EXPERIMENTAL EVALUATION OF INTEGRATED PATH ESTIMATORS

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ABSTRACT

We describe the results of numerical experiments evaluating the efficiency of variance estimators based on integrated sample paths. The idea behind the estimators is to compute a vector of integrated paths and combine them to form an estimator of the time-average variance constant that is used, for example, in the construction of confidence intervals. When used in conjunction with batching, the approach generalizes the method of non-overlapping batch means. Compared with non-overlapping batch means, the estimators require longer to compute, have smaller variance and larger bias. We show that for long enough simulation run lengths, the efficiency (the reciprocal of running time multiplied by mean-squared error) of integrated path estimators can be much greater than that of non-overlapping batch means; the numerical experiments show an efficiency improvement by up to a factor of ten.

1 INTRODUCTION

In steady-state discrete-event simulation, we are often interested in estimating the variance parameter associated with a stationary output process. Many methods have been proposed, such as batch means (non-overlapping and overlapping), spectral methods, and the regenerative method; see for example Law and Kelton (2000). In this paper we describe a method based on computing a vector of integrated simulation paths, an approach introduced in Calvin (2005).

Suppose that the discrete-event simulation generates a real-valued output sequence Y_1, Y_2, \ldots . We assume that the process satisfies a functional central limit theorem of the following form. Assume that there exist constants $\mu \in \mathbb{R}$ and $\sigma \in (0, \infty)$ such that the sequence of processes

$$X_n(t) = \sigma^{-1} n^{-1/2} \sum_{i=1}^{\lceil nt \rceil} (Y_i - \mu), \quad 0 \le t \le 1,$$

converges in distribution to a standard Brownian motion, where $\lceil x \rceil$ denotes the smallest integer not less than *x*. Here we take convergence to be in the space *D* of right-continuous processes with left hand limits, endowed with the Skorohod metric; see Billingsley (1999). Under this assumption,

$$n^{1/2}\left(\frac{1}{n}\sum_{i=1}^{n}Y_{i}-\mu\right) \xrightarrow{\mathcal{D}} \mathcal{N}(0,\sigma^{2}),$$
(1)

where $\xrightarrow{\mathcal{D}}$ denotes convergence in distribution. A suitable estimate of σ^2 enables the use of the central limit theorem (1) to construct asymptotically valid confidence intervals for the steady-state mean μ . An estimate of σ^2 can also be used in adaptive methods for comparing the performance of alternative systems.

2 OVERVIEW OF ESTIMATORS

We define a family of estimators indexed by a positive integer parameter k, which we call the integration count. The memory required to compute the estimators increases linearly with k, and the overall computation time increases roughly affinely with k. The parameter k should be small compared to the square root of the simulation run length.

The estimator that we consider in this paper is a two-pass estimator. See Calvin (2005) for a one-pass version.

In the first phase, a simulation is run producing output Y_1, Y_2, \ldots, Y_n . Let

$$\mu_n = \frac{1}{n} \sum_{i=1}^n Y_i$$

be the sample mean. The construction of the estimator will be based on the "bridged" path

$$W_i^0 = \sum_{j=1}^i Y_j - i\mu_n, \quad 1 \le i \le n.$$

The idea is to compute the *r*-times integrated paths, for $1 \le r \le k$, and use the limit distribution of the normalized vector of integrated paths. For $1 \le r \le k$, set

$$W_{i}^{r} = \sum_{l=1}^{i} W_{l}^{r-1}$$
(2)

and

$$\widetilde{W}_{n}^{r} = n^{-r-1/2} W_{n}^{r} - \sum_{j=1}^{r-1} (-1)^{r-j} s(r,j) \frac{j!}{r!} \widetilde{W}_{n}^{j},$$

where the s(n,i) are the Stirling numbers of the first kind, satisfying the recurrence

$$s(n+1,m) = s(n,m-1) - ns(n,m), \quad 1 \le m \le n$$

and s(n,n) = 1, and s(0,0) = 1, s(n,0) = 0 for $n \ge 1$. For $1 \le r \le k$, set

$$Z_n^r = \sum_{j=1}^r A_{rj} n^{-j-1/2} \widetilde{W}_n^j,$$

where

$$A_{ij} = \frac{(-1)^{i+j}(i+j)!\sqrt{2i+1}}{j!(i-j)!}$$
(3)

if $1 \le j \le i$ and $A_{ij} = 0$ otherwise.

We define our estimator of σ^2 based on a simulation of length *n* by

$$V_n = \frac{1}{k} \sum_{r=1}^k (Z_n^r)^2.$$
 (4)

Theorem 1 As $n \to \infty$,

$$V_n \xrightarrow{\mathcal{D}} \sigma^2 \frac{\chi_k^2}{k},\tag{5}$$

where χ_v^2 denotes a chi-squared random variable with v degrees of freedom.

The asymptotic variance of V_n as $n \to \infty$ is therefore $2\sigma^4/k$.

We now consider the bias of the estimator V_n . We will assume that $\{Y_i\}$ is a second order stationary process with $EY_i = 0$ and $EY_iY_{i+j} = \gamma_j$, $j \ge 0$. We further assume that

$$\sum_{j=1}^{\infty} j |\gamma_j| < \infty$$

and define

$$\lambda = \sum_{j=1}^{\infty} j \gamma_j$$

With these assumptions we have the representation

$$\sigma^2 = \gamma_0 + 2\sum_{j=1}^{\infty} \gamma_j.$$

Theorem 2 For fixed k, we have

$$n\left(EV_n-\sigma^2\right)\to-2k\lambda$$

as $n \to \infty$.

Theorems 1 and 2 are proved in Calvin (2005).

3 BATCHING

In this section we describe how the integrated path estimator can be used in a batching context. Suppose that the simulation length *n* can be expressed as n = mb, where *b* is the batch size and *m* is the number of batches. The integrated path estimator of the previous section can be applied to each batch (subtract from W^0 the linear interpolation between W_{jb}^0 and $W_{(j+1)b-1}^0$ for each $0 \le j < m$). Apply the standard method of (non-overlapping) batch means to W^0 , obtaining a batch means estimator B_n^m . As simulation run length $n \to \infty$ (with the number of batches *b* held fixed and batch size $m \to \infty$),

$$B_n^m \xrightarrow{\mathcal{D}} \sigma^2 \frac{\chi_{b-1}^2}{b-1};$$

see for example Chien, Goldsman, and Melamed (1997). Let V_n^i be the integrated path estimator for batch *i*. Our integrated path estimator with batching is defined by

$$V_{b,n} = \frac{k \sum_{i=1}^{b} V_n^i + (b-1)B_n^m}{kb+b-1},$$

for which we have

$$V_{b,n} \stackrel{\mathcal{D}}{\to} \sigma^2 \frac{\chi^2_{kb+b-1}}{kb+b-1}$$

as $n \to \infty$.

4 EFFICIENCY

In addition to studying the variance and bias of the estimators, our goal is to examine their efficiency. We take the efficiency of an estimator with bias B and variance V, that takes time

t to compute, to be

$$\frac{1}{t(B^2+V)};$$

that is, the efficiency of a simulation estimator is the reciprocal of the mean-squared error multiplied by the running time. Increasing the parameter k increases the running time, while decreasing the variance and increasing the bias.

In order to get a feeling for the efficiency with large values of *n* and *k*, let us consider a simple computational model for the simulation. Suppose that the time to perform an add/store is α , and the time to generate one step of the simulation data is β . In general we would expect β to be much larger than α , but we do not assume that is the case. The *k* terms $\{W_n^r : 1 \le r \le k\}$ can be computed in time $kn\alpha$; adding the time $n\beta$ to generate the simulation, we have a total computation time of $n(k\alpha + \beta)$. (The computation of V_n requires additional work of $O(k^2)$, which we ignore since $k^2 = o(n)$.) From Theorems 1 and 2, we expect that the efficiency is therefore approximately

$$\frac{1}{n(k\alpha+\beta)\left(\frac{4\lambda^{2}k^{2}}{n^{2}}+\frac{2\sigma^{4}}{k}\right)}$$
$$=\frac{1}{2\sigma^{4}n(\alpha+\beta/k))(1+\mathcal{O}(n^{-2}))}.$$

Let us consider increasing run length with increasing $k = k_n$, where $k_n = o(n^{1/2})$. Then as $n \to \infty$, the relative efficiency of the integrated path estimator compared with the standard non-overlapping batch means estimator is

$$\frac{\alpha+\beta}{\alpha+\beta/k}.$$

Thus asymptotically as $n \to \infty$ efficiency is increasing in k (still assuming that $k = o(n^{1/2})$). As k increases, the limiting ratio is

$$1+\frac{\beta}{\alpha}$$
.

If the time to generate a step of the simulation β is much longer than the time to perform an addition and store α , then the potential efficiency improvement would be correspondingly large.

Of course, for fixed n there will be a point beyond which increasing k degrades performance.

5 EXPERIMENTS

This section reports the results of numerical experiments on a first-order autoregressive process. We ran experiments calculating the sample variance, sample bias, and running time. Based on these data we also computed the efficiency.

In the experiments we computed the relative increase in efficiency compared with the base case of k = 0, which is the standard method of batch means. The AR(1) model is inexpensive to simulate; the efficiency increases would be larger for more computationally intensive simulations.

The AR(1) model is a stationary Gaussian process defined by $Y_0 \sim N(0,1)$ and

$$Y_i = \varphi Y_{i-1} + \varepsilon_i, \quad i \ge 1,$$

where $-1 < \varphi < 1$ and the $\{\varepsilon_i\}$ are independent, $\varepsilon_i \sim N(0, 1 - \varphi^2)$. For this process $\gamma_k = \varphi^k$,

$$\lambda = \sum_{k=1}^{\infty} k \gamma_k = \frac{\varphi}{(1-\varphi)^2}$$

and

$$\sigma^2 = \gamma_0 + 2\sum_{k=1}^{\infty} \gamma_k = \frac{1+\varphi}{1-\varphi}.$$

For the experiment we took $\varphi = 0.9$, so $\sigma^2 = 19$ and

$$\lambda = \frac{\phi}{(1-\phi)^2} = 90$$

The model and these calculations are described in Alexopoulos, Argon, Goldsman, Steiger, Tokol, and Wilson (2005).

The experiments consisted of 1,000 independent replications, with each simulation split into b = 20 batches. In Table 1 we show the bias, variance, and mean-squared error for k between 0 and 10 and simulation run length n = 20,000. In Table 2 we show the same performance characteristics, but with a longer run length of n = 200,000and for k ranging from 0 to 20. Notice that with the longer run length, efficiency increases with larger values of k. In both cases, efficiency decreases with k after some point.

6 CONCLUSIONS

The integrated path estimators considered in this paper have aymptotic variance proportional to 1/k, where *k* is the fixed integration count parameter which should be chosen small compared to the square root of the simulation run length. When used in conjunction with batching, the method generalizes the popular method of (non-overlapping) batch means.

Compared with the standard non-overlapping batch means estimator, the integrated path estimators have lower mean-squared error, and for long enough simulation run lengths the efficiency of the estimators is increasing in the

k	variance	bias	MSE	rel. eff.
0	35.80	-0.28	35.88	1.00
1	18.42	-0.43	18.61	1.80
2	11.75	-0.58	12.09	2.36
3	8.71	-0.72	9.22	3.00
4	6.65	-1.08	7.83	3.34
5	5.64	-1.15	6.96	3.48
6	4.25	-1.43	6.31	3.75
7	3.67	-1.48	5.86	3.59
8	3.51	-1.77	6.66	3.16
9	2.92	-1.83	6.26	3.16
10	2.87	-2.07	7.16	2.65

Table 1: Performance of Integrated-Path Estimators for Different Parameters k, Simulation Run Length 20,000

Table 2: Performance of Integrated-Path Estimators for Different Parameters *k*, Simulation Run Length 200,000

k	variance	bias	MSE	rel. eff.
0	36.35	0.09	36.35	1.00
1	18.80	0.07	18.81	1.73
2	12.50	-0.14	12.52	2.39
3	9.47	0.13	9.48	2.99
4	7.33	-0.12	7.34	3.66
5	5.43	-0.13	5.44	4.64
6	5.47	-0.01	5.47	4.42
7	4.55	-0.13	4.57	5.05
8	4.02	-0.18	4.05	5.40
9	3.57	-0.09	3.58	5.86
10	3.23	-0.21	3.27	6.15
11	2.92	-0.27	2.99	6.47
12	2.57	-0.26	2.63	7.04
13	2.49	-0.24	2.55	8.89
14	2.33	-0.28	2.41	9.07
15	2.28	-0.22	2.32	9.13
16	2.04	-0.37	2.17	9.50
17	1.72	-0.36	1.85	10.85
18	1.84	-0.33	1.94	10.05
19	1.90	-0.40	2.06	9.19
20	1.66	-0.44	1.85	9.99

parameter k. In numerical examples, the efficiency increases by up to a factor of 10.

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