P}(dx) =: \clubsuit.
$$
 (9)

Now Eq. [9](#page-2-0) gives the claimed formula but we need to prove Eq. [9](#page-2-0) is finite: by Kipnis a[n](#page-9-0)d Varadhan [\(1986](#page-9-0)) finiteness of the integral in Eq. [9](#page-2-0) implies a CLT for *f* and  $P_{\mu}$ . Observe that

$$
|G(x)| \le 1
$$
 for all  $x \in [-1, 1]$ ,  
 $G(x) \le \mu(0) + x(1 - \mu(0))$  for  $x \ge 0$ .

Moreover, if (i) holds, then

$$
G(x) \le \sum_{k \text{ even}} \mu(k) x^k \le 1 - \mu_{\text{odd}} \quad \text{for} \quad x \le 0,
$$

hence we can write

$$
\begin{aligned}\n\blacklozenge &= \int_{[-1,0)} \frac{1 + G_{\mu}(x)}{1 - G_{\mu}(x)} E_{f,P}(dx) + \int_{[0,1]} \frac{1 + G_{\mu}(x)}{1 - G_{\mu}(x)} E_{f,P}(dx) \\
&\leq \frac{1}{\mu_{\text{odd}}} \int_{[-1,0)} 2E_{f,P}(dx) + \frac{1}{1 - \mu(0)} \int_{[0,1]} \frac{2}{1 - x} E_{f,P}(dx).\n\end{aligned} \tag{10}
$$

The first integral in Eq. 10 is finite by Eq. [7](#page-2-0) and the second by Eq. [8](#page-2-0) and we are done with (i).

Next assume that (ii) holds. By  $S(P)$  denote the spectrum of P and let  $s_P :=$  $\sup\{|\lambda| : \lambda \in S(P)\}\$  $\sup\{|\lambda| : \lambda \in S(P)\}\$  $\sup\{|\lambda| : \lambda \in S(P)\}\$  be the spectral radius. From Roberts and Rosenthal [\(1997\)](#page-10-0) we know that since *P* is reversible and geometrically ergodic, it has a spectral gap, i.e.  $s_P < 1$ . Hence for  $x \in [-s_P, 0]$ , we can write

$$
G_{\mu} \leq \mu(0) + \sum_{k \text{ even}} \mu(k) x^{k} \leq \mu(0) + s_{P}(1 - \mu(0)).
$$

Consequently

$$
\begin{split} \clubsuit &= \int_{[-s_P,0)} \frac{1 + G_\mu(x)}{1 - G_\mu(x)} E_{f,P}(dx) + \int_{[0,s_P]} \frac{1 + G_\mu(x)}{1 - G_\mu(x)} E_{f,P}(dx) \\ &\le \frac{1}{1 - \mu(0)} \int_{[-s_P,0)} \frac{2}{1 - s_P} E_{f,P}(dx) + \frac{1}{1 - \mu(0)} \int_{[0,s_P]} \frac{2}{1 - x} E_{f,P}(dx). \end{split} \tag{11}
$$

The first integral in Eq. 11 is finite by Eq. [7](#page-2-0) and the second by Eq. [8.](#page-2-0)

The most important special case of Theorem 2 is underlined and computed explicitly in the next corollary.

**Corollary 1** *Let P be a reversible and ergodic transition kernel with stationary measure*  $\pi$ , *and assume that for f and P the CLT* (*Eq.* [1](#page-0-0)) *holds. For*  $\varepsilon \in (0, 1)$  *let the*  *lazy version of P be defined as*  $P_{\varepsilon} := \varepsilon I d + (1 - \varepsilon) P$ . Then the CLT holds for f and *P*<sup>ε</sup> *and*

$$
\sigma_{f,P_{\varepsilon}}^2 = \frac{1}{1-\varepsilon} \sigma_{f,P}^2 + \frac{\varepsilon}{1-\varepsilon} \sigma_f^2. \tag{12}
$$

*Proof* We use Theorem 2 with  $\mu(0) = \varepsilon$ ,  $\mu(1) = 1 - \varepsilon$ . Hence  $G_{\mu} = \varepsilon + (1 - \varepsilon)x$ , and consequently

$$
\sigma_{f,P_{\varepsilon}}^2 = \int_{[-1,1]} \frac{1+\varepsilon + (1-\varepsilon)x}{1-\varepsilon - (1-\varepsilon)x} E_{f,P}(dx)
$$
  
\n
$$
= \int_{[-1,1]} \frac{1}{1-\varepsilon} \left(\frac{1+x}{1-x} + \varepsilon\right) E_{f,P}(dx)
$$
  
\n
$$
= \frac{1}{1-\varepsilon} \int_{[-1,1]} \frac{1+x}{1-x} E_{f,P}(dx) + \frac{\varepsilon}{1-\varepsilon} \int_{[-1,1]} 1 E_{f,P}(dx)
$$
  
\n
$$
= \frac{1}{1-\varepsilon} \sigma_{f,P}^2 + \frac{\varepsilon}{1-\varepsilon} \sigma_f^2.
$$

Efficiency of time sampled Markov chains can be compared using the following corollary from Theorem 2.

**Corollary 2** *Let P and f be as in Theorem 2. If P is positive as an operator on*  $L^2(\pi)$ *and*  $\mu_1$  *dominates stochastically*  $\mu_2$  *(i.e.*  $\mu_1 \geq_{st} \mu_2$ *), then*  $P_{\mu_1}$  *dominates*  $P_{\mu_2}$  *in the*  $\textit{efficiency ordering, i.e. } \sigma_{f, P_{\mu_1}}^2 \leq \sigma_{f, P_{\mu_2}}^2.$ 

*Proof* If *P* is positive self-adjoint then supp $E_{f,P} \subseteq [0, 1]$ . Moreover

$$
\mu_1 \geq_{st} \mu_2 \Rightarrow G_{\mu_1}(x) \leq G_{\mu_2}(x) \qquad \text{for} \quad x \in [-1, 1].
$$

The conclusion follows from Eq. [6.](#page-2-0)  $\Box$ 

In another direction of studying CLTs, the *variance bounding* property of Markov chains has been introduced in Roberts and Rosentha[l](#page-10-0) [\(2008\)](#page-10-0) and is defined as follows. *P* is variance bounding if there exists  $K < \infty$  such that  $Var(f, P) < KVar_\tau(f)$ for all *f*. Here *Var*(*f*, *P*) is defined in Eq. [2](#page-1-0) and Var<sub>π</sub>(*f*) =  $\pi f^2 - (\pi f)^2$ . We prove that for time-sampled Markov chains the variance bounding property propagates the same way the CLT does.

**Theorem 3** *Assume P is reversible and variance bounding. Then P*<sup>μ</sup> *is variance bounding if any of the following conditions hold*

(i)  $\mu_{\text{odd}} := \mu({1, 3, 5, \dots}) > 0$ ,

(ii)  $\mu(0) < 1$  *and P is geometrically ergodic.* 

*Proof* For any *f* such that  $Var_{\pi} f < \infty$ , the Kipnis–Varadhan condition holds due to variance bounding property of *P* and thus the assumptions of Theorem 2 are met. Hence for every  $f \in L^2(\pi)$  there is a CLT for f and  $P_\mu$ . Therefore  $P_\mu$  is variance bounding by Theorem 7 of Roberts and Rosentha[l](#page-10-0) [\(2008\)](#page-10-0). 

 $\Box$ 

The next example shows that in case of Markov chains that are not geometrically ergodic, the condition  $\mu_{\text{odd}} > 0$  is necessary.

*Example 1* We set  $f(x) = x$  and give an example of an ergodic and reversible transition kernel *P* on  $\mathcal{X} = [-1, 1]$ , and such that there is a CLT for *P* and *f* but *not* for  $P^2$  and *f*[.](#page-9-0) We shall rely on Theorem 4.1 of Bednorz et al. [\(2008\)](#page-9-0) that provides if and only if conditions for Markov chains CLTs in terms of regenerations. It will be apparent that the condition  $\mu_{odd} > 0$  in Theorem 2 is necessary.

Set  $s(x) := \sqrt{1 - |x|}$ , let  $U(\cdot)$  be the uniform distribution on [−1, 1], and let the kernel *P* be of the form

$$
P(x, \cdot) = (1 - s(x))\delta_{-x}(\cdot) + s(x)U(\cdot), \qquad \text{hence} \tag{13}
$$

$$
P^{2}(x, \cdot) = (1 - s(x))^{2} \delta_{x}(\cdot) + (2s(x) - s(x)^{2}) U(\cdot).
$$
 (14)

To find the stationary distribution of  $P$  (and also  $P^2$ ), we verify reversibility with  $\pi(x) \propto 1/s(x)$ .

$$
\pi(\mathrm{d}x)P(x,\mathrm{d}y) \propto \frac{1}{s(x)}\delta_{-x}(y) + \delta_{-x}(y) + U(\mathrm{d}y)
$$

$$
= \frac{1}{s(y)}\delta_{-y}(x) + \delta_{-y}(x) + U(\mathrm{d}x) \propto \pi(\mathrm{d}y)P(y,\mathrm{d}x).
$$

Hence  $\pi(x)$  is a reflected Beta(1,  $\frac{1}{2}$ ). Clearly  $\pi(f^2) < \infty$ .

Recall now the split chain construction (Nummeli[n](#page-10-0) [1978;](#page-10-0) Athreya and Ne[y](#page-9-0) [1978\)](#page-9-0) of the bivariate Markov chain  $\{X_n, \Gamma_n\}$  on  $\{0, 1\} \times \mathcal{X} = \{0, 1\} \times [0, 1]$ . If  $(X_n)_{n>0}$ evolves according to *P* defined in Eq. 14, we have the following transition rule from  ${X_{n-1}, \Gamma_{n-1}}$  to  ${X_n, \Gamma_n}$  for the split chain.

$$
\tilde{\mathbb{P}}(X_n \in \cdot | \Gamma_{n-1} = 1, X_{n-1} = x) = U(\cdot),
$$
  

$$
\tilde{\mathbb{P}}(X_n \in \cdot | \Gamma_{n-1} = 0, X_{n-1} = x) = \delta_{-x}(\cdot),
$$
  

$$
\tilde{\mathbb{P}}(\Gamma_n = 1 | \Gamma_{n-1}, X_n = x) = s(x),
$$
  

$$
\tilde{\mathbb{P}}(\Gamma_n = 0 | \Gamma_{n-1}, X_n = x) = 1 - s(x).
$$

The notation  $\check{\mathbb{P}}$  above indicates that we consider the extended probability space for  $(X_n, \Gamma_n)$ , not the original one of  $X_n$ . The appropriate modification of the above holds if the dynamics of  $X_n$  is  $P^2$ , namely

$$
\tilde{\mathbb{P}}(X_n \in | \Gamma_{n-1} = 1, X_{n-1} = x) = U(\cdot),
$$
  

$$
\tilde{\mathbb{P}}(X_n \in | \Gamma_{n-1} = 0, X_{n-1} = x) = \delta_x(\cdot),
$$
  

$$
\tilde{\mathbb{P}}(\Gamma_n = 1 | \Gamma_{n-1}, X_n = x) = 2s(x) - s^2(x),
$$
  

$$
\tilde{\mathbb{P}}(\Gamma_n = 0 | \Gamma_{n-1}, X_n = x) = (1 - s(x))^2.
$$

We refer to to the original papers for more details on the split chain construction and to Bednorz et al[.](#page-9-0) [\(2008](#page-9-0)) and Roberts and Rosentha[l](#page-10-0) [\(2004](#page-10-0)) for central limit theorems in this context. Denote

$$
\tau := \min \{ k \ge 0 : \Gamma_k = 1 \}. \tag{15}
$$

<span id="page-6-0"></span>By Theorem 4.1 of Bednorz et al[.](#page-9-0) [\(2008](#page-9-0)), the CLT for *P* and *f* holds if and only if the following expression for the asymptotic variance is finite.

$$
\sigma_{f,P}^2 = \int_{[-1,1]} s(x)\pi(x)dx \, \check{\mathbb{E}}_U \left(\sum_{k=0}^{\tau} f(X_n)\right)^2, \tag{16}
$$

where  $(X_n, \Gamma_n)$  follow the dynamics of *P*. Respectively, the CLT for  $P^2$  and *f* holds in our setting, *if and only if*

$$
\sigma_{f,P^2}^2 = \int_{[-1,1]} (2s(x) - s^2(x)) \pi(x) dx \, \check{\mathbb{E}}_U \left( \sum_{k=0}^{\tau} f(X_n) \right)^2 \tag{17}
$$

is finite, where  $(X_n, \Gamma_n)$  follow the dynamics of  $P^2$ .

Now observe that if  $(X_n)_{n\geq 0}$  evolves according to *P*, then  $(\sum_{k=0}^{\tau} f(X_n))^2$  equals 0 if  $\tau$  is odd, or  $(\sum_{k=0}^{\tau} f(X_n))^2 = X_0^2$ , if  $\tau$  is even. Consequently Eq. 16 is finite. However, if  $(X_n)_{n\geq 0}$  evolves according to  $P^2$ , then  $(\sum_{k=0}^{\tau} f(X_n))^2 = (\tau + 1)^2 X_0^2$  and the distribution of  $\tau$  is geometric with parameter  $2s(X_0) - s^2(X_0) = 1 - (1 - s(x))^2$ . Therefore we compute  $\sigma_{f,P^2}^2$  in Eq. 17 as

$$
\sigma_{f,P^2}^2 = \int_{[-1,1]} \left( 2s(x) - s^2(x) \right) \pi(x) dx \int_{[-1,1]} \frac{2 - \left( 1 - \left( 1 - s(x) \right)^2 \right)}{2 \left( 1 - (1 - s(x))^2 \right)^2} x^2 dx
$$
  
=  $C \int_{[-1,1]} \frac{\left( 1 + (1 - s(x))^2 \right) x^2}{2 \left( 1 - |x| - 2\sqrt{1 - |x|} \right)^2} dx$   
 $\ge C \int_{[-1,1]} \frac{x^2}{8(1 - |x|)} dx = \infty.$ 

#### **3 Barker's Algorithm**

When assessing efficiency of Markov chain Monte Carlo algorithms, the asymptotic variance criterion is one of natural choices. Peskun ordering (Pesku[n](#page-10-0) [1973\)](#page-10-0) (see also Tierne[y](#page-10-0) [1998;](#page-10-0) Mira and Geye[r](#page-10-0) [1999](#page-10-0)) provides a tool to compare two reversible transition kernels  $P_1$ ,  $P_2$  with the same limiting distribution  $\pi$  and is defined as follows.  $P_1 \succ P_2 \iff$  for  $\pi$  –almost every  $x \in \mathcal{X}$  and all  $A \in \mathcal{B}(\mathcal{X})$  holds  $P_1(x, A {f(x)} \ge P_2(x, A - {x})$ . If  $P_1 > P_2$  then  $\sigma_{f,P_1}^2 \le \sigma_{f,P_2}^2$  for every  $f \in L^2(\pi)$ .

Consider now a class of algorithms where the transition kernel *P* is defined by applying an irreducible proposal kernel Q and an acceptance rule  $\alpha$ , i.e. given  $X_n =$ *x*, the value of  $X_{n+1}$  is a result of performing the following two steps.

- 1. Draw a proposal  $y \sim Q(x, \cdot),$
- 2. Set  $X_{n+1} := y$  with probability  $\alpha(x, y)$  and  $X_{n+1} = x$  otherwise,

where  $\alpha(x, y)$  is such that the resulting kernel P is reversible with stationary distributio[n](#page-10-0)  $\pi$ . It follows Peskun [\(1973\)](#page-10-0) and Tierne[y](#page-10-0) [\(1998](#page-10-0)) that for a given proposal kernel *Q* the standard Metropolis–Hastings (Metropolis et al[.](#page-9-0) [1953;](#page-9-0) Hasting[s](#page-9-0) [1970\)](#page-9-0) acceptance rule

$$
\alpha^{(\text{MH})}(x, y) = \min\left\{1, \frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}\right\}
$$
\n(18)

yields a transition kernel  $P^{(MH)}$  that is maximal with respect to Peskun ordering and thus minimal with respect to asymptotic variance. In particular, the Barker's algorithm (Barke[r](#page-9-0) [1965](#page-9-0)) that uses acceptance rule

$$
\alpha^{(\text{B})}(x, y) = \frac{\pi(y)q(y, x)}{\pi(y)q(y, x) + \pi(x)q(x, y)}
$$
(19)

is inferior to Metropolis–Hastings when the asymptotic variance is considered. In the above notation we assume that all the involved distributions have common denominating measure and  $q(x, \cdot)$  are transition densities of *Q*. See Tierne[y](#page-10-0) [\(1998\)](#page-10-0) for a more general statement and discussion.

Exact Algorithms introduced in Beskos et al[.](#page-9-0) [\(2006a,](#page-9-0) [b,](#page-9-0) [2008\)](#page-9-0) and Beskos and Robert[s](#page-9-0) [\(2005\)](#page-9-0) allow for inference in diffusion models without Euler discretization error. In recent advances in Exact MCMC inference for complex diffusion models a particular setting is reoccurring, where the Metropolis–Hastings acceptance step requires a specific Bernoulli Factory and is not possible to execute. However, in this diffusion context the Barker's algorithm (Eq. 19) is feasible, as well as the 'lazy' version of the Metropolis–Hastings kernel

$$
P_{\varepsilon}^{\text{(MH)}} := \varepsilon Id + (1 - \varepsilon) P^{\text{(MH)}}.
$$
\n(20)

We refer to Gonçalves et al[.](#page-9-0)  $(2011)$  and Łatuszyński et al.  $(2011a, b)$  $(2011a, b)$  $(2011a, b)$  $(2011a, b)$  for the background on exact MCMC inference for diffusions and the Bernoulli Factory problem. This motivates us to investigate performance of these alternatives in comparison to the standard Metropolis–Hastings.

**Theorem 4** *Let*  $P^{(B)}$  *denote the transition kernel of the Barker's algorithm and let*  $P^{(MH)}$  *and*  $P_{\varepsilon}^{(MH)}$  *be as defined in Eq.* 20*. If the CLT (Eq. [1](#page-0-0)) holds for f and*  $P^{(MH)}$ , *then it holds also for*

(i)  $f$  and  $P_s^{(MH)}$  with

$$
\sigma_{f,P_{\varepsilon}^{(MH)}}^2 = \frac{1}{1-\varepsilon} \sigma_{f,P^{(MH)}}^2 + \frac{\varepsilon}{1-\varepsilon} \sigma_f^2. \tag{21}
$$

(ii)  $f$  *and*  $P^{(B)}$  *with* 

$$
\sigma_{f, P^{(MH)}}^2 \leq \sigma_{f, P^{(B)}}^2 \leq \sigma_{f, P_{1/2}^{(MH)}}^2 = 2\sigma_{f, P^{(MH)}}^2 + \sigma_f^2. \tag{22}
$$

*Proof* The first claim (i) is a restatement of Corollary 1 for Metropolis–Hastings chains. To obtain the second claim (ii), note that  $P_{1/2}^{(MH)}$  can be viewed as an algorithm that uses proposals from *Q* and acceptance rule

$$
\alpha(x, y) = \min\left\{\frac{1}{2}, \frac{\pi(y)q(y, x)}{2\pi(x)q(x, y)}\right\}.
$$

<span id="page-8-0"></span>Now since

$$
\min\left\{1,\frac{\pi(y)q(y,x)}{\pi(x)q(x,y)}\right\} \geq \frac{\pi(y)q(y,x)}{\pi(y)q(y,x)+\pi(x)q(x,y)} \geq \min\left\{\frac{1}{2},\frac{\pi(y)q(y,x)}{2\pi(x)q(x,y)}\right\},\,
$$

the result follows from Peskun ordering and Corollary 1. 

### **4 Numerical Examples**

To illustrate the theoretical findings, we consider two numerical examples. The first focuses on time sampling, the second on efficiency of the Barker's algorithm.

4.1 Time Sampled Contracting Normals

Consider the contracting normals example, i.e. a Markov chain with transition probabilities

$$
P(x, \cdot) = N(\theta x, 1 - \theta^2)
$$
 (23)

for some  $\theta \in (-1, 1)$ . It is easy to check that the stationary distribution is  $\pi(\cdot)$  = *N*(0, 1). Moreover the transition kernel is geometrically ergodic and reversible for all  $\theta \in (-1, 1)$  $\theta \in (-1, 1)$  $\theta \in (-1, 1)$  and als[o](#page-9-0) positive for  $\theta \in [0, 1)$  (Baxendale [2005;](#page-9-0) Łatuszyński and Niemiro [2011\)](#page-9-0). For the target function we take  $f(x) = x$  and estimate the asymptotic variance using the batch means estimator of Jones et al[.](#page-9-0) [\(2006](#page-9-0)) based on a trajectories of length 10<sup>7</sup>. We set  $\theta$  to 0.9 and −0.9 in the following settings:

- CN: Contracting normals;
- LCN: Lazy contracting normals with  $\varepsilon = 0.5$ ;
- TSCN1: Time sampled contracting normals for sampling distribution

$$
\mu = 1 + Pois(1);
$$

– TSCN2: Time sampled contracting normals for sampling distribution

$$
\mu = 1 + Pois(5).
$$

The first two columns of Table 1 report how laziness increases asymptotic variance and illustrate Corollary 1. Note that the stationary variance  $\sigma_f^2 = 1$  is substantial compared to the asymptotic variance of contracting normals for  $\theta = -0.9$  and thus the lazy version LCN becomes severely inefficient compared to CN. The stochastic ordering of the sampling distributions in the above scenarios is LCN  $\lt_{st}$  CN  $\lt_{st}$ TSCN1  $\lt_{st}$  TSCN2 therefore the simulation shows how the asymptotic variance decreases for stochastically bigger sampling distributions (Corollary 2) in case of positive operators ( $\theta = 0.9$ ) and how this property fails if the operator is not positive, i.e for  $\theta = -0.9$ .

**Table 1** Estimated asymptotic variance of the contracting normals Markov chain for different sampling scenarios

	CN	LCN	TSCN1	TSCN2
$\theta = 0.9$	19.1	38.5	9.28	3.43
$\theta = -0.9$	0.053	1.14	$0.80\,$	0.96

<span id="page-9-0"></span>**Table 2** Estimated asymptotic variance of the Metropolis, Barker's and lazy Metropolis algorithms

	Metropolis	Parker's	Lazy Metropolis
Asymptotic variance	3.69	5.67	R 77

## 4.2 Efficiency of the Barker's Algorithm

We compare the estimated asymptotic variance of the random walk Metropolis algorithm, the Barker's algorithm and lazy version of the random walk Metropolis with  $\varepsilon = 0.5$  to illustrate the bounds of Theorem 4. For the stationary distribution we take  $N(0, 1)$  and the increment proposal is  $U([-2, 2])$ . The results based on a simulation length  $10<sup>7</sup>$  are reported in Table 2.

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