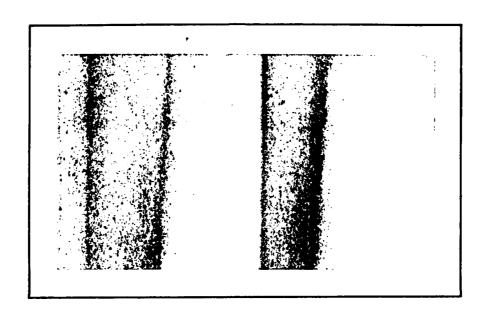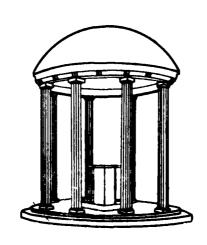END

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SUPEREFFICIENT SIMULATION

OF MARKOV CHAINS AND

SEMI-MARKOV PROCESSES

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Abstract

This paper describes a method of simulating a Markov chain for the purpose of estimating functions of the chain and functions of associated semi-Markov processes. In particular, special attention is devoted to the estimation of the probability density function of first passage time from, say, state a to state b. Rotation sampling is used to achieve variances of estimators of order $O(1/k^2)$ (k squared), where k is the number of replications, which compares with $O(1/k)$ when independently sampled replications are used. Since both independent and rotation sampling have computation time complexity $O(k)$, the relative advantage of rotation sampling is clear as $k \rightarrow \infty$ (infinity). The paper presents two examples to illustrate the method.

Introduction

Consider a positive recurrent aperiodic Markov chain with state space $S = (0,1,\ldots,n)$ and transition probability matrix $\underset{\sim}{p}_n = || \, p_{ij} \, ||$ where p_{ij} denotes the probability of moving from state i to state j in one step for $i,j \in S$. Let s_{ij} denote the frequency of one-step transitions from i to j during a first passage from state a to state b $a,b \in S$ and let $\underset{\sim}{s}$ denote a $1\times(n+1)^2$ vector with s_{ij} in column $n(i-1) + j$. Also let $p(\underset{\sim}{s};a,b)$ denote the probability of observing the frequency vector $\underset{\sim}{s}$ during a first passage.

The need to know $p(\underset{\sim}{s};a,b)$ arises in many areas of applied probability and operations research. For example, consider a semi-Markov process with Markov chain $\underset{\sim}{p}_n$ and holding time probability density function (p.d.f.) $f_{ij}(t)$ on $[0,\infty)$ for one-step transitions from i to j $i,j \in S$. Let $f_{ij}(t|s)$ denote the s-fold convolution of $f_{ij}(t)$ with itself. Then the semi-Markov process has first passage time p.d.f.

$$g(t;a,b) = \sum_{\underset{\sim}{s}} p(\underset{\sim}{s};a,b) \; f(t|\underset{\sim}{s}) \qquad (1)$$

where $f(t|\underset{\sim}{s})$ denotes the convolution of the p.d.fs. $f_{ij}(t|s_{ij})$ for all $i,j \in S$ such that $s_{ij} > 0$.

Although one can write down systems of equations to represent (1), it is difficult to solve these systems. In particular, it is difficult to derive computationally convenient expressions for $p(\underset{\sim}{s};a,b)$. The purpose of this paper is to propose a method for estimating $p(\underset{\sim}{s};a,b)$ by means of a *superefficient* Monte Carlo sampling method and then showing how these estimates can be used to estimate an important class of reward functions, of which (1) is a special case. In k independent Monte Carlo replications or sampling experiments, the variances of estimators usually are $O(1/k)$. The

sampling plan proposed here leads to variances of order $O(1/k^2)$. Since the computation time complexity of the proposed scheme is $O(k)$, which also holds for independent replications, the proposed sampling plan is termed *superefficient* .

The sampling plans use a special case of the antithetic variate method (Hammersley and Handscomb 1964) called *rotation sampling* which is described in detail in Fishman and Huang (1980). The technique has already been applied to the direct simulation of Markov chains in Fishman (1981a, 1981b, 1982a). The present paper extends the technique to the estimation of the more complex probabilities $p(\underset{\sim}{s};a,b)$.

Section 1 describes the procedure in detail and Section 2 describes how it applies for Gamma distributed holding times. Section 3 presents two examples, one of which is the estimation of the p.d.f. of busy time for the M/M/1 queueing model. The results of this example are compared with the theoretical solution in Cox and Smith (1961, p. 148). These examples use the MCHAIN FORTRAN subprogram (Fishman 1982b) which enables one to simulate k replications of the chain in parallel, using rotation sampling.

For consistency with the earlier work in Fishman (1981a, 1981b, 1982a), we add several modelling details. We assume that there exists a positive integer $\delta \leq (n-1)/2$ such that

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

and

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

Also, let s_j denote the total number of states that have positive transition probabilities from state j and let $\{m_{jr}; r = 1,\ldots,s_j\}$ denote the ordered sequence $(m_{jr} < m_{j,r+1}; r = 1,\ldots,s_j -1)$ of the s_j states to which entry can occur from state j. Then one has the representation

$$p_{jm_{jr}} > 0 \qquad\qquad r = 1,\ldots,s_j$$

$$\sum_{r=1}^{s_j} p_{jm_{jr}} = 1 \qquad\qquad\qquad (2)$$

$$\delta \geq \max \left(|m_{j1} - j| , |m_{js_j} - j| \right) \qquad j = 0,1,\ldots .$$

The value of this alternative, but equivalent, representation becomes apparent when actually generating sample paths by simulation on a computer. See Fishman (1982b).

1. Simulation of a Markov Chain

Reward Functions

Let I denote the set of all one-step (i,j) transition pairs with $p_{ij} > 0$. Suppose one wants to use simulation to study the behavior of the chain during an interval that begins with exit from state a and ends with entry to state b where $a,b \in S$. Let

$$N_i = \begin{array}{l} \text{frequency of transitions of } \textit{type} \text{ i during} \\ \text{first passage on an arbitrarily selected} \\ \text{sample run} \end{array} \qquad (3a)$$

and

$$A(j_1,\ldots,j_r;\underline{\theta}) = \begin{array}{l} \text{reward received during first passage for} \\ j_1,\ldots,j_r \text{ transitions of types } 1,\ldots,r \\ \text{respectively.} \end{array} \qquad (3b)$$

A type denotes all the one-step (i,j) transition pairs which lead to the exact same reward. Here there are r distinct types. This notation proves convenient later in reducing the dimensionality of the estimation problem.

On k replications the sample mean reward is

$$R_k = \frac{1}{k} \sum_{\ell=1}^{k} A(N_1^{(\ell)},\ldots,N_r^{(\ell)};\underline{\theta}) \qquad (4)$$

where the superscript (ℓ) denotes replication ℓ. The reward function A can assume many alternative forms. For example, if

$$A(j_1,\ldots,j_r;\underline{\theta}) = \sum_{s=1}^{r} j_s a_s \qquad (5)$$

for given $\underline{\theta} = (a_1, \ldots, a_r)$, R_k is linear in $S_1, \ldots, S_r$ where

$$S_j = \sum_{\ell=1}^{k} N_j^{(\ell)}. \tag{6}$$

This case has been studied in detail from the point of view of simulation in Fishman (1981a, 1981b, 1982a). As a second example, consider a semi-Markov process with Markov chain $\underline{p}_n$ and continuous holding time p.d.fs. $f_1, \ldots, f_r$ for the r types of transitions in I. Let

$$g_i(t|j) = \overbrace{f_i(t) * f_i(t) * \ldots * f_i(t)}^{j} \quad 0 \le t < \infty \tag{7}$$

denote the j-fold convolution (j > 0) of f_i. Then for given $N_i = j_i$ i = 1,...,r the p.d.f. of first passage time from a to b is

$$A(j_1, \ldots, j_r; \underline{\theta}) = g_1(t|j_1) * g_2(t|j_2) * \ldots * g_r(t|j_r) \tag{8}$$

where the convolution includes only those g_i's for which $j_i > 0$ and $\underline{\theta} = t$.

Aggregation Across Replications

Although (4) proves useful for computation of R_k, an alternative representation considerably simplifies the derivation of results. Let

$$K_{j_1, \ldots, j_r} = \sum_{\ell=1}^{k} \prod_{s=1}^{r} \delta(N_s^{(\ell)} - j_s) \tag{9}$$

where

$$\delta(x) = 1 \qquad \text{if } x = 0$$
$$\quad\quad = 0 \qquad \text{otherwise,}$$

so that one can write (4) as

$$R_k = \frac{1}{k} \sum_{j_1, \ldots, j_r=0}^{\infty} K_{j_1, \ldots, j_r} A(j_1, \ldots, j_r; \underline{\theta}) .$$

Note that

$$\Delta K_{bm} = \sum_{\substack{j_1, \ldots, j_r=0 \\ j_1 + \ldots + j_r = m}}^{m} K_{j_1, \ldots, j_r}$$

is the number of replications that enter b on step m. More importantly, note that $K_{j_1,\ldots,j_r}/k$ is an unbiased estimator of $p(\underline{s};a,b)$ in (1) with frequency vector $\underline{s} = (j_1,\ldots,j_r)$ in the case in which there are $r = (n + 1)^2$ distinct types of transitions. Although we hereafter discuss the properties of R_k it should be recognized that a reward function

$$A(j_1,\ldots,j_r;\underline{\theta}) = \Pi \, {}^r_{i=1} \, \delta(j_i - j_i^*)$$

specializes the analysis to the estimation of $p(\underline{s};a,b)$ where $\underline{s} = (j_1^*,\ldots,j_r^*)$.

Serial Simulation

Presumably, the objective of simulation is to perform k replications sufficient to achieve an acceptable accuracy for R_k as an estimate of ER_k. In the case of k independent replications in series, with a≠b, one can ensure that each replication begins with an exit from a and ends with a first entry into b by replacing $\{p_{bj}; j=0,1,\ldots,n\}$ by $p_{ba}=1$, and $p_{bs}=0$ for $\forall$ s≠a. For the case a=b there is no need to modify the probabilities. In the independent case one has var $R_k=O(1/k)$ and computation time complexity $O(k)$.

Parallel Simulation

To speed up the convergence rate of var R_k we turn to parallel simulation using rotation sampling. Hereafter, a prime superscript denotes parallel rotation sampling. Consider k replications each beginning with an exit from state a and set $p_{bb}=1$ and $p_{bs}=0$ for $\forall$ s≠b. If a≠b this modification of $\{p_{bs}\}$ should be performed after the first transition. This modification makes the chain absorbing with transient states $j \in S_b$, where $S_b = S-b$, and absorbing state b. Let T_m denote the set of transient states with at least one resident replication at the end of step m and let K'_{jm} denote the number of such replications in state $j \in T_m$. Let $\{U_{jm}; \, j \in T_m\}$ denote a sequence of i.i.d. random variables uniformly distributed on $[0,1)$ and define for

$i=1,\ldots,K'_{jm}$

$$V_{ijm} = U_{jm} + (i-1)/K'_{jm} \qquad \text{if } U_{jm} < 1-(i-1)/K'_{jm}$$
$$= U_{jm} + (i-1)/K'_{jm}-1 \qquad \text{otherwise.} \tag{10}$$

Also define

$$q_{js} = \textstyle\sum_{\ell=0}^{S} p_{j\ell} \qquad\qquad s \in S \tag{11}$$

and

$$q_{j,-1} = 0.$$

Then at step m+1 replication i in state j goes to state s if

$q_{j,s-1} \leq V_{ijm} < q_{js}.$ Since $q_{jn}=1$, a destination is guaranteed.

Note that although $V_{1jm},\ldots,V_{K'_{jm}jm}$ are each uniformly distributed on [0,1], they are not independent. Therefore, the sample path of each replication from a to b has the correct probability law, but the k paths are not independent. The assignment in (10) is called *rotation sampling* and produces a clear benefit in simulation. For a reward function as in (5), the use of (4) leads to

$$\text{var } R'_k \leq 0((\ln k/k)^2) \qquad n < \infty$$

and (12)

$$\text{var } R'_k \leq 0((\ln k)^4/k^2) \qquad n \to \infty \quad,$$

which improve on $0(1/k)$ for independent replications. Moreover, for (5) one can show that the computation time complexity is $0(\ln k)$ for $n < \infty$ and $0((\ln k)^2)$ for $n \to \infty$. This last result follows from a more compact sampling scheme, than that in (10), that can be used when there is no need to keep track of the distinct sample paths on each replication. See .Fishman (1981a, 1981b, 1982a). For the more general reward function (4), keeping sample path data to compute $\{N_j^{(\ell)}; j \in I\}$ for $\ell=1,\ldots,k$ is necessary and therefore the computation time complexity is $0(k)$.

One additional result is of importance. Let K'_{ijm} denote the number of replications that move from i to j on step m. Then it is shown in Fishman (1981a) that as $k \rightarrow \infty$

$$\text{var } K'_{ijm} = O(1) \quad i,j \in S \quad m = 1,2, \ldots . \tag{13}$$

We use this result next when bounding var R'_k for the general reward function (4). Observe that by analogy with (9)

$$\Delta K'_{bm} = \sum_{\substack{j_1,\ldots,j_r=0 \\ j_1+\ldots+j_r=m}}^{m} K'_{j_1,\ldots,j_r} = \sum_{i \in S_b} K'_{ibm} \tag{14}$$

so that for given m and $k \rightarrow \infty$

$$\sum_{\substack{i_1,\ldots,i_r=0 \\ i_1+\ldots+i_r=m}}^{m} \sum_{\substack{j_1,\ldots,j_r=0 \\ j_1+\ldots+j_r=m}}^{m} \text{cov}(K'_{i_1,\ldots,i_r}, K'_{j_1,\ldots,j_r})$$

$$= \sum_{i,j \in S_b} \text{cov}(K'_{ibm}, K'_{jbm}) \tag{15}$$

$$= O(1) \quad .$$

Then it can be shown that as $k \rightarrow \infty$

$$\text{cov } (K'_{i_1,\ldots,i_r}, K'_{j_1,\ldots,j_r}) = O(1) \tag{16}$$

so that our estimate $K'_{j_1},\ldots, K'_{j_r}/k$ of $p(\underline{s};a,b)$ with $\underline{s} = (j_1,\ldots,j_r)$ has variance $O(1/k^2)$. Proof of (16) follows from Proposition 1.

<u>Proposition 1.</u> Let $X_1,\ldots,X_t$ denote random variables with

$$\text{var } X_i = \sigma_i^2(z) \ ,$$

$$\text{cov } (X_i, X_j) = \sigma_{ij}(z) \quad i \neq j \quad i,j = 1,\ldots,t$$

and define

$$Y_j = \sum_{i=1}^{j} X_i$$

with

$$\text{var } Y_j = \omega_j^2(z) \qquad j=1,\ldots,t .$$

If

$$\lim_{z\to\infty} \omega_j^2(z) = c < \infty \qquad \forall j,$$

then

$$\lim_{z\to\infty} \sigma_i^2(z) \leq \text{constant} \qquad \forall i. \qquad (17)$$

Proof. Observe that

$$\sigma_t^2(z) = \omega_t^2(z) - \omega_{t-1}^2(z) - 2C_t(z)$$

where

$$C_t(z) = \text{cov } (X_t, Y_{t-1}) \quad t>1 .$$

Since

$$|C_t(z)| \leq \sigma_t(z) \, \omega_{t-1}(z),$$

one has

$$\sigma_t^2(z) - 2 \, \sigma_t(z) \, \omega_{t-1}(z) + \omega_{t-1}^2 (z) - \omega_t^2(k) =$$

$$[\sigma_t(z) - \omega_{t-1}(z) - \omega_t(z)] \, [\sigma_t(z) - \omega_{t-1}(z) + \omega_t(z)] \leq 0$$

so that

$$\omega_{t-1}(z) - \omega_t(z) \leq \sigma_t(z) \leq \omega_{t-1}(z) + \omega_t(z) \qquad (18)$$

Taking the limit as $z\to\infty$ gives (17). The result in (16) follows directly.

We now derive var R_k' for the important case

$$\sum_{j_1,\ldots,j_r=0}^{\infty} A(j_1,\ldots,j_r; \underset{\sim}{\theta}) \leq \text{constant} \qquad (19a)$$

and

$$A(j_1,\ldots,j_r;\underset{\sim}{\theta}) \geq 0 \qquad \forall j_1,\ldots,j_r. \qquad (19b)$$

Suppose that a transition of type $i \in I$ has the Gamma p.d.f.

$$f_i(t) = \frac{\lambda_i^{\alpha_i} t^{\alpha_i - 1} e^{-\lambda_i t}}{\Gamma(\alpha_i)} \qquad \begin{array}{l} \alpha_i \geq 1, \quad \lambda_i > 0, \\ 0 \leq t < \infty \end{array} \qquad (24)$$

denoted by $G(\alpha_i, \lambda_i)$. Let us also assume that all transition pairs (i,j) with the same p.d.f. are regarded as one type in I and that $\lambda_1 < \ldots < \lambda_r$. For an arbitrary replication with N_i transitions of type i, the corresponding total holding time has the Gamma distribution $G(\alpha_i N_i, \lambda_i)$ with p.d.f.

$$g_i(t|N_i) = \frac{\lambda_i^{\alpha_i N_i} t^{\alpha_i N_i - 1} e^{-\lambda_i t}}{\Gamma(\alpha_i N_i)} \qquad \begin{array}{l} \alpha_i, N_i \geq 1, \lambda_i > 0, \\ 0 \leq t < \infty \end{array} . \quad (25)$$

Then the estimated first passage time p.d.f. is

$$R_k'(t) = \frac{1}{k} \sum_{j_1,\ldots,j_r=0}^{\infty} K_{j_1,\ldots,j_r}' \; g(t|j_1,\ldots,j_r) \quad (26a)$$

where

$$g(t|j_1,\ldots,j_r) = g_1(t|j_1) * \ldots * g_r(t|j_r) \qquad (26b)$$

and the convolution is taken only over those types i for which $j_i > 0$.

In practice, it is more convenient to compute $R_k'(t)$ from

$$R_k'(t) = \frac{1}{k} \sum_{\ell=1}^{k} \; g(t|N_1^{(\ell)},\ldots,N_r^{(\ell)}) \qquad (27)$$

which is algebraically equivalent to (26a). Note that the sample frequencies (9) for the parallel simulation, need not be computed when (27) is used. However, the computation of $g(t|N_1^{(\ell)},\ldots,N_r^{(\ell)})$ remains a difficult one when $\lambda_1,\ldots,\lambda_r$ are unequal. By using the Taylor series expansion of e^θ, one can write (27) equivalently as

Proposition 2. Let the reward function A satisfy (19a) and (19b). Then

$$\text{var } R'_k \leq O(1/k^2). \tag{20}$$

Proof. Let $B = \sup\limits_{j_1,\ldots,j_r} \text{var } K'_{j_1,\ldots,j_r}$. Since these variances are

bounded, clearly

$$\text{var } R'_k \leq [\textstyle\sum_{j_1,\ldots,j_r=0}^{\infty} A(j_1,\ldots,j_r)]^2 \, B/k^2$$

$$\leq O(1/k^2). \tag{21}$$

We now show that the result (20) applies for the case of the first

passage time p.d.f. in (8). Observe that one can write

$$\sum_{j_1,\ldots,j_r=0}^{\infty} A(j_1,\ldots,j_r; t) =$$
$$h_1(t) * h_2(t) * \ldots * h_r(t) \tag{22}$$

where h_i is the *renewal density function*

$$h_i(t) = \sum_{j=0}^{\infty} g_i(t|j) \qquad 0 \leq t < \infty \tag{23}$$

and

$$g_i(t|0) = 0 \qquad\qquad i=1,\ldots,r.$$

Since each of the renewal densities can be bounded from above, it is clear

that for $t \in [0,\infty)$ (22) is also bounded, thus establishing (20).

2. Gamma Distributed Holding Times

Although our estimator of $p(\underline{s};a,b)$ based on rotation sampling has

a clear advantage over an estimator based on independent replications,

computational problems remain in using either estimator to estimate the

first passage time p.d.f. in (1). In this section we describe and illustrate

how these problems can be overcome for the common case of Gamma holding times.

$$g(t|N_1,\ldots,N_r) =$$

$$\sum_{i_1=0}^{\infty}\cdots\sum_{i_{s-1}=0}^{\infty} [\prod_{j=1}^{s-1} p_j(i_j|I_{j-1})]\, g_s(t|M_s + I_{s-1}) \qquad (28)$$

where

$$s = \max\,(i: N_i > 0),$$

$$I_0 = 0$$

and for $j = 1,\ldots,s$

$$I_j = I_{j-1} + i_j,$$

$$M_j = \sum_{m=1}^{j} \alpha_m N_m,$$

$$p_j(i_j|I_{j-1}) = \delta(i_j) \qquad\qquad\qquad\qquad \text{if } N_j = 0$$

$$= \frac{\Gamma(M_j + I_j)}{i_j!\; \Gamma(M_j+I_{j-1})}\, \omega_j^{M_j + I_{j-1}}(1-\omega_j)^{i_j} \qquad \text{if } N_j > 0$$

and

$$\omega_j = \frac{\lambda_j}{\lambda_\ell} \qquad\qquad \ell = \min(i: i > j,\, N_i > 0).$$

More concisely, (28) is equivalent to

$$g(t|N_1,\ldots,N_r) = \sum_{I_{s-1}=0}^{\infty} q_{s-1}\,(I_{r-1})\, g_s(t|M_s + I_{s-1}) \quad (29)$$

where

$$q_1(I_1) = p_1(i_1|0) \qquad\qquad\qquad\qquad\qquad (30)$$

$$q_j(I_j) = \sum_{I_{j-1}=0}^{I_j} p_j(I_j-I_{j-1}|I_{j-1})q_{j-1}(I_{j-1}) \quad j=2,\ldots,s-1.$$

Finally (28) has the equivalent form

$$g(t|N_1,\ldots,N_r) = \frac{(\lambda_s t)^{M_s} e^{-\lambda_s t}}{t\, \Gamma(M_s)}\left\{ q_{s-1}(0) + \sum_{j=1}^{\infty}\left[\frac{q_{s-1}(j)(\lambda_s t)^j}{\prod_{\ell=1}^{j}(M_s + \ell - 1)} \right] \right\}. \quad (31)$$

Expression (31) is exact and can be used in (27) with $N_i^{(\ell)}$ replacing N_i $i = 1,\ldots,r$ to compute an estimate of the p.d.f. Note that the term in brackets in (31) is eventually a decreasing function of j for given t. This fact enables one to truncate the summation on j at a point where the remainder is relatively incidental.

3. Examples

Consider an M/M/1 queueing model with arrival rate λ and service rate ω. Suppose one wants to estimate the p.d.f. of the busy period. Cox and Smith (1961, p. 148) give this p.d.f. as

$$g(t) = \frac{e^{-(\lambda+\omega)t}}{t(\lambda/\omega)^{\frac{1}{2}}} \; I_1(2t\sqrt{\lambda\omega}) \qquad 0 \le t < \infty \qquad (32)$$

where I_1 denotes the Bessel function of imaginary argument and first order. In this example, a=b=0, n=∞ and r=1, since all holding time distributions from states i>0 are exponential with identical rate $\lambda+\omega$. If N is the total number of transitions on an arbitrarily selected replication, excluding the initial transition from state 0, then

$$A(N,t) = g(t|N) = \frac{(\lambda+\omega)^N t^{N-1} e^{-(\lambda+\omega)t}}{\Gamma(N)} \qquad (33)$$

and the sample mean based on parallel simulation is

$$R_k'(t) = \frac{1}{k}\sum_{\ell=1}^{k} \frac{(\lambda+\omega)^{N^{(\ell)}} t^{N^{(\ell)}-1} e^{-(\lambda+\omega)t}}{\Gamma(N^{(\ell)})}$$

$$= \frac{1}{k}\sum_{j=1}^{\infty} K_{j+1}' \frac{(\lambda+\omega)^j t^{j-1} e^{-(\lambda+\omega)t}}{\Gamma(j)} \qquad (34)$$

where

$$K_j' = \sum_{\ell=1}^{k} \delta(N^{(\ell)}-j).$$

Experimental Design

We distinguish between *microreplications* and *macroreplications.* In particular, each of L independent macroreplications of the simulation contains k parallel microreplications that use (10). The L independent data blocks enable us to estimate var $R_k'(t)$ for each value of k considered. The global factor levels are $\lambda=0.9$, $\omega=1$ and $t=0.5j$; $j=1,\ldots,10$. For these, L=100 macroreplications were run for six experiments with $k_j=2^{7+j}$ microreplications on experiments $j=1,\ldots,6$. The macroreplications were used to estimate var $R_k'(t)$ for each t and k considered. Also, for these λ,ω and t's, L=1000 macroreplications were run each for k=1 microreplication to get a baseline estimate of var $R_1'(t)$, the variance without rotation sampling.

Table 1 shows $g(t)$ from (32) and $R_{256}'(t)$ for comparative purposes.

Insert Table 1 about here.

To measure variance reduction we use the ratio

$$V_k = \frac{\text{var } R_1'(t)}{k \text{ var } R_k'(t)} \quad .$$

Our earlier results indicate that this quantity is linear in k as $k\to\infty$. Now when assessing variance reduction for the estimation of a function, it should be noted that the variance reductions for all 10 values of t in Table 1 need not be identical for each k . Therefore for each k we plotted the minimal and maximal V_k's in Fig. 1, noting that all remaining variance reductions lie between them. In general, the graphs agree with theory. Moreover, we observed that for fixed k the V_k's decreased with

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Insert Figure 1 about here.

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decreasing coefficients of variations computed for the estimates derived in the baseline case of independent replications. This result is reassuring for it indicates that the benefits of rotation sampling are most apparent precisely where needed, namely where the larger coefficients of variation arise.

Our second example illustrates the estimation technique based on (31). It uses the same Markov chain as in example 1 but now with $\lambda=0.5$, $\omega=1$ and holding time distributions $G(1,\lambda_m)$ $m=1,\ldots,4$. Table 2 lists the transition types. The objective was to estimate the first passage time

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Insert Table 2 about here.

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for $a=b=0$ at times $t=0.1j$ $j=1,\ldots,40$. For these parameters, $L=100$ macroreplications were run for nine experiments with $k_j=2^{1+j}$ microreplications on experiment $j=1,\ldots,9$. Also, $L=1000$ macroreplications were run each with $k=1$ microreplication to get a baseline estimate of var $R_1'(t)$. Figure 2 shows the graphs of minimal and maximal variance reduction V_k versus k on logarithmic scales. Again the graphs essentially agree with theory. For each k the same relationship between variance reduction and coefficients of variation were observed as in example 1.

4. Conclusions

This paper demonstrates how one can estimate by a superefficient method the probability of observing $s_1,\ldots,s_r$ transitions of types $1,\ldots,r$ during a first passage from state a to state b in a positive recurrent aperiodic Markov chain with state space $S = (0,1,\ldots,n)$. It then shows how these results can be used to estimate a class of mean reward functions of which

first passage time p.d.fs. are a special case. Section 2 specializes the analysis to the case of Gamma holding times, showing how one derives expression (31) which is convenient for numerical calculation. Section 3 demonstrates the technique by two examples.

In order to implement the proposals of this paper, one needs a package that generates the transition frequencies $\{N_{ij}^{(\ell)}$; $i,j \in S\}$ $\ell=1,\ldots,k$ for k parallel replications based on rotation sampling. The MCHAIN FORTRAN program in Fishman (1982b) will generate these data.

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Table 1

Results for Example 1

$\lambda=.9$, $\omega=1$, $n=\infty$, and L=100

t	.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5
g(t)	.4319	.2276	.1399	.0955	.0701	.0542	.0434	.0358	.0302	.0258
$R'_{256}(t)$	.4320	.2278	.1399	.0956	.0702	.0543	.0435	.0359	.0302	.0258

Table 2

Transition Types for Example 2

type m	transition pairs	λ_m
1	(0,1)	0.5
2	(1,0), (1,2), (2,1)	1.5
3	(2,3), (3,2), (3,4), (4,3)	2.0
4	(i,j) j=i-1, i+1; i=5,6,...	3.0

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This paper describes a method of simulating a Markov chain for the purpose of estimating functions of the chain and functions of associated semi-Markov processes. In particular, special attention is devoted to the estimation of the probability density function of first passage time from,

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say, state a to state b . Rotation sampling is used to achieve variances of estimators of order $O(1/k^2)$, where k is the number of replications, which compares with $O(1/k)$ when independently sampled replications are used. Since both independent and rotation sampling have computation time complexity $O(k)$, the relative advantage of rotation sampling is clear as $k \to \infty$. The paper presents two examples to illustrate the method.

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