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VARIANCE REDUCTION TECHNIQUES FOR THE SIMULATION OF MARKOV PROC--ETC(U)
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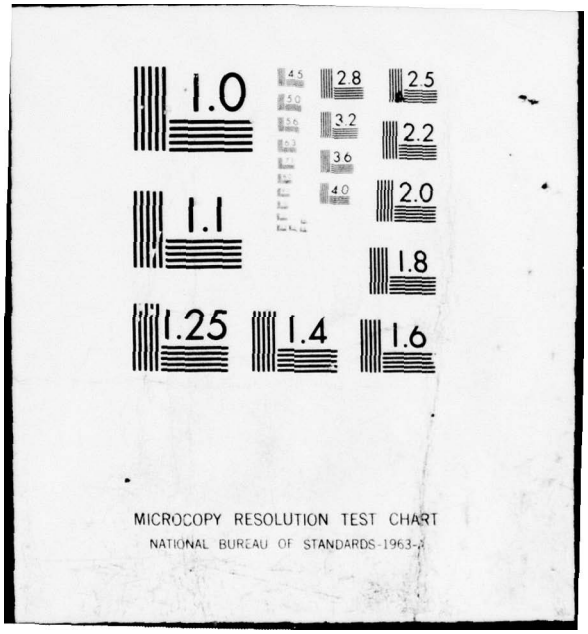
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(6) VARIANCE REDUCTION TECHNIQUES FOR THE SIMULATION OF MARKOV PROCESSES, III. INCREASING THE FREQUENCY OF REGENERATIONS.

by

(10) Philip Heidelberger*

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1. Introduction

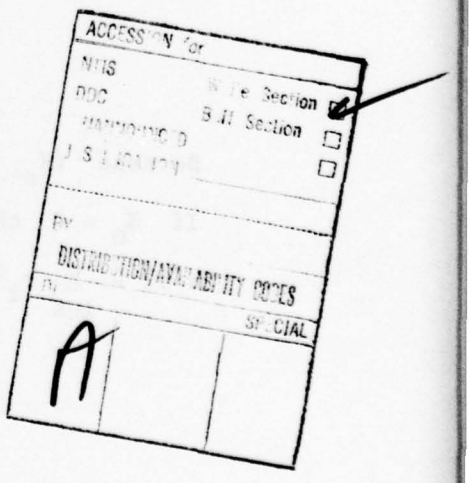
In this paper we consider a class of methods which are designed to increase the computational efficiency of computer simulations. This increased efficiency is obtained by simulating a stochastic process which is related to, but different from, the stochastic process of interest. Each event in the new process will correspond to several events in the original process. The simulation of this new process will then, in some sense, proceed at a faster rate than that of the original process.

The types of processes for which this technique may be applied are positive recurrent Markov chains in both discrete and continuous time as well as semi-Markov processes. These are all examples of regenerative processes (see Çinlar (1975) or Crane and Iglehart (1975)), and the method to be proposed relies heavily on this fact. Under the regenerative assumption a single simulation run may be broken up into randomly spaced i.i.d. (independent and identically distributed) blocks, or cycles. This allows the techniques of classical statistics to be applied in analyzing the output of the simulation.

One of the main difficulties with regenerative simulations is that even though it may be known that the process being simulated is regenerative, the regenerations may be few and far between. Thus even for very long simulation runs, only a relatively few i.i.d. cycles are observed. In this case it becomes difficult to form reliable point and interval estimates. One possible remedy to this problem is the use of approximate

regenerations (see Crane and Iglehart (1975a) or Gunther (1975)). The idea here is to break the simulation run up into blocks which are "almost" i.i.d. by defining a sequence of "almost" regenerations. These blocks are then treated as if they are i.i.d. (although they are not). Since "almost" regenerations are defined so that they occur more frequently than actual regenerations, one obtains more blocks using the approximation than is otherwise possible. Presumably this facilitates the formation of point and interval estimates, although this has never been demonstrated satisfactorily. Because this method lacks a strong theoretical foundation, it should be used with caution.

The method proposed here also seeks to increase the number of blocks obtained during a simulation, but does so without resorting to any approximations. Instead, a new Markov chain is simulated for which regenerations occur more often than for the original chain. This new chain is constructed in such a way that point estimates and confidence intervals may still be formed for certain parameters of the original chain.



2. Derivation of the Modified Markov Chain

We now state this basic problem. Let $\{X_n, n \geq 0\}$ be an irreducible, aperiodic, positive recurrent Markov chain with state space $E = \{0,1,2,\ldots\}$ and transition matrix $P = \{p_{ij} : i,j \in E\}$. It is then well known that there exists a probability distribution $\pi = \{\pi_i : i \in E\}$ on E and a random variable X, having distribution π, such that $X_n \Rightarrow X$ ($\Rightarrow$ denotes weak convergence). π is called the stationary distribution of the process and is usually unknown or difficult to calculate. Let f be a real valued function on E and define $r = \pi f = E[f(X)] = \sum_{i \in E} \pi_i f(i)$. We shall be interested in estimating r.

Pick some state, say 0, in E and let $T_0 = 0$. Define

$$T_m = \inf\{n > T_{m-1} : X_n = 0\}, \qquad m \geq 1.$$

We say that a regeneration occurs at time T_m and the time between T_{m-1} and $T_m - 1$ is referred to as the mth cycle. If $\tau_m = T_m - T_{m-1}$, then τ_m is the length of the mth cycle. Let

$$Y_m = \sum_{n=T_{m-1}}^{T_m - 1} f(X_n), \qquad m \geq 1.$$

Because $\{X_n, n \geq 0\}$ is positive recurrent $E_i[\tau_m] = E[\tau_m | X_0 = i] < \infty$. If $X_0 = 0$ then $\{(Y_m, \tau_m), m \geq 1\}$ are i.i.d. It is also known that if $\pi|f| = \sum_{i \in E} \pi_i |f(i)| < \infty$, then

(2.1) $$r = E_0[Y_m]/E_0[\tau_m]$$

(see Crane and Iglehart (1975)). Let

$$Z_m = Y_m - r\tau_m \quad .$$

By equation (2.1), $E_0[Z_m] = 0$. Let $\sigma^2 = E_0[Z_m^2]$ and assume that $0 < \sigma^2 < \infty$. Define

(2.2) $$\hat{r}(M) = \sum_{m=1}^{M} Y_m / \sum_{m=1}^{M} \tau_m \quad ,$$

and

(2.3) $$\hat{x}(N) = \sum_{n=0}^{N} f(X_n)/N+1 \quad .$$

Then $\hat{r}(M) \to r$ a.s. (almost surely) as $M \to \infty$ and $\hat{x}(N) \to r$ a.s. as $N \to \infty$. Because $\{Z_m, m \geq 1\}$ are i.i.d. (assuming $X_0 = 0$) it is easy to prove the central limit theorems

(2.4) $$\frac{\sqrt{M}\,(\hat{r}(M) - r)}{\sigma/E_0[\tau_1]} \Rightarrow N(0,1) \qquad \text{as} \quad M \to \infty$$

(2.5) $$\frac{\sqrt{N}\,(\hat{x}(N) - r)}{\sigma/E_0[\tau_1]^{1/2}} \Rightarrow N(0,1) \qquad \text{as} \quad N \to \infty \ ,$$

where $N(0,1)$ is a normally distributed random variable with mean 0 and variance 1. Point estimates for r can be given by either (2.2) or (2.3) and confidence intervals for r can be based on (2.4) or (2.5).

We now show how to define a modified Markov chain which will have a shorter expected cycle length and from which point estimates and confidence intervals for r may be derived. Introduce a new state Δ, and let $E^{\Delta} = E \cup \Delta$. The addition of the state Δ will enable us to use Dynkin's formula, which is the basis of the method. Define a new transition matrix $\tilde{P} = \{\tilde{p}_{ij} : i,j \in E^{\Delta}\}$ where

$$\tilde{p}_{ij} = \begin{cases} 0 & j = 0 \\ p_{ij} & i \in E,\ j \in E,\ j \neq 0 \\ p_{i0} & i \in E,\ j = \Delta \\ 1 & i = j = \Delta \end{cases}$$

$\tilde{P}$ is then basically the same as P, the major difference being that column 0 of P has been placed in column Δ of $\tilde{P}$ and column 0 of $\tilde{P}$ is set equal to 0. If $E = \{0, 1, \ldots, m\}$, then $\tilde{P}$ may be written as

$$\tilde{P} = \begin{array}{c} \\ 0 \\ 1 \\ \vdots \\ m \\ \Delta \end{array} \begin{array}{c} \begin{array}{cccc} 0 & 1 & \cdots & m \end{array} \quad \Delta \\ \begin{pmatrix} 0 & p_{01} & \cdots & p_{0m} & p_{00} \\ 0 & p_{11} & \cdots & p_{1m} & p_{10} \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & p_{m1} & \cdots & p_{mm} & p_{m0} \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix} \end{array}$$

Following the notation of Hordijk, Iglehart and Schassberger (1976) denote the submatrix of $\tilde{P}$ consisting of all rows and columns except for row and column Δ by ${}_0P$. Let $\{\tilde{X}_n, n \geq 0\}$ be a Markov chain with state space E^{Δ} and transition matrix $\tilde{P}$. For this Markov chain each state in E is transient and Δ is an absorbing state. Extend the definition of any vector (or function) g on E to E^{Δ} by setting $g(\Delta) = 0$. Define the absorption time $\tilde{\tau}$ by

$$\tilde{\tau} = \inf\{n \geq 0 : \tilde{X}_n = \Delta\}$$

and let

$$\tilde{Y} = \sum_{n=0}^{\tilde{\tau}-1} f(\tilde{X}_n) \quad .$$

Notice that if $X_0 = \tilde{X}_0$ a.s. then the pairs (Y_1, τ_1) and $(\tilde{Y}, \tilde{\tau})$ have the same distribution (in fact if we simulated these two processes using the same stream of random numbers then $(Y_1, \tau_1) = (\tilde{Y}, \tilde{\tau})$). Let $y(i) = E_i[Y_1] = E_i[\tilde{Y}]$ and $t(i) = E_i[\tau_1] = E_i[\tilde{\tau}]$. By equation (2.1) $r = y(0)/t(0)$. Since $\tilde{X}_n = \Delta$ for all $n \geq \tilde{\tau}$ and $f(\Delta) = 0$ then

$$\tilde{Y} = \sum_{n=0}^{\infty} f(\tilde{X}_n) \ .$$

By taking expectations we find that

$$y = \sum_{n=0}^{\infty} \tilde{P}^n f \quad . \tag{2.6}$$

Similarly if $e(i) = 1$ for all $i \in E$ then

$$t = \sum_{n=0}^{\infty} \tilde{P}^n e \quad . \tag{2.7}$$

The interchanges of summation needed in (2.6) and (2.7) are justified by the assumption that $\pi|f| < \infty$. Define the potential matrix $A = \{a_{ij} : i,j \in E^{\Delta}\}$ by

$$A = \sum_{n=0}^{\infty} \tilde{P}^n \quad .$$

Then

$$a_{ij} \begin{cases} < \infty , & j \in E \\ = \infty , & j = \Delta , \end{cases}$$

and a_{ij} is the expected number of visits of the Markov chain $\{\tilde{X}_n, n \geq 0\}$ to state j given that $\tilde{X}_0 = i$. If we interpret $\infty \, 0 = 0$ then (2.6) and (2.7) may be written as $y = Af$ and $t = Ae$.

The derivation of the new Markov chain to be simulated will be based on Dynkin's formula, which is given in the following proposition. For the definition of a stopping time see page 118 of Çinlar (1975).

(2.8) PROPOSITION. Let S be any stopping time for the Markov chain $\{\tilde{X}_n, n \geq 0\}$ such that $d(i) = E[S|\tilde{X}_0 = i] < \infty$ for each i. If $\pi|f| < \infty$ then

$$y(i) = E\left[\sum_{n=0}^{S-1} f(\tilde{X}_n)|\tilde{X}_0 = i\right] + E[y(\tilde{X}_S)|\tilde{X}_0 = i] \quad .$$

PROOF. See page 201 of Çinlar (1975). □

Let

$$h(i) = E\left[\sum_{n=0}^{S-1} f(\tilde{X}_n) | \tilde{X}_0 = i\right]$$

and let

$$\bar{R} = \{\bar{r}_{ij} : i,j \in E^{\Delta}\}$$

where

$$\bar{r}_{ij} = P\{\tilde{X}_S = j | \tilde{X}_0 = i\} .$$

Then Dynkin's formula is

$$y = h + \bar{R}y .$$

Similarly

$$t = d + \bar{R}t .$$

If we assume that $\bar{R}^n y \to 0$ and $\bar{R}^n t \to 0$ as $n \to \infty$, then

$$y = \sum_{n=0}^{\infty} \bar{R}^n h \tag{2.9}$$

and

$$t = \sum_{n=0}^{\infty} \bar{R}^n d .$$

Let $\{\bar{C}_n,\ n \geq 0\}$ be a Markov chain with state space E^{Δ} and transition matrix $\bar{R}$. This Markov chain also has Δ as an absorbing state. Let

$$\bar{\tau} = \inf\{n \geq 0 : \bar{C}_n = \Delta\} ,$$

$$\bar{Y} = \sum_{n=0}^{\bar{\tau}-1} h(\bar{C}_n) ,$$

and

$$\bar{\delta} = \sum_{n=0}^{\bar{\tau}-1} d(\bar{C}_n) \quad .$$

Since $E[\bar{Y}] = \sum_{n=0}^{\infty} \bar{R}^n h$, equation (2.9) implies that $E[\bar{Y}|\bar{C}_0 = i] = y(i)$. Similarly $E[\bar{\delta}|\bar{C}_0 = i] = t(i)$.

We now remove the state Δ. Assume that $\bar{r}_{i0} = P\{\tilde{X}_S = 0|\tilde{X}_0 = i\} = 0$ for all i (this will be the case for all interesting stopping times S). Define the transition matrix $R = \{r_{ij} : i,j \in E\}$ where

$$r_{ij} = \begin{cases} \bar{r}_{i\Delta} , & j = 0 \\ \bar{r}_{ij} , & j \neq 0 . \end{cases}$$

R is obtained from $\bar{R}$ by placing column Δ of $\bar{R}$ in column 0 of R, deleting row and column Δ of R, and leaving $\bar{R}$ otherwise unchanged. Now let $\{C_n,\ n \geq 0\}$ be a Markov chain with transition matrix R. Define $T'_0 = 0$,

$$T'_m = \inf\{n > T'_{m-1} : C_n = 0\} , \qquad m \geq 1 ,$$

$$\tau'_m = T'_m - T'_{m-1} , \qquad m \geq 1 ,$$

$$Y'_m = \sum_{n=T'_{m-1}}^{T'_m - 1} h(C_n) , \qquad m \geq 1 ,$$

$$\delta'_m = \sum_{n=T'_{m-1}}^{T'_m - 1} d(C_n) , \qquad m \geq 1 ,$$

and

$$Z'_m = Y'_m - r\delta'_m , \qquad m \geq 1 .$$

As before if $C_0 = \bar{C}_0$ a.s., then $(Y'_1, \delta'_1, \tau'_1)$ has the same distribution as $(\bar{Y}, \bar{\delta}, \bar{\tau})$. In particular $E[Y'_1|C_0 = i] = y(i) = E[Y_1|X_0 = i]$ and $E[\delta'_1|C_0 = i] = t(i) = E[\tau_1|X_0 = i]$, so that $E_0[Z'_1] = 0$ Furthermore the times $\{T'_m, m \geq 1\}$ are regenerations for $\{C_n, n \geq 0\}$ so that if $C_0 = 0$, $\{(Y'_m, \delta'_m, \tau'_m, Z'_m), m \geq 1\}$ are i.i.d.

The Markov chain $\{C_n, n \geq 0\}$ is the one that will finally be simulated. The use of the state Δ in defining the stopping time S automatically ensures that the return state 0 cannot be inadvertently "skipped" during the simulation of $\{C_n, n \geq 0\}$.

Defining

$$\hat{r}'(M) = \sum_{m=1}^{M} Y'_m \Big/ \sum_{m=1}^{M} \delta'_m \tag{2.10}$$

and

$$\hat{x}'(N) = \sum_{n=0}^{N} h(C_n) \Big/ \sum_{n=0}^{N} d(C_n) , \tag{2.11}$$

then $\hat{r}'(M) \to r$ a.s. as $M \to \infty$ and $\hat{x}'(N) \to \tau$ a.s. as $N \to \infty$. Let $\sigma'^2 = E_0[Z'^2_m]$ and assume that $0 < \sigma'^2 < \infty$. It is straightforward to derive the central limit theorems;

$$(2.12) \qquad \frac{\sqrt{M}\,(\hat{r}'(M) - r)}{\sigma'/E_0[\delta'_m]} \Rightarrow N(0,1) , \qquad \text{as } M \to \infty ,$$

and

$$(2.13) \qquad \frac{\sqrt{N}\,(\hat{x}'(N) - r)}{\sigma' E_0[\tau'_1]^{1/2}/E_0[\delta'_m]} \Rightarrow N(0,1) \qquad \text{as } N \to \infty .$$

Point estimates for r are now given by either (2.10) or (2.11) and confidence intervals can be based on (2.12) or (2.13). Once the transition matrix R and functions h and d have been calculated, the formation of point estimates and confidence intervals is essentially the same as in the regenerative method.

3. Numerical Discussion

To determine the amount of variance reduction obtained by simulating the chain $\{C_n, n \geq 0\}$ rather than $\{X_n, n \geq 0\}$ we need only compare the variance terms in the central limit theorems (2.12) and (2.5). This variance reduction, which will be denoted by R_S^2, is

$$R_S^2 = \frac{\sigma'^2 \, E_0[\tau_1']/E_0[\delta_1']^2}{\sigma^2/E_0[\tau_1]} ,$$

which, since $E_0[\delta_1'] = E_0[\tau_1]$, simplifies to

$$R_S^2 = \frac{\sigma'^2 \, E_0[\tau_1']}{\sigma^2 \, E_0[\tau_1]} .$$

If σ' and σ are approximately equal then $R_S^2 \approx E_0[\tau_1']/E_0[\tau_1]$, the ratio of the expected cycle lengths for the two processes. This suggests that S be made as large as possible, however by doing so the amount of work needed to compute R, h and d may be prohibitive. Each transition in the chain $\{C_n, n \geq 0\}$ corresponds to $E[S|C_n]$ transitions in the chain $\{X_n, n \geq 0\}$, so that we expect transitions for $\{C_n, n \geq 0\}$ to be relatively expensive to generate. The stopping time S should therefore be chosen so that R, h and d may be readily computed and the sample paths of $\{C_n, n \geq 0\}$ may be easily generated. We give several examples of such stopping times.

(3.1) EXAMPLE. Constant S.

If $S = m$, a constant, then $h = \sum_{n=0}^{m-1} {}_0P^n f$, $d = \sum_{n=0}^{m-1} {}_0P^n e$ and R is given by

$$r_{ij} = \begin{cases} {}_0P_{ij}^m , & j \neq 0 \\ 1 - \sum_{k \neq 0} {}_0P_{ik}^m , & j = 0 . \end{cases}$$

If P is relatively sparse the work involved in computing R, h and d should not be too great for small values of m. If $S = 1$, then $R = P$, $h = f$ and $d = e$, so that this choice of S reduces to straighforward simulation of the original Markov chain $\{X_n, n \geq 0\}$. If m is small and if $p_{i0} = 0$ for most $i \in E$ then

$$d = \sum_{n=0}^{m-1} {}_0P^n e \approx \sum_{n=0}^{m-1} P^n e = me .$$

Since

$$E[\tau_1] = \sum_{n=0}^{\infty} {}_0P^n e = \sum_{n=0}^{\infty} {}_0R^n d \approx m \sum_{n=0}^{\infty} {}_0R^n e = mE[\tau_1'] ,$$

we expect that $R_S^2 \approx 1/m$. Tables 1 and 2 bear out this speculation for two birth and death processes, the finite capacity M/M/1 queue and the repairman problem. The repairman problem has birth and death parameters

$$\lambda_i = \begin{cases} n\lambda , & 0 \le i \le s \\ (n+s-i)\lambda , & s < i \le n+s \end{cases}$$

$$\mu_i = \begin{cases} i\mu , & 1 \le i \le c \\ c\mu , & c < i \le s+n , \end{cases}$$

where n is the number of operating units, s is the number of spare units, c is the number of repairmen, and λ and μ are the failure and repair rates respectively of the units. These continuous time problems have been transformed into discrete time using the methods of Hordijk, Iglehart and Schassberger (1976).

(3.2) EXAMPLE. Exit Times of Sets

Suppose E is partitioned into N_B disjoint blocks B_i; i.e., $E = \bigcup_{i=0}^{N_B} B_i$ and $B_i \cap B_j = \emptyset$, the empty set, for $i \neq j$. Let $|B_i|$ denote the number of elements in B_i and assume that $|B_i| < \infty$. Define the stopping time S_B to be the first exit time from the initial block; i.e.,

$$S_B = \inf\{n > 0 : \tilde{X}_n \notin B_k\} , \qquad \text{for } \tilde{X}_0 \in B_k .$$

Let $f_i = \{f(j) : j \in B_i\}$, $e_i = \{e(j) : j \in B_i\}$ and ${}_0P_{ij} = \{{}_0P_{k\ell} : k \in B_i, \ell \in B_j\}$. Let I_{ii} denote the identity matrix of size $|B_i|$ by $|B_i|$. Then

$$h_i = (I_{ii} - {}_0P_{ii})^{-1} f_i$$

$$d_i = (I_{ii} - {}_0P_{ii})^{-1} e_i$$

and

$${}_0R_{ij} = \begin{cases} 0 , & i = j \\ (I_{ii} - {}_0P_{ii})^{-1} {}_0P_{ij} , & i \neq j \end{cases}$$

where $h_i = \{h(j) : j \in B_i\}$, $d_i = \{d(j) : j \in B_i\}$ and ${}_0R_{ij} = \{{}_0r_{k\ell} : k \in B_i, \ell \in B_j\}$. The transition matrix R is found by setting

$$r_{ij} = \begin{cases} {}_0r_{ij} , & j \neq 0 \\ 1 - \sum_{k \in E} {}_0r_{ik} , & j = 0 . \end{cases}$$

The matrix ${}_0R$ is the block Jacob matrix for solving the set of equations $y = f + {}_0Py$ (see Varga (1962)). The Markov chain $\{C_n, n \geq 0\}$ is the same one that appears when using the techniques of Heidelberger (1978). Tables 1 and 2 give R_S^2 and R_S for the finite capacity M/M/1 queue and the repairman problem respectively.

(3.3) EXAMPLE. Continuous Time Markov Chains and Semi-Markov Processes.

By applying this technique to continuous time Markov chains, the discrete time methods of Hordijk, Iglehart and Schassberger (1976) are obtained as a special case. Let $\{X_t, t \geq 0\}$ be an irreducible, positive recurrent continuous time Markov chain with infinitesimal matrix $Q = \{q_{ij} : i,j \in E\}$.

Set $q_i = \sum_{j \neq i} q_{ij}$ $(q_i = -q_{ii})$. Dynkin's formula remains valid for continuous time Markov chains (with an integral replacing the sum in (2.18)). Define the stopping time $S = \inf\{t > 0 : X_t \neq X_0\}$. We then simulate a discrete time Markov chain $\{C_n, n \geq 0\}$ with $r_{ij} = q_{ij}/q_i$, $i \neq j$, $h(i) = f(i)/q_i$ and $d(i) = 1/q_i$. Hordijk, Iglehart and Schassberger (1976) have shown that in this case $\sigma' \leq \sigma$. These techniques may also be used to reduce semi-Markov processes to discrete time. Once in discrete time, the method may be applied again to obtain further variance reductions.

TABLE 1

Variance Reductions, R_S^2 and R_S, for Finite Capacity M/M/1 Queue Obtained by Simulating the Modified Markov Chain:

r = E(X), Return State = 0

ρ	Stopping Time S		
	2	3	S_B *
.25	.4264 .6530	.2923 .5406	.2942 .5424
.50	.4590 .6775	.3620 .6016	.4441 .6664
.75	.4841 .6957	.3585 .5987	.4037 .6353
.90	.4888 .6991	.3422 .5850	.3624 .6020
.95	.4893 .6995	.3370 .5805	.3510 .5925
.99	.4895 .6996	.3333 .5773	.3429 .5856

* Block sizes = (1, 3, 3, 3, 3, 2)

TABLE 2

Variance Reductions, R_S^2 and R_S, for Repairman Problem
Obtained by Simulating the Modified Markov Chain:
r = E(X), Return State = 0

c	μ	Stopping Time S: 2	3	S_B *
1	12	.4676	.3358	.3602
		.6837	.5795	.6002
2	6	.4597	.3128	.2821
		.6780	.5593	.5311
3	4	.4532	.2950	.2447
		.6732	.5431	.4947
4	3	.4476	.2821	.2432
		.6691	.5311	.4932

n = 10

s = 4

λ = 1

* Block sizes = (1, 3, 3, 3, 3, 2)

4. Conclusions

The variance reduction technique proposed in this paper shows promise for processes with relatively long cycle lengths. Examples of such processes may be found in both open and closed queueing networks. By simulating the modified Markov chain $\{C_n, n \geq 0\}$ an increased number of i.i.d. cycles are obtained for a prespecified run length than is possible with the original chain $\{X_n, n \geq 0\}$. Assuming that the chains $\{C_n, n \geq 0\}$ and $\{X_n, n \geq 0\}$ are approximately equally variable over a cycle, this increase in the number of cycles translates directly into a variance reduction. Since the sample paths of $\{C_n, n \geq 0\}$ will usually be more expensive to generate than those of $\{X_n, n \geq 0\}$, the simulator must be careful to ensure that the variance reduction obtained is sufficient to produce an overall computational savings. The method has the best chance of being computationally efficient when the transition matrix of the Markov chain is relatively sparse.

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One of the main difficulties with the regenerative method of simulation is that even though a process may be known to be regenerative, regenerations may occur quite infrequently. A class of methods, based on Dynkin's formula, is considered that increases the frequency of regenerations when the process being simulated is a Markov chain. Instead of simulating the original Markov chain, a new Markov chain is simulated from which point estimates and confidence intervals for parameters of the original chain's stationary distribution may be formed. Because regenerations occur more frequently in the new chain, such confidence intervals will usually be shorter than is otherwise possible.

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