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A COMPREHENSIVE REVIEW OF METHODS FOR SIMULATION OUTPUT ANALYSIS

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ABSTRACT

This paper reviews statistical methods for analyzing output data from computer simulations. Specifically, it focuses on the estimation of steady-state system parameters. The estimation techniques include the replication/deletion approach, the regenerative method, the batch means method, and methods based on standardized time series.

1 INTRODUCTION

A primary goal of most simulation studies is the approximation of prescribed system parameters with the objective of identifying parameter values that optimize some system performance measures. Since the input processes driving a simulation are often random, the output data are also random and runs of the simulation program only result in *estimates* of system performance measures.

A simulation study consists of several steps such as data collection, coding and verification, model validation, experimental design, output data analysis, and implementation. This paper reviews statistical methods for computing confidence intervals for system performance measures from output data. Statistical methods for determining the best system from a set of alternatives are the subject of the tutorial by Benson et al. (2006) in this volume. This tutorial does not aim at replacing "standard" texts, such as Fishman (2001) or Law (2006). A comprehensive coverage of the topics reviewed herein is presented in Chapters 8, 15, and 16 of the recent handbook edited by Henderson and Nelson (2006) and in the entry by Alexopoulos et al. (2006d).

There are two types of simulations with regard to output analysis:

Finite-horizon simulations. In this case the simulation starts in a specific state and is run until some terminating event occurs. The output process is not expected to achieve any steady-state behavior and any parameter estimated from the output data will be transient in the sense that its value will depend upon the initial conditions. An example is the simulation of a vehicle storage and distribution facility for a week.

Steady-state simulations. The purpose of a steady-state simulation is the study of the long-run behavior of the system of interest. A performance measure of a system is called a *steady-state parameter* if it is a characteristic of the equilibrium distribution of an output stochastic process. An example is the simulation of a continuously operating communication system where the objective is the computation of the mean delay of a data packet.

Section 2 discusses methods for analyzing output from finite-horizon simulations. Section 3 presents techniques for point and interval estimation of steady-state parameters.

2 FINITE-HORIZON SIMULATIONS

Suppose that we simulate a system until n output data $X_1, X_2, \ldots, X_n$ are collected with the objective of estimating $\mu \equiv \mathrm{E}(\bar{X}_n)$, where $\bar{X}_n \equiv \frac{1}{n}\sum_{i=1}^{n} X_i$ is the sample mean of the data. For example, X_i may be the transit time of unit i through a network of queues or the total time station i is busy during the ith hour. Clearly, $\bar{X}_n$ is an unbiased estimator for μ. Unfortunately, the X_i are generally dependent random variables making the estimation of the variance $\mathrm{Var}(\bar{X}_n)$ a nontrivial problem. Let $S_n^2(X) \equiv \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2$ be the sample variance of the data. The presence of autocorrelation makes the familiar estimator $S_n^2(X)/n$ a biased estimator of $\mathrm{Var}(\bar{X}_n)$. In particular, if the X_i are positively correlated, one has $\mathrm{E}(S_n^2(X)/n) < \mathrm{Var}(\bar{X}_n)$ (see Section 3).

To overcome this problem, one can run k independent replications of the system simulation. Assume that run i produces the output data $X_{i1}, X_{i2}, \ldots, X_{in}$. Then the replicate averages $Y_i = \frac{1}{n}\sum_{j=1}^{n} X_{ij}$ are independent and identically distributed (IID) random variables, their sample mean $\bar{Y}_k = \frac{1}{k}\sum_{i=1}^{k} Y_i$ is also an unbiased estimator of μ, and their sample variance $\hat{V}_R = S_k^2(Y)$ is an unbiased

estimator of $\mathrm{Var}(\bar{X}_n)$. If in addition k is sufficiently large, an approximate $1-\alpha$ confidence interval (CI) for μ is

$$\bar{Y}_k \pm t_{k-1,1-\alpha/2}\sqrt{\hat{V}_R/k}\,, \tag{1}$$

where $t_{d,\delta}$ represents the δ-quantile of Student's t distribution with d degrees of freedom.

Alexopoulos and Seila (1998, Section 7.2.2) review sequential procedures for determining the number of replications required to estimate μ with a fixed absolute or relative precision. The procedure for constructing a $1-\alpha$ CI for μ with a small absolute error $|\bar{Y}_k-\mu|\le\beta$ is based on Chow and Robbins (1965). It starts with $k\ge 5$ runs and stops when the halfwidth $t_{k-1,1-\alpha/2}\sqrt{\hat{V}_R/k}\le\beta$. Law (2006, pp. 501–502) describes an empirical method for obtaining an estimate whose relative error satisfies $\Pr(|\bar{Y}_k-\mu|/|\mu|\le\gamma)\ge 1-\alpha$, with $\alpha\le 0.15$. The method starts with $k\ge 10$ runs and stops when the relative halfwidth $t_{k-1,1-\alpha/2}|\bar{Y}_k|^{-1}\sqrt{\hat{V}_R/k}$ drops below $\gamma/(1+\gamma)$.

The method of replications can also be used for estimating performance measures other than means. Let Y be the total cost incurred in an inventory system during a certain time window, and let $y_p\equiv\inf\{y:\Pr(Y\le y)\ge p\}$ denote the p-quantile of Y. To estimate y_p, we can make k independent replications, denote by Y_i the cost observed during replication i, and let $Y_{(1)}<Y_{(2)}<\cdots<Y_{(k)}$ be the order statistics corresponding to the Y_i. Then a point estimate for y_p is $\hat{\xi}_p=Y_{(kp)}$ if kp is an integer or $\hat{y}_p=Y_{(\lfloor kp+1\rfloor)}$ otherwise ($\lfloor\cdot\rfloor$ is the floor function). A CI for y_p is described in Alexopoulos and Seila (1998, Section 7.3.2).

3 STEADY-STATE ANALYSIS

We focus on methods for computing point and interval estimators for the mean of a discrete-time stationary process. Analogous methods for analyzing continuous-time output data are described in a variety of texts (Fishman 2001; Law 2006). The process $X=\{X_i\}$ is called *stationary* if the joint distribution of $X_{i+j_1},X_{i+j_2},\ldots,X_{i+j_k}$ is independent of i for all indices $j_1,j_2,\ldots,j_k$ and all $k\ge 1$. If $\mathrm{E}(X_i)=\mu$, $\mathrm{Var}(X_i)\equiv\sigma_X^2<\infty$ for all i, and the $\mathrm{Cov}(X_i,X_{i+j})$ is independent of i, then X is called *weakly stationary*. We denote the autocovariance function of X by $R_j\equiv\mathrm{Cov}(X_1,X_{1+j})$ $(j=0,\pm1,\pm2,\ldots)$. Notice that $R_0=\sigma_X^2$. Alexopoulos et al. (2006d) give a detailed overview of the properties of stationary processes that are central to simulation output analysis and proceed with a detailed description of the majority of the methods in this section.

Let $\bar{X}_n$ and $S_n^2(X)$ be the sample mean and sample variance of n observations, say $X_1,\ldots,X_n$. Clearly $\bar{X}_n$ is not only unbiased for μ, but also strongly consistent by the ergodic theorem (see Durrett 2005).

Under the assumption that $\bar{X}_n$ is approximately normally distributed (which is reasonable for sufficiently large n), the usual construction of a CI for μ requires the derivation of an estimator for $\mathrm{Var}(\bar{X}_n)$. A little algebra yields (Anderson 1984),

$$\mathrm{E}\left[\frac{S_n^2(X)}{n}\right]=\frac{\frac{n}{a_n}-1}{n-1}\mathrm{Var}(\bar{X}_n), \tag{2}$$

where $a_n=1+(2/\sigma_X^2)\sum_{j=1}^{n-1}(1-j/n)R_j$. Then for processes that are positively correlated ($R_i>0$), Equation (2) implies that $\mathrm{E}[S_n^2(X)/n]<\mathrm{Var}(\bar{X}_n)$. Hence the "classical" $1-\alpha$ CI for IID data $\bar{X}_n\pm t_{n-1,1-\alpha/2}\frac{S_n(X)}{\sqrt{n}}$ can have coverage probability that can be considerably below the nominal value $1-\alpha$.

A common assumption facilitating the derivation of a CI for μ is as follows:

Functional Central Limit Theorem (FCLT) Assumption. Suppose that the series

$$\sigma^2\equiv\sigma_X^2+2\sum_{j=1}^{\infty}R_j \tag{3}$$

is absolutely convergent and $\sigma^2>0$. Let

$$X_n(t)\equiv\frac{\lfloor nt\rfloor(\bar{X}_{\lfloor nt\rfloor}-\mu)}{\sigma\sqrt{n}},\quad t\ge 0.$$

Then $X_n(\cdot)\Longrightarrow\mathcal{W}$, where $\{\mathcal{W}(t):t\ge 0\}$ is a standard Brownian motion process. We call σ^2 the *(asymptotic) variance parameter* of X.

This assumption holds under several conditions (see Durrett 2005). Examples are a condition involving conditional second moments of X and the stronger φ-mixing condition: X is *φ-mixing* if there are $\varphi_k\downarrow 0$ such that, for each $k\ge 0$, $A\in\mathcal{F}_{-\infty}^{j}$, and $B\in\mathcal{F}_{j+k}^{\infty}$,

$$|\Pr(A\cap B)-\Pr(A)\Pr(B)|\le\varphi_k\Pr(A).$$

Here $\mathcal{F}_i^j$ $(i\le j)$ denotes the σ-field generated by $X_i,X_{i+1},\ldots,X_j$.

Remark 1 Contrary to popular belief, many stochastic processes encountered in simulation output analysis are *not* φ-mixing. Examples are autoregressive processes, regenerative processes (see Section 3.3) with regenerations not occurring uniformly fast over the state space, and virtually all open queueing networks (Glynn and Iglehart 1985).

The variance of the sample mean in terms of the autocovariance function is

$$\mathrm{Var}(\bar{X}_n)=\frac{1}{n}\left[\sigma_X^2+2\sum_{j=1}^{n-1}(1-j/n)R_j\right]. \tag{4}$$

Assumption $0 < \sigma^2 < \infty$ along with Equation (4) imply $\lim_{n\to\infty} n\mathrm{Var}(\bar{X}_n) = \sigma^2$ and $\lim_{n\to\infty} \mathrm{Var}(\bar{X}_n) = 0$; hence $\bar{X}_n$ is also consistent (in mean square error). Our focus will be on methods for obtaining CIs for μ, which involve estimating σ^2.

Finally, the "little-oh" notation $f(m) = o(g(m))$ means that $f(m)/g(m) \to 0$ as $m \to \infty$; and the "big-oh" notation $f(m) = O(g(m))$ means that there is a positive integer m_0 such that $|f(m)/g(m)| \le C$ for some constant C and all $m \ge m_0$.

3.1 Dealing with the Initial Conditions

Several problems arise when the process X does not start in steady-state. For example, $\bar{X}_n$ is not an unbiased estimator of the mean μ. The removal of the effect of the initial conditions is a challenging problem.

The most commonly used method for eliminating the bias of $\bar{X}_n$ identifies an index l and *truncates* the observations $X_1, \ldots, X_l$. Several procedures have been proposed for the detection of a cutoff index l (see Fishman 2001; Law 2006; Ockerman 1995; Wilson and Pritsker 1978a,b).

The graphical procedure of Welch (1983) uses k independent replications, with the ith replication producing observations $X_{i1}, X_{i2}, \ldots, X_{in}$, and computes the "across-runs" averages $\bar{X}_j = \frac{1}{k}\sum_{i=1}^{k} X_{ij}$, $j = 1, \ldots, n$. Then for a given time window w, the procedure plots the *moving averages*

$$\bar{X}_j(w) = \begin{cases} \frac{1}{2w+1}\sum_{m=-w}^{w} \bar{X}_{j+m} & w+1 \le j \le n-w \\ \frac{1}{2j-1}\sum_{m=-j+1}^{j-1} \bar{X}_{j+m} & 1 \le j \le w \end{cases}$$

against j. If the plot is reasonably smooth, then l is chosen to be the value of j beyond which the sequence of moving averages converges. Otherwise, a different time window is chosen and a new plot is drawn. The choice of w may be a difficult problem for congested systems with output time series having autocorrelation functions with long tails (see Alexopoulos and Seila 1998, Example 7).

3.2 The Replication/Deletion Approach

This intuitive approach runs k independent replications, each of length $l + n$ observations, and discards the first l observations from each run. One then uses the IID sample means $Y_i(l, n) = \frac{1}{n}\sum_{j=l+1}^{l+n} X_{ij}$ from the k runs to compute the point estimate $\bar{Y}_k(l, n) = \frac{1}{k}\sum_{i=1}^{k} Y_i(l, n)$ and the following approximate $1 - \alpha$ CI for μ:

$$\bar{Y}_k(l, n) \pm t_{k-1,1-\alpha/2}\sqrt{\hat{V}_R(l, n)/k}, \qquad (5)$$

where $\hat{V}_R(l, n)$ is the sample variance of the $Y_i(l, n)$.

The method is simple and general, but involves the choice of three parameters, l, n and k. Here are a few points the user should be aware of: (a) As l increases for fixed n, the "systematic" error in each $Y_i(l, n)$ due to the initial conditions decreases. (b) As n increases for fixed l, the systematic and sampling errors in $Y_i(l, n)$ decrease. (c) The systematic error in the sample means $Y_i(l, n)$ *cannot* be reduced by increasing the number of replications k. (d) For fixed n and under some mild moment conditions that are satisfied by a variety of simulation output processes, the CI (5) is asymptotically valid only if $l/\ln k \to \infty$ as $k \to \infty$ (Fishman 2001). This means that as one makes more runs in an attempt to compute a narrower CI, the truncation index l must increase faster than $\ln k$ for the CI to achieve the nominal coverage. This requirement is hard to implement in practice. (e) This method is also potentially wasteful of data as the truncated portion is removed from each replication. Additional shortcomings of this method are presented in Alexopoulos and Goldsman (2004).

The regenerative method (Section 3.3) and the batch means method (Section 3.4) seek to overcome the aforementioned issues. For a thorough comparison between the methods of independent replications and batch means, see Alexopoulos and Goldsman (2004).

3.3 The Regenerative Method

This method assumes the identification of time indices at which the process X probabilistically *starts over* and uses these regeneration epochs for obtaining IID random variables which can be used for computing point and interval estimates for the mean μ. The method was proposed by Crane and Iglehart (1975) and Fishman (1973, 1974). More precisely, assume that there are (random) time indices $1 \le T_1 < T_2 < \cdots$ such that the portion $\{X_{T_i+j}, j \ge 0\}$ has the same distribution for each i and is independent of the portion prior to time T_i. The portion of the process between two successive regeneration epochs is called a *cycle*. Let $Y_i = \sum_{j=T_i}^{T_{i+1}-1} X_j$ and $Z_i = T_{i+1} - T_i$ for $i = 1, 2, \ldots$ and assume that $\mathrm{E}(Z_i) < \infty$. Then the steady-state mean μ is given by $\mu = \mathrm{E}(Y_1)/\mathrm{E}(Z_1)$.

Now suppose that one simulates the process X over n cycles and collects the observations $Y_1, \ldots, Y_n$ and $Z_1, \ldots, Z_n$. Then $\hat{\mu} = \bar{Y}_n/\bar{Z}_n$ is a strongly consistent estimator of μ. Furthermore, CIs for μ can be constructed by using the IID random variables $Y_i - \mu Z_i, i = 1, \ldots, n$ and the central limit theorem (see Iglehart 1975).

The regenerative method is difficult to apply in practice because the majority of simulations have either no regenerative points or very long cycle lengths. Two classes of systems this method has successfully been applied to are inventory systems and highly reliable communications systems with repairs.

3.4 The Batch Means Method

The method of nonoverlapping batch means (NBM) is a popular approach for computing point and CI estimators for the mean μ of a stationary process. Original accounts on the method were given by Conway (1963), Fishman (1978), and Law and Carson (1979); see Alexopoulos and Goldsman (2004) and Fishman (2001) for detailed coverage.

Suppose that the sample $X_1, \ldots, X_n$ is divided into k contiguous batches, each consisting of m observations (for simplicity, we assume $n = km$). For $i = 1, \ldots, k$, the ith batch consists of the observations $X_{(i-1)m+1}, X_{(i-1)m+2}, \ldots, X_{im}$ and the ith batch mean $Y_{i,m} = \frac{1}{m}\sum_{j=1}^{m} X_{(i-1)m+j}$ is the sample average from batch i. The NBM-based estimator of the mean is the grand sample mean

$$\bar{X}_n = \frac{1}{k}\sum_{i=1}^{k} Y_{i,m} = \frac{1}{n}\sum_{i=1}^{n} X_i. \tag{6}$$

Clearly, the stationarity of X implies $\mathrm{E}(\bar{X}_n) = \mu$ and the stationarity of the batch means sequence $\{Y_{i,m} : i \geq 1\}$.

The motivation behind the NBM method is simple. First, under the FCLT, one can show that as $m \to \infty$, the batch means become uncorrelated (Law and Carson 1979) and normally distributed. Since the grand mean $\bar{X}_n$ is the sample average of the batch means, one has the approximation

$$n\mathrm{Var}(\bar{X}_n) \doteq n\mathrm{Var}(Y_{1,m})/k = m\mathrm{Var}(Y_{1,m}).$$

Hence the NBM estimator for σ^2 is

$$\hat{V}_B(k,m) \equiv \frac{m}{k-1}\sum_{i=1}^{k}(Y_{i,m} - \bar{X}_n)^2, \tag{7}$$

which is m times the sample variance of the batch means. An approximate $1-\alpha$ CI for μ is

$$\bar{X}_n \pm t_{k-1,1-\alpha/2}\sqrt{\frac{\hat{V}_B(k,m)}{n}}. \tag{8}$$

Of course, the fundamental issue is the choice of the batch size and the number of batches. Several early studies (e.g., Fishman 1978; Schmeiser 1982) addressed this issue, but without the rigor of recent studies.

To motivate the description of the modern procedures, we focus on the mean squared error (MSE) of $\hat{V}_B(k,m)$ and the coverage of the CI (8). Here we let $\sigma_n^2 \equiv n\mathrm{Var}(\bar{X}_n)$, and define the "center of gravity" constant

$$\gamma \equiv -\sum_{j=-\infty}^{\infty} jR_j = -2\sum_{j=1}^{\infty} jR_j. \tag{9}$$

One can show that

$$\mathrm{E}[\hat{V}_B(k,m)] = \frac{1}{k-1}(k\sigma_m^2 - \sigma_n^2).$$

If in addition $\mathrm{E}(X_1^4) < \infty$, and the process X is φ-mixing with $\varphi_j = O(j^{-4-\epsilon})$ for some $\epsilon > 0$, then γ exists and

$$\sigma_n^2 = \sigma^2 + \gamma/n + o(1/n). \tag{10}$$

Combining the last two equations we obtain

$$\mathrm{E}[\hat{V}_B(k,m)] = \sigma^2 + (k+1)\gamma/n + o(1/n). \tag{11}$$

Hence, $\hat{V}_B(k,m)$, usually has negative first-order bias for positively autocorrelated processes.

Also, the additional assumptions $\mathrm{E}(X_1^{12}) < \infty$ and $\varphi_j = O(j^{-9})$ allow one to write (Chien et al. 1997)

$$\begin{aligned}\mathrm{Var}[\hat{V}_B(k,m)] &= \frac{2\sigma^4(k+1)}{(k-1)^2} + O(1/(km^{1/4})) \\ &\quad + O(1/k^2).\end{aligned} \tag{12}$$

Then the MSE of the variance estimator $\hat{V}_B(k,m)$ has the form

$$\mathrm{MSE}[\hat{V}_B(k,m)] = O(1/(km^{1/4})) + O(1/k^2) \to 0, \tag{13}$$

as $m, k \to \infty$. Property (13) implies weak consistency for the estimator $\hat{V}_B(k,m)$, but does not guarantee the asymptotic validity of the CI in Equation (8). Before we discuss batching rules that yield the last property, we briefly examine how the variance estimator $\hat{V}_B(k,m)$ approaches σ^2. As in Fishman (2001, p. 251), Equation (11) allows us to write

$$\begin{aligned}\hat{V}_B(k,m) - \sigma^2 = {} & \underbrace{\sigma_n^2 - \sigma^2}_{\substack{\text{error due to} \\ \text{finite } n}} \\ & - \underbrace{\sigma_n^2 \frac{1 - \sigma_m^2/\sigma_n^2}{1 - m/n}}_{\substack{\text{error due to} \\ \text{ignoring correlations} \\ \text{between batch means}}} + \underbrace{\epsilon_n}_{\substack{\text{error due to} \\ \text{random sampling}}},\end{aligned} \tag{14}$$

where the error ϵ_n has mean zero and variance given by Equation (12). We call the first two terms on the right-hand side of Equation (14) a systematic error; by Equation

(10) this error behaves as $O(1/m)$. On the other hand, Equation (12) implies that the standard deviation of ϵ_n behaves as $O(1/k^{1/2})$. These growth rates reveal the tradeoff between the two types of error induced by k and m. Since σ_n^2 approaches σ^2 from below for a variety of systems with positive autocorrelation functions, the systematic error induces a negative bias in $\hat{V}_B(k,m)$ that dissipates as the batch size increases. Then the error due to random sampling fluctuates around zero and decreases at rate $O(1/k^{1/2})$.

The recent literature contains a variety of rules for selecting batch sizes $\{m_\ell\}$ and batch counts $\{k_\ell\}$ as the sample size increases. The most intuitive rule fixes the number of batches and doubles the batch size at each iteration. This assignment is computationally attractive because at every iteration, pairs of existing batch means are averaged to compute the new batch means.

Fixed Number of Batches (FNB) Rule. Start with k batches of size m_1. At stage $\ell \geq 2$, use batch size $m_\ell = 2m_{\ell-1}$ and sample size $n_\ell = km_\ell$.

Under the FCLT assumption, one can show that for fixed k and $m \to \infty$, $\hat{V}_B(k,m) \xrightarrow{d} \sigma^2 \chi^2_{k-1}/(k-1)$, where χ^2_d denotes a chi-square random variable with d degrees of freedom; and the CI in Equation (8) is asymptotically valid (Glynn and Whitt 1991). If we assume uniform integrability for $\hat{V}_B^2(k,m)$ (see Billingsley 1968), we have $\lim_{m\to\infty} \mathrm{E}[\hat{V}_B(k,m)] = \sigma^2$ and $\lim_{m\to\infty} \mathrm{Var}[\hat{V}_B(k,m)] = 2\sigma^4/(k-1)$; hence the FNB rule does not yield a consistent variance estimator. This is in agreement with Equation (14) as the error $O(k^{-1/2})$ due to random sampling does not diminish. Therefore the CI in Equation (8) tends to be wider than CIs based on consistent variance estimators.

3.5 Consistent Batch Means Estimation Methods

Alternative rules that yield strongly consistent estimators for $\hat{V}_B(k,m)$ are based on the following assumption:

Assumption of Strong Approximation (ASA). There exists a constant $\lambda \in (0, 1/2]$ and a finite random variable C such that, as $n \to \infty$,

$$|\sqrt{n}(\bar{X}_n - \mu)/\sigma - \mathcal{W}(n)/\sqrt{n}| \leq Cn^{-\lambda}, \quad \text{w.p.1},$$

where $\mathcal{W}$ is a standard Brownian motion process defined on the same space as the standardized process $\{\bar{X}_n\}$.

A λ close to $1/2$ indicates a marginal normal distribution and low correlation among the X_i. Conversely, a λ close to zero indicates the absence of at least one of these properties (Philipp and Stout 1975). The following theorem proposes batching assumptions which along with ASA yield a strongly consistent estimator for σ^2. (Notice that the batching sequences are indexed by the sample size.)

Theorem 1 *(Damerdji 1994a) Suppose that the ASA holds and that $\{m_n\}$ and $\{k_n\}$ are deterministic sequences of batch sizes and batch counts, respectively, such that $m_n \to \infty$, $k_n \to \infty$, $n^{1-2\lambda}\ln(n)/m_n \to 0$ (as $n \to \infty$), and $\sum_{n=1}^{\infty} k_n^{-q} < \infty$ for some finite integer $q \geq 1$. Then, as $n \to \infty$, $\hat{V}_B(k_n, m_n) \to \sigma^2$, w.p.1 and*

$$Z(k_n, m_n) \equiv \frac{\sqrt{n}(\overline{X}_n - \mu)}{\sqrt{\hat{V}_B(k_n, m_n)}} \xrightarrow{d} N(0,1), \qquad (15)$$

where $N(0,1)$ is a standard normal random variable.

Suppose that $m_n \doteq n^\theta$, for some $\theta \in (0,1)$. One can verify that the conditions of Theorem 1 are satisfied if $\theta \in (1-2\lambda, 1)$. In particular, the square root (SQRT) rule that uses $m_n \doteq k_n \doteq \sqrt{n}$ ($\theta = 1/2$) yields a strongly consistent variance estimator when $1/4 < \lambda < 1/2$. In addition to the derivation of a strongly consistent estimator for σ^2, the SQRT rule induces an optimal property: Assuming that $\mathrm{E}(X_1^{20}) < \infty$ and that X is φ-mixing with $\varphi_j = O(j^{-13})$, Chien (1989) showed that the CDF of the standardized statistic $Z(k,m)$ converges to the standard normal CDF at the fastest possible rate. Unfortunately, the CIs for μ that result from an implementation of the SQRT rule often exhibit low coverage for small sample sizes (see Example 11 in Alexopoulos and Seila 1998).

Although both the FNB and SQRT rules yield asymptotically valid CIs for μ, each has desirable properties and limitations. To close the gap, Fishman and Yarberry (1997) proposed the LABATCH.2 suite of algorithms. Among the two recommended algorithms, LBATCH and ABATCH, we present the latter because it is more conservative with regard to the coverage of the resulting CI (8). This method uses von Neumann's test (von Neumann 1941) to assess the hypothesis H_0: "the batch means are independent." The associated test statistic is

$$\Gamma(k,m) \equiv \sqrt{\frac{k^2-1}{k-2}} \left[1 - \frac{\sum_{i=1}^{k-1}(Y_{i,m} - Y_{i+1,m})^2}{2\sum_{i=1}^{k}(Y_{i,m} - \bar{X}_n)^2} \right].$$

Assume that the hypothesis H_0 is true. If the batch means are normally distributed, the distribution of $\Gamma(k,m)$ is very close to $N(0,1)$ for k as small as 8. On the other hand, if the batch means are nonnormal, the first four cumulants of $\Gamma(k,m)$ converge to the respective cumulants of the $N(0,1)$ distribution as $k \to \infty$. Hence, under H_0, $\Gamma(k,m) \approx N(0,1)$ for large m (the batch means become approximately normal) or large k. To guard against positive correlation, one can use a one-sided test and reject H_0 at level β when $\Gamma(k,m) > z_{1-\beta}$, where z_δ is the δ-quantile of the standard normal distribution.

The ABATCH algorithm evolves as follows. For a complete description, see Fishman (2001).

Algorithm ABATCH

- Select initial batch size m_1, initial batch count k_1, confidence level $1-\alpha$, and type I error β for von Neumann's test.
- On iteration $\ell \geq 1$:
  Compute von Neumann's statistic $\Gamma(k_\ell, m_\ell)$. If $\Gamma(k_\ell, m_\ell) > z_{1-\beta}$, reject H_0 and use the FNB rule on iteration $\ell+1$. Otherwise, use the SQRT rule on iteration $\ell+1$.

Since the ABATCH algorithm uses random m_ℓ's and k_ℓ's, Theorem 6.6 of Fishman (2001) lists conditions that imply strong consistency for $\hat{V}_B(k_\ell, m_\ell)$ and asymptotic validity for the CI $\bar{X}_n \pm z_{1-\alpha/2}\sqrt{\hat{V}_B(k_\ell, m_\ell)/n_\ell}$. The FNB and SQRT rules can be implemented easily within the ABATCH algorithm by setting $\beta = 0$ or $\beta = 1$, respectively. Two features of the LABATCH.2 suite that are often overlooked are algorithm efficiency and low space requirements: each algorithm requires $O(n)$ *total* time and $O(\log_2 n)$ space. Although like complexities are known for static fixed-batch-size algorithms (e.g., all the methods in the remainder of this paper have a linear time complexity per iteration), the dynamic setting of ABATCH offers an important additional advantage not present in the static approach: as the analysis evolves with increasing sample path length, it allows a user to assess how well the estimated variance of the sample mean stabilizes, in linear total time. This assessment is essential to gauge the quality of the variance parameter estimates and the CI for the mean. C, FORTRAN and SIMSCRIPT II.5 codes of LABATCH.2 can be downloaded via anonymous ftp from the site <http://www.or.unc.edu/~gfish/labatch.2.html>.

Steiger et al. (2004) proposed a sequential NBM approach, ASAP3, that delivers a CI for μ that satisfies user-specified requirements on absolute or relative precision as well as coverage probability. This approach takes advantage of the fact that the batch means often become approximately multivariate normal random variables before achieving independence. ASAP3 operates as follows: the batch size is progressively increased until the batch means pass the Shapiro-Wilk test for multivariate normality; and then ASAP3 fits a first-order autoregressive (AR(1)) time series model to the batch means. If necessary, the batch size is further increased until the autoregressive parameter in the AR(1) model does not significantly exceed 0.8. Next ASAP3 computes the terms of an inverted Cornish-Fisher expansion for the classical batch means t-ratio based on the AR(1) parameter estimates; and finally ASAP3 delivers a correlation-adjusted CI based on this expansion. Although ASAP3 does not possess the computational efficiency of the LABATCH.2 algorithms, it performs very well with regard to conformance to the precision and coverage probability requirements as well as with regard to the mean and variance of the half-length of the delivered CI. Related papers, experimental results, and the ASAP3 software are accessible from the site <http://www.ie.ncsu.edu/jwilson>. A detailed experimental study of sequential NBM procedures is presented in Lada et al. (2006).

A reasonable compromise between the methods of independent replications (IR) in Section 2 and NBM has been proposed recently by Argon and Andradóttir (2006). The *replicated batch means* (RBM) method uses a few independent replications of equal length, each containing the same number of batches, and estimates the variance parameter σ^2 my m times the sample variance of all batch means. When the output process is stationary, the RBM method appears to exhibit performance characteristics that fall between the constituent IR and NBM methods. The recent paper by Alexopoulos et al. (2006a) studies the performance of the RBM variance estimator in the presence of an additive transient bias.

Overlapping Batch Means

An interesting variation of the traditional batch means method is the method of *overlapping* batch means (OBM) proposed by Meketon and Schmeiser (1984). For given batch size m, this method uses all $n-b+1$ overlapping batches to estimate μ and $\mathrm{Var}(\bar{X}_n)$. The first batch consists of observations $X_1, \ldots, X_m$, the second batch consists of $X_2, \ldots, X_{m+1}$, etc. The OBM estimator of μ is

$$\bar{Y}_O = \frac{1}{n-m+1}\sum_{i=1}^{n-m+1} Y'_{i,m},$$

where $Y'_{i,m} = \frac{1}{m}\sum_{j=i}^{i+m-1} X_j$ $(i = 1, \ldots, n-m+1)$ are the respective batch means. The OBM-based estimator of σ^2 is

$$\hat{V}_O(k,m) = \frac{nm}{(n-m+1)(n-k)}\sum_{i=1}^{n-m+1}(Y'_{i,m} - \bar{X}_n)^2,$$

with $k \equiv n/m$. The OBM variance estimator is almost identical to Bartlett's spectral estimator (see Anderson 1984).

Under conditions similar to those required to derive Equations (11) and (12) one has (Song and Schmeiser 1995)

$$\mathrm{E}[\hat{V}_O(k,m)] = \sigma^2 + \gamma/m + o(1/m) \qquad (16)$$

and, as $m \to \infty$,

$$\mathrm{Var}[\hat{V}_O(k,m)] \to \frac{2(2k^2-3k-3)\sigma^4}{3(k-1)^2} \doteq \frac{4\sigma^4}{3k}. \qquad (17)$$

Equations (11) and (16) show that the estimators $\hat{V}_B(k,m)$ and $\hat{V}_O(k,m)$ have the same asymptotic means (as $k, m \to \infty$). However a comparison between Equations (12) and

(17) reveals that

$$\frac{\mathrm{Var}[\hat{V}_O(k,m)]}{\mathrm{Var}[\hat{V}_B(k,m)]} \to \frac{2}{3}, \quad \text{as } k, m \to \infty.$$

Thus, the OBM method gives better (asymptotic) performance than NBM with regard to MSE. Also, the behavior of $\mathrm{Var}[\hat{V}_O(k,m)]$ appears to be less sensitive to the choice of the batch size than does the behavior of $\mathrm{Var}[\hat{V}_B(k,m)]$ (see Song and Schmeiser 1995, Table 1).

An approximate $1-\alpha$ CI for μ is

$$\bar{X}_n \pm t_{d,1-\alpha/2}\sqrt{\hat{V}_O(k,m)/n},$$

with the degrees of freedom d chosen so that $\hat{V}_O(k,m)$ is asymptotically $\sigma^2\chi_d^2/d$. Meketon and Schmeiser (1984) use the value $d = 1.5(k-1)$ whereas, based on Monte Carlo studies, Schmeiser (1986) recommends the larger value $d = 1.5(k-1)[1+(k-1)^{-0.5-0.6k}]$.

The OBM method can also yield a consistent variance estimator. If X satisfies ASA, and the deterministic sequences satisfy the assumptions of Theorem 1 and $\lim_{n\to\infty}(k_n^2/n) = 0$, then $\mathrm{Var}[\hat{V}_O(k_n,m_n)] \to \sigma^2$, w.p.1 (Damerdji 1994a).

Using Equations (16) and (17), one can show that for a sample size n, the batch size that minimizes the $\mathrm{MSE}[\hat{V}_O(k,m)]$ is given by

$$m^* = \left(\frac{3\gamma^2 n}{2\sigma^4}\right)^{1/3}. \tag{18}$$

Song (1996) developed methods for estimating the ratio γ^2/σ^4 for a variety of processes, including moving average processes and autoregressive processes. Then one can obtain an estimator for m^* by plugging the ratio estimator into Equation (18).

Welch (1987) noted that both traditional batch means and overlapping batch means are special cases of spectral estimation at frequency 0 and, more importantly, suggested that overlapping batch means yield near-optimal variance reduction when one forms sub-batches within each batch and applies the method to the sub-batches. For example, a batch of size 64 is split into 4 sub-batches and the first (overlapping) batch consists of observations $X_1,\ldots,X_{64}$, the second consists of observations $X_{17},\ldots,X_{80}$, etc.

3.6 The Standardized Time Series Method

Now we turn to estimators based on standardized time series (STS). We start with estimators based on the entire sample, and then present estimators based on standardized time series applied to batches.

The STS for the sample $X_1,\ldots,X_n$ is formed as follows (see Schruben 1983): One defines $D_{0,n} \equiv 0$ and $D_{i,n} \equiv \bar{Y}_i - \bar{Y}_n$, for $i = 1,\ldots,n$; scales the sequence $\{D_{i,n}\}$ by $i/(\sigma\sqrt{n})$; and then scales the time index i of the resulting sequence to the unit interval by setting $t = i/n$. The resulting STS is

$$T_n(t) \equiv \frac{\lfloor nt \rfloor(\bar{X}_n - \bar{X}_{\lfloor nt \rfloor})}{\sigma\sqrt{n}}, \quad 0 \le t \le 1.$$

If X satisfies a FCLT, it can be shown that, as $n \to \infty$,

$$(\sqrt{n}(\bar{X}_n - \mu), \sigma T_n) \Longrightarrow (\sigma\mathcal{W}(1), \sigma\mathcal{B}), \tag{19}$$

where $\mathcal{B}$ is a standard Brownian bridge process on $[0,1]$ defined by $\mathcal{B}(t) = \mathcal{W}(t) - t\mathcal{W}(1)$. For a set of sufficient conditions, see Glynn and Iglehart (1990). In addition, the STS $T_n(\cdot)$ is asymptotically independent of $\bar{X}_n$. Recall that all finite-dimensional joint distributions of $\mathcal{B}$ are normal with $\mathrm{E}(\mathcal{B}(t)) = 0$ and $\mathrm{Cov}(\mathcal{B}(s),\mathcal{B}(t)) = \min(s,t) - st$, $0 \le s,t \le 1$.

The Weighted Area Estimator

We start with the weighted area estimator (Goldsman, Meketon, and Schruben 1990; Goldsman and Schruben 1990; Schruben 1983). Suppose that the function f is twice continuously differentiable on the interval $[0,1]$ and normalized so that $\mathrm{Var}(\int_0^1 f(t)\mathcal{B}(t)\,dt) = 1$. Then $\int_0^1 f(t)\mathcal{B}(t) \sim \sigma N(0,1)$. The square of the weighted area under the STS is defined by

$$A(f;n) \equiv \left[\frac{1}{n}\sum_{i=1}^{n} f(i/n)\sigma T_n(i/n)\right]^2.$$

Under mild conditions, the continuous mapping theorem (see Billingsley 1968, Theorem 5.1) implies

$$A(f;n) \xrightarrow{d} A(f) \equiv \left[\int_0^1 f(t)\sigma\mathcal{B}(t)\,dt\right]^2 \sim \sigma^2\chi_1^2,$$

as $n \to \infty$. For this reason, we call $A(f;n)$ the *weighted area* estimator for σ^2.

The following theorem gives expressions for the mean and variance of the weighted area estimator.

Theorem 2 *(Foley and Goldsman 1999; Goldsman et al. 1990) Suppose that X is φ-mixing and satisfies a FCLT, the constant γ in (9) exists, and $A^2(f;n)$ is uniformly integrable. Then, as $n \to \infty$,*

$$\mathrm{E}[A(f;n)] = \sigma^2 + \frac{[(F(1)-\bar{F}(1))^2 + \bar{F}^2(1)]\gamma}{2n} + o(1/n)$$

and

$$\mathrm{Var}[A(f;n)] \to \mathrm{Var}[A(f)] = \mathrm{Var}(\sigma^2\chi_1^2) = 2\sigma^4,$$

where $F(s) \equiv \int_0^s f(t)\ dt$, $0 \le s \le 1$, *and* $\bar{F}(u) \equiv \int_0^u F(s)\ ds$, $0 \le u \le 1$.

Notice that the limiting variance does not depend on the weight function f.

Example 1 Schruben (1983) studied the area estimator with constant weight function $f_0(t) \equiv \sqrt{12}$, for $t \in [0,1]$; in this case, Theorem 2 implies that $\mathrm{E}[A(f_0;n)] = \sigma^2 + 3\gamma/n + o(1/n)$.

If one chooses weights having $F(1) = \bar{F}(1) = 0$, the resulting estimator is *first-order unbiased* for σ^2, i.e., its bias is $o(1/n)$. An example of a weight function yielding a first-order unbiased estimator for σ^2 is $f_2(t) \equiv \sqrt{840}(3t^2 - 3t + 1/2)$ (see Goldsman, Meketon, and Schruben 1990; Goldsman and Schruben 1990).

Other examples of weight functions yielding first-order unbiased estimators for σ^2 are given by the family $f_{\cos,j}(t) = \sqrt{8}\pi j \cos(2\pi jt)$, $j = 1, 2, \ldots$. Foley and Goldsman (1999) showed that this "orthonormal" sequence of weights produces area estimators $A(f_{\cos,1}, n), A(f_{\cos,2}, n), \ldots$ that are not only first-order unbiased, but asymptotically independent; that is, $A(f_{\cos,1}), A(f_{\cos,2}), \ldots$ are IID $\sigma^2\chi_1^2$.

Batched Area Estimators

Up to now, the STS-based variance estimators have been constructed directly from a single long run of n observations. We now examine what happens if we (a) divide the run into contiguous, nonoverlapping *batches*; (b) form an STS estimator from each batch; and (c) take the average of the estimators.

The STS from batch i ($i = 1, \ldots, k$) is

$$T_{i,m}(t) \equiv \frac{\lfloor mt \rfloor (Y_{i,m} - Y_{i,\lfloor mt \rfloor})}{\sigma\sqrt{m}}, \quad 0 \le t \le 1,$$

where $Y_{i,j} = \frac{1}{j}\sum_{\ell=1}^{j} X_{(i-1)m+\ell}$. Under the same mild conditions as before, one has

$$\begin{aligned}&(\sqrt{m}(Y_{1,m} - \mu), \sqrt{m}(Y_{2,m} - \mu), \ldots,\\ &\sqrt{m}(Y_{k,m} - \mu); \sigma T_{1,m}, \sigma T_{2,m}, \ldots, \sigma T_{k,m})\\ &\quad \Longrightarrow (\sigma Z_1, \sigma Z_2, \ldots, \sigma Z_k; \sigma\mathcal{B}_0, \sigma\mathcal{B}_1, \ldots, \sigma\mathcal{B}_{k-1}),\end{aligned}$$

where the Z_i are IID standard normal random variables, and $\mathcal{B}_s$ denotes a standard Brownian bridge on $[s, s+1]$, for $s \in [0, k-1]$. That is,

$$\mathcal{B}_s(t) = \mathcal{W}(s+t) - \mathcal{W}(s) - t[\mathcal{W}(s+1) - \mathcal{W}(s)], \quad 0 \le t \le 1.$$

One can easily show that the Brownian bridges $\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_k$ are independent.

The area estimator from batch i is

$$A_i(f;m) \equiv \left[\frac{1}{m}\sum_{\ell=1}^{m} f(\ell/m)\sigma T_{i,m}(\ell/m)\right]^2, \quad i = 1, \ldots, k,$$

and the *batched area* estimator for σ^2 is

$$\hat{V}_A(f;k,m) \equiv \frac{1}{k}\sum_{i=1}^{k} A_i(f;m). \tag{20}$$

Since the $T_{i,m}$, $i = 1, \ldots, k$, converge to independent Brownian bridges as m becomes large (with fixed k), we shall assume that the the $A_i(f;m)$ are asymptotically independent as $m \to \infty$. Then by the discussion above, we have $\hat{V}_A(f;k,m) \xrightarrow{d} \sigma^2\chi_k^2/k$, and an approximate $1-\alpha$ CI for μ is $\bar{X}_n \pm t_{k-1,1-\alpha/2}\sqrt{\hat{V}_A(k,m)/n}$.

Theorem 2 implies

$$\begin{aligned}\mathrm{E}[\hat{V}_A(f;k,m)] &= \mathrm{E}[A_1(f;m)]\\ &= \sigma^2 + \frac{[(F(1) - \bar{F}(1))^2 + \bar{F}^2(1)]\gamma}{2m}\\ &\quad + o(1/m).\end{aligned} \tag{21}$$

Further, if we assume uniform integrability of $\hat{V}_A^2(f;k,m))$, we can also make an analogous statement concerning the variance of the batched area estimator: As $m \to \infty$,

$$\begin{aligned}\mathrm{Var}[\hat{V}_A(f;k,m)] &= k^{-1}\mathrm{Var}[A_1(f;m)]\\ &\to k^{-1}\mathrm{Var}[A(f)] = 2\sigma^4/k.\end{aligned} \tag{22}$$

Equations (21) and (22) indicate that the batched area estimator has a bit more bias than the area estimator obtained from the entire sample, but smaller asymptotic variance (by a factor of k). Sargent et al. (1992) present an extensive experimental study for various CIs mentioned in this section.

It is worth mentioning that, under the assumptions of Theorem 1, Damerdji (1994ab) showed that the batched area estimator $\hat{V}_A(f;k,m)$ is strongly consistent.

Another class of estimators is based on the weighted area under the square of the STS (Goldsman et al. 1999). Also, additional benefits result from combining NBM-based and area estimators (Schruben 1983) or by forming estimators based on STS from overlapping batches (Alexopoulos et al. 2006bc).

Remark 2 Methods based on NBM and STS can also be used for computing point and CI estimators for continuous nonlinear functions of steady-state means (Muñoz and Glynn 1997; Chang 2004).

3.7 Quantile Estimation

A variety of methods have been proposed for estimating quantiles of steady-state data (see Iglehart 1976; Moore 1980; Seila 1982ab; Heidelberger and Lewis 1984). The methods differ in the way the variance of the sample quantile is estimated. It should be mentioned that quantile estimation is typically a harder problem than the estimation of steady-state means.

3.8 Density Estimation

In addition to point and interval estimates, users are often interested in estimating the density functions (or CDFs) of random variables generated by a computer simulation. Several simulation packages can generate histograms, but such plots are often "poor" estimates of the unknown density function because their shape depends heavily on the chosen origin and the bin width. Although the statistical literature contains many state-of-the-art density estimation techniques, such as those based on kernel functions, the simulation literature (in particular texts) barely mentions such techniques, and only within the context of independent input data. The book chapter by Alexopoulos (2006) attempts to close the gap between the statistical and simulation literatures by reviewing univariate kernel density estimators based on independent samples and sample paths of stationary dependent processes.

3.9 Multivariate Estimation

Frequently, the output from a single simulation run is used for estimating several system parameters. The estimators of these parameters are typically correlated. As an example, consider the average customer delays at two stations on a path of a queueing network. In general, Bonferroni's inequality can be used for computing a conservative confidence coefficient for a set of CIs. Indeed, suppose that D_i is a $1-\alpha$ CI for the parameter μ_i, $i = 1, \ldots, m$. Then $\Pr[\cap_{i=1}^{m}\{\mu_i \in D_i\}] \geq 1 - \sum_{i=1}^{m} \alpha_i$.

This result can have serious implications as for $m = 10$ and $\alpha_i = 0.10$ the r.h.s. of the above inequality is equal to 0. If the overall confidence level must be at least $1-\alpha$, then the α_i can be chosen so that $\sum_{i=1}^{m} \alpha_i = \alpha$. Multivariate estimation methods are described in Charnes (1989, 1990, 1991) and Chen and Seila (1987).

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