Output Analysis Procedures for Computer Simulations

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〈 개 요 〉

시뮬레이션 연구에서는 출력 데이터의 적절한 분석이 무엇보다도 중요하다. 출력 데이터에 내재하는 자동상관관계는 출력 결과의 평균에 대한 구간추정을 어렵게 하고 있다. 이러한 관점에서 본 논문은 이산형-사건 시뮬레이션의 출력 데이터에 대한 통계분석 방법론에 대하여 다루었다. 우선 종결형 시뮬레이션과 정상상태 시뮬레이션의 차이점을 규명한 후, 시뮬레이션의 정상상태 평균에 대한 6가지 범주의 구간추정기법인 독립 반복법, 구간평균법, 재생주기 기법, ARMA표현법, 스펙트럼 분석법, 표준시계열 분석법에 대하여 상론하였다. 그리고 마지막으로 이 6가지 범주 중에서 가장 흔히 사용되는 분석기법인 구간평균법에 대하여 최근에 시도되는 수정안들을 소개하고 시뮬레이션 출력분석 분야의 최신 연구동향을 조명하였다.

Ⅰ. Introduction

Computer simulation is a powerful and widely used technique for addressing problems in the areas of operations and management. We may be interested, for example, in the daily production of a newly planned manufacturing process, customers' waiting time in a banking service system, monthly transportation costs in many alternative logistic systems, response time in a field service system, and so on. The above-mentioned quantities, being affected by many variables, both stochastic and deterministic, are variables themselves and evolve overtime. The sequence of such a variable over time is called a *stochastic process*. Some characteristic or parameter of this process may be of interest. To find this value, we translate the problem into a mathematical model, and attempt to solve it with analytical methods. However, the class of models that have analytically tractable solutions

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is very limited. Usually, management problems are so complex that analytical solutions are not available. Computer simulation is an appropriate technique for studying such problems because there is little limit on the complexity of the simulation models and thus we can build a model that represents the problem in a more valid way.

An important problem in a simulation study is that of estimating the steady-state expected value (process mean) of simulation output process. The choice of a point estimator for the process mean is usually clear: the sample mean of the simulation output data is an unbiased estimator for the process mean if the simulation is in steady state. However, interval estimation - constructing a confidence interval (c.i.), which we need as a measure of the precision of the point estimator - for the process mean is a difficult problem owing to the autocorrelation inherent in ordinary simulation output process.

Suppose we make observations $\{X_1, X_2, \cdots, X_n\}$ from a simulation run of length n. (In this dissertation, the term *run length* denotes the number of observations generated by a simulation run, and thus has the same meaning as *sample size*.)

If the X_i's were independent and identically distributed (i.i.d.),then an interval estimator for the process mean μ is given by:

$$\overline{X} \pm t_{1-\alpha/2,n-1}\,\hat{\sigma}_{\overline{X}}, \qquad (1)$$

where

$$\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

is the sample mean, and

$$\hat{\sigma}^2_{\overline{X}} = \frac{1}{n(n-1)}\sum_{i=1}^{n}(X_i - \overline{X})^2$$

is an estimator of the variance of the sample mean (in short, variance estimator), and $t_{1-\alpha/2,n-1}$ is the upper $1-\alpha/2$ critical point of the t distribution with $n-1$ degrees of freedom. This interval estimator is based on the assumption that $(\overline{X}-\mu)/\hat{\sigma}_{\overline{X}}$ has a t

distribution with $n-1$ degrees of freedom, which is valid if $\overline{X}$ has a normal distribution, $n\ \hat{\sigma}^2_{\overline{X}}/\ \sigma^2_{\overline{X}}$ has a χ^2_{n-1} distribution, and these two statistics are independent.

In general, though, the X_i's will be neither independent, identically distributed, nor normal. For example, X_i might be the delay in queue of the i-th arriving customer, so that X_{i+1} would be dependent on the value of X_i. The normality assumption of $\overline{X}$ may approximately hold for a long run length owing to various central limit theorems for correlated data. But autocorrelation in the X_i's makes the usual variance estimator $\hat{\sigma}^2_{\overline{X}}$ biased for Var($\overline{X}$). Correcting for this bias is the primary focus of this dissertation.

Actually, the fact that the simulation output process is in general nonstationary is another source of the bias in $\hat{\sigma}^2_{\overline{X}}$ (as well as in $\overline{X}$ as an estimator of μ). The nonstationarity problem exists because the simulation is started at a state that is not taken from the steady-state probability distribution of the process. This study concentrates on the problem related to the bias in variance estimation caused by autocorrelation. Therefore, we assume that our simulation starts at a steady-state, or has been run long enough so that steady-state conditions in the first moment are approximately attained.

II. Terminating vs. Steady-State Simulation

We begin by introducing two types of simulations: *terminating* and *steady-state*. They each require different basic approaches for interval estimation of the process mean. A terminating simulation is one for which the termination event is defined as a part of modeling the system under analysis. For example, we may be interested in the performance of a single 8-hour shift of a manufacturing facility that starts out with all machines idle and no parts present, and ends exactly 8 hours later regardless of whether parts are still in the system. In this case each simulation run or *replication*, being one complete succession from starting to termination time, provides an unbiased and i.i.d. observation for the transient process mean, being the object of study. Thus, classical

statistical methods can be directly applied to analyze the output from a set of terminating simulation runs, leaving only the problem of determining the number of runs to ensure the desired precision of the estimation. The problem of analyzing output from terminating simulations is considered to be solved (Law 1980), at least in principle. We will not treat terminating simulations further in this paper.

A steady-state simulation is one in which the parameters to be estimated are defined as limits as simulated time goes to infinity: thus, the system being modeled has no specific termination event. In the earlier manufacturing example, we might instead be interested in the long-run production per shift if the facility never shuts down. Thus, the estimation of interest is that for the steady-state or long-run expected value μ of the performance of the system. The autocorrelation problem is concerned with this type of simulation. Steady-state simulations are the object of study in this paper.

III. Commonly Used C.I. Construction Procedures

We identify six types of c.i. procedures for data from a steady-state simulation: independent replications, batch means, regeneration cycles, autoregressive moving average representation, spectral analysis, and standardized time series. Taken broadly, they may be classified into two groups: one including the former three methods, and the other one having the latter three methods. Those in the first group try to obtain approximately independent random variables by aggregating data over the observations in each replication, batch, or regeneration cycle, in the hope of making simple classical statistical techniques applicable. Those in the second group try to use information on the dependence structure rather than trying to destroy it through data aggregation.

3.1 Independent Replications

Suppose we can take n observations on the process. One simple approach to

constructing a c.i. is to obtain k i.i.d. random variables from k independent replications of length $m = n/k$ (Suppose that we take n so that it is divisible by m). Each replication starts from the same initial conditions, and uses an independent random-number stream. If $X_j(m)$ denotes the sample mean of the m observations in the j-th replication (replication mean), then the $X_j(m)$'s are i.i.d. random variables with expectation $\mu(m) = E[X_j(m)]$. Assuming that $\mu(m) = \mu$, we use

$$\overline{X} = \frac{1}{k}\sum_{j=1}^{k} X_j(m),$$

as an unbiased point estimator for the process mean, and we estimate $\hat{\sigma}^2_{\overline{X}} = \mathrm{Var}(\overline{X})$ by $\hat{\sigma}^2_{\overline{X}} = \frac{1}{k(k-1)}\sum_j [X_j(m) - \overline{X}]^2$

If we assume further that $X_j(m)$ has a normal distribution, then the ratio

$$\frac{\overline{X}-\mu}{\hat{\sigma}_{\overline{X}}}$$

has a t distribution with $k-1$ degrees of freedom. Thus we can construct a $100(1-\alpha)$ c.i. as presented in the equation (1) with n replaced by k.

This c.i. procedure is easy to understand and use, and completely free of the autocorrelation problem. However, $\mu(m) \neq \mu$ in general owing to the effect of the initial conditions which are not from the steady-state probability distribution of the process, and thus $\overline{X}$ is a biased estimator for μ (Law 1977). This so-called *initial bias problem* tends to be serious with the replication method because the simulation runs have to start anew for each replication, refreshing the effect of the initial conditions. Therefore, the actual probability of coverage of the c.i.'s constructed by this procedure may turn out to be much lower than the desired level if we increase k for fixed m, unless the initial conditions are properly chosen, m is sufficiently large, or a large number of initial observations in each replication are thrown away. Law and Kelton (1984) argue in effect that, until there is are liable means of eliminating the initial bias problem, this method has a dangerous potential for misleading the analyst in interpreting the results of a simulation study.

3.2 Batch Means

We assume again that we can make n observations, with $n = mk$ As opposed to independent replications, we make a single long simulation run of length n, and then group the n observations into k batches such that each batch has m consecutive observations. We denote $X_j(m)$ as the j-th *batch mean* (the sample mean of the observations in the j-th batch), and define $\overline{X}$ and $\hat{\sigma}^2_{\overline{X}}$ as in the method of independent replications. Then we form a $100(1-\alpha)\%$ c.i. by (1.1) with n replaced by k, assuming that the ratio $(\overline{X}-\mu)/\hat{\sigma}_{\overline{X}}$ has a t distribution with $k-1$ degrees of freedom.

Compared to the method of independent replications, this method suffers from the initial bias problem much less by starting the simulation just once instead of k times. However, the assumption that the $X_j(m)$'s are i.i.d. becomes valid only when m is sufficiently large. Otherwise, the $X_j(m)$'s may be correlated and thus $\sigma^2_{\overline{X}}$ may be underestimated by $\hat{\sigma}^2_{\overline{X}}$, leading to a serious degradation in the coverage of the c.i.'s for μ (Lawand Kelton 1984) Thus, procedures which seek to find an acceptably large batch size have been developed (Mechanic and McKay 1966, Law and Carson 1979, and Fishman 1978b).

3.3 Regeneration Cycles

This method, developed simultaneously by Crane and Iglehart (1974, 1974b, 1975, 1975b)] and by Fishman (1973), (1974) is applicable only to regenerative processes.

A process $\{X_t, t=1,2,\cdots\}$ is said to be *regenerative* if there is an increasing sequence of *regeneration points* $1 \le t_1 < t_2 < \cdots$ such that the process $\{X_t, t \ge t_j\}$ starts over probabilistically at each $j=1,2,\cdots$. Thus, the process

$\{X_t, t \ge t_j\}$ is independent of the process $\{X_t, t < t_j\}$ and is probabilistically identical for each $j=1,2,\cdots$. Now, divide the process $\{X_t, t=1,2,\cdots\}$ into a sequence of *regeneration cycles* $\{X_t, t_j \le t < t_{j+1}\}$ of length $N_j = t_{j+1}-t_j$, $j=1,2,\cdots$.

Denote $Y_j = \sum_{t=t_j}^{t_{j+1}-1} X_t$.

Then Y_j's are i.i.d. random variables (Crane and Iglehart 1975). Suppose that $E(N_j)<\infty$, $E(|Y_j|)<\infty$, and we simulate for exactly k regeneration cycles. Let

$$\mathrm{Cov}\begin{pmatrix} Y_1 \\ N_1 \end{pmatrix} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix}$$

$$Z_j = Y_j - \mu N_j$$

$$\overline{Y} = \frac{1}{k}(Y_1 + \cdots + Y_k)$$

$$\overline{N} = \frac{1}{k}(N_1 + \cdots + N_k)$$

Then the Z_j's are i.i.d. random variables with mean zero and variance

$$\sigma^2_Z = \sigma_{11} - 2\mu\sigma_{12} + \mu^2\sigma_{22}$$

And thus, by the central limit theorem, we have

$$\frac{\overline{Z}}{\sigma_Z/\sqrt{k}} \rightarrow N(0,1), \text{ as } k \rightarrow \infty,$$

provided that $0 < \sigma^2_Z < \infty$, where $\rightarrow$ denotes convergence in distribution, and $N(0,1)$ is a standard normal random variable. Based on the above properties, we can construct an asymptotically valid classical c.i. by (Law and Kelton 2000)

$$\hat{\mu}_C \pm z_{1-\alpha/2}\frac{\hat{\sigma}_Z}{\overline{N}\sqrt{k}},$$

where $z_{1-\alpha/2}$ is the upper $1-\alpha/2$ critical point of the $N(0,1)$ distribution, $\hat{\mu}_C = \overline{Y}/\overline{N}$ is a strongly consistent point estimator for μ, $\hat{\sigma}_Z = \{\hat{\sigma}_{11} - 2\hat{\mu}_C\hat{\sigma}_{12} + \mu^2_C\hat{\sigma}_{22}\}^{1/2}$, and $\hat{\sigma}_{11}$, $\hat{\sigma}_{12}$, and $\hat{\sigma}_{22}$ are strongly consistent estimates for σ_{11}, σ_{12} and σ_{22}, respectively.

This method (as well as the method of standardized time series) is founded on a solid mathematical basis. There is no decision (except that on the number of cycles, k) to be made arbitrarily when we apply this method, while the other methods have some rules-of-thumb involved.

However, use of this method is very limited because it is applicable only to regenerative processes for which the expected length of the regeneration cycles is

sufficiently small so that enough cycles become available within the budget, which is rarely the case for complex systems often encountered in real-world studies.

3.4 Autoregressive Moving Average (ARMA) Representation

As in the other c.i. procedures, we use the sample mean $\overline{X}$ as a point estimator for μ. However, in this c.i. procedure we do not try to obtain i.i.d. random variables from given simulation output data to estimate $\sigma^2_{\overline{X}} = \mathrm{Var}(\overline{X})$. Instead, we try to represent the process by an ARMA model, and we use a limiting property related to $\sigma^2_{\overline{X}}$ and the ARMA parameters of the model representing the data.

This method, developed by Fishman (1971, 1972, 1973) as the AR representation and extended by Schriber and Andrews (1984) as the ARMA representation, has an underlying assumption that the process is covariance stationary (i.e., $\gamma_t = \mathrm{Cov}(X_i, X_{i+t})$ is independent of i and is thus a function of t only).

In the AR *representation*, we model the process $\{X_i, i \geq 1\}$ of interest as

$$\sum_{t=0}^{p} \phi_t (X_{i-t} - \mu) = \varepsilon_i \quad \cdots\cdots (2)$$

where $\phi_0 = 1$ and $\{\varepsilon_i\}$is a sequence of uncorrelated random variables with mean 0 and variance σ^2_ε. The process defined by equation (2) is called an AR process of order p, or, in short, an AR(p) process. It has been shown (Fishman 1978) that $\hat{\sigma}^2_{\overline{X}} \rightarrow \sigma^2_\varepsilon / (\sum_{t=0}^{p} \phi_t)^2$ as $n \rightarrow \infty$, provided that

$$\sum_{t=-\infty}^{\infty} |\gamma_t| < \infty$$

Therefore, we can estimate $\sigma^2_{\overline{X}}$ by

$$\hat{\sigma}^2_A = \hat{\sigma}^2_\varepsilon / [n\, \hat{b}(r)]$$

where

$$\hat{b}(r) = \sum_{t=0}^{r} \hat{\phi}^2_t,$$

r is a specified value for p, and $\hat{\sigma}_\varepsilon^2$ and the $\hat{\phi}_t$'s are estimates for σ_ε^2 and the ϕ_t's, respectively. If we assume that the distribution of $(\overline{X}-\mu)/\hat{\sigma}_A$ can be approximated by a t distribution with

$$\hat{f}=\{n\hat{b}(r)/[(2r+1)\hat{b}(r)-4\sum_{t=1}^{r} t\hat{\phi}_t(r)]\}-1$$

degrees of freedom (Fishman 1978), then we form a $100(1-\alpha)\%$ c.i. as

$\overline{X} \pm t_{\hat{f},1-\alpha/2}\,\hat{\sigma}_A$.

In this method, it is critically important to choose right value of r as an estimate of the true AR order p, which is seldom a simple task. Also, there are several possible sources of error, as Law and Kelton (1984) state "… the process is assumed to be covariance stationary and to satisfy (2): neither will generally be the case in practice. Further, the assumption of a t distribution necessary to specify the c.i. will generally be violated. Hence, the true probability of coverage of the c.i. proposed here need not be $1-\alpha$, as claimed."

In the ARMA representation, the process is assumed to be represented by a more flexible ARMA(p,q) model, where the AR order p and the MA order q are identified from the data. This c.i. procedure is closely related to the one developed in this paper.

3.5 Spectral Analysis

Suppose the simulation output process is covariance stationary and we have data $\{X_1, X_2, \ldots, X_n\}$ taken from this process. Then the variance of the sample mean is given by (Fishman 1978)

$$\sigma^2_{\overline{X}} = \frac{1}{n}\sum_{t=-n+1}^{n-1}\left(1-\frac{|t|}{n}\right)C(t), \quad \cdots\cdots (3)$$

where $\hat{C}(t) = Cov(X_i, X_{i+t})$. This formula suggests using

$$\hat{\sigma}^2_{\overline{X}} = \frac{1}{n}\sum_{t=-n+1}^{n-1}\left(1-\frac{|t|}{n}\right)\hat{C}(t), \quad \cdots\cdots (4)$$

where

$$\hat{C}(t)=\frac{1}{n-t}\sum_{i=1}^{n-t}[X_i-\overline{X}][X_{i+t}-\overline{X}], \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots (5)$$

as an estimator for Var($\overline{X}$). However, this idea has problems: First, it would take a lot of computation to estimate $n-1$ covariances when n is large. Perhaps more importantly, the covariance estimators ($\hat{C}(t)$'s) would be based only a few observations for t near n, so will be highly variable. Therefore, it is reasonable to ask if there is a weighting function other than $(1 - |t|/n)$ in Eq. (4) that allows approximation to Var($\overline{X}$) in Eq. (3) by a linear combination of considerably few autocovariances. Based on spectral analysis, several alternative variance estimators of the following form have been proposed:

$$\hat{\sigma}^2{}_S(l) = \frac{1}{n}\sum_{t=1}^{l-1} w_l(t)\,\hat{C}(t),$$

where $l < n$ and is prespecified, and the $\hat{C}(t)$'s are as shown in Eq. (5) with $1/(n - t)$ replaced by $1/n$. The weighting function $w_l(t)$ is called *spectral window*. One example is the Tukey-Hanning window

$$w_l(t) = \begin{cases} 0.5(1+\cos(\pi t/l) & |t|<k \\ 0 & \text{otherwise} \end{cases}$$

Fishman (1978) suggests that $(\overline{X}-\mu)/\hat{\sigma}_S(l)$ be treated as having a t distribution with the "*effective degrees of freedom*" $\hat{f}$, and derives that $\hat{f}=2.667n/l$ for the Tukey-Hanning window.

Thus, the 100(1- α)% c.i. for μ is given by

$\overline{X} \pm t_{\hat{f},1-\alpha/2}\,\hat{\sigma}_S(l)$.

One drawback of this method is that derivation of the spectral window is based on highly sophisticated statistical knowledge and thus may not be so intuitive for those who are not familiar with thinking in the frequency domain. Moreover, there is no definitive rule to choose l, while it is an important issue.

In the experiments executed by Law and Kelton (1984), this method turns out to be the only competitor against the usual batch-means method with large value of l (Note

that the standardized time-series method was not available at the time of their survey).

This finding suggests that the performance of this method is sensitive to the specification of l, and that we may have to allocate much computing time to estimating $l-1$ covariances.

3.6 Standardized Time Series

In the standardized time series (STS) method, developed originally by Schruben (1983), we transform the entire time series in order to use properties of the limiting process of the transformed process.

Supposing again that we can make $n=mk$ observations on a process with mean μ, we may make k replications of length m each, or group (into k batches) the observations obtained through a single simulation run of length n. Consider the j-th *batch*$\{X_{(j-1)m+s},\ s=1,2,\cdots,m\}$ (or replication), which will be called the j-th time series). This series can be centered to have mean zero by the transformation:

$$S(i) = \overline{X}_m - \overline{X}_i,$$

where $\overline{X}_i = \frac{1}{i}\sum_{s=1}^{i} X_{(j-1)m+s}$ denotes the cumulative average of the first i observations in this series, and thus $\overline{X}_m$ is the j-th batch mean (or replication mean). The resulting series is then scaled by being divided by $\sigma\sqrt{m}/i$, where

$$\sigma^2 = \lim_{m\to\infty} m\,\mathrm{Var}(\overline{X}_m).$$

Also, the time index i is transformed to $t = i/m \in [0,1]$. Through these steps, we have the STS,

$$T(t) = \lceil mt \rceil\, S(\lceil mt \rceil)/(\sigma\sqrt{m}),\quad 0\le t\le 1,$$

where $\lceil \cdot \rceil$ denotes the greatest integer function.

It is shown (Schruben 1984) that the limiting (as $n\to\infty$) model of this STS is a *Brownian bridge*(a standard Wiener process on the unit interval conditioned to start and end at zero) and that known properties of this limiting Brownian bridge process lead to many alternative methods for constructing asymptotically valid c.i.'s for the process mean μ.

A strength of this method is that it requires only the mild assumption that the original process is phi-mixing (i.e., the "distant" future becomes essentially independent of the past or present). Schruben shows that all finite-state discrete-event computer simulations satisfy this assumption. According to his empirical results, the c.i. procedures based on the notion of the STS seem to perform well, at least, with fairly large run length. However, their success for short or moderate run lengths is less clear.

Ⅳ. Modifications of the Batch-Means Method

As mentioned earlier, the batch-means (BM) method may be the simplest and most popular among all the c.i. procedures for the process mean developed to date. A few procedures have recently been or are being developed to improve the quality of the variance estimator of the sample mean. One of them is the *overlapping batch-means* method proposed by Meketon and Schmeiser (1984). Another one is the *weighted batch-means* method (Bischak 1988).

The batch-means method before modifications will be referred to as the *usual* BM method from now on, to be differentiated from its modifications.

The overlapping BM estimator of Var($\overline{X}$) is defined by

$$\tilde{\sigma}^2_{\overline{X}}(m) = \frac{m}{n} \sum_{j=1}^{n-m+1} \frac{(X_j(m)-\overline{X})^2}{n-2m+1}$$

where

$$X_j(m) = \frac{1}{m} \sum_{i=0}^{m-1} X_{j+i}$$

is the batch mean of size m beginning with observation X_j. Because of the role of batch independence in the usual batch means, the idea of using the overlapping BM estimator may appear unnatural, since the common observations in the overlapping batches cause substantial positive correlation. However, this idea in many ways is a good one. It has been shown that the overlapping BM variance estimator, based on the same assumptions and batch size as the usual BM variance estimator, has essentially the same mean and

only 2/3 the asymptotic variance of the usual BM variance estimator.

However, it should be noticed that the above statement is only asymptotically valid. Sargent, Kang, and Goldsman (1987) show that the degradation in coverage for short run lengths is even worse with the overlapping BM method compared to the usual BM method, even though the former method results in shorter intervals without sacrificing coverage for long run lengths.

V. Conclusions

Proper analysis of output is one of the most important aspects of any simulation study. Since simulation output is never i.i.d. normal, the experimenter must be careful when making conclusions about such data. Indeed, the purpose of this tutorial has been to inform the experimenter about some of the issues and techniques relevant to conducting valid analyses.

There are many interesting sides of output analysis that we have not had space to discuss in this paper, e.g., multi-variate parameter estimation, sequential methods, and other variance reduction techniques. Fortunately, a number of excellent general resources are available that devote substantial discussion to the subject, e.g., Banks (1998), Banks, Carson, and Nelson (1995), Bratley, Fox, and Schrage (1987), Fishman (1978), Law and Kelton (2000).

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