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ACCELERATED CONVERGENCE IN THE SIMULATION OF COUNTABLY INFINITE-ETC(U)

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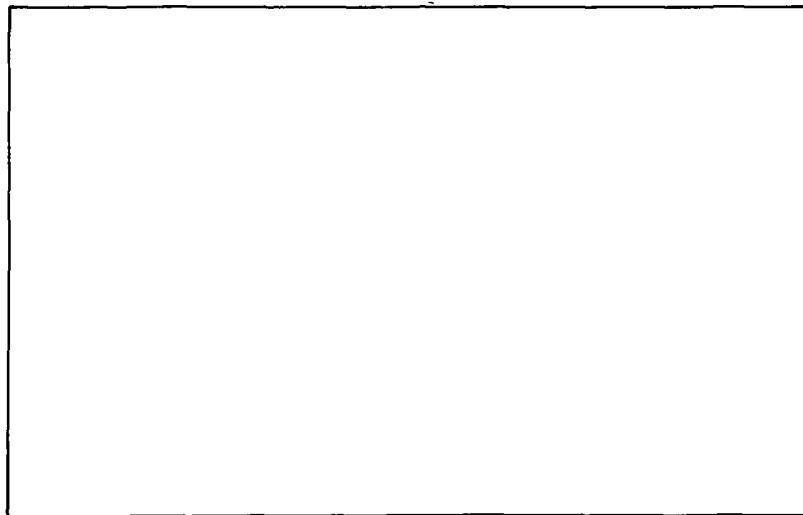
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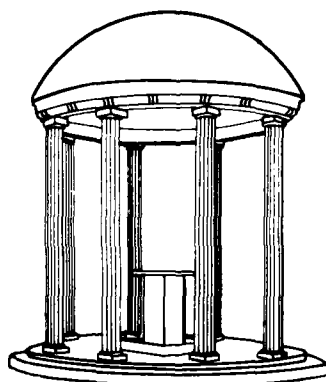
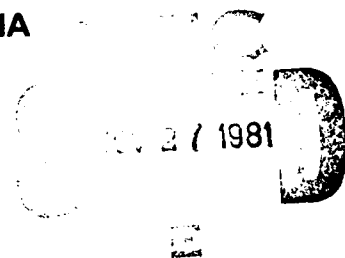
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ACCELERATED CONVERGENCE IN THE SIMULATION OF
COUNTABLY INFINITE STATE MARKOV CHAINS

George S. Fishman

Technical Report No. 81-4
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Curriculum in Operations Research
and Systems Analysis

University of North Carolina at Chapel Hill

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Acknowledgment

I wish to express my appreciation to Professor Louis R. Moore for many enlightening discussions on this topic.

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Abstract

This paper describes a method of obtaining results from the simulation of a countably infinite state positive recurrent aperiodic Markov chain at a cost considerably below the cost required to achieve the same accuracy with pure random sampling. By reorganizing k independent epochs or tours simulated serially into k replications simulated in parallel, one can induce selected joint distributions across replications that produce the cost-saving benefits. The joint distributions follow from the use of rotation sampling, a special case of the antithetic variate method. The chains considered are of the band type so that for the state space $S = (0, 1, 2, \dots)$ there exists an integer δ such that transition from a state i can move no further than to states $i - \delta$ and $i + \delta$.

The paper shows that an estimator of interest has variance bounded above by $O(\delta^2 (\ln k)^4 / k^2)$ when using rotation sampling, as compared to a variance $O(1/k)$ for independent sampling. Moreover, the mean cost of simulation based on rotation sampling has an upper bound $O((\delta \ln k)^2)$ as compared to at least $O(k)$ for independent sampling.

The paper also describes how one can exploit special structure in a model together with rotation sampling to improve the bound on variance for essentially the same mean cost.

KEYWORDS: Markov chains; rotation sampling; simulation; variance reduction.

Introduction

A recent paper (Fishman 1981) describes how one can use rotation sampling, a special case of the antithetic variate method, to induce substantial variance reduction in the simulation of a finite state Markov chain. Since many discrete event simulations have an underlying Markov structure or one close to being Markov, this variance reducing proposal has clear appeal. Moreover, for large and possibly ill-conditioned transition matrices, one may prefer the Monte Carlo or simulation method with appropriate variance reducing plans to numerical analysis when solving for steady-state and first passage time distributions. In fact, it may be the only feasible method for some problems. The present paper extends the earlier results for rotation sampling to Markov chains with countably infinite state space. Here the willingness to rely on the simulation method for solution increases because the convenience of an efficient computer code for matrix inversion is no longer a relevant issue.

The earlier work derived its cost-saving potential from viewing the simulation of k tours in *series* of a finite $(n+1)$ state positive recurrent aperiodic Markov chain as equivalent to the simulation of k replications of the Markov chain in *parallel*. Although the marginal distributions that arise with the two alternative formulations are necessarily the same for corresponding variables, the parallel formulation allows one to induce joint distributions across replications that lead to a significant cost saving. The induced joint distributions follow from

the use of rotation sampling, as described in detail in Fishman and Huang (1980). The cost saving arises in two ways. Firstly, for fixed n , run time in the correlated case is $O(\ln k)$ in contrast to $O(k)$ for the serial simulation. Secondly, for fixed n the variance of an estimator of interest has an upper bound $O((\ln k/k)^2)$ for the correlated case compared to $O(1/k)$ for the serial case.

In the present paper we replace the specification $n < \infty$ with the assumption that transition from a state can go to no more than $2\delta + 1$ states where δ is an integer. Then it is shown that the mean cost of simulation has an upper bound $O((\delta \ln k)^2)$ and the variance of the corresponding estimator has an upper bound $O(\delta^2 (\ln k)^4 / k^2)$. These results compare favorably with those using independent sampling to simulate the behavior of a Markov chain where mean cost is, at best, $O(k)$ and variance is proportional to $1/k$.

The paper also shows how one can combine rotation sampling with special structure in the chain to achieve additional variance reduction without any essential increase in cost. The relevance of this result becomes more apparent as the number of states occupied by the k parallel replications increases at a given step. The benefit is achieved by inducing an appropriate joint distribution for the transition paths of *all* replications from *all* states at each transition while preserving the correct marginal distribution for each replication. By contrast, in the earlier use of rotation sampling we preserved the marginal distributions

but merely induced an appropriate joint distribution for the transition paths of the replications in a given state on a given transition, leaving the sets of paths for different exited states conditionally independent.

Section 1 introduces the Markov chain notation. It also formulates the experiment as k independent tours where a tour begins with an exit from state 0 and ends upon first entry into state a . A reformulation in terms of k independent parallel tours or replications is presented and then extended to the case of k correlated replications using rotation sampling. Results for mean number of transitions, expected cost and variance are then derived. Section 2 derives the comparable results when combining rotation sampling with special structure. Section 3 demonstrates how the results apply to a simulation of a nearest neighbor Markov chain.

1. The Infinite State Chain

Consider a positive recurrent aperiodic Markov chain with state space $S = (0,1,2,\dots)$ and transition probabilities $\{p_{ij}; i,j = 0,1,\dots\}$ where there exists a positive integer δ such that

$$p_{ij} = 0 \quad \text{for } |i-j| > \delta$$

and

$$\sum_{j=\max(0,i-\delta)}^{i+\delta} p_{ij} = 1 \quad (1)$$

It is convenient to describe an alternative, but equivalent, representation to (1) whose value is apparent when actually generating sample paths by simulation on a computer. Let s_j denote the total number of states that have positive transition probabilities from state j and let $m_{jr}; r = 1, \dots, s_j$ denote the ordered sequence ($m_{jr} < m_{j,r+1}; r = 1, \dots, s_j - 1$) of the s_j states to which entry can occur from state j . Then one has the representation

$$p_{jm_{jr}} > 0 \quad r = 1, \dots, s_j$$

$$\sum_{r=1}^{s_j} p_{jm_{jr}} = 1$$

$$\delta \geq \max (|m_{j1} - j|, |m_{js_j} - j|) \quad j = 0, 1, \dots$$

Let A_{ij} denote the reward received when a jump occurs from state i to state j and assume for the moment that $|A_{ij}| \leq O(1)$. Suppose one wishes to estimate μ_{0a} , the mean reward received on a path begun with a departure from state 0 and terminated with the first entry into state a . If $N_{ij}^{(m)}$ gives the number of transitions from i to j on the m th of k independent replications and $S_a = S - a$, then

$$R_k = \frac{1}{k} \sum_{m=1}^k \sum_{i \in S_a} \sum_{j \in S} A_{ij} N_{ij}^{(m)} \quad (2)$$

is an unbiased estimator of μ_{0a} and $\text{var } R_k \propto 1/k$. Here each

replication begins with a departure from state 0 and ends upon entry into state a. To simulate this chain on a computer for k consecutive independent replications or epochs, one need only set $p_{a0} = 1$ and $p_{aj} = 0$ for $j = 1, 2, \dots$.

Let T_k denote the number of transitions in k epochs. Clearly $E T_k = O(k)$. Let S_k denote the cost of simulating k replications in series. In the case of (1) with a finite state space of $n + 1$, one has $O(k) \leq E S_k \leq O(\delta k)$. The lower bound applies if one can store all the distributions and the *aliases* required to use the alias method of Walker (1977). Also see Kronmal and Peterson (1979). As n increases the feasibility of this approach diminishes. The upper bound $O(\delta k)$ results from application of the inverse transform method to determine the branch taken from each state. Since in the infinite state case one can conceive of using the alias method for a finite set of commonly entered states and the inverse transform method for less frequented states, taking $E S_k \geq O(k)$ is a useful bound for comparative purposes.

Consider simulating the Markov chain with replications executed in parallel. Simulation begins with an exit of all k replications from state 0. Then one sets $p_{aa} = 1$ and $p_{aj} = 0$ $j \in S_a$, if state a is to be absorbing state. Note that the chain is absorbing with S_a a transient set of states. The simulation ends with the entry of the last of the k replications into state a. Let K_{ijl} denote the number of

independent replications that move from i to j on transition ℓ and let $K_{j\ell}$ denote the number of replications in state j after transition ℓ . Then

$$\dot{R}_k = \frac{1}{k} \sum_{\ell=1}^{\infty} \sum_{i,j \in S} A_{ij} K_{ij\ell}$$

is an unbiased estimator of μ_{0a} with $\text{var } \dot{R}_k = \text{var } R_k$. Note that

$$\sum_{\ell=1}^{\infty} \sum_{i,j \in S} K_{ij\ell} = \sum_{m=1}^k \sum_{i \in S_a} \sum_{j \in S} N_{ij}^{(m)}. \quad (3)$$

Let

$$\dot{T}_k = \min (\ell: K_{a\ell} = k).$$

From Theorem 1 of Fishman (1981), one has $E \dot{T}_k^2 \leq O(k)$. Now one easily sees that at transition ℓ no more than $\min(k, \delta\ell)$ states are occupied. Therefore, no more than $\delta t(t+1)/2$ states are occupied in t transitions and the expected number of occupied states has upper bound $\frac{\delta}{2} \cdot (E \dot{T}_k^2 + E \dot{T}_k) \leq O(\delta k)$. Let $\dot{S}_k$ denote the cost of simulating k independent replications in parallel and note that no more than $2\delta + 1$ states can be entered from a given state. If one uses a sampling program as in Ahrens and Dieter (1979) or in Fishman (1979), which have bounded computation times, to generate

the binomial variates $K_{jm_{jr}^\ell}$ for $j \in S$, $r = 1, \dots, s_j$ and $\ell = 1, 2, \dots$, then

$$E \dot{S}_k \leq O(\ell^2 k) \quad .$$

This observation is peripheral to our main interest and we merely mention it for completeness.

Once the replications are to be run in parallel an opportunity exists to induce a desirable form of correlation across replications while preserving the required distributional behavior along the sample path of each replication. Define

$$q_{jw} = \sum_{r=1}^w p_{jm_{jr}} \quad w = 1, \dots, s_j ; j = 0, 1, \dots \quad (4)$$

Let $U, U_1, \dots, U_{K_{j\ell}}$ be i.i.d. random variables from $U(0,1)$ where $K_{j\ell} > 0$ is given. Then for parallel replications one has

$$K_{jm_{jr}^{\ell+1}} = \sum_{m=1}^{K_{j\ell}} I_{[q_{j,r-1}, q_{jr})}(U_m) \quad (5)$$

where

$$q_{j0} \equiv 0$$

and

$$\begin{aligned} I_{[u,v)}(x) &= 1 & u \leq x < v \\ &= 0 & \text{otherwise} \quad . \end{aligned}$$

Observe that on each transition (ℓ) a Bernoulli trial determines the path that each replication follows, independent of the paths of other replications. Moreover, $\text{var}(K_{jm_{jr}\ell+1}|K_{j\ell}) = K_{j\ell} p_{jm_{jr}} (1 - p_{jm_{jr}})$. Although the Bernoulli property must be maintained to assure that the sample paths for each replication follows the correct probability law, the independence across replications is but a consequence of the independence of $U_1, \dots, U_{K_{j\ell}}$. Hereafter we use a prime superscript $(')$ to denote parallel correlated replications.

Suppose that for $r = 1, \dots, K'_{j\ell}$

$$\begin{aligned} U_m &= U + \frac{r-1}{K'_{j\ell}} & U < 1 - \frac{r-1}{K'_{j\ell}} \\ &= 1 + \frac{r-1}{K'_{j\ell}} - 1 & \text{otherwise} \end{aligned} \quad (6a)$$

so that

$$K'_{jm_{jr}\ell+1} = \sum_{m=1}^{K'_{j\ell}} I_{[q_{j,r-1}, q_{jr})}(U_m) \quad r=1, \dots, s_j. \quad (6b)$$

We refer to this representation as *rotation sampling*. See Fishman and Huang (1980). Using the notation $\bar{x} \equiv x \pmod{1}$ and $[x] = x - \bar{x}$, one then has from Theorem 5 in Fishman (1981):

(i) For $r = 1, \dots, s_j$

$$\begin{aligned} K'_{jm_{jr}^{l+1}} &= [Q] - [P] - 1 && \text{w.p. } \max(\bar{P}, \bar{Q}) - \bar{Q} \\ &= [Q] - [P] && \text{w.p. } 1 - \max(\bar{P}, \bar{Q}) + \min(\bar{P}, \bar{Q}) \\ &= [Q] - [P] + 1 && \text{w.p. } \max(\bar{P}, \bar{Q}) - \bar{P} \end{aligned} \quad (7a)$$

where $P \equiv K'_{j\ell} q_{j,r-1}$, $Q \equiv K'_{j\ell} q_{jr}$.

$$(ii) \quad \text{var}(K'_{jm_{jr}^{l+1}} | K'_{j\ell}) = \overline{(K'_{j\ell} p_{jm_{jr}})} (1 - \overline{K'_{j\ell} p_{jm_{jr}}}) \leq 1/4.$$

$$(iii) \quad \text{var } K'_{jm_{jr}^{l+1}} = O(1).$$

Since only two of the three outcomes in (i) have positive probability at a time, $K'_{jm_{jr}^{l+1}}$ has the Bernoulli property. Most importantly, note in (ii) that the variance is independent of $K'_{j\ell}$, in contrast to the linear dependence on $K_{j\ell}$ in the case of independent replications. Also, the required Bernoulli property for each replication is preserved.

As an alternative to (6b), (i) enables one to write for $r = 1, \dots, s_j$

$$\begin{aligned} K'_{jm_{jr}^{l+1}} &= [Q] - [P] + I_{[\bar{P}, \bar{Q})}(U) && \bar{P} \leq \bar{Q} \\ &= [Q] - [P] - I_{[\bar{Q}, \bar{P})}(U) && \bar{P} > \bar{Q}. \end{aligned} \quad (7b)$$

This expression is considerably more efficient to use than (6b) is in practice for its cost depends only on the number of occupied states and not on the number of nonabsorbed replications. Hereafter, we assume that (7b) is used.

Let

$$R'_{k\ell} = \sum_{j,m \in S} A_{jm} K'_{jm\ell} \quad (8a)$$

$$R'_k = \frac{1}{k} \sum_{\ell=1}^{\infty} R'_{k\ell} \quad (8b)$$

Here $R'_{k\ell}$ denotes the sample contribution to reward on transition ℓ . Using the results in (7) one can easily show that $\text{var } R'_{k\ell} \leq O(\delta^2 \ell^2)$, which is independent of k . In the case of a finite state space Fishman (1981), shows that for $T'_k = \min(t: K'_{at} = k)$ and cost S'_k $E T'_k \leq E S'_k \leq O(\ln k)$ and $\text{var } R'_k \leq O((\ln k/k)^2)$. However, one cannot carry over these results directly for the case of an unbounded state space. Before deriving the corresponding results for this case, we study an interesting property of T'_k which holds for both finite and infinite state models. Because of the restrictions on the p_{ij} 's, at most $\delta + \min(a, \delta)$ transient states have nonzero entries on transition $T'_k - 1$. In fact, absorption can occur only when all the nonzero entries are in states $a - \min(a, \delta), \dots, a-1$ and $a+1, \dots, a+\delta$ in the way specified in Lemma 1.

Lemma 1. In order for total absorption to occur on transitions $\ell+1, \ell+2, \dots$, necessary and sufficient conditions at the end of transition ℓ are

$$(a) \quad K'_{j\ell} = 0 \qquad |j - a| > \delta$$

$$(b) \quad K'_{j\ell} \leq 1/(1 - p_{ja}) \qquad |j - a| \leq \delta.$$

Proof. Condition (a) is a consequence of $p_{ja} = 0$ for $|j-a| > \delta$. For part (b) we note that total absorption using rotation sampling implies

$$K'_{ja,\ell+1} = [K'_{j\ell} p_{ja}] + 1 = K'_{j\ell} \qquad |j - a| \leq \delta.$$

For a specific j this occurs with positive probability if and only if $K'_{j\ell} \leq 1/(1-p_{ja})$.

Lemma 1 provides the basis for an initial characterization of absorption time in Lemma 2.

Lemma 2. Let $k > 1/(1-\alpha)$ where $\alpha = \sup_{j \in S_a} p_{ja}$.

Let

$$T_k^* = \min(\ell: \text{conditions (a) and (b) of Lemma 1 obtain})$$

and

$$Y_k = T'_k - T_k^* .$$

Then

- (i) $E T'_k = E T_k + E Y_k .$
- (ii) Y_k is independent of k .

Proof. Part (i) follows by inspection. Part (ii) makes use of the fact that since all $K'_{j\ell} \leq 1/(1-\alpha) < k$ for $\ell = T_k^* + 1, T_k^* + 2, \dots$, then the remaining time to absorption Y_k must be independent of k . In effect, rotation sampling is nonoperative for $t > T_k^*$.

Theorem 1 provides a more comprehensive characterization of absorption time T'_k .

Theorem 1. Let

$p_{ij}^{(\ell)}$ = probability of moving from i to j in ℓ steps.

$$M_{ij\ell} = K'_{tj\ell} - K'_{i,\ell-1} p_{ij} .$$

Then

$$(i) \quad K'_{jt} = k p_{0j}^{(t)} + Z_{jt}$$

where

$$Z_{jt} = \sum_{i \in S_a} M_{ijt} + \sum_{\ell=1}^{t-1} \sum_{i, m \in S_a} M_{im\ell} p_{mj}^{(t-\ell)} \quad j \in S_a$$

and

$$K'_{at} = k(1 - \sum_{\ell=1}^t p_{0a}^{(\ell)}) + Z_{at}$$

where

$$Z_{at} = \sum_{m \in S_a} M_{mat} + \sum_{\ell=1}^{t-1} \sum_{i, m \in S_a} M_{im\ell} \left(1 - \sum_{r=1}^{t-\ell} p_{ma}^{(r)}\right).$$

$$(ii) \quad T'_k = O(\ln k) \text{ w.p.1.}$$

$$(iii) \quad E(T'_k)^r = O((\ln k)^r) \quad r = 1, 2, \dots$$

See the Appendix for proof.

Theorem 2 shows the benefit of rotation sampling for the representation in (1).

Theorem 2. For the simulation of a Markov chain as in (1) using rotation sampling as in (6a) and (7b):

$$(i) \quad E S'_k \leq O((\delta \ln k)^2).$$

$$(ii) \quad \text{var } R'_k \leq O(\delta^2 (\ln k)^4 / k^2).$$

$$(iii) \quad V(R_k, R'_k) = \frac{E S_k \cdot \text{var } R_k}{E S'_k \cdot \text{var } R'_k} \geq O(k^2 / \delta^4 (\ln k)^6).$$

See the Appendix for the proof. The expression $V(R_k, R'_k)$ gives a measure of the relative efficiency of rotation sampling based on (7b) as compared to independently sampled replications for simulating the chain (1).

It is of interest to compare these results with those in Fishman (1981) for an $n + 1$ state chain. Although those results hold for the absorbing state $a = 0$, they also apply, with minor adjustment, more generally. In particular, $E S'_k \leq O(n^2 \ln k)$ and $\text{var } R'_k \leq O((n \ln k)^2/k^2)$. These are consistent with (i) and (ii) of Theorem 2 when one notes that the mean number of transient states entered has an upper bound $\min(O(n \ln k), O(\delta(\ln k)^2))$ and the number of states to which a transition can occur has an upper bound $\min(n+1, 2\delta+1)$.

Although the results for $\text{var } R'_k$ hold for bounded $\{A_{ij}\}$, the results for the variance reduction measure $V(R_k, R'_k)$ and the absorption time T'_k apply more generally. For example, the relative desirability of the proposed sampling plan continues to grow with k for the family of reward functions $\{A_{ij} = c_0 + \sum_{\ell=1}^P (c_\ell i^\ell + d_\ell j^\ell)\}$. Section 2 uses a reward function of this type to show how one can achieve additional variance reduction.

2. Exploiting Special Structure

Although Theorem 2 shows that for large k rotation sampling offers a clear advantage over independent serial replications, the factors δ^2 and $(\ln k)^4$ in the bound on $\text{var } R'_k$ are sufficiently broad to make one look for improved convergence for moderate k . Consider the sampling at transition ℓ . Recall that rotation sampling applies to the $K'_{j\ell}$ transitions from state j , but transitions from different states are independent, given $\{K'_{j\ell}; j \in S_a\}$. We now describe how a modification of this independent sampling can

for special cases of $\{A_{jm}; j, m = 0, 1, 2, \dots\}$ lead to a considerable reduction in variance. Theorem 3 provides the basis for the approach.

Theorem 3. Let

$$\begin{aligned}
 0 &< p_i < 1 \\
 q_{-1} &= 0 \\
 q_i &= q_{i-1} + p_i & i = 0, 1, \dots \\
 x_i &= I_{[\bar{q}_{i-1}, \bar{q}_i)}(U) & \text{if } \bar{q}_{i-1} \leq \bar{q}_i \\
 &= 1 - I_{[\bar{q}_i, \bar{q}_{i-1})}(U) & \text{if } \bar{q}_{i-1} > \bar{q}_i \\
 Y_s &= \sum_{i=0}^s x_i & s = 1, 2, \dots
 \end{aligned} \tag{9}$$

where $U \sim U(0, 1)$. Then

$$\begin{aligned}
 \text{(i)} \quad Y_s &= \lfloor q_s \rfloor + I_{[0, \bar{q}_s)}(U) & s = 1, 2, \dots \\
 \text{(ii)} \quad Z_{s,t} &= Y_t - Y_s = \lfloor q_t \rfloor - \lfloor q_s \rfloor + J_{s,t}(U) & t > s
 \end{aligned}$$

where

$$\begin{aligned}
 J_{s,t}(U) &= I_{[\bar{q}_s, \bar{q}_t)}(U) & \text{if } \bar{q}_s \leq \bar{q}_t \\
 &= -I_{[\bar{q}_t, \bar{q}_s)}(U) & \text{if } \bar{q}_s > \bar{q}_t
 \end{aligned}$$

See the Appendix for the proof. The significance of this result becomes apparent shortly.

Consider a Markov chain for which $s_0 = s_1 = \dots = 2$ so that one has

$$R'_{k,l+1} = \sum_{j \in S_a} (B_j K'_{jm_{j1}l+1} + A_j K'_{jl}) \quad (10)$$

where $A_j = A_{jm_{j2}}$ and $B_j = A_{jm_{j1}} - A_{jm_{j2}}$ for $j = 0, 1, \dots$ and

$B_{-1} = 0$. Recall that

$$K'_{jm_{j1}l+1} = [K'_{jl} p_{jm_{j1}}]^J + I_{[0, p_j)}(U_j),$$

where $p_j = \frac{K'_{jl}}{K'_{jl} p_{jm_{j1}}}$ and $U_0, U_1, U_2, \dots$ are i.i.d. from $U(0,1)$, so

that

$$R'_{k,l+1} = C_l + \sum_{j \in S_a} B_j I_{[0, p_j)}(U_j) \quad (11)$$

where

$$C_l = \sum_{j \in S_a} (B_j [K'_{jl} p_{jm_{j1}}]^J + A_j K'_{jl}).$$

Let

$$j_l^* = \max(j: K'_{jl} > 0).$$

Then from Theorem 1

$$\text{var}(R'_{k,\ell+1} | K'_{j\ell} \quad j \in S_a) \leq \frac{1}{4} \sum_{j=0}^{j_\ell^*} B_j^2. \quad (12)$$

Now one can write (11) equivalently as

$$R'_{k,\ell+1} = C_\ell + \sum_{j=0}^{j_\ell^*} (B_j - B_{j-1}) \sum_{m=j}^{j_\ell^*} I_{[0,p_m)}(U_m) \quad (13)$$

where one should note that

$$\begin{aligned} I_{[0,p_m)}(U_m) &= I_{[\bar{q}_{m-1}, \bar{q}_m)}(U_m) && \text{if } \bar{q}_{m-1} \leq \bar{q}_m \\ &= 1 - I_{[\bar{q}_m, \bar{q}_{m-1})}(U_m) && \text{if } \bar{q}_{m-1} > \bar{q}_m. \end{aligned} \quad (14)$$

As an alternative to i.i.d. $U_0, U_1, \dots$, set $U_0 = U_1 = \dots = U$ where $U \sim U(0,1)$. From Theorem 3, one has (13) as

$$R'_{k,\ell+1} = C_\ell + \sum_{j=0}^{j_\ell^*} (B_j - B_{j-1}) [Lq_{j_\ell^*} - Lq_{j-1} + J_{j-1, j_\ell^*}(U)] \quad (15)$$

Now observe that

$$\text{var}(R'_{k,\ell+1} | K'_{j\ell} \quad j \in S_a) \leq \frac{1}{4} \left[\sum_{j=0}^{j_\ell^*} |B_j - B_{j-1}|^2 \right], \quad (16)$$

which is to be compared with (12). However, a more appealing case exists. If for $j = 0, 1, \dots$ either $B_j \geq B_{j-1}$ or $B_j \leq B_{j-1}$, then one has

$$\text{var}(R'_{k, \ell+1} | K'_{j\ell} \quad j \in S_a) \leq B_{j\ell}^{2*}/4.$$

As an example, consider the reward

$$A_{jm_{jr}} = c_1 j + c_2 m_{jr} + c_3.$$

Then

$$B_j = A_{jm_{j1}} - A_{jm_{j2}} = c_2(m_{j1} - m_{j2})$$

so that (15) has for either $m_{j1} > m_{j2}$ or $m_{j1} < m_{j2}$ for $j = 0, 1, \dots$

$$\text{var}(R'_{k, \ell+1} | K'_{j\ell} \quad j \in S_a) \leq [c_2 (m_{j\ell}^{*1} - m_{j\ell}^{*2})/2]^2 \leq [c_2(2\delta + 1)/2]^2 = O(\delta^2)$$

whereas (11), based on independent $U_0, U_1, \dots$, has

$$\text{var}(R'_{k, \ell+1} | K'_{j\ell} \quad j \in S_a) \leq \frac{c_2^2}{4} \sum_{j=0}^{j_\ell^*} (m_{j1} - m_{j2})^2 \leq O(\delta^2 j_\ell^* + 1)^2.$$

The extent to which one can exploit special structure for more general $\{A_{jm_jr} : r=1, \dots, s_j; s_j=2 \ j=0,1, \dots\}$ and for the case $\{s_j \geq 2\}$ remains a topic for future research.

3. An Illustration

This section describes a simulation designed to show how the theoretical results of Sections 1 and 2 fare in practice. Consider a single server queueing system with independent and identically distributed exponential interarrival times with rate λ , independent and identically distributed exponential service times with rate $\omega > \lambda$ and infinite capacity. As an alternative to this continuous time representation one can view this system as a nearest neighbor Markov chain with $p_{j,j-1} = \omega/(\lambda+\omega)$ $j = 1,2, \dots$. Here $\delta = 1$, $s_j = 2$ for $j = 1,2, \dots$ and the absorbing state is $a = 0$.

The objective is to estimate the mean number of customers in system, $\mu = \lambda/(\omega-\lambda)$ (e.g. see Gross and Harris 1974, p. 67). In the serial model we estimate this quantity by

$$\hat{\mu}_k = \frac{\frac{1}{k} \left[\frac{1}{\lambda+\omega} \sum_{m=1}^k \sum_{j=1}^{\infty} j(N_{j,j-1}^{(m)} + N_{j,j+1}^{(m)}) \right]}{\frac{1}{k} \left[\frac{k}{\lambda} + \frac{1}{\lambda+\omega} \sum_{m=1}^k \sum_{j=1}^{\infty} (N_{j,j-1}^{(m)} + N_{j,j+1}^{(m)}) \right]} \quad (17)$$

In the parallel model using rotation sampling we estimate μ by

$$\mu'_k = \frac{\frac{1}{k} \left[\frac{1}{\lambda + \omega} \sum_{\ell=1}^{T'_k} \sum_{j=1}^{\infty} 1(K'_{j,j-1,\ell} + K'_{j,j+1,\ell}) \right]}{\frac{1}{k} \left[\frac{k}{\lambda} + \frac{1}{\lambda + \omega} \sum_{\ell=1}^{T'_k} \sum_{j=1}^{\infty} (K'_{j,j-1,\ell} + K'_{j,j+1,\ell}) \right]} \quad (18)$$

Note that (17) and (18) are *ratio* estimators in contrast to (2) and (8b) which are *linear* estimators. As a result, (17) and (18) are biased estimators of μ . Therefore, our evaluation focuses on mean-square error rather than on variance alone. The motivation for considering ratio estimators arises from the observations that they commonly arise in regenerative simulation.

For convenience and without loss of generality we set $\omega = 1$. Table 1 gives the number of independent macroreplications performed for each value of k and experimental layout (ρ). Table 2 presents

Table 1
Experimental Layout
($k = 2^m$)

$\rho = \lambda/\omega$	Number of Macroreplications	
	1000	100
0.5	$m = 1, \dots, 11$	$m = 12, \dots, 14$
0.9	$m = 1, \dots, 11$	$m = 12, \dots, 14$

ratios of interest. Here c_i and MSE_i denote the CPU time and mean-square error for model i where $i = 1$ denotes k independent tours in series, $i = 2$ denotes parallel replication with (7b) and $i = 3$ denotes parallel replication using (7b) and (14).

For $\rho = 0.5$ Table 1 reveals that $k = 16$ is the first sample size that gives benefits for both models 2 and 3. Also, note the strong favorable performance for $k \geq 256$. For $\rho = 0.9$ the benefits of both models 2 and 3 do not arise until $k = 1024$. The behavior thereafter shows substantive variance reduction. In presenting results for small values of k we merely sought to provide a comprehensive picture of how the models behaved. In practice one normally would expect to use a considerably larger k so that the risk of an unfavorable variance reduction is small. Since limited time was spent on the computer code for models 2 and 3, one also suspects that careful attention to programming efficiency would move the indifference points to smaller values of k for both $\rho = 0.5$ and 0.9 .

Table 2
Simulation Results for Example

k	$\rho=0.5$		$\rho=0.9$	
	$\frac{c_1 \cdot \text{MSE}_1}{c_2 \cdot \text{MSE}_2}$	$\frac{c_1 \cdot \text{MSE}_1}{c_3 \cdot \text{MSE}_3}$	$\frac{c_1 \cdot \text{MSE}_1}{c_2 \cdot \text{MSE}_2}$	$\frac{c_1 \cdot \text{MSE}_1}{c_3 \cdot \text{MSE}_3}$
	(1)	(2)	(3)	(4)
2	.50	.54	.18	.22
4	.58	.44	.22	.20
8	.83	.67	.23	.19
16	1.30	1.00	.17	.28
32	1.32	2.07	.22	.25
64	2.23	3.69	.29	.33
128	4.53	5.82	.33	.42
256	7.70	14.71	.42	.67
512	16.46	32.06	.54	1.40
1024	37.99	64.38	1.00	2.07
2056	71.32	174.11	1.95	4.59
4096	230.02	583.63	3.70	10.38
8192	451.79	1476.74	4.98	22.70
16384	696.20	3783.70	15.46	42.82
32768	2366.17	10280.72	17.42	63.00
65536	8526.68	22743.06	37.21	143.30

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Appendix

Proof of Theorem 1 (i) comes from applying rotation sampling to k replications in state $j = 0$ on transition $\ell = 1$, then applying it to each K'_{j2} for states $j = 0, \dots, \delta$ on transition $\ell = 2$, etc. One then regroups the resulting terms to give $\{K'_{jt}, j \in S\}$.

For (ii) note that

$$|M_{ij\ell}| \leq 1 \quad i \in S_a \quad j \in S$$

$$\sum_{i \in S_a} \sum_{j \in S} M_{ij\ell} = 0$$

$$E Z_{jt} = 0$$

$$-k p_{0j}^{(t)} \leq Z_{jt} \leq k(1 - p_{0j}^{(t)}) \quad j \in S_a$$

and

$$-k(1 - \sum_{\ell=1}^t p_{0a}^{(\ell)}) \leq Z_{at} \leq k \sum_{\ell=1}^t p_{0a}^{(\ell)}.$$

Most importantly, observe that Z_{jt}/k does not depend on k . Also, one has

$$T'_k = \min [t: Z_{at} = -k(1 - \sum_{\ell=1}^t p_{0a}^{(\ell)})].$$

Now for the absorbing state there exists $\rho \in (0,1)$ such that

$$1 - \sum_{i=1}^i p_{0a}^{(\ell)} = O(\rho^t)$$

so that

$$\begin{aligned} T'_k &= \min[t: \ln O(\rho^t) = \ln(-Z_{at}) - \ln k] \\ &= \min[t: t \ln O(\rho^{-1}) = -\ln(-Z_{at}) + \ln k] \end{aligned}$$

from which it is clear that $T'_k = O(\ln k)$ w.p.1. (iii) is a direct consequence of (ii) and is relevant when deriving $\text{var } R'_k$.

Proof of Theorem 2. Recall that no more than $\delta \ell$ steps are visited at transition ℓ and no more than $\delta t(t+1)/2$ are visited in t transitions. Also, at state j one needs to determine which of the $2\delta + 1$ possible states are entered by the $K'_{j\ell}$ replications at transition $\ell + 1$. Using (iii) of Theorem 1 gives

$$E S'_k \leq \frac{1}{2} (2\delta + 1)\delta E[T'_k(T'_k + 1)] \leq O((\delta \ln k)^2),$$

which proves (i).

For (ii), observe that

$$K'_{ij\ell} = k p_{0i}^{(\ell-1)} p_{ij} + W_{ij\ell}$$

where

$$W_{ijl} = Z_{i,l-1} - r_{ijl} + I_{[0, r_{ijl})}(U_{il})$$

$$r_{ijl} = (k p_{0i}^{(l-1)} + Z_{i,l-1}) p_{ij}$$

and U_{il} is the uniform deviate used to determine paths from state i on transition l . Note that $E W_{ijl} = 0$ and more generally that, like $Z_{i,l-1}$, W_{ijl} is not a function of the magnitude of k . Recall that

$$\text{var } R'_{kl} \leq O(\delta^2 l^2) .$$

Now, one can write

$$R'_{kl} = \sum_{i \in S_a} \sum_{j \in S} A_{ij} (k p_{0i}^{(l-1)} p_{ij} + W_{ijl})$$

and

$$\text{var } R'_k = E_{T'_k} \text{var}(R'_k | T'_k) + E_{T'_k} H_{T'_k}^2$$

where

$$H_{T'_k} = \frac{1}{k} \sum_{i \in S_a} \sum_{j \in S} \sum_{l=1}^{T'_k} E(W_{ijl} | T'_k) .$$

Since

$$\text{var}(R'_{kl} | T'_k) \leq O((\delta T'_k)^2)$$

and

$$k |H_{T'_k}| \leq O(\delta (T'_k)^2)$$

one has

$$k^2 \text{var}(R'_k | T'_k) \leq O(\delta^2 (T'_k)^4)$$

$$k^2 H_{T_k}^2 \leq O(\delta^2 (T'_k)^4)$$

so that

$$k^2 \text{var} R'_k \leq O(\delta^2 (\ln k)^4) .$$

Part (iii) follows by substitution.

Proof of Theorem 3. Clearly $X_i \sim \text{Ber}(p_i)$ $i = 1, \dots, m$. Let $r = \lfloor q_s \rfloor$.

Let $i_1, \dots, i_r$ denote the indices at which $\bar{q}_{i_t} < \bar{q}_{i_t-1}$ for $t = 1, \dots, r$.

Then one can represent Y_s as

$$Y_s = \sum_{t=1}^r \{ [1 - I_{[\bar{q}_{i_t}, \bar{q}_{i_t}-1]}(U)] + \sum_{\substack{i=1 \\ i \neq i_t}}^s I_{[\bar{q}_{i-1}, \bar{q}_i)}(U) \} .$$

Now straightforward evaluation gives (i) so that $Y_s - \lfloor q_s \rfloor \sim \text{Ber}(\bar{q}_s)$.

In particular, $\text{var} Y_s = \bar{q}_s(1 - \bar{q}_s) = O(1)$.

For part (ii) we have

$$Y_{s_2} - Y_{s_1} = \lfloor q_{s_2} \rfloor - \lfloor q_{s_1} \rfloor + I_{[0, \bar{q}_{s_2})}(U) - I_{[0, \bar{q}_{s_1})}(U)$$

Since

$$\begin{aligned}
 I_{[0, \bar{q}_{s_2})}(U) - I_{[0, \bar{q}_{s_1})}(U) &= I_{[\bar{q}_{s_1}, \bar{q}_{s_2})}(U) && \text{if } \bar{q}_{s_2} \geq \bar{q}_{s_1} \\
 &= -I_{[\bar{q}_{s_2}, \bar{q}_{s_1})}(U) && \text{if } \bar{q}_{s_2} < \bar{q}_{s_1} .
 \end{aligned}$$

(ii) obtains .

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case of the antithetic variate method. The chains considered are of the band type so that for the state space $S = (0,1,2,\dots)$ there exists an integer δ such that transition from a state i can move no further than to states $i - \delta$ and $i + \delta$.

The paper shows that an estimator of interest has variance bounded above by $O(\delta^2(\ln k)^4/k^2)$ when using rotation sampling, as compared to a variance $O(1/k)$ for independent sampling. Moreover, the mean cost of simulation based on rotation sampling has an upper bound $O((\delta \ln k)^2)$ as compared to at least $O(k)$ for independent sampling.

The paper also describes how one can exploit special structure in a model together with rotation sampling to improve the bound on variance for essentially the same mean cost.

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