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RATE OF CONVERGENCE FOR DERIVATIVE ESTIMATION OF DISCRETE-TIME MARKOV CHAINS VIA FINITE-DIFFERENCE APPROXIMATION WITH COMMON RANDOM NUMBERS*

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Abstract. The scheme of *common random numbers* (CRN) is a very popular method for variance reduction in simulation. *Finite difference* (FD) is a conventional technique for derivative estimation. In this paper, we examine the effectiveness of CRN for improving the rates of convergence for FD estimates over infinite horizon for homogeneous discrete-time Markov chains. For direct FD estimates, we give sufficient conditions for the effectiveness of CRN. Based on these conditions, we also suggest several simulation schemes with guaranteed effectiveness. For ratio estimates based on regenerative structures, we prove that the use of CRN is always advantageous.

Key words. discrete-time Markov chain, simulation, derivative estimation, infinite horizon, common random number

AMS subject classifications. 60J10, 60G17, 62C20

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1. Introduction.

Computer simulation, or simulation for short, has been widely used for performance analysis of complex systems. Since simulation is often very time consuming and costly, it is desirable to use simulation efficiently. Efficiency is measured by different criteria in different problems. Hammersley and Handscomb (1964, p. 22) proposed that "the efficiency of a Monte Carlo process may be taken as inversely proportional to the product of the sampling variance and the amount of labour expended in obtaining this estimate" (see Glynn and Whitt (1992) for a detailed discussion). When comparing two alternative designs, consequently, the estimation variance of the difference of their performance functions is an important indicator of efficiency. Without increasing "the amount of labour expended in obtaining this estimate," reduction in variance can be interpreted as an increase of efficiency according to the previously mentioned principle. The use of the same sequence of random numbers to drive different experiments, widely known as the scheme of *common random numbers* (CRN), is perhaps the most popular method for variance reduction. CRN is easy for implementation and does not increase computational load. It is intuitively appealing since different designs should be compared under same conditions in order to stress the difference in design rather than the difference of random factors. Analysis and guidelines on the use of CRN can be found, for example, in Bratley, Fox, and Schrage (1987). Other techniques for variance reduction can be found in Bratley, Fox, and Schrage (1987); Fishman (1978); and Kleijnen (1974).

We are concerned with the use of CRN in *finite-difference* (FD) approximation. FD is a traditional technique for estimating derivatives of performance functions. Such derivative information is very useful for sensitivity analysis and optimization. To be precise, consider a general stochastic system with a parameterized family of performance functions of the form $J(\theta) = E_\xi[L(\theta, \xi)] \in R$, where R is the set of real numbers, ξ represents the underlying random factors defined on some probability

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space, and θ is a scalar parameter, $\theta \in (\underline{\theta}, \bar{\theta}) = \Theta$. We assume that the analytic form of $J(\theta)$ is not available, which is true for systems studied in simulation. However, the sample function $L(\theta, \xi) \in R$ is available from realizations of ξ. Let $\theta \in \Theta$ and $\delta > 0$ be a small increment satisfying $\theta + \delta \in \Theta$. The FD estimator uses

$$\frac{L(\theta + \delta, \xi_1) - L(\theta, \xi_2)}{\delta}$$

as an approximation to $J'(\theta)$, the derivative of $J(\theta)$. The FD estimator is biased with a bias of $(J(\theta+\delta) - J(\theta))/\delta - J'(\theta)$. However, this bias vanishes asymptotically when δ goes to zero. When the two experiments at θ and $\theta+\delta$ are performed independently, the variance of an FD estimator is about $2Var[L(\theta, \xi)]/\delta^2$, which grows quadratically as δ goes to zero, assuming that $Var[L(\theta, \xi)] > 0$ is continuous on Θ. Since two experiments are needed in FD, it is natural to employ the scheme of CRN to reduce the estimation variance. Roughly speaking, CRN requires that we calculate the performance functions at θ and $\theta + \delta$ from the same sequence of random numbers which are usually uniformly distributed on $[0, 1)$. Unfortunately, this is an ill-posed definition. It hints nothing about the implementation of these two simulation experiments, which may significantly affect the effectiveness of CRN, as we shall demonstrate in the paper. In this paper, the meaning of CRN will be specified in subsection 3.2. Please be advised that CRN is not guaranteed effective for variance reduction. One example will be presented in Remark 3.2. Nevertheless, there are many situations where CRN indeed works (see, e.g., Bratley, Fox, and Schrage (1987)). So it is practically important to know when CRN works and when it does not. As far as FD is concerned, we want to find out when the reduction in variance can yield an increase in the rates of convergence for FD. Such rates cannot be improved without reduction in variance.

Zazanis and Suri (1993) investigated the rates of convergence for FD estimates without the use of CRN. They mainly considered the case of finite-horizon functions. For infinite-horizon functions, they considered the case of ratio estimates for systems with regenerative structures. Other issues regarding the asymptotic efficiency of FD estimates without the use of CRN were investigated by Fox and Glynn (1989), Glynn (1989), and Glynn and Whitt (1992). When the scheme of CRN is used, Glasserman and Yao (1992) and L'Ecuyer and Perron (1994) studied the variance properties of finite-horizon performance functions that are sufficiently smooth for the infinitesimal perturbation analysis to apply. Glynn (1989) examined the rates of convergence for FD estimates for finite-horizon performances and L'Ecuyer (1992) examined the rates for infinite-horizon performances, both under a priori assumptions on the effectiveness of CRN. Dai (1994) proved under very mild conditions that CRN is effective for improving rates of convergence for FD estimates when the number of independent replications goes to infinity. For finite-horizon performance functions, results of Dai (1994) provide a fairly clear answer to the effectiveness of CRN and also give conditions on how effective CRN may be.

For relatively complex Markov chains it may be numerically infeasible or inefficient to solve the stationary distribution equation to evaluate a given performance function. For these types of systems, simulation is a very competitive, or even the only practical, alternative. In this paper, we are concerned with the effectiveness of CRN in FD for homogeneous finite-state Markov chains with infinite-horizon performance functions. Our goal is to find answers to the following questions. (1) Is CRN always effective for accelerating the convergence of an FD estimator? (2) Can we provide simulation methods that guarantee the effectiveness of CRN? (3) How effective could CRN be? We show that the answers to (1) and (2) are "no" and "yes," respectively. We will give answers to (3).

We have arranged our discussions in the following order. In section 2, we introduce some preliminaries of Markov chains that are necessary for later sections. In section 3, we first examine the rates of convergence for FD estimates in the case of independent replications without the use of CRN. Our discussion is not based on ratio estimates. We then show that CRN is not always effective for improving the rates of convergence for FD estimates. We present general conditions under which CRN is effective. In section 4, we give several simulation methods which are variations of CRN that are guaranteed to yield faster rates of convergence for FD estimates than independent simulations. In section 5, we study the effectiveness of CRN in ratio estimates by taking advantage of the regenerative structure of finite Markov chains. In this case, we prove that CRN is always helpful in improving the rates of convergence when the number of regenerative cycles goes to infinity.

2. Preliminaries. The following notations will be used:

$\mathcal{S} = \{s_0, s_1, ..., s_{d-1}\}$, a *finite* set of d states that does not depend on θ;

$\mathcal{D} = \{(x,x) : x \in \mathcal{S}\}$;

$\mathcal{F} = \{f(x,\theta) : \mathcal{S} \times \Theta \to R;\ f(x,\theta)$ is uniformly bounded, twice continuously differentiable in θ with uniformly bounded first-order derivative on $\Theta\}$;

$\mathcal{U}$ = the set of random numbers that are uniformly distributed on $[0,1)$.

Consider a discrete-time Markov chain $\{X_n \in \mathcal{S}, n \geq 0\}$ with state transition matrix $P(\theta)$ and a performance function $J(N,\theta) = E[L(N,\theta,\xi)] \in R$, where

$$L(N,\theta,\xi) = \frac{1}{N}\sum_{n=1}^{N} f(X_n,\theta),$$

$f(x,\theta) \in \mathcal{F}$ is the cost or reward function, and N is a deterministic positive integer. The performance function $J(N,\theta)$ represents the average cost or reward of making N state transitions. Each element $p_\theta(x,y) \geq 0, x,y \in \mathcal{S}$, of $P(\theta)$ is the probability of making a state transition from x to y. Denote $\Gamma(x) = \{y \in \mathcal{S} \mid p_\theta(x,y) > 0\} \subset \mathcal{S}$. Then, for each $x \in \mathcal{S}$, $\sum_{y\in\Gamma(x)} p_\theta(x,y) = 1$.

We assume that the initial state $X_0 \in \mathcal{S}$ is fixed. If the Markov chain under study contains exactly one aperiodic positive recurrent class of states, then it is geometrically ergodic and there exists a stationary distribution $\pi_\theta = [\pi_\theta(x) > 0]$ such that (Iosifescu (1980, p. 126))

$$|p_\theta^{(n)}(x) - \pi_\theta(x)| \leq \alpha\beta^n \quad \forall\, x \in \mathcal{S},\ X_0 \in \mathcal{S}, \tag{1}$$

where $\alpha > 0$, $0 \leq \beta < 1$, and $p_\theta^{(n)}(x)$ is the probability of state being x at the nth transition. We assume that α and β can be chosen independent of $\theta \in \Theta$. In this case, we have

$$\lim_{N\to\infty} L(N,\theta,\xi) = J(\theta) \text{ almost surely (a.s.)} \quad \text{and} \quad \lim_{N\to\infty} J(N,\theta) = J(\theta), \tag{2}$$

where the stationary performance function $J(\theta) = E_{\pi_\theta}[f(X,\theta)]$ is the mean cost or reward of making one transition. Moreover, there exists a constant $\gamma > 0$ such that

$$|J(N,\theta) - J(\theta)| \leq \frac{\gamma}{N}. \tag{3}$$

Let $e \in R^d$ be a vector all of whose components are unity. If the Markov chain contains exactly one aperiodic positive recurrent class of states, the fundamental matrix $Z(\theta) = [z_\theta(x,y)] = [I - P(\theta) + e\pi_\theta]^{-1}$ always exists. For any $x, y \in \mathcal{S}$, define

$$d(x,y) = \pi_\theta(x)z_\theta(x,y) + \pi_\theta(y)z_\theta(y,x) - \pi_\theta(x)\delta(x,y) - \pi_\theta(x)\pi_\theta(y)$$

with $\delta(x, y) = 1$ if $x = y$, $= 0$ if $x \neq y$. Then we have (see, e.g., Iosifescu (1980, p. 138))

$$\left| \frac{1}{N} Var\left[\sum_{n=1}^{N} f(X_n, \theta) \right] - a(\theta) \right| \leq \frac{b(\theta)}{N}, \tag{4}$$

where

$$a(\theta) = \sum_{x, y \in \mathcal{S}} d(x, y) f(x, \theta) f(y, \theta),$$

$b(\theta) \in R$ does not depend on N. The previous (2) and (4) establish the convergence and the rate of convergence of sample performance functions.

Remark 2.1. Sharper estimates of the distribution of $L(N, \theta, \xi)$ are available. As a matter of fact, by using the *large deviation techniques*, it is possible to derive an asymptotic expansion on the probability $\text{Prob}[L(N, \theta, \xi) - J(N, \theta) \leq y]$ (see, e.g., Dembo and Zeitouni (1993)). Such expansion provides additional insights on the convergence of $L(N, \theta, \xi)$. However, the bounds (3) and (4) are sufficient for us since we are interested only in the effectiveness of CRN on FD. In fact, we need only the existence of γ, $a(\theta)$, and $b(\theta)$.

Finally, by differentiating the stationary distribution equation $\pi_\theta = \pi_\theta P(\theta)$, we get

$$\pi'_\theta = \pi'_\theta P(\theta) + \pi_\theta P'(\theta) \quad \text{and} \quad \pi''_\theta = \pi''_\theta P(\theta) + 2\pi'_\theta P'(\theta) + \pi_\theta P''(\theta).$$

Cramer's rule guarantees that π_θ is twice continuously differentiable on Θ if $P(\theta)$ is. Therefore, $J(\theta)$ is twice continuously differentiable for any $f(x, \theta) \in \mathcal{F}$ if $P(\theta)$ is.

We will use the notation $g(s) = O(s)$ which says that $g(s)/s$ is bounded for all s ($g(s) = o(s)$ means that $g(s)/s$ goes to zero as s goes to zero or infinity depending on the context). The notions $O(1)$ and $o(1)$ are meant to be uniform with respect to $\theta \in \Theta$ unless otherwise stated.

3. FD estimates for discrete-time Markov chains. We are interested in the following FD estimator:

$$h^{FD}(N, \delta) = \frac{L(N, \theta + \delta, \xi_2) - L(N, \theta, \xi_1)}{\delta}, \tag{5}$$

where $\delta > 0$ is a small positive increment and ξ_1 and ξ_2 represent two realizations of simulation experiments. According to (2) we know that

$$\lim_{\delta \to 0^+} \lim_{N \to \infty} h^{FD}(N, \delta) = J'(\theta), \quad \text{a.s.}$$

For the sake of efficiency, we would like to choose δ as a function of N and make $h^{FD}(N, \delta)$ convergent to $J'(\theta)$ as fast as possible. A common criterion to measure the behavior of an estimator such as (5) is the *root mean square error* (RMSE) which is defined as (Zazanis and Suri (1993))

$$\text{RMSE}[h^{FD}(N, \delta)] = (E[(h^{FD}(N, \delta) - J'(\theta))^2])^{1/2}.$$

RMSE measures the accuracy of an estimate. Our goal is to find the best possible rate of convergence for $\text{RMSE}[h^{FD}(N, \delta)]$ and how to achieve the best rate by choosing an appropriate increment δ. If there exist a δ_N and a $\sigma > 0$ such that $\mathrm{RMSE}[h^{FD}(N, \delta_N)] = O(N^{-\sigma})$, we say that the rate of convergence for the expression $\mathrm{RMSE}[h^{FD}(N, \delta_N)]$ is $N^{-\sigma}$. Naturally, σ should be as large as possible. The largest σ gives the best possible rate of convergence. A more convenient form of $\mathrm{RMSE}[h^{FD}(N, \delta)]$ is

$$(6)\quad \mathrm{RMSE}[h^{FD}(N,\delta)] = \left\{ Var[h^{FD}(N,\delta)] + \left(\frac{J(N,\theta+\delta) - J(N,\theta)}{\delta} - J'(\theta) \right)^2 \right\}^{1/2}.$$

The first term inside the square root measures how fast the estimation variance goes to zero. The second term measures how fast the bias vanishes. Both the variance and the bias must go to zero for consistent estimates. Therefore, (6) implies that we need to balance the rates for the bias and the variance to go to zero so that we can obtain the best overall rate for $\mathrm{RMSE}[h^{FD}(N, \delta)]$.

3.1. Independent simulations. We use $\{X_n \in \mathcal{S}\}$ and $\{Y_n \in \mathcal{S}\}$ to denote sample paths of Markov chains governed by transition matrices $P(\theta)$ and $P(\theta + \delta)$, respectively. Then $L(N, \theta, \xi_1)$ and $L(N, \theta + \delta, \xi_2)$ are their corresponding sample performance functions. For independent simulations, $L(N, \theta, \xi_1)$ and $L(N, \theta + \delta, \xi_2)$ are independent. In this case, we have

$$(7)\quad \begin{aligned} \frac{1}{N} Var\left[\sum_{n=1}^{N} (f(X_n,\theta) - f(Y_n,\theta+\delta))\right] &= \frac{1}{N} Var\left[\sum_{n=1}^{N} f(X_n,\theta)\right] \\ &\quad + \frac{1}{N} Var\left[\sum_{n=1}^{N} f(Y_n,\theta+\delta)\right], \end{aligned}$$

from which we can prove the following result.

THEOREM 3.1. *Assume that $\{X_n\}$ is irreducible and aperiodic for all $\theta \in \Theta$, $f(x, \theta) \in \mathcal{F}$, $P(\theta)$ is twice continuously differentiable, $J''(\theta) \neq 0$, and $a(\theta), b(\theta) > 0$ are continuous on Θ. Then for any $\theta \in \Theta$, the best possible rate of convergence for $\mathrm{RMSE}[h^{FD}(N, \delta)]$ is $N^{-1/4}$, which can be achieved by choosing $\delta = cN^{-1/4}$, where c is any positive constant.*

Proof. When $L(N, \theta, \xi_1)$ and $L(N, \theta + \delta, \xi_2)$ are independent, we know from (4) and (7) that

$$\left| \frac{1}{N} Var\left[\sum_{n=1}^{N} (f(X_n,\theta) - f(Y_n,\theta+\delta))\right] - a(\theta) - a(\theta+\delta) \right| \leq \frac{b(\theta) + b(\theta+\delta)}{N}.$$

Since both $a(\theta)$ and $b(\theta)$ are continuous on Θ, $a(\theta+\delta) = a(\theta)(1+o(1))$ and $b(\theta+\delta) = b(\theta)(1 + o(1))$ for sufficiently small δ. Therefore,

$$Var[h^{FD}(N,\delta)] = \frac{2a(\theta)}{N\delta^2}(1 + o(1))$$

and

$$(8)\quad (\mathrm{RMSE}[h^{FD}(N,\delta)])^2 = \frac{2a(\theta)}{N\delta^2}(1 + o(1)) + \left(\frac{J(N,\theta+\delta) - J(N,\theta)}{\delta} - J'(\theta) \right)^2.$$

In order to have $\mathrm{RMSE}[h^{FD}(N,\delta)] \to 0$ we must choose δ such that the first term of (8) goes to zero, i.e., $N\delta^2 \to \infty$. By applying Jensen's inequality $a + b \geq 2(ab)^{1/2}$ for any nonnegative a, b, we get

$$(\mathrm{RMSE}[h^{FD}(N,\delta)])^2 \geq 2\left\{\frac{2a(\theta)}{N\delta^2}(1+o(1))\left(\left|\frac{1}{2}J''(\theta)\delta + o(\delta)\right| - \frac{2\gamma}{N\delta}\right)^2\right\}^{1/2}$$
$$\to [2a(\theta)]^{1/2}|J''(\theta)|N^{-1/2}$$

as $N \to \infty$, which shows that for $\mathrm{RMSE}[h^{FD}(N,\delta)]$ the best possible rate of convergence is $N^{-1/4}$. The small increment that achieves the asymptotically minimal $\mathrm{RMSE}[h^{FD}(N,\delta)]$ is given by

$$\delta^* = (8a(\theta)/(J''(\theta))^2)^{1/4}N^{-1/4}.$$

According to (8), the rate $N^{-1/4}$ is achievable by any $\delta = cN^{-1/4}$. □

The rate $N^{-1/4}$ is the same as that of the case of finite-horizon performance functions without using CRN (Zazanis and Suri (1993)).

3.2. Simulation with the use of CRN. By CRN, we mean that the generation of $\{X_n\}$ and $\{Y_n\}$ satisfies the following two conditions:

(1) For each n, X_n and Y_n are generated by the same $\xi_n \in \mathcal{U}$ (or a vector of such random numbers). For any $i \neq j$, ξ_i and ξ_j are independent.

(2) When $\delta = 0$ and $X_0 = Y_0 \in \mathcal{S}$, $X_n = Y_n$, a.s., for all $n \geq 1$.

These two conditions are satisfied if $\xi_1 = \xi_2$. (We will run the program twice using the same random seed but only change the value of θ.) Although such a definition does not cover all aspects of CRN, such as generating Y_n depending on all $\{X_i, i \leq n\}$, it is sufficiently general for most simulations.

We study the convergence of an FD estimator (5) with the use of the previously defined CRN by considering the coupled Markov chain $\{\tilde{X}_n = (X_n, Y_n) \in \mathcal{S} \times \mathcal{S}, n \geq 0\}$. Let $\mathcal{A} \subset \mathcal{S} \times \mathcal{S}$ be the minimal closed set of communicating states of $\{\tilde{X}_n\}$ containing $\mathcal{D}$. When the initial state $(X_0, Y_0) \in \mathcal{D}$, $\{\tilde{X}_n\}$ defines an irreducible Markov chain with state space $\mathcal{A}$.

Let $\tilde{P}(\theta,\delta)$ be the state transition matrix for $\{\tilde{X}_n\}$. Then CRN requires that, by suitably numbering the states, $\tilde{P}(\theta,\delta)$ is of the form

$$\tilde{P}(\theta,\delta) = \begin{bmatrix} P(\theta) + \Delta P_1(\theta,\delta) & \Delta P_2(\theta,\delta) \\ Q_1(\theta,\delta) & Q_2(\theta,\delta) \end{bmatrix},$$

where $\Delta P_i(\theta,\delta), Q_i(\theta,\delta)$, $i = 1,2$, are of appropriate dimensions, $\Delta P_i(\theta, 0) = 0$, $i = 1, 2$. If $\tilde{P}(\theta,\delta)$ is analytic in δ in a small neighborhood of $\delta = 0$, the set $\mathcal{A}$ remains the same for all sufficiently small $\delta > 0$.

LEMMA 3.1. *Define* $F_n = f(Y_n, \theta+\delta) - f(X_n,\theta) \in R$ *and*

$$g_n(X_n, Y_n) = E\left[\sum_{i=0}^{N-n}(F_{n+i} - (J(\theta+\delta) - J(\theta)))|X_n, Y_n\right] \in R. \tag{9}$$

Then

$$Var\left[\sum_{n=1}^{N}(f(Y_n,\theta+\delta) - f(X_n,\theta))\right] = \sum_{n=1}^{N} E[Var[g_n(X_n,Y_n)|X_{n-1},Y_{n-1}]]. \tag{10}$$

Proof. For any two random variables X and Y, we have (see, e.g., Shiryayev, (1984, p. 81))

$$Var[X] = E[Var[X|Y]] + Var[E[X|Y]].$$

By repeated use of the previous identity and the Markovian property, we obtain

$$\begin{aligned}
&Var\left[\sum_{n=1}^{N}(f(Y_n,\theta+\delta)-f(X_n,\theta))\right]\\
&= E[Var[F_N|X_{N-1},Y_{N-1}]] + Var\left[\sum_{n=1}^{N-1}F_n + E[F_N|X_{N-1},Y_{N-1}]\right]\\
&= \cdots\\
&= \sum_{n=1}^{N} E\left[Var\left[E\left[\sum_{i=n}^{N}F_i|X_n,Y_n\right]|X_{n-1},Y_{n-1}\right]\right]\\
&= \sum_{n=1}^{N} E[Var[g_n(X_n,Y_n)|X_{n-1},Y_{n-1}]],
\end{aligned}$$

which is exactly what we want. □

LEMMA 3.2. *Assume that $f(x,\theta)\in\mathcal{F}$, $P(\theta)$ is twice continuously differentiable on Θ, and $\tilde{P}(\theta,\delta)$ is analytic in δ in a small neighborhood of zero with bounded first-order derivatives. If the chain $\{X_n\}$ is irreducible and aperiodic and $\{\tilde{X}_n\}$ contains exactly one aperiodic positive recurrent class of states when $\delta=0$, then for any $\theta\in\Theta$ there exists a constant $M>0$ such that*

$$Var\left[\sum_{n=1}^{N}(f(Y_n,\theta+\delta)-f(X_n,\theta))\right]\le MN\delta \tag{11}$$

for all $N\ge 1$ and all sufficiently small $\delta>0$.

Proof. The proof is completed in three steps.

Step 1. *Evaluation of the stationary distribution of $\{\tilde{X}_n\}$*

Let $\tilde{\pi}_\delta$ denote the stationary distribution of $\{\tilde{X}_n\}$. Since $\{\tilde{X}_n\}$ contains exactly one aperiodic positive recurrent class of states and $\mathcal{D}$ is closed, all the states in $\mathcal{A}\setminus\mathcal{D}$ are transient when $\delta=0$. Then $\tilde{\pi}_0=[\pi_\theta,0]$. Therefore, we have (Schweitzer (1968); Louchard and Latouche (1990))

$$\tilde{\pi}_\delta = \tilde{\pi}_0 + \tilde{\pi}_0(\tilde{P}(\theta,\delta)-\tilde{P}(\theta,0))\tilde{Z}[I-(\tilde{P}(\theta,\delta)-\tilde{P}(\theta,0))\tilde{Z}]^{-1}, \tag{12}$$

where the $|\mathcal{A}|\times|\mathcal{A}|$-dimensional fundamental matrix

$$\tilde{Z} = [I-\tilde{P}(\theta,0)+e\tilde{\pi}_0]^{-1}$$

always exists. By the assumption that all the first-order derivatives of $\tilde{P}(\theta,\delta)$ are bounded, there exists a constant $c_1>0$ such that the Euclidean norm $||\tilde{P}(\theta,\delta)-\tilde{P}(\theta,0)||\le c_1\delta$. In light of (12), we know that there exists a $c_2>0$ such that

$$|\tilde{\pi}_\delta(x,y)-\pi_\theta(x)|\le c_2\delta \ \ \forall\ (x,y)\in\mathcal{D} \tag{13}$$

and

$$|\tilde{\pi}_\delta(x,y)|\le c_2\delta \ \ \forall\ (x,y)\in\mathcal{A}\setminus\mathcal{D} \tag{14}$$

for arbitrarily sufficiently small $\delta>0$.

Step 2. Evaluation of $g_n(X_n, Y_n)$

Consider the $g_n(x, y)$ defined in (9). It is the bias between sample and stationary performance functions as a result of nonstationary initial state $(x, y) \in \mathcal{A}$. According to (1), we have

$$\begin{aligned} |g_n(X_n, Y_n)| &\le \sum_{i=0}^{N-n} |E[F_{n+i} - (J(\theta+\delta) - J(\theta))|X_n, Y_n]| \\ &\le 2 \sup_{x\in\mathcal{S},\theta\in\Theta} \{|f(x,\theta)|\} \sum_{i=0}^{N-n} d\alpha\beta^i \\ &\le 2 \sup_{x\in\mathcal{S},\theta\in\Theta} \{|f(x,\theta)|\} d\alpha(1-\beta)^{-1} = M_1, \end{aligned} \tag{15}$$

where the constant $M_1 > 0$ does not depend on n, N, and $\delta > 0$.

Furthermore, for any $(X_n, Y_n) \in \mathcal{D}$ we have

$$\begin{aligned} g_n(X_n, Y_n) &= \sum_{i=0}^{N-n} E[f(Y_{n+i}, \theta+\delta) - J(\theta+\delta)|X_n, Y_n] \\ &\quad - \sum_{i=0}^{N-n} E[f(X_{n+i}, \theta) - J(\theta)|X_n, Y_n] \\ &= \sum_{i=0}^{N-n} (e_{Y_n} P^i(\theta+\delta) - \pi_{\theta+\delta}) f(\theta+\delta) - \sum_{i=0}^{N-n} (e_{X_n} P^i(\theta) - \pi_\theta) f(\theta) \\ &= \sum_{i=0}^{N-n} e_{Y_n} (P(\theta+\delta) - e\pi_{\theta+\delta})^i f(\theta+\delta) - \sum_{i=0}^{N-n} e_{X_n} (P(\theta) - e\pi_\theta)^i f(\theta) \\ &= e_{Y_n}[I - (P(\theta+\delta) - e\pi_{\theta+\delta})^{N-n+1}] Z(\theta+\delta) f(\theta+\delta) \\ &\quad - e_{X_n}[I - (P(\theta) - e\pi_\theta)^{N-n+1}] Z(\theta) f(\theta), \end{aligned} \tag{16}$$

where

$$f(\theta) = \begin{bmatrix} f(s_0, \theta) \\ f(s_1, \theta) \\ \cdots \\ f(s_{d-1}, \theta) \end{bmatrix}$$

and e_x is a row vector of zeros except for the unity component corresponding to the state $x \in \mathcal{S}$.

Since the stationary distribution π_θ satisfies $\pi_\theta = \pi_\theta P(\theta)$, we know that

$$\pi_\theta P'(\theta) = \pi'_\theta(I - P(\theta)) = \pi'_\theta(I - P(\theta) + e\pi_\theta).$$

Therefore,

$$\pi'_\theta = \pi_\theta P'(\theta) Z(\theta).$$

Under the assumption that the first-order derivatives of $p_\theta(x, y)$ and $f(x, \theta)$ are uniformly bounded on Θ, each entry of the following two column vectors

$$(Z(\theta)f(\theta))' \quad \text{and} \quad (P'(\theta) - e\pi'_\theta) Z(\theta) f(\theta)$$

is bounded on Θ by a constant, say, $c_3 > 0$. On the other hand, the derivative of

$$e_{X_n}[I - (P(\theta) + e\pi_\theta)^{N-n+1}] Z(\theta) f(\theta)$$

equals

$$e_{X_n}[I-(P(\theta)-e\pi_\theta)^{N-n+1}](Z(\theta)f(\theta))'$$
$$-e_{X_n}(N-n+1)(P(\theta)-e\pi_\theta)^{N-n}(P'(\theta)-e\pi'_\theta)Z(\theta)f(\theta),$$

which is bounded by

$$c_3\left(1+\sum_{x\in\mathcal{S}}|\pi_\theta^{(N-n+1)}(x)-\pi_\theta(x)|\right)+c_3(N-n+1)\sum_{x\in\mathcal{S}}|\pi_\theta^{(N-n)}(x)-\pi_\theta(x)|$$
$$\leq c_3(1+d\alpha\beta^{N-n+1})+c_3d(N-n+1)\alpha\beta^{N-n}\leq M_2,$$

where $M_2>0$ is a constant independent of N, n, and $\delta>0$. Combining the previous inequality with (16), we get

$$|g_n(X_n,Y_n)|\leq M_2\delta \;\;\forall\,(X_n,Y_n)\in\mathcal{D}. \tag{17}$$

Step 3. *Evaluation of* $E[Var[g_n(X_n,Y_n)|X_{n-1},Y_{n-1}]]$

First, (15) and (17) show that, for any $(X_{n-1},Y_{n-1})\in\mathcal{D}$,

$$Var[g_n(X_n,Y_n)|X_{n-1},Y_{n-1}]\leq E[g_n^2(X_n,Y_n)|X_{n-1},Y_{n-1}]$$

$$\leq\sum_{(X_n,Y_n)\in\mathcal{D}}M_2^2\delta^2+\sum_{(X_n,Y_n)\in\mathcal{A}\backslash\mathcal{D}}M_1^2\Delta P_2(\theta,\delta)((X_{n-1},Y_{n-1}),(x,y))\leq M_3\delta, \tag{18}$$

where $M_3>0$ is a constant. Moreover, we know from (15) that there exists a constant $M_4>0$ such that $Var[g_n(X_n,Y_n)]\leq M_4$. In light of (18), we have

$$E[Var[g_n(X_n,Y_n)|X_{n-1},Y_{n-1}]]$$
$$\leq\sum_{(X_{n-1},Y_{n-1})\in\mathcal{D}}Var[g_n(X_n,Y_n)|(X_{n-1},Y_{n-1})]\tilde{\pi}_\delta^{(n-1)}(X_{n-1},Y_{n-1})$$
$$+\sum_{(X_{n-1},Y_{n-1})\in\mathcal{A}\backslash\mathcal{D}}Var[g_n(X_n,Y_n)|(X_{n-1},Y_{n-1})]\tilde{\pi}_\delta^{(n-1)}(X_{n-1},Y_{n-1})$$
$$\leq\sum_{(X_{n-1},Y_{n-1})\in\mathcal{D}}M_3\delta+\sum_{(X_{n-1},Y_{n-1})\in\mathcal{A}\backslash\mathcal{D}}M_4c_2\delta\leq M\delta,$$

where $M=dM_3+(|\mathcal{A}|-d)c_2M_4$.

By substituting the previous inequality into (10), we immediately obtain (11). □

Lemma 3.2 also demonstrates that when N is fixed, CRN is always helpful for variance reduction for very small $\delta>0$ under the conditions of the lemma.

THEOREM 3.2. *Under the assumptions of Lemma* 3.2, RMSE$[h^{FD}(N,\delta)]$ *converges to zero at a rate of at least* $N^{-1/3}$ *if we choose* $\delta=cN^{-1/3}$, *where* $c>0$ *is a constant.*

Proof. When $\delta=cN^{-1/3}\to 0$, we know from (3), (6), and (11) that

$$(\mathrm{RMSE}[h^{FD}(N,\delta)])^2\leq\frac{M}{N\delta}+\left(\left|\frac{J(\theta+\delta)-J(\theta)}{\delta}-J'(\theta)\right|+\frac{2\gamma}{N\delta}\right)^2$$
$$\leq\frac{M}{N\delta}+\left(\frac{1}{2}|J''(\theta)\delta|+|o(\delta)|+\frac{2\gamma}{N\delta}\right)^2$$
$$=(M/c)N^{-2/3}+\left(\frac{1}{2}|J''(\theta)|cN^{-1/3}+|o(N^{-1/3})|+(2\gamma/c)N^{-2/3}\right)^2$$
$$=O(N^{-2/3}).$$

This proves that RMSE$[h^{FD}(N,\delta)]$ converges at a rate of at least $N^{-1/3}$. □

A comparison of the proofs of Theorems 3.1 and 3.2 reveals that CRN increases the rate of convergence for RMSE$[h^{FD}(N,\delta)]$ by reducing the variance of $Var[h^{FD}(N,\delta)]$ by a factor of δ. Without such variance reduction, the rate increase would be impossible. The following theorem shows that the rate of $N^{-1/3}$ cannot be improved in general.

THEOREM 3.3. *Let $\theta \in \Theta$. Assume that $P(\theta)$ is twice differentiable and $J''(\theta) \neq 0$. If there exist some $(x', y') \in \mathcal{D}, (x'', y'') \in \mathcal{A}/\mathcal{D}$ such that*

$$\Delta P_2(\theta,\delta)((x',y'),(x'',y'')) \geq k\delta, \quad k > 0,$$

then there exists a cost function $f(x,\theta) \in \mathcal{F}$ and a constant $\bar{M} > 0$ such that

$$\text{RMSE}[h^{FD}(N,\delta)] \geq \bar{M}N^{-1/3}$$

for all sufficiently large N and all sufficiently small $\delta > 0$.

Proof. Define

$$A = \begin{bmatrix} 0 \\ 1 \\ \cdots \\ d-1 \end{bmatrix}, \quad f(\theta) = Z^{-1}A = (I - P(\theta) + e\pi_\theta)A.$$

Then the cost function defined in this way satisfies $f(x,\theta) \in \mathcal{F}$.

Since $\{\tilde{X}_n\}$ contains exactly one aperiodic positive recurrent class of states when $\delta = 0$, all but the simple 1 eigenvalues of $\tilde{P}(\theta, 0)$ are within the unit circle on the complex plane. For the same reason as that used in the proof of Theorem 3.1, there exists a $0 \leq \beta_2 < 1$ independent of δ such that all but the simple 1 eigenvalues of $\tilde{P}(\theta,\delta)$ are within a circle of radius β_2 centered at the origin on the complex plane. Thus, $\tilde{\pi}_\delta^{(n)}$ converges to $\tilde{\pi}_\delta$ uniformly in δ and for any β_1, $1 > \beta_1 > \beta_2$, there exists an $\alpha_1 > 0$ such that

$$|\tilde{\pi}_\delta^{(n)}(x,y) - \tilde{\pi}_\delta(x,y)| \leq \alpha_1\beta_1^n \tag{19}$$

for all $n \geq 0$, all $(x,y) \in \mathcal{A}$, and all sufficiently small $\delta > 0$. Hence, according to (13) and (19), for any $(X_{n-1}, Y_{n-1}) \in \mathcal{D}$,

$$\tilde{\pi}_\delta^{(n-1)}(X_{n-1}, Y_{n-1}) \geq \pi_\theta(X_{n-1}) - \alpha_1\beta_1^{n-1} - c_2\delta. \tag{20}$$

Consider the $g_n(x,y)$ defined in (9). Since $\pi_\theta^{(n)} = \pi_\theta^{(0)}P^n(\theta)$, we know from (16) that

$$\begin{aligned} g_n(x,y) &= \sum_{i=0}^{N-n} e_y(P(\theta+\delta) - e\pi_{\theta+\delta})^i f(\theta+\delta) - \sum_{i=0}^{N-n} e_x(P(\theta) - e\pi_\theta)^i f(\theta) \\ &= [e_y - e_x]A - e_y(P(\theta+\delta) - e\pi_{\theta+\delta})^{N-n+1}A + e_x(P(\theta) - e\pi_\theta)^{N-n+1}A \\ &= [e_y - e_x]A - [e_yP^{N-n+1}(\theta+\delta) - \pi_{\theta+\delta}]A + [e_xP^{N-n+1}(\theta) - \pi_\theta]A. \end{aligned}$$

Combining the previous equation with (1), we obtain

$$|g_n(x,y)| \geq 1 - 2(d-1)d\alpha\beta^{N-n+1} \ \ \forall\, (x,y) \in \mathcal{A} \setminus \mathcal{D}$$

and

$$\begin{aligned} E[g_n^2(X_n,Y_n)|X_{n-1} = x', Y_{n-1} = y'] &\geq \sum_{(x,y)\in\mathcal{A}\setminus\mathcal{D}} g_n^2(x,y)\Delta P_2(\theta,\delta)((x',y'),(x,y)) \\ &\geq k\delta[1 - 2(d-1)d\alpha\beta^{N-n+1}]. \end{aligned}$$

On the other hand, (17) shows that

$$|E[g_n(X_n, Y_n)|X_{n-1}, Y_{n-1}]| \leq M_2\delta.$$

Therefore,

$$Var[g_n(X_n, Y_n)|X_{n-1} = x', Y_{n-1} = y'] \geq k\delta[1 - 2(d-1)d\alpha\beta^{N-n+1}] - M_2^2\delta^2.$$

Consequently, for any $n \geq 1$ we have

$$\begin{aligned} &E[Var[g_n(X_n, Y_n)|X_{n-1}, Y_{n-1}]] \\ &\geq \tilde{\pi}_\delta^{(n-1)}(x', y')[k\delta(1 - 2(d-1)d\alpha\beta^{N-n+1}) - M_2^2\delta^2]. \end{aligned}$$

By combining the previous inequality with (20), we get

$$\begin{aligned} &E[Var[g_n(X_n, Y_n)|X_{n-1}, Y_{n-1}]] \\ &\geq k\pi_\theta(x')\delta[1 - 2(d-1)d\alpha\beta^{N-n+1}] - \pi_\theta(x')M_2^2\delta^2 - (\alpha_1\beta_1^{n-1} + c_2\delta)k\delta. \end{aligned}$$

The substitution of the previous expression into (10) shows that

$$\begin{aligned} &Var\left[\sum_{n=1}^{N}(f(Y_n, \theta+\delta) - f(X_n, \theta))\right] \\ &\geq Nk\pi_\theta(x')\delta - N(\pi_\theta(x')M_2^2 + c_2k)\delta^2 - k\delta\alpha_1\beta_1(1-\beta_1)^{-1} - [2kd(d-1)\alpha\beta(1-\beta)^{-1}]\delta. \end{aligned}$$

Thus, for sufficiently small δ and very large N, we have

$$Var\left[\sum_{n=1}^{N}(f(Y_n, \theta+\delta) - f(X_n, \theta))\right] \geq 0.5k\pi_\theta(x')N\delta,$$

from which, together with (6), we get

$$(\text{RMSE}[h^{FD}(N, \delta)])^2 \geq \frac{k\pi_\theta(x')}{2N\delta} + \left(\frac{1}{2}|J''(\theta)\delta| - |o(\delta)| - \frac{2\gamma}{N\delta}\right)^2.$$

We have already proved in Theorem 3.2 that the right-hand side converges at a rate of at least $N^{-2/3}$. Thus δ must not go to zero faster than $N^{-1/3}$, which means that $1/(N\delta^2)$ must go to zero. Using Jensen's inequality again, $a+b+c \geq 3(abc)^{1/3}$ for any $a, b, c \geq 0$, the right-hand side of the previous inequality is bounded from below by

$$\begin{aligned} &3\left[\left(\frac{k\pi_\theta(x')}{4N\delta}\right)^2\left(\frac{1}{2}|J''(\theta)\delta| - |o(\delta)| - \frac{2\gamma}{N\delta}\right)^2\right]^{1/3} \\ &= 3\left[\left(\frac{k\pi_\theta(x')}{4N}\right)^2\left(\frac{1}{2}|J''(\theta)| - |o(1)| - \frac{2\gamma}{N\delta^2}\right)^2\right]^{1/3} \geq \left(\frac{k\pi_\theta(x')|J''(\theta)|}{8N}\right)^{2/3}, \end{aligned}$$

for sufficiently large N, showing the conclusion is true for $\bar{M}=(k\pi_\theta(x')|J''(\theta)|/4)^{1/3}$. □

COROLLARY 3.1. *Assume that $f(x,\theta) \in \mathcal{F}$, $P(\theta)$ is twice differentiable and $J''(\theta) \neq 0$. If there exists a pair of states $x, y \in \mathcal{S}$ satisfying $p'_\theta(x,y) \neq 0$, then the conclusion of Theorem* 3.3 *is valid for any simulations satisfying the two CRN conditions.*

Proof. Since $p'_\theta(x,y) \neq 0$, we know that there is a $k_1 > 0$ such that

$$|p_{\theta+\delta}(x,y) - p_\theta(x,y)| \geq k_1\delta$$

when δ is sufficiently small. Furthermore, X and Y are two random variables defined on the same state space $\mathcal{S}$ with probability distribution $P_X(x)$ and $P_Y(y)$, respectively. Then we have (Lindvall (1992, p. 18))

$$\text{Prob}\{X \neq Y\} \geq \frac{1}{2}\sum_{x\in\mathcal{S}} |P_X(x) - P_Y(x)|.$$

Applying the previous inequality to our problem, we know that for any simulation satisfying the first requirement of CRN

$$\sum_{(x',y')\in\mathcal{A}\setminus\mathcal{D}} \Delta P_2(\theta,\delta)((x,x),(x',y')) = \text{Prob}\{(x',y') \in \mathcal{A}\setminus\mathcal{D}\}$$

$$\geq \frac{1}{2}\sum_{z\in\mathcal{S}} |p_{\theta+\delta}(x,z) - p_\theta(x,z)| \geq \frac{1}{2}k_1\delta.$$

Thus, there must exist a constant $k > 0$ and a pair of states $(x'', y'') \in \mathcal{A}\setminus\mathcal{D}$ such that

$$\Delta P_2(\theta,\delta)((x,x),(x'',y'')) \geq k\delta,$$

which implies that the conclusion of Theorem 3.3 is valid with $(x',y') = (x,x)$. □

The conclusion of Corollary 3.1 is very strong. It requires nothing of the details of the implementation of CRN. All it needs is that the simulation is performed using the scheme of CRN according to the two very mild conditions specified at the beginning of this section.

Several remarks are in order.

Remark 3.1. *The inadequacy of* $P(\theta)$.

Generally speaking, the transition matrix $P(\theta)$ alone cannot determine the rate of convergence for RMSE$[h^{FD}(N,\delta)]$, as illustrated by the following example.

Example 3.1. Consider a Markov chain with $\mathcal{S} = \{1,2\}$ and

$$P(\theta) = \begin{bmatrix} \theta & 1-\theta \\ 1-\theta & \theta \end{bmatrix},$$

where $\theta \in (0, 0.5)$. The function $f(x,\theta)$ is defined as $f(x,\theta) = \theta^x$, $x \in \mathcal{S}$. Then $0 \leq f(x,\theta) \leq 1$, $\pi_\theta = [0.5,\ 0.5]$, $J(\theta) = (1/2)(\theta + \theta^2)$, and $J''(\theta) = 1$.

(i) Assume that in simulation the state transition at the nth step is determined by a $\xi_n \in \mathcal{U}$ in the following way.

When $X_{n-1} = 1$,

$$X_n = \begin{cases} 1 & \text{if } \xi_n < \theta, \\ 2 & \text{otherwise.} \end{cases}$$

When $X_{n-1} = 2$,

$$X_n = \begin{cases} 1 & \text{if } \xi_n < 1-\theta, \\ 2 & \text{otherwise.} \end{cases}$$

Then the state transition matrix of the coupled chain $\{\tilde{X}_n\}$ is

$$\tilde{P}(\theta,\delta) = \begin{bmatrix} \theta-\delta & 1-\theta & \delta & 0 \\ 1-\theta & \theta-\delta & 0 & \delta \\ \theta & \theta-\delta & 0 & 1-2\theta+\delta \\ \theta-\delta & \theta & 1-2\theta+\delta & 0 \end{bmatrix}.$$

Direct verification shows that the assumptions of Theorems 3.2 and 3.3 are satisfied, and thus the best possible rate of convergence for $\text{RMSE}[h^{FD}(N,\delta)]$ is $N^{-1/3}$.

(ii) We modify the simulation in (i) by changing the state transition for $X_{n-1} = 2$ to

$$X_n = \begin{cases} 2 & \text{if } \xi_n < \theta, \\ 1 & \text{otherwise.} \end{cases}$$

The new state transition matrix of the coupled chain is

$$\tilde{P}(\theta,\delta) = \begin{bmatrix} \theta-\delta & 1-\theta & \delta & 0 \\ 1-\theta & \theta-\delta & 0 & \delta \\ \delta & 0 & \theta-\delta & 1-\theta \\ 0 & \delta & 1-\theta & \theta-\delta \end{bmatrix}.$$

In this case, the assumptions of Theorem 3.2 are violated. Since $\tilde{\pi}_\delta$ is discontinuous at $\delta = 0$, $\tilde{\pi}_\delta^{(n)}$ does not converge uniformly to the stationary distribution $\tilde{\pi}_\delta$ in any neighborhood around $\delta = 0$. By solving

$$\tilde{\pi}_\delta^{(n+1)} = \tilde{\pi}_\delta^{(n)} \tilde{P}(\theta,\delta)$$

and direct calculating, we obtain (see the appendix for a detailed derivation)

$$(\text{RMSE}[h^{FD}(N,\delta)])^2 = \frac{\theta^3(1-\theta)}{2N\delta^2}\left[1 - \frac{1}{2N\delta}(1-(1-2\delta)^N)\right](1+o(1)) + \left(\frac{\delta}{2} + \frac{1}{4N}\right)^2. \tag{21}$$

The first term on the right-hand side of (21) clearly indicates that

$$\frac{1}{N} Var\left[\sum_{n=1}^{N}[f(Y_n,\theta+\delta) - f(X_n,\theta)]\right] = \frac{\theta^3(1-\theta)}{2N}\left[1 - \frac{1}{2N\delta}(1-(1-2\delta)^N)\right](1+o(1))$$

does not converge to zero as $\delta \to 0$ uniformly in N. However, it does go to zero as $\delta \to 0$ for any fixed N. Thus, the use of CRN is indeed helpful for variance reduction.

A detailed analysis shows that the best possible rate of convergence for (21) is achieved when $\delta = cN^{-1/4}$. The corresponding rate of convergence for $\text{RMSE}[h^{FD}(N,\delta)]$ is $N^{-1/4}$ and

$$\begin{aligned} \text{RMSE}[h^{FD}(N,\delta)] &\to \left[\frac{\theta^3(1-\theta)}{2c^2} + \left(\frac{c}{2}\right)^2\right]^{1/2} N^{-1/4} \\ &= \left[\frac{\theta^3(1-\theta)}{2c^2} + \frac{c^2}{4}\right]^{1/2} N^{-1/4}. \end{aligned} \tag{22}$$

On the other hand, by calculating the exact form of $a(\theta)$ in (4),

$$a(\theta) = \frac{\theta}{4(1-\theta)}(f(1,\theta) - f(2,\theta))^2 = \frac{1}{4}\theta^3(1-\theta),$$

we know from (8) that for independent simulations and if $\delta = cN^{-1/4}$, the asymptotic form of $\text{RMSE}[h^{FD}(N,\delta)]$ is given by

$$\begin{aligned} &\left[\frac{\theta}{2(1-\theta)c^2}(f(2,\theta) - f(1,\theta))^2 + c^2\left(\frac{1}{2}J''(\theta)\right)^2\right]^{1/2} N^{-1/4} \\ &= \left[\frac{\theta^3(1-\theta)}{2c^2} + \frac{c^2}{4}\right]^{1/2} N^{-1/4}, \end{aligned}$$

which is exactly the same as that in (22). CRN is not effective for improving the rate of convergence and for reducing the asymptotic variance.

This example shows that for the same original transition matrix $P(\theta)$, slightly different simulations, both using CRN, may yield two different rates of convergence for FD estimates.

Remark 3.2. *The case of symmetric difference.*

Another variation of finite difference is the *symmetric difference* (SD) of the form

$$h^{SD}(N,\delta) = \frac{L(N,\theta+\delta,\xi_2) - L(N,\theta-\delta,\xi_1)}{2\delta}.$$

In this case, we have

$$\mathrm{RMSE}[h^{SD}(N,\delta)] = \left\{ Var[h^{SD}(N,\delta)] + \left(\frac{J(N,\theta+\delta) - J(N,\theta-\delta)}{2\delta} - J'(\theta) \right)^2 \right\}^{1/2}.$$

The estimation bias of an SD estimator is

$$\frac{J(N,\theta+\delta) - J(N,\theta-\delta)}{2\delta} - J'(\theta) = \frac{J(\theta+\delta) - J(\theta-\delta)}{2\delta} - J'(\theta) + O\left(\frac{1}{N\delta}\right)$$

$$= \frac{1}{6} J'''(\theta)\delta^2(1+o(1)) + O\left(\frac{1}{N\delta}\right),$$

which converges to zero faster than that of an FD when δ goes to zero. An analysis similar to that used in the proof of Theorems 3.1–3.3 yields the following result on the rates of convergence for SD estimates.

THEOREM 3.4. (i) *Assume all the assumptions of Theorem* 3.1 *except that* $J''(\theta) \neq 0$ *is replaced by* $J'''(\theta) \neq 0$. *Then for independent simulations, the best possible rate of convergence for* $\mathrm{RMSE}[h^{SD}(N,\delta)]$ *is* $N^{-1/3}$, *which is achievable by setting* $\delta = cN^{-1/6}$ *with any positive constant c.* (ii) *Under the assumptions of Theorem* 3.2, *if* $J(\theta)$ *is triple continuously differentiable, then the rate of convergence for* $\mathrm{RMSE}[h^{SD}(N,\delta)]$ *is at least* $N^{-2/5}$, *which can be achieved by* $\delta = cN^{-1/5}$.

Remark 3.3. *Comparison with independent simulations.*

Under the assumptions of Theorem 3.2, CRN is helpful for accelerating the convergence of both FD and SD estimates. The increase in the rates of convergence can often be interpreted as an increase of simulation efficiency since CRN does not require extra effort in simulation. However, as shown in Remark 3.1, we generally cannot guarantee that CRN is helpful for accelerating the convergence of FD or SD estimates.

Remark 3.4. *About the assumption that* $\{\tilde{X}_n\}$ *contains exactly one aperiodic positive recurrent class of states.*

The key step to the proof of Theorem 3.2 is the inequality (14) which implies that a small perturbation δ should produce only small effect in stationary distribution. If $\{\tilde{X}_n\}$ contains exactly one aperiodic positive recurrent class of states when $\delta = 0$, sample paths of $\{X_n\}$ and $\{Y_n\}$ started from different states in $\mathcal{A} \setminus \mathcal{D}$ agree with probability one as $\delta \to 0$ after only a finite number of transitions, which in turn means that small perturbations can only cause higher-order effect.

Theorem 3.1 gives only sufficient conditions on the effectiveness of CRN. The same procedure, but in more detail and more tedious, as that is used in the appendix can yield precise conditions under which CRN is effective for the acceleration of FD or SD estimates. However, as demonstrated in section 4, we can easily design simulation schemes that guarantee the effectiveness of CRN. As a result of the existence of such better simulation schemes, we are not interested in deriving these exact conditions. Finally, we would like to point out that, in general, CRN is unlikely to be effective in increasing the rates of convergence without the assumption that $\{\tilde{X}_n\}$ contains exactly one aperiodic positive recurrent class of states.

4. Convergence of some simulation schemes.

(1) *The scheme of CRN.* The most natural way to simulate a discrete-time Markov chain is the following scheme.

Scheme I. Following the nth state transition, we generate a $\xi_n \in \mathcal{U}$. Let order $\Gamma(X_{n-1})$ as $s_{n_1}, s_{n_2}, \ldots, s_{n_{|\Gamma(X_{n-1})|}} \in \mathcal{S}$ and define

$$\rho_\theta(X_{n-1}, s_{n_0}) = 0, \quad \rho_\theta(X_{n-1}, s_{n_i}) = \sum_{j=1}^{i} p_\theta(X_{n-1}, s_{n_j}), \quad i = 1, 2, \ldots, |\Gamma(X_{n-1})|.$$

Then the next state X_n is s_{n_i} if $\xi_n \in [\rho_\theta(X_{n-1}, s_{n_{i-1}}), \rho_\theta(X_{n-1}, s_{n_i}))$. For any $x = s_{n_i} \in \mathcal{S}$ we use x_- to denote the state $s_{n_{i-1}}$.

The CRN conditions are satisfied if Scheme I is used to generate X_n and Y_n by *the same* ξ_n with $P(\theta)$ and $P(\theta+\delta)$, respectively. The state transition probability

$$\mathrm{Prob}\{\tilde{X}_n = (x, y) \mid \tilde{X}_{n-1} = (x', y')\}$$

of the coupled chain is determined by

$$(\min\{\rho_\theta(x', x), \rho_{\theta+\delta}(y', y)\} - \max\{\rho_\theta(x', x_-), \rho_{\theta+\delta}(y', y_-)\})^+,$$

where $(x)^+ = \max\{x, 0\}$. The effectiveness of CRN for this simulation scheme depends on the matrix $\tilde{P}(\theta, \delta)$, as we have already demonstrated in Remark 3.2.

Consider the simulation of the embedded Markov chain of the M/M/1/K queue. Let θ be the arrival rate and μ be the service rate, $\theta < \mu$. Then the state transition matrix of this Markov chain is

$$P(\theta) = \begin{bmatrix} 1-p & p & & & & \\ 1-p & 0 & p & & & \\ & 1-p & 0 & & & \\ & & \cdots & & & \\ & & & 1-p & 0 & p \\ & & & & 1-p & p \end{bmatrix},$$

where $p = \theta/(\mu+\theta)$. Let Scheme I be implemented by

$$X_n = \begin{cases} X_{n-1} + 1 & \text{if } \xi_n < p, \\ (X_{n-1} - 1)^+ & \text{otherwise.} \end{cases}$$

Direct verification shows that all the assumptions of Theorem 3.2 are satisfied. Hence, CRN is indeed effective in this case.

For simulation Scheme I, CRN is not guaranteed to be helpful for either FD or SD estimates. Next we investigate several alternatives with guaranteed effectiveness.

(2) *Simulation based on maximal coupling.* Our first choice is simulation based on maximal coupling. For any two random variables X and Y with given marginal distributions, we say that their samples are maximally coupled if the probability that their samples are the same is maximized, i.e., $\max \mathrm{Prob}\{X = Y\}$. Coupling is a very useful method in simulation. The readers are referred to Devroye (1990) and Lindvall (1992) for a detailed discussion on the coupling method and to Bremaud (1993) for its use in sensitivity analysis.

Scheme II. We simultaneously simulate $\{X_n\}$ and $\{Y_n\}$ with maximal coupling. We generate the nth transition from (X_{n-1}, Y_{n-1}) to (X_n, Y_n) in the following way: Let $P_1(x)$ and $P_2(y)$ be the distribution of X_n and Y_n, respectively, for any given pair X_{n-1}, Y_{n-1}. Define $s = 0.5 \sum_{x \in \Gamma(X_{n-1}) \bigcup \Gamma(Y_{n-1})} |P_1(x) - P_2(x)|$ and generate four random variables $U \in \{0,1\}$, $V, W, Z \in \mathcal{S}$ such that $P\{U=1\} = 1 - P\{U=0\} = 1-s$, $P\{V=x\} = \min\{P_1(x), P_2(x)\}/(1-s)$, $P\{W=x\} = (P_1(x) - P_2(x))^+/s$, and $P\{Z = x\} = (P_2(x) - P_1(x))^+/s$. Define $X_n = UV + (1-U)W$ and $Y_n = UV + (1-U)Z$. Then X_n and Y_n generated in this way have the desired marginal distributions and, more importantly, maximize the probability $P\{X_n = Y_n\}$ (Devroye (1990)).

THEOREM 4.1. *If $\{X_n\}$ is irreducible and aperiodic and $\delta = 0$, under the simulation based on maximal coupling, any $(x,y) \in (\mathcal{S} \times \mathcal{S}) \setminus \mathcal{D}$ is transient and eventually gets absorbed in $\mathcal{D}$.*

Proof. Consider the coupled Markov chain $\{\tilde{X}_n\}$ when $\delta = 0$. For any $(X_{n-1}, Y_{n-1}) \in \mathcal{D}$, $s = 0$ and $(X_n, Y_n) \in \mathcal{D}$, a.s. Therefore, $\mathcal{D}$ is closed and irreducible. Consider any $(X_{n-1}, Y_{n-1}) = (x,y) \in (\mathcal{S} \times \mathcal{S}) \setminus \mathcal{D}$. If $\Gamma(x) \bigcap \Gamma(y) \neq \emptyset$, then $s < 1$ and

$$P\{\tilde{X}_n \in \mathcal{D}\} = P\{U = 1\} = 1 - s > 0.$$

With a positive probability (x,y) gets absorbed in $\mathcal{D}$; that is, (x,y) is transient. If $\Gamma(x) \bigcap \Gamma(y) = \emptyset$, then $s = 1$ and the maximal coupling method is equivalent to independent simulations of X_n and Y_n starting from x and y. $\{X_n\}$ is irreducible and aperiodic, with a positive probability that $\{\tilde{X}_{n+i}, i \geq 0\}$ will reach a state (x', y') such that $\Gamma(x') \bigcap \Gamma(y') \neq \emptyset$ or even $(x', y') \in \mathcal{D}$. The state (x,y) is also transient in this case. Thus we have proved that all states in $(\mathcal{S} \times \mathcal{S}) \setminus \mathcal{D}$ are transient. □

(3) *Simulation based on maximal correlation.* Our purpose of introducing the maximal coupling method in Scheme II is to reduce the variance of $Var[L(N, \theta + \delta) - L(N, \theta)]$. For any two random variables X and Y with respective marginal distributions $F(t)$ and $G(t)$, the variance $Var[X - Y]$ is minimized (or the correlation $Cov[X, Y]$ is maximized) if X and Y are generated according to $X = F^{-1}(\xi), Y = G^{-1}(\xi)$, where $F^{-1}(.)$ is the inverse function, $\xi \in \mathcal{U}$.

Scheme I is a variation of simulation based on maximal correlation. The following simulation scheme is another one which ensures the transience of all states in $(\mathcal{S} \times \mathcal{S}) \setminus \mathcal{D}$.

Scheme III. Consider the nth state transition.

(a) If $(X_{n-1}, Y_{n-1}) \in \mathcal{D}$, generate a $\xi_n \in \mathcal{U}$ and determine the next states X_n and Y_n using the same ξ_n according to maximal correlation.

(b) If $(X_{n-1}, Y_{n-1}) \in \mathcal{A} \setminus \mathcal{D}$ and there is a state $s \in \Gamma(X_{n-1}) \bigcap \Gamma(Y_{n-1})$, we order the sets $\Gamma(X_{n-1})$ and $\Gamma(Y_{n-1})$ starting with s; i.e., $\Gamma(X_{n-1}) = \{s, ...\}$ and $\Gamma(Y_{n-1}) = \{s, ...\}$. Then generate X_n and Y_n according to (a).

(c) If $(X_{n-1}, Y_{n-1}) \in \mathcal{A} \setminus \mathcal{D}$ and $\Gamma(X_{n-1}) \bigcap \Gamma(Y_{n-1}) = \emptyset$, generate X_n and Y_n independently using (a), requiring two independent random numbers.

Direct verification shows that, under Scheme III and when $\delta = 0$, any $(x,y) \in (\mathcal{S} \times \mathcal{S}) \setminus \mathcal{D}$ is transient and eventually gets absorbed in $\mathcal{D}$. Step (b) can be eliminated while preserving the state transience; that is, if $(X_{n-1}, Y_{n-1}) \in (\mathcal{S} \times \mathcal{S}) \setminus \mathcal{D}$, we generate two independent samples for X_n and Y_n until they reach $\mathcal{D}$. However, this modification is less efficient since we passively wait for (X_n, Y_n) to reach $\mathcal{D}$ rather than forcing (X_n, Y_n) to go to $\mathcal{D}$ as fast as possible.

For simulations using Schemes II and III, Theorem 3.2 is applicable, ensuring faster convergence for the FD and SD estimates than independent simulations.

Schemes II and III are applicable to any irreducible, aperiodic Markov chains. Their disadvantage is that we have to generate sample paths with θ and $\theta + \delta$ simultaneously, which is more complicated than running two experiments with the same sequence of random numbers. Nevertheless, they are not difficult for implementation in simulation.

5. Regenerative structure. An irreducible Markov chain has the regenerative structure which can be used to increase the efficiency of estimation. Zazanis and Suri (1993) studied the convergence of FD and SD estimates without the use of CRN. In this section, we show how CRN accelerates the convergence of these estimates.

Let us fix a state, say, $\bar{x} \in \mathcal{S}$, and the simulation starts from $X_0 = \bar{x}$. Let $n_0 = 0, n_i, i \geq 1$, be the ith regenerative transition that the chain $\{X_n\}$ visits $\bar{x}$. Define

$$h_i(\theta) = \sum_{n=n_{i-1}}^{n_i-1} f(X_n, \theta), \quad T_i(\theta) = n_i - n_{i-1}, \quad i = 1, 2, \ldots.$$

Then $\{h_i(\theta), T_i(\theta)\}$ is a sequence of independently and identically distributed (i.i.d.) random variables, and the following is a consistent ratio estimate for the stationary performance function $J(\theta)$ (Zazanis and Suri (1993))

$$\lim_{N\to\infty} \frac{\sum_{i=1}^N h_i(\theta)}{\sum_{i=1}^N T_i(\theta)} = \frac{E[h_1(\theta)]}{E[T_1(\theta)]} = E_{\pi_\theta}[f(X, \theta)] = J(\theta), \quad \text{a.s.}$$

We construct the following FD estimator for $J'(\theta)$

$$h^{RFD}(N, \delta) = \frac{1}{\delta}\left[\frac{\sum_{i=1}^N h_i(\theta+\delta)}{\sum_{i=1}^N T_i(\theta+\delta)} - \frac{\sum_{i=1}^N h_i(\theta)}{\sum_{i=1}^N T_i(\theta)}\right].$$

Since $\{X_n\}$ and $\{Y_n\}$ are sample paths with respective parameters θ and $\theta+\delta$, we need to align these two sample paths in a manageable manner. For regenerative simulations, we require that Scheme I be used in simulation, and for every i the same sequence of random numbers is employed to simulate the ith regenerative cycles of both $\{X_n\}$ and $\{Y_n\}$. It is quite possible that $T_i(\theta) \neq T_i(\theta+\delta)$. However, for different regenerative cycles, simulations are carried out independently; i.e., $\{(h_i(\theta), h_i(\theta+\delta), T_i(\theta), T_i(\theta+\delta))\}$ is a sequence of i.i.d. random vectors.

LEMMA 5.1. *Assume that $f(x, \theta) \in \mathcal{F}$, $E[T_1^i(\theta)]$, $i = 1, 2$, are uniformly bounded for all $\theta \in \Theta$ and every entry of $\Delta P_2(\theta, \delta)$ is continuously differentiable in δ with bounded first-order derivatives on Θ. Then there exist two constants k_1 and k_2 such that*

$$Var[h_1(\theta+\delta) - h_1(\theta)] \leq k_1\delta \text{ and } Var[T_1(\theta+\delta) - T_1(\theta)] \leq k_2\delta.$$

Proof. Since every entry of $\Delta P_2(\theta, \delta)$ is continuously differentiable with bounded first-order derivatives, there is a constant $k > 0$ such that $\text{Prob}\{X_n \neq Y_n | (X_{n-1}, Y_{n-1}) \in \mathcal{D}\} \leq k\delta$ for all n and any $(X_{n-1}, Y_{n-1}) \in \mathcal{D}$. Since $f(x, \theta) \in \mathcal{F}$, $f'(x, \theta)$, the derivative of $f(x, \theta)$ with respect to θ, is continuous on Θ and there exists a $\bar{k} > 0$ such that $|f'(x, \theta)| \leq \bar{k}$ for any $x \in \mathcal{S}$ and for any $\theta \in \Theta$. Furthermore, since $E[T_1^2(\theta)]$ is uniformly bounded on Θ and $f(x, \theta)$ is a bounded function, there exists a $B > 0$ such that, for every i, $0 \leq i < n_1$, $E[h_1^2(\theta) | X_j, j \leq i] \leq B/4$ for any $\theta \in \Theta$, which implies that for any $0 \leq i \leq \min\{T_1(\theta), T_1(\theta+\delta)\} - 1$ and, for any $X_{i-1} \in \mathcal{S}$,

$$E\left[\left(\sum_{n=i}^{T_1(\theta+\delta)-1} f(Y_n, \theta+\delta) - \sum_{n=i}^{T_1(\theta)-1} f(X_n, \theta)\right)^2 | X_j = Y_j, j \leq i\right]$$
$$\leq 2E[h_1^2(\theta+\delta) | Y_j, j \leq i] + 2E[h_1^2(\theta) | X_j, j \leq i] \leq B.$$

Therefore, starting from $X_0 = Y_0 = \bar{x}$,

$$E[(h_1(\theta+\delta) - h_1(\theta))^2] = E\left[\left(\sum_{n=0}^{T_1(\theta+\delta)-1} f(Y_n, \theta+\delta) - \sum_{n=0}^{T_1(\theta)-1} f(X_n, \theta)\right)^2\right]$$

$$= E_{X_1}\left[\sum_{Y_1 \neq X_1} E\left[\left(\sum_{n=0}^{T_1(\theta+\delta)-1} f(Y_n, \theta+\delta) - \sum_{n=0}^{T_1(\theta)-1} f(X_n, \theta)\right)^2 |Y_1 \neq X_1\right] P\{Y_1 \neq X_1\}\right.$$

$$\left. + E\left[\left(\sum_{n=0}^{T_1(\theta+\delta)-1} f(Y_n, \theta+\delta) - \sum_{n=0}^{T_1(\theta)-1} f(X_n, \theta)\right)^2 |Y_1 = X_1\right] P\{Y_1 = X_1\}\right]$$

$$\leq E_{X_1}\left[dBk\delta + E\left[\left(\sum_{n=0}^{T_1(\theta+\delta)-1} f(Y_n, \theta+\delta) - \sum_{n=0}^{T_1(\theta)-1} f(X_n, \theta)\right)^2 |Y_j = X_j, j \leq 1\right]\right]$$

$$\leq E_{X_1,X_2}\left[dBk\delta + E\left[\left(\sum_{n=0}^{T_1(\theta+\delta)-1} f(Y_n, \theta+\delta) - \sum_{n=0}^{T_1(\theta)-1} f(X_n, \theta)\right)^2 |Y_j = X_j, j \leq 2\right]\right]$$

$$\leq \cdots$$

$$\leq E[T_1]dBk + E\left[\left(\sum_{n=0}^{T_1(\theta)-1} f(X_n, \theta+\delta) - f(X_n, \theta)\right)^2\right]$$

$$\leq k_1\delta$$

(23)

for sufficiently small δ, where $k_1 = E[T_1]dBk + \bar{k}^2\delta E[T^2(\theta)]$.

Setting $f(x, \theta) = 1$, we know immediately from (23) that there exists a k_2 satisfying

$$Var[T_1(\theta+\delta) - T_1(\theta)] \leq E[(T_1(\theta+\delta) - T_1(\theta))^2] \leq k_2\delta.$$

Thus we have completed the proof of Lemma 5.1. □

THEOREM 5.1. *Suppose all the assumptions of Lemma* 5.1 *and, in addition,* $E[T_1^4(\theta)]$ *and* $E[h_1^4(\theta)]$ *are finite,* $E[T_1(\theta)]$ *and* $E[h_1(\theta)]$ *are continuous on* Θ, *and* $J(\theta)$ *is twice differentiable with* $J''(\theta) \neq 0$. *Then, for any* $\theta \in \Theta$, RSME$[h^{RFD}(N, \delta)]$ *converges at rate at least* $N^{-1/3}$, *which is achieved by* $\delta = cN^{-1/3}$ *with any constant* $c > 0$.

Proof. We need to rewrite the form of $h^{RFD}(N, \delta)$ as

$$h^{RFD}(N, \delta) = \frac{1}{\delta} \frac{[\sum_{i=1}^N \Delta h_i(\theta)][\sum_{i=1}^N T_i(\theta)] - [\sum_{i=1}^N h_i(\theta)][\sum_{i=1}^N \Delta T_i(\theta)]}{[\sum_{i=1}^N T_i(\theta)][\sum_{i=1}^N \Delta T_i(\theta) + \sum_{i=1}^N T_i(\theta)]},$$

where $\Delta h_i(\theta) = h_i(\theta+\delta) - h_i(\theta)$ and $\Delta T_i(\theta) = T_i(\theta+\delta) - T_i(\theta)$. By applying the asymptotic properties of ratio estimates, under the assumption that $E[T_1^4(\theta)]$ and $E[h_1^4(\theta)]$ are finite, we have (see, e.g., Zazanis and Suri (1993))

$$E[h^{RFD}(N, \delta)] = \frac{J(\theta+\delta) - J(\theta)}{\delta} + O\left(\frac{1}{N\delta}\right) \quad (24)$$

and

$$\begin{aligned}
&Var[h^{RFD}(N,\delta)] \\
&= \frac{1}{N\delta^2} Var[a_1 \Delta h_1(\theta) + a_2 \Delta T_1(\theta) + a_3 h_1(\theta) + a_4 T_1(\theta)] + O(N^{-3/2}\delta^{-2}) \\
&\leq \frac{4}{N\delta^2}\{a_1^2 Var[\Delta h_1(\theta)] + a_2^2 Var[\Delta T_1(\theta)] + a_3^2 Var[h_1(\theta)] + a_4^2 Var[T_1(\theta)]\} \\
&\quad + O(N^{-3/2}\delta^{-2}), \qquad (25)
\end{aligned}$$

where

$$a_1 = \frac{1}{E[T_1(\theta+\delta)]},$$

$$a_2 = \frac{-E[h_1(\theta)]}{E^2[T_1(\theta+\delta)]},$$

$$a_3 = \frac{E[T_1(\theta+\delta)] - E[T_1(\theta)]}{E[T_1(\theta+\delta)]E[T_1(\theta)]},$$

$$a_4 = \frac{E[h_1(\theta)](E^2[T_1(\theta+\delta)] - E^2[T_1(\theta)]) - (E[h_1(\theta+\delta)] - E[h_1(\theta)])E^2[T_1(\theta)]}{E^2[T_1(\theta+\delta)]E^2[T_1(\theta)]}.$$

Since $E[T_1(\theta)]$ and $E[h_1(\theta)]$ are continuous on Θ, $a_1 = O(1)$, $a_2 = O(1)$, $a_3 = O(\delta)$, and $a_4 = O(\delta)$. According to Lemma 5.1, $Var[\Delta h_1(\theta)] \leq k_1\delta$ and $Var[\Delta T_1(\theta)] \leq k_2\delta$. Hence, we know from (25) that $Var[h^{RFD}(N,\delta)] = O((N\delta)^{-1}) + O(N^{-3/2}\delta^{-2})$ and, consequently, from (24),

$$\begin{aligned}
&(\mathrm{RMSE}[h^{RFD}(N,\delta)])^2 \\
&= O(N^{-1}\delta^{-1}) + O(N^{-3/2}\delta^{-2}) + \left(\frac{J(\theta+\delta)-J(\theta)}{\delta} - J'(\theta) + O\left(\frac{1}{N\delta}\right)\right)^2 \\
&= O(N^{-1}\delta^{-1}) + O(N^{-5/2}\delta^{-2}) + \frac{1}{2}\left(J''(\theta)\delta + o(\delta) + O\left(\frac{1}{N\delta}\right)\right)^2.
\end{aligned}$$

Hence, $\mathrm{RMSE}[h^{RFD}(N,\delta)]$ converges at a rate at least $N^{-1/3}$ if we choose $\delta = cN^{-1/3}$. □

If

$$Var[a_1 \Delta h_1(\theta) + a_2 \Delta T_1(\theta) + a_3 h_1(\theta) + a_4 T_1(\theta)] = \lambda(\theta)(1+o(1))$$

and $\lambda(\theta) > 0$, then (24) and (25) show that the rate of $N^{-1/3}$ cannot be improved.

Unlike the cases examined in sections 3 and 4, CRN is always effective for improving the rates of convergence for regenerative ratio estimates. The reason is that, if the regenerative cycles are finite in up to the fourth moments, the effect of the small perturbation caused by δ is kept proportional to δ. It is also obvious from Lemma 5.1 and Theorem 3.4 that CRN is also effective for SD ratio estimates. In this case, CRN can increase the rate of convergence from $N^{-1/3}$ for independent simulation to $N^{-2/5}$.

Appendix. In this appendix, we outline an asymptotic expansion of

$$\frac{1}{N}Var\left[\sum_{n=1}^{N} F_n\right] \quad \text{and} \quad \frac{J(N,\theta+\delta)-J(N,\theta)}{\delta} - J'(\theta)$$

for the case examined in Example 3.1 (ii). We assume that $\delta > 0$ goes to zero when $N \to \infty$. In this example, $\tilde{P}(\theta,\delta)$ has four eigenvalues $\lambda_1 = 1-2\delta,\ \lambda_2 = 2\theta-1,$ $\lambda_3 = 2\theta-1-2\delta,\ \lambda_4 = 1.0$.

Define

$$T = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Then $T^{-1} = (1/4)T$ and

$$\tilde{P}(\theta,\delta) = T^{-1}\operatorname{diag}(\lambda_4,\lambda_1,\lambda_2,\lambda_3)T = \frac{1}{4}T\operatorname{diag}(\lambda_4,\lambda_1,\lambda_2,\lambda_3)T.$$

By solving the transition equation

$$\tilde{\pi}_\delta^{(n+1)} = \tilde{\pi}_\delta^{(n)}\tilde{P}(\theta,\delta),$$

we obtain

$$\tilde{\pi}_\delta^{(n)} = \tilde{\pi}_\delta^{(0)}\tilde{P}^n(\theta,\delta) = \tilde{\pi}_\delta + \tilde{\pi}_\delta^{(0)}D_1\operatorname{diag}(\lambda_1^n,\lambda_2^n,\lambda_3^n)D_2, \tag{26}$$

where $\tilde{\pi}_\delta = [0.25, 0.25, 0.25, 0.25]$ is the stationary distribution and

$$D_1 = \frac{1}{4}\begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}, \qquad D_2 = \begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Assume that $\tilde{\pi}_\delta^{(0)} = [1\ 0\ 0\ 0]$. With expression (26), we can directly calculate that

$$Cov[F_n, F_{n+j}] = \frac{1}{4}\theta^2(\theta-1)^2[(1-\lambda_1^n)(\lambda_2^j+\lambda_3^j) + (\lambda_2^n-\lambda_3^n)(\lambda_2^{n+j}-\lambda_3^{n+j})].$$

Therefore, omitting terms of higher order, we have

$$\sum_{n=1}^{N}\sum_{j=1}^{N-n} Cov[F_n,F_{n+j}] = \frac{1}{4}\theta^2(\theta-1)^2\left(\frac{\lambda_2}{1-\lambda_2}+\frac{\lambda_3}{1-\lambda_3}\right)\left[N-\frac{\lambda_1}{1-\lambda_1}(1-\lambda_1^N)\right].$$

Similarly,

$$\sum_{j=1}^{N} Var[F_n] = \frac{1}{2}\theta^2(\theta-1)^2\left[N-\frac{\lambda_1}{1-\lambda_1}(1-\lambda_1^N)\right].$$

Hence,

$$\begin{aligned}\frac{1}{N}Var\left[\sum_{n=1}^{N}F_n\right] &= \frac{1}{N}\sum_{j=1}^{N}Var[F_n] + \frac{2}{N}\sum_{n=1}^{N}\sum_{j=1}^{N-n}Cov[F_n,F_{n+j}] \\ &= \frac{1}{2}\theta^2(\theta-1)^2\left(\frac{1}{1-\lambda_2}+\frac{\lambda_3}{1-\lambda_3}\right)\left[1-\frac{\lambda_1}{N(1-\lambda_1)}(1-\lambda_1^N)\right] \\ &= \frac{1}{2}\theta^3(1-\theta)\left[1-\frac{1}{2N\delta}(1-(1-2\delta)^N)\right].\end{aligned}$$

Direct computation using (26) yields that, omitting terms of higher order,

$$J(N,\theta) = \frac{1}{2}(\theta + \theta^2) + \frac{\theta}{4N}.$$

and

$$\frac{J(N,\theta+\delta) - J(N,\theta)}{\delta} - J'(\theta) = \frac{\delta}{2} + \frac{1}{4N}.$$

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