Proceedings of the 1992 Winter Simulation Conference
ed. J. J. Swain, D. Goldsman, R. C. Crain, and J. R. Wilson

SMOOTHING METHODS FOR VARIANCE REDUCTION IN SIMULATION OF MARKOV CHAINS

Sigrún Andradóttir

Department of Industrial Engineering
University of Wisconsin – Madison
1513 University Avenue
Madison, WI 53706, U.S.A.

Daniel P. Heyman
Teunis J. Ott

Bell Communications Research
445 South Street
Morristown, NJ 07962, U.S.A.

ABSTRACT

This paper is concerned with the problem of applying simulation to efficiently estimate the long-run average cost m associated with a Markov chain $\{X_n\}$ when a cost $F(X_{n-1}, X_n)$ is incurred during the nth state transition, $n = 1, 2, \ldots$ Our approach is to replace the cost structure F by a (smoother) cost structure F' which provably results in the same long-run average cost m, and (hopefully) results in easier simulation. We show that the smoothing techniques proposed in this paper lead to variance reduction when applied to two state Markov chains, and we also present empirical results that show that the application of these techniques can lead to variance reduction on more general Markov chains.

1 INTRODUCTION

Let $\{X_n\}$ be a discrete time Markov chain with state space $S = \{0, \ldots, K\}$, initial distribution μ, and a transition probability matrix P. Suppose that for all $i, j \in S$, a cost $F(i, j)$ is incurred whenever the Markov chain $\{X_n\}$ makes a transition from the state i to the state j, and that we are interested in estimating the long-run average cost

$$m = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} F(X_{n-1}, X_n).$$

We assume that the Markov chain $\{X_n\}$ has a unique stationary distribution π. Then it is possible to show that

$$m = \sum_{i=0}^{K} \pi(i) \sum_{j=0}^{K} P(i, j) F(i, j) \text{ a.s.}$$

One way of estimating the long-run average cost m is by applying what we refer to as "naive" simulation: choose a suitably large time horizon N, generate X_0 using the initial distribution μ and $X_1, \ldots, X_N$ using the transition probability matrix P, and use

$$\hat{m}(N) = \frac{1}{N} \sum_{n=1}^{N} F(X_{n-1}, X_n)$$

as an estimate for m. Unfortunately, $\hat{m}(N)$ sometimes has a high variance (this is particularly the case in rare event simulation, where m is very small), so the development of more efficient methods for estimating m is presently an active area of research. Importance sampling is a technique that has been developed for this purpose (see for instance Glynn and Iglehart (1989), Siegmund (1976) and Andradóttir, Heyman and Ott (1991, 1992b)). This method involves conducting the simulation of the Markov chain $\{X_n\}$ with an alternative initial distribution μ' and transition probability matrix P' and then using the likelihood ratio random variable to translate the results into an unbiased estimate for m. Control variates can also be used to obtain more efficient estimates of m (see for instance Lavenberg and Welch (1981), Rubinstein and Marcus (1985) and Andradóttir, Heyman and Ott (1992a)). In this paper, we will focus on smoothing methods for estimating m. These methods involve replacing the original cost structure F with an alternative cost structure F' in such a way that the long-run average cost m remains unchanged. For more detail on the smoothing methods that are discussed in this paper, the reader is referred to Andradóttir, Heyman and Ott (1992a).

This paper is organized as follows: in Section 2, we present some methods for smoothing the cost structure F, in Section 3, we show how these methods compare with naive simulation when applied to Markov chains on two states, and Section 4 contains empirical results, both for the example of Section 3 and for an example taken from Heyman (1992). Finally, Section 5 contains some concluding remarks.

2 SMOOTHING

The essential idea behind smoothing is that if F' is an alternative cost structure having the property that the long-run average cost

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} F'(X_{n-1}, X_n)$$

associated with the cost structure F' equals m almost surely, and if F' is smoother than F in the sense that the random variables $F'(X_{n-1}, X_n)$ are in general closer to m than the random variables $F(X_{n-1}, X_n)$, then it is reasonable to expect that

$$\frac{1}{N}\sum_{n=1}^{N} F'(X_{n-1}, X_n)$$

has a lower variance than $\hat{m}(N)$.

One way of smoothing the (matrix) cost structure F is by replacing it with a (vector) cost structure f, where

$$f(i) = \sum_{j=0}^{K} P(i,j)F(i,j) \tag{1}$$

for all $i \in S$. (This smoothing technique is closely related to a variance reduction scheme proposed earlier by Heidelberger (1980).) It is easy to show that

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} f(X_{n-1}) = m \text{ a.s.},$$

so this method for smoothing the original cost structure F does not affect the long-run average cost. We can therefore generate X_0 using the initial distribution μ and $X_1, \ldots, X_N$ using the transition probability matrix P, and use

$$\hat{m}_f(N) = \frac{1}{N+1}\sum_{n=0}^{N} f(X_n)$$

as an estimate of m. In Section 3, we show that when $K = 1$ and for $i = 0, 1$, $F(i,0) = 1$ and $F(i,1) = 0$, this smoothing method will always result in variance reduction.

Another method for (possibly) smoothing the (matrix) cost structure F is by replacing it by a (matrix) cost structure H, where

$$H(i,j) = F(i,j) - g(i) + g(j) \tag{2}$$

for all $i, j \in S$, and where g is an arbitrary vector. It is possible to show that

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} H(X_{n-1}, X_n) = m \text{ a.s.}$$

(see Andradóttir, Heyman and Ott (1992a)), so this smoothing method does not affect the long-run average cost. We can now combine the smoothing methods of equations (1) and (2) and replace the (matrix) cost structure F by the (vector) cost structure h, where

$$\begin{aligned} h(i) &= \sum_{j=0}^{K} P(i,j)H(i,j) \\ &= \sum_{j=0}^{K} P(i,j)[F(i,j) - g(i) + g(j)] \end{aligned} \tag{3}$$

for all $i \in S$. It is easy to show that

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} h(X_{n-1}) = m \text{ a.s.},$$

so this method for smoothing the cost structure F does not affect the long-run average cost. We now present a good way of selecting the vector g of equation (3).

It is clear that we would like to select the vector g in such a way that the vector h of equation (3) becomes as smooth as possible. The ideal situation would be to select the vector g in such a way that all the elements of h are equal to a constant c. In that situation equation (3) implies that

$$ce + (I - P)g = Me, \tag{4}$$

where $e^T = (1, \ldots, 1)$ and the (i,j)th element of the matrix M is

$$M(i,j) = P(i,j)F(i,j)$$

for all $i, j \in S$. Equation (4) is often referred to as Poisson's equation, and it is well known that this equation determines the constant $c = m$ uniquely and the vector g up to an additive constant (see for instance Theorem 4-13 in Heyman and Sobel (1984)). If it is possible to solve equation (4), then it is clearly not necessary to apply simulation to estimate m. However, in the situation where it is either very difficult or impossible to solve equation (4), we can obtain an approximate solution g and then generate X_0 using the initial distribution μ and $X_1, \ldots, X_N$ using the transition probability matrix P, and use

$$\hat{m}_g(N) = \frac{1}{N+1}\sum_{n=0}^{N} h(X_n)$$

as an estimate of m. The following iterative procedure can be used to obtain a sequence $\{g^{(k)}\}$ of approximate solutions to equation (4): Let a be an

arbitrary constant and let u be an arbitrary vector having the property that $u^T e = 1$. If $g^{(0)}$ is an arbitrary vector, and if, for all $k \geq 0$,

$$g^{(k+1)} = (aI + M)e + (P - eu^T)g^{(k)}, \qquad (5)$$

then it is possible to show that the sequence $\{g^{(k)}\}$ converges to a solution of equation (4) under general conditions (see Andradóttir, Heyman and Ott (1992a)). Moreover, it is possible to show that when k is large enough, $\hat{m}_{g^{(k)}}(N)$ has a lower asymptotic variance than $\hat{m}(N)$ (see Andradóttir, Heyman and Ott (1992a)). In Section 3, we show that when $K = 1$ and for $i = 0, 1$, $F(i, 0) = 1$ and $F(i, 1) = 0$, then $\hat{m}_{g^{(k)}}(N)$ has a lower asymptotic variance than $\hat{m}_f(N)$ when k is large enough; in one important special case, $k = 1$ is large enough.

3 MARKOV CHAINS WITH TWO STATES

For the simple case of two states, we can do the manipulations needed to effectively compute the variances of $\hat{m}(N)$, $\hat{m}_f(N)$ and $\hat{m}_{g^{(k)}}(N)$, $k = 1, 2, \ldots$, and then make comparisons. Let the transition matrix be

$$P = \begin{bmatrix} 1-c & c \\ d & 1-d \end{bmatrix}$$

with $0 < c, d < 1$ to ensure irreducibility.

Suppose we want to estimate $\pi(0)$, so

$$F = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$$

Let $M_i(N)$ be the the number of visits to state i by time N (that is $M_i(N) = \sum_{n=1}^{N} I_{\{X_n = i\}}$, where I_A is the indicator random variable), $i = 0, 1$. For naive simulation, $\hat{m}(N) = M_0(N)/N$ and

$$\sigma^2(N) = \mathrm{Var}[\hat{m}(N)] = \frac{\mathrm{Var}[M_0(N)]}{N^2}$$

From $M_0(N) + M_1(N) = N$, it is immediate that

$$\sigma^2(N) = \frac{\mathrm{Var}[M_1(N)]}{N^2} = -\frac{\mathrm{Cov}[M_0(N), M_1(N)]}{N^2}$$

When the vector cost structure $f = (1-c, d)^T$ is used, the variance $\sigma_f^2(N)$ of $\hat{m}_f(N)$ is given by

$$\begin{aligned} \sigma_f^2(N) &= (1-c)^2 \frac{\mathrm{Var}[M_0(N)]}{N^2} + d^2 \frac{\mathrm{Var}[M_1(N)]}{N^2} \\ &\quad + 2(1-c)d \frac{\mathrm{Cov}[M_0(N), M_1(N)]}{N^2} \\ &= (1-c-d)^2 \sigma^2(N) \qquad (6) \\ &< \sigma^2(N), \end{aligned}$$

so the smoothing method (1) always results in variance reduction in this situation.

Now we turn to the estimator $\hat{m}_{g^{(k)}}(N)$. Let $h^{(k)}$ be the cost structure obtained by using the vector $g^{(k)}$ of equation (5) in equation (3):

$$h^{(k)}(i) = \sum_{j=0}^{K} P(i, j) H^{(k)}(i, j)$$

for all $i \in S$, where

$$H^{(k)}(i, j) = F(i, j) - g^{(k)}(i) + g^{(k)}(j)$$

for all $i, j \in S$. Take $u^T = (v, 1-v)$, so the iteration matrix in (5) is

$$A = P - eu^T = \begin{bmatrix} 1-c-v & c+v-1 \\ d-v & v-d \end{bmatrix}$$

The eigenvalues of A are 0 and $\lambda = 1 - c - d$, and the Cayley-Hamilton theorem implies that $A^j = \lambda^{j-1} A$, for all j. Thus, the solution of (5) is

$$g^{(k)} = \left(\sum_{j=0}^{k-1} A^j \right) \alpha + A^k g^{(0)}, \qquad (7)$$

$k = 1, 2, \ldots$, where

$$\alpha = \begin{bmatrix} a+1-c \\ a+d \end{bmatrix}$$

The matrix $H^{(k)} = [H^{(k)}(i, j)]$ is given by

$$H^{(k)} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} + (g^{(k)}(1) - g^{(k)}(0)) \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \qquad (8)$$

The variance of the estimator $\hat{m}_{g^{(k)}}(N)$, $\sigma^2_{g^{(k)}}(N)$, is given by

$$\begin{aligned} \sigma^2_{g^{(k)}}(N) &= \frac{\mathrm{Var}[h^{(k)}(0) M_0(N) + h^{(k)}(1) M_1(N)]}{N^2} \\ &= [h^{(k)}(1) - h^{(k)}(0)]^2 \sigma^2(N). \qquad (9) \end{aligned}$$

From (7) and (8) we obtain

$$h^{(k)}(0) - h^{(k)}(1) = b\lambda^k, \qquad (10)$$

where

$$b = 1 - (c+d)[1 - g^{(0)}(1) + g^{(0)}(0)].$$

Substituting (10) into (9) yields

$$\sigma^2_{g^{(k)}}(N) = b^2 \lambda^{2k} \sigma^2(N). \qquad (11)$$

We have $\sigma^2_{g^{(k)}}(N) < \sigma_f^2(N)$ if and only if

$$b^2 \lambda^{2k-2} < 1. \qquad (12)$$

This condition holds whenever

$$0 < (c+d)[1 - g^{(0)}(1) + g^{(0)}(0)] < 2 \qquad (13)$$

(this makes $b^2 < 1$). In particular, (13) is valid when $g^{(0)}(0) = g^{(0)}(1) = 0$. In general, (12) holds when

$$k > 1 - \frac{\log b}{\log |\lambda|}$$

This contains $k = 1$ when λ is sufficiently small.

Remark: Extending the results in this section to Markov chains with three states is difficult. This is primarily because for three state Markov chains, the transition probability matrix P has six parameters, the matrix $A = P - eu^T$ has two non-zero eigenvalues that are roots of a quadratic equation, and we don't have a simple relationship between the variance and covariance terms of $M_i(N)$, $i = 0, 1, 2$.

4 EMPIRICAL WORK

In this section, we compare the performance of naive simulation with the performance of two of the smoothing methods that were discussed in Section 2: replacing the (matrix) cost structure F by the vector cost structure f of equation (1), and replacing the (matrix) cost structure F by the (vector) cost structure h of equation (3) with the vector g being an approximate solution to equation (4) obtained by using the iterative procedure (5). For each example and each sample path length N, common random numbers are used to be able to compare the performance of the three techniques more meaningfully. In order to compute the sequence $\{g^{(k)}\}$ of equation (5), we let $e = 1$, $u^T = (1, 0, \ldots, 0)$ and $(g^{(0)})^T = (0, \ldots, 0)$. We show in Andradóttir, Heyman and Ott (1992a) that the asymptotic variance of $\hat{m}_{g^{(k)}}(N)$ does not depend on e and u, so this choice is not critical.

Example 1 Consider the two state Markov chain of Section 3 with $c = 0.9$ and $d = 0.2$. We want to apply the three simulation techniques mentioned above to estimate $\pi(0) = \frac{2}{11} \simeq 0.181818$. Tables 1 and 2 show the average values and the sample variances of the point estimators $\hat{m}(N)$, $\hat{m}_f(N)$ and $\hat{m}_{g^{(k)}}(N)$, $k = 1, 2, 3$, obtained after 100 replications, for $N = 100$ and $N = 10^5$ respectively.

In both Tables 1 and 2, the variances have the form $\beta \times 10^{-p}$, where β is a constant. The reason is that using common random numbers makes the 100 realizations of $M_0(N)$ the same over all estimators (this accounts for β), our choices for c and d make $\lambda = -0.1$,

Table 1: Simulation Results for a Two State Markov Chain with $N = 100$

Estimate	Mean	Variance
$\hat{m}(N)$	0.1867	1.184×10^{-3}
$\hat{m}_f(N)$	0.1813	1.184×10^{-5}
$\hat{m}_{g^{(1)}}(N)$	0.181867	1.184×10^{-7}
$\hat{m}_{g^{(2)}}(N)$	0.181813	1.184×10^{-9}
$\hat{m}_{g^{(3)}}(N)$	0.1818187	1.184×10^{-11}

Table 2: Simulation Results for a Two State Markov Chain with $N = 100,000$

Estimate	Mean	Variance
$\hat{m}(N)$	0.18178	1.254×10^{-6}
$\hat{m}_f(N)$	0.18182	1.254×10^{-8}
$\hat{m}_{g^{(1)}}(N)$	0.1818178	1.254×10^{-10}
$\hat{m}_{g^{(2)}}(N)$	0.1818182	1.254×10^{-12}
$\hat{m}_{g^{(3)}}(N)$	0.1818182	1.254×10^{-14}

and our choice for $g^{(0)}$ makes $b = \lambda$ (accounting for the 10^{-p} term). The empirical variances conform to the formulas (6) and (11) in Section 3 exactly.

Example 2 Consider the five hundred state Markov chain having the transition probability matrix given below equation (10) in Heyman (1992), where $C_{max} = 250$, $u = 0.2$, $v = 0.7$, and, for all k, a_k is the probability a binomial variable with parameters $N = 4$ and $p = 0.9$ equals k. We want to apply the three simulation techniques mentioned above to estimate $\pi(0) \simeq 2.963 \times 10^{-5}$. Table 3 shows the average values and the sample variances of the point estimators $\hat{m}(N)$, $\hat{m}_f(N)$ and $\hat{m}_{g^{(k)}}(N)$, $k = 3, 50, 100$, obtained after 30 replications, for $N = 3 \times 10^5$.

Table 3: Simulation Results for a Five Hundred State Markov Chain with $N = 300,000$

Estimate	Mean	Variance
$\hat{m}(N)$	2.82×10^{-5}	7.03×10^{-11}
$\hat{m}_f(N)$	2.88×10^{-5}	1.49×10^{-11}
$\hat{m}_{g^{(3)}}(N)$	2.88×10^{-5}	1.44×10^{-11}
$\hat{m}_{g^{(50)}}(N)$	3.04×10^{-5}	6.22×10^{-12}
$\hat{m}_{g^{(100)}}(N)$	3.04×10^{-5}	6.08×10^{-12}

The variance of $\hat{m}_{g^{(50)}}(N)$ is an order of magnitude smaller than the variance of $\hat{m}(N)$. The approximately 50% decrease in the variance of $\hat{m}_{g^{(50)}}(N)$

compared to the variance of $\hat{m}_{g(3)}(N)$ conforms to the prediction made from Theorem 6.2 (as shown in the graph in Section 10) in Andradóttir, Heyman and Ott (1992a). That graph also predicts that diminishing returns has sat in when $k = 50$, as demonstrated by the small additional variance reduction achieved by increasing k to 100.

5 CONCLUSION

We have presented methods for smoothing the original cost structure F that can lead to variance reduction over naive simulation. When these methods are applied to two state Markov chains, they are guaranteed to result in variance reduction, and we have shown empirically that they can also result in variance reduction when applied to more general Markov chains.

A major strength of the smoothing methods discussed in this paper is that they can be applied mechanically. This is not the case for importance sampling, another variance reduction technique that can be applied in this context. Moreover, when these techniques are applied to two state Markov chains, smoothing always results in variance reduction, whereas importance sampling may result in a variance increase (see Andradóttir, Heyman and Ott (1991)).

ACKNOWLEDGEMENT

The work of the first author was supported by the National Science Foundation under Grant No. DDM-9210679.

REFERENCES

Andradóttir, S., D. P. Heyman, and T. J. Ott. 1991. On the choice of alternative measure in importance sampling with Markov chains. Submitted for publication.

Andradóttir, S., D. P. Heyman, and T. J. Ott. 1992a. Variance reduction through smoothing and control variates. Working paper.

Andradóttir, S., D. P. Heyman, and T. J. Ott. 1992b. Potentially unlimited variance reduction in importance sampling with Markov chains. Working paper.

Glynn, P. W., and D. L. Iglehart. 1989. Importance sampling for stochastic simulations. *Management Science* 35:1367-1392.

Heidelberger, P. 1980. Variance reduction techniques for the simulation of Markov processes, I: multiple estimates. *IBM Journal of Research and Development* 24:570-581.

Heyman, D. P., and M. J. Sobel. 1984. *Stochastic models in operations research, vol. II: stochastic optimization.* New York: McGraw-Hill.

Heyman, D. P. 1992. A performance model of the credit manager algorithm. *Computer Networks and ISDN Systems* 24:81-91.

Lavenberg, S. S., and P. D. Welch. 1981. A perspective on the use of control variables to increase the efficiency of Monte Carlo simulations. *Management Science* 27:322-335.

Rubinstein, R. Y., and R. Marcus. 1985. Efficiency of multivariate control variates in Monte Carlo simulation. *Operations Research* 33:661-677.

Siegmund, D. 1976. Importance sampling in the Monte Carlo study of sequential tests. *The Annals of Statistics* 4:673-684.

AUTHOR BIOGRAPHIES

SIGRÚN ANDRADÓTTIR is an Assistant Professor of Industrial Engineering at the University of Wisconsin - Madison. She received a B.S. in Mathematics from the University of Iceland in 1986, an M.S. in Statistics from Stanford University in 1989, and a Ph.D. in Operations Research from Stanford University in 1990. Her research interests include stochastic optimization, simulation and stochastic processes. She is presently a member of ORSA and TIMS.

DANIEL P. HEYMAN did his undergraduate work in Industrial and Electrical Engineering at Rensselaer Polytechnic Institute (1960). He received an M.I.E. degree from Syracuse University (1962) and his Ph.D. in Operations Research from the University of California - Berkeley in 1966, and then joined Bell Laboratories. He transferred to Bellcore at the epoch of the AT&T divestiture. His research areas are numerical analysis of stochastic processes, queueing theory, and performance models of data communications systems.

TEUNIS J. OTT is Director of Operations Research and Computational Analysis at Bell Communications Research. He obtained a "Doctoraal" in Mathematics at the University of Amsterdam in 1970 and a Ph.D. in Operations Research at the University of Rochester in 1974. After teaching at Case Western Reserve University and at the University of Texas, he joined Bell Laboratories in 1978, and at divestiture he went to Bellcore. His current research interest is in the traffic theory of broadband communications systems, including efficient simulation of such systems.