A PROCEDURE FOR BUILDING CONFIDENCE INTERVAL ON THE MEAN OF SIMULATION OUTPUT DATA

S. T. Akhavan-Niaki

Department of Industrial Engineering
Sharif University of Technology
Tehran, Iran

Abstract  One of the existing methods to build a confidence interval (c.i.) for the mean response in a single steady state simulation system is the batch means method. This method, compared to the other existing methods (autoregressive representation, regenerative cycles, spectrum analysis, standardized time series), is quite easy to understand and to implement and performs relatively well. However, the most serious source of error is the underestimation of the variance of the sample mean due to the correlation of batch means. In the new method, which is essentially based on the batch means approach, weights are assigned to the batch means such that they become uncorrelated. Then based on the assumption that the output data are obtained from steady-state simulation, as expression is developed for obtaining the confidence interval on the mean.

Key Words  Simulation, Output Analysis, Batch Means

INTRODUCTION

One of the most serious problems encountered in a real-world simulation study is that of constructing a confidence interval (c.i.) for the steady-state mean \( \mu \) of a stochastic process. The information contained in such a confidence interval provides the decision-maker with a measure of how precisely \( \mu \) is estimated. However, constructing the c.i. is difficult because of the non-stationarity and serial correlation of the output data from a simulation model; hence direct use of the classical statistical techniques is precluded. This problem has received considerable attention in the literature, and many methodologies have been proposed. At present, there are still several output-analysis problems for which there is no completely accepted solution, and the solutions that do exist are often too complicated to apply. To alleviate some of the existing problems, a new procedure is offered here.

LITERATURE REVIEW

There are basically six different approaches in constructing a c.i. for the average response in a single steady-state simulation model. Each of these procedures involves some basic assumptions on the process being simulated, which may not be realized, in general, in real-world systems. Some of these methods, such as the one of independent replications, are
wasteful in term of the information obtained from the data [1]. Others, such as spectrum analysis, autoregression representation, and standardized time series place a heavy requirement on the user to be familiar with sophisticated methods of time series analysis. Other methods, like the regenerative method, are simple and easy to understand, but cannot be applied to most real life simulation systems. The last approach suggested in the literature, the batch means method, is easy to understand and to apply and is based on the assumption of i.i.d. observations being available. However, the key to the batch means method appears to be the determination of the number of observations per batch [7, 3]. This determination needs to rely on a test of independence of batch means if the resulting estimate is to be consistent with the assumptions involved in the method. However, such test procedures are reported to require a large number of batches (at least 100) to be reliable [4]. On the other hand, since the total number of observations is not unlimited, increasing number of batches requires decreasing the number of observations per batch which may result in violation of the assumption of the independence of batch means. In addition to the above difficulties, having a relatively large number of observations is the key element for all of the above procedures.

**RESEARCH OBJECTIVE**

The main objective of this research is to develop a procedure for determining confidence intervals for the average response in a single steady-state simulation system. This procedure should require a relatively small number of observations and produce c.i.'s that have good coverages, and that are easy to understand and implement.

**RESEARCH DEVELOPMENT**

Batching, discussed as early as 1963 [5], is a conceptually straightforward method for computing confidence intervals on the mean response of a steady-state simulation by transforming correlated observations \(X_1, X_2, \ldots, X_n\) into fewer, almost uncorrelated, and almost normally distributed random variables. In this method it is assumed that \(n\) observations can be taken from a covariance stationary process with the mean, \(\mu\), and lag s covariance, \(C_s = \text{Cov}(X, X_{s+n})\), starting from some initial conditions and making a single long run of the length \(n\), then dividing the run into \(k\) "batches" of \(m\) consecutive observations each \((n=km)\). Let \(X_{i,j}\) (\(i=1, 2, \ldots, m\), and \(j=1, 2, \ldots, k\)) be the \(i\)'th observation from the \(j\)'th batch, defined as

\[
\overline{X}_j(m) = \frac{1}{m} \sum_{i=1}^{m} X_{i,j}
\]

be the \(j\)'th batch mean, and \(C_s(m)\) be the lag \(s\) covariance between the batch means. Law and Carson [6] showed that if:

\[
0 < \sum_{s=\infty}^{\infty} C_s(m) < \infty
\]

then:

\[
\lim_{m \to \infty} \frac{C_s(m)}{C_0(m)} \to 0 \quad \text{for } s=1, 2, \ldots, k-1
\]

Thus, the batch means will be approximately uncorrelated for sufficiently large \(m\). Furthermore, using central limit theorem, it is not unreasonable to assume that the batch means \(\overline{X}_j(m)\)'s will be approximately normally distributed. Hence, when \(m\) is large enough, the batch means are uncorrelated and normally distributed, i.e., they will be i.i.d. normal random variables with the mean, \(\mu\), (by the assumption of covariance stationarity), so that the classical statistical methods can be applied, and a 100(1-\(\alpha\))% c.i. for \(\mu\) would be:
\[ X(k,m) = \frac{1}{k} \sum_{j=1}^{k} X_j(m) \]

where \( t_{(k-1,1-\alpha/2)} \) is the upper 1-\( \alpha/2 \) critical point of the \( t \) distribution with \( k-1 \) degrees of freedom (d.f.).

\[ \sigma^2(k,m) = \frac{\sum_{j=1}^{k} [\sum_{j=1}^{k} X_j(m) - \bar{X}(k,m)]^2}{k(k-1)} \]  

(1)

is a point estimate of \( \mu \), and

is a point estimate of the \( \text{Var} [\bar{X}(k,m)] \).

In summary, the assumptions involved in the method of Batch means are:

i) Initial transient effects have been removed; i.e., the output is covariance stationary with mean, \( \mu \), the variance, \( \sigma^2 \), and lag s covariance \( C_s \), \( s = 1,2, \ldots \).

ii) For a run length of \( n \), there exists a number of batches \( k^* \) with an associated batch size \( m^* = n/k^* \) such that the dependency and the nonnormality of the batch means are negligible, and

iii) The problem of \( n/k^* \) not being integer is insignificant.

Hence, there are three potential sources of error when one uses batch means to construct a c.i. for \( \mu \):

1) \( X_{1,m}, X_{1,m+1}, \ldots \) (for a fixed and nonnegative integer \( L \)) will not be exactly covariance stationary.

2) If \( m \) is not large enough, the batch means \( \bar{X}_j(m) \)'s, may not be approximately normally distributed.

3) If \( m \) is not large enough, \( \bar{X}_j(m) \)'s may be highly correlated and the estimate of the variance of the mean of their means given by Equation 1 will be a severely biased estimator.

The assumption of independence between batch means is typically made in simulation analyses even though there exists an autocorrelation between the values at the end of one subinterval and those at the beginning of the next subinterval. In particular, if the \( X \)'s are positively correlated (the case usually encountered in practice), the batch means will be positively correlated as well, giving a variance estimate that is biased low and a c.i. that is too small. By making the batch size \( m \) larger, the covariance between batch means should decrease. It was concluded in Law [2] that underestimation of \( \text{Var} [\bar{X}(m,k)] \), due to small value of \( m \), is the principal source of error in this method. As empirical results in Law and Kelton [7] indicate that, at least for sample systems like an M/M/1 queue, the correlation between the batch means is the most serious source of error and it is better to make a few large batches rather than many small batches; the batch means in the latter case being too heavily correlated to obtain a good estimate of the variance of the sample mean (see also Schneising [8]).

The actual coverage of a nominal 90% c.i. for \( \mu \) in an M/M/1 queue with traffic intensity of \( \rho = 0.8 \) when \( k = 20 \) and \( n = 420 \) has been shown to be 0.49 [7]. In order for the method of batch means to be a reliable approach for steady-state analyses, a procedure for determining the batch size \( m \), such that the covariance between adjacent batch means is insignificant, is needed. One approach which has been suggested in the literature for obtaining uncorrelated batch means is given by Fishman [9]. This method is based on Von Neumann's test for the presence of correlation. However, when tested on the M/M/1 queue with \( \rho = 0.8 \) or \( \rho = 0.9 \), the method produced c.i.'s with coverage below the desired value, if the total run length \( n \) was too small. While Fishman's
procedure allows the number of batches to be as small as eight, Kleijnen et al. [4] recommended that the number of batches should be at least 100 when using Von Neumann's test to ensure a test for correlation with sufficiently high power. Schmeiser [8] quantified the effects of using different batch sizes on the c.i. coverage. He concluded that a value of $m$ between $10 \leq m \leq 30$ is reasonable for most simulation situations, however, it is important to note that a large number of batches may be required to determine a batch size for which the corresponding batch means will be approximately uncorrelated (see Kleijnen et al. [4], and Law and Carson [6]). Also Adam and Klein [10] concluded that the coverage probability for the process mean decreases significantly at moderate levels of autocorrelation, and unless the number of batches is large, neither the Von Neumann ratio test, nor its rank version is good as a test of zero autocorrelation. Their results tend to agree with the recommendation of Kleijnen et al. [4] that a large number of batches (perhaps at least 100) be used when testing for first-order autocorrelation.

Other papers that discuss the method of batch means have been developed by Adam [11], Kang and Goldsman [12], Mechanic and McKay [13], and Schriber and Andrews [3] which have proposed a modification to Fishman's algorithm.

Law [7] encouraged researchers to develop a new procedure for choosing the batch size for the method of batch means such that the corresponding batch means are approximately uncorrelated and normally distributed. He also recommended to investigate the possibility suggestion of leaving some observations between batches that are actually used for estimation purposes, or more generally to assign possibly different weights to the observations within a batch. The goal of such schemes would be to try to reduce the correlation between batch means.

In this paper we develop a c.i. procedure for the mean of the output data from a single steady-state stochastic process which is essentially based on the batch means approach and Law’s recommendations. The main idea is to find some weight schemes for the batch means such that the batch means are i.i.d. random variables and the classical statistical methods can be applied. Thus, the most potential source of error involved in the batch means approach will be eliminated and hopefully the actual coverage of the new confidence interval procedure will be more efficient than the ordinary batch means method. The new method, even though general, will be specially helpful in situations where the ordinary batch means method fails. It will also be helpful in the situations in which the estimation of c.i.’s for simulation outputs where observations are hard or expensive to obtain and only limited data are available.

**DERIVATION OF THE NEW C.I. METHOD**

Since the variance-covariance matrix $\mathbf{K}_b$ associated with the batch means vector is real and symmetric, it has a full set of orthonormal eigenvectors and can be easily diagonalized to $\mathbf{U}^T \mathbf{K}_b \mathbf{U} = \mathbf{\Lambda}$ once $\mathbf{U}$ is known [14]. The columns of $\mathbf{U}$ are just the unit eigenvectors of $\mathbf{K}_b$ and these can be obtained once the eigenvalues are known. In other words, we will have:

$$
\mathbf{U}^T \mathbf{K}_b \mathbf{U} = \mathbf{\Lambda} = \begin{bmatrix}
\lambda_1 & 0 & \ldots & 0 \\
0 & \lambda_2 & \ldots & 0 \\
& \ddots & \ddots & \ddots \\
0 & \ldots & \ldots & \lambda_n
\end{bmatrix}
$$

where:

$$
\mathbf{U} = \begin{bmatrix}
\mathbf{K}_1 \\
\downarrow \\
\mathbf{K}_2 \\
\downarrow \\
\mathbf{K}_n
\end{bmatrix}
$$

and $\mathbf{K}_i$'s are the orthonormal eigenvectors associated
with \( K_\xi \) such that:

\[
K_i^T K_j = \begin{cases} 
1 & : i = j \\
0 & : i \neq j 
\end{cases}
\]

i.e.; \( U \) is an orthogonal matrix and we have \( U^T K_\xi U = \Lambda \). On the other hand, since we are looking for some weight schemes for the correlated batch means such that the weighted batch means (random variables) are uncorrelated, we want to have a linear transformation of the form, \( Y = D \bar{X} \) such that the variance-covariance matrix associated with the random vector \( Y \) is diagonal. i.e.; \( K_Y = \Lambda \), and \( D \) is the weight matrix.

The mean vector \( \mu_Y \) and the variance-covariance matrix \( (K_Y) \) associated with the random vector \( Y \) can be derived as follows:

\[
\mu_Y = E(Y) = E(D \bar{X}) = DE(\bar{X}) = D \mu_X
\]
\[
K_Y = E[(Y-\mu_Y)(Y-\mu_Y)^T] = E[(Y-D \mu_X)(Y-D \mu_X)^T] = E[D(\bar{X}-\mu_X)(\bar{X}-\mu_X)^T] = DE(\bar{X}-\mu_X)(\bar{X}-\mu_X)^T] = DK_\xi D^T
\]

and we want \( K_Y = \Lambda \), i.e., \( D K_\xi D^T = \Lambda \). We have seen above that \( U^T K_\xi U = \Lambda \). Then the comparison of the last two equations \( D \) must equal \( U^T \).

### The New Confidence Interval Method

Given the random vectors \( \bar{X} \Delta (\bar{X}_1(m), \bar{X}_2(m), \ldots, \bar{X}_k(m))^T \) and \( Y \Delta (Y_1, Y_2, \ldots, Y_k)^T \), we have seen that if we apply the linear transformation to the random vector \( \bar{X} \), \( (Y=D \bar{X}) \), where \( D=U^T \) and \( U \) is a matrix with the unit eigenvectors of \( K_\xi \) along its columns, then \( Y \) will be an uncorrelated random vector, i.e., all of its \( k \) random components will be uncorrelated.

Now if we assume that the \( X_i \) (m)'s \( (i=1,2,\ldots,k) \) are normally distributed but correlated random variables (an assumption which is not far from reality according to the central limit theorem, when each batch mean contains a large number of observations), then under this linear transformation, the random vector \( Y \) will also have a normal distribution. However, the components of \( Y \) will be uncorrelated (and in the case of normal distribution they will also be independent, hence they will be i.i.d jointly normally distributed random variables). Now \( Y = D \bar{X} \) in expanded form is:

\[
Y_i = D_1 \bar{X}_1 + D_2 \bar{X}_2 + \ldots + D_k \bar{X}_k \quad i = 1,\ldots, k
\]

If we add the left hand sides of the above \( k \) equations we obtain:

\[
\sum_{i=1}^{k} Y_i = \sum_{j=1}^{k} \sum_{i=1}^{k} D_{ij} \bar{X}_j
\]

Now defining the weights \( W_i (i=1,2,\ldots,k) \) as the sum of the \( i \)th column of the \( D \) matrix, we have:

\[
\sum_{i=1}^{k} Y_i = \sum_{i=1}^{k} W_i \bar{X}_i
\]

Since the \( Y \)'s components are i.i.d normal random variables, the variance of their summation is simply the summation of the \( \Lambda \) matrix diagonal entries, i.e.:

\[
\text{Var} \left( \sum_{i=1}^{k} Y_i \right) = \sum_{i=1}^{k} \text{Var} (Y_i) = \sum_{i=1}^{k} \lambda_i
\]

where the \( \lambda_i \)'s are the eigenvalues of the variance-covariance matrix associated with the random vector \( \bar{X} \). The mean of the summation of the \( Y \)'s components can be derived from the mean of the process response (for which we are looking to construct a c.i.). Knowing that the sample mean is an unbiased estimator of the real process mean:

\[
E[\bar{X}_i] = \mu_{x_i} \quad i = 1,2,\ldots,k
\]

and also since we assumed that the observations come from a steady-state simulation...
system i.e.:

\[ \mu_{x_i} = \mu \quad i = 1, 2, ..., k \]

then:

\[ E \left( \sum_{i=1}^{k} Y_i \right) = \left( \sum_{i=1}^{k} W_i \right) \mu \]

Now since \( Y_i \)'s are i.i.d. normal random variables, their summation will also be a normal random variable with a mean of:

\[ \left( \sum_{i=1}^{k} W_i \right) \mu \]

and a variance of:

\[ \sum_{i=1}^{k} \lambda_i \]

and we can have:

\[
\begin{align*}
P \left[ \sum_{i=1}^{k} W_i \bar{X}_i - \left( \sum_{i=1}^{k} \lambda_i \right) \frac{1}{2} Z_{\alpha/2} \leq \left( \sum_{i=1}^{k} W_i \right) \mu \leq \sum_{i=1}^{k} W_i \bar{X}_i + \left( \sum_{i=1}^{k} \lambda_i \right) \frac{1}{2} Z_{\alpha/2} \right] &= 1 - \alpha \\
\sum_{i=1}^{k} W_i &< \mu < \sum_{i=1}^{k} W_i 
\end{align*}
\]

If the summation of the weights is positive, we will have:

\[
\begin{align*}
P \left[ \sum_{i=1}^{k} W_i \bar{X}_i - \left( \sum_{i=1}^{k} \lambda_i \right) \frac{1}{2} Z_{\alpha/2} \leq \sum_{i=1}^{k} W_i \bar{X}_i + \left( \sum_{i=1}^{k} \lambda_i \right) \frac{1}{2} Z_{\alpha/2} \right] &= 1 - \alpha \\
\sum_{i=1}^{k} W_i &< \sum_{i=1}^{k} W_i 
\end{align*}
\]

However, when the summation of the weights is negative we will have:

\[
\begin{align*}
P \left[ \sum_{i=1}^{k} W_i \bar{X}_i - \left( \sum_{i=1}^{k} \lambda_i \right) \frac{1}{2} Z_{\alpha/2} \leq \sum_{i=1}^{k} W_i \bar{X}_i + \left( \sum_{i=1}^{k} \lambda_i \right) \frac{1}{2} Z_{\alpha/2} \right] &= 1 - \alpha \\
\sum_{i=1}^{k} W_i &< \sum_{i=1}^{k} W_i 
\end{align*}
\]

where \( \bar{X}_i \) is the \( i \)th batch mean, \( W_i \) is equal to the sum of the \( i \)th column of the \( \mathbf{D} \) matrix. \( \lambda_i \)'s are non-negative eigenvalues of the variance-covariance matrix associated with the random vector containing the batch means, and \( Z_{\alpha/2} \) is the upper \((1-\alpha/2)\)% percentile of the standard normal distribution. Recall that the \( \mathbf{D} \) matrix is the transpose of the matrix of which the columns are the unit eigenvectors of the variance-covariance matrix of the batch means. Also note that since the eigenvalues are all non-negative, their summation will also be non-negative and there will not exist any difficulty computing the square root.

The application of the new methodology will be clearer through the following example in which the variance-covariance matrix is assumed to be known. However from the realization of a given stochastic process (simulation output sequence) we need to have an estimation of the variance-covariance matrix which are discussed in [9, 14 - 18].

**Numerical Example**

Suppose that we make a single simulation run and obtain \( n=1000 \) steady state observations on the system performance (response). We want to obtain the point and interval estimates for the average response (\( \mu \)) based on the sample observations \( X_1, X_2, ..., X_{1000} \).

Let the sample mean \( \bar{X}(n)=3 \) which in general is a good point estimate because \( \bar{X}(n) \) is an unbiased estimator of \( \mu \). Suppose that we divide the sample data into \( k=2 \) batches of size \( m=500 \) each. Let \( \bar{X}_1=2 \) and \( \bar{X}_2=4 \) be the two batch means obtained from \( m=500 \) observations in each batch. Also suppose that we know that the variance-covariance matrix \( (\mathbf{K}_a) \) associated with the batch means has the following values:

\[
\mathbf{K}_a = \begin{bmatrix} 3 & -1 \\ -1 & 3 \end{bmatrix}
\]
The non-negative eigenvalues $\lambda_1$ and $\lambda_2$ associated with the positive definite matrix $K_X$ can be obtained as follows:

$$\det(K_X - \lambda I) = 0$$

$$\Rightarrow \det \left( \begin{array}{ccc} 3 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 3-\lambda \end{array} \right) = \det \left( \begin{array}{ccc} -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & 3-\lambda \end{array} \right) = 0$$

$$(3-\lambda)^2 - 1 = 0 \Rightarrow \lambda_1 = 4, \lambda_2 = 2$$

and we have:

$$\sum_{i=1}^{k=2} \lambda_i = 4 + 2 = 6$$

The unit eigenvectors $K_1$ and $K_2$ can be obtained as follows:

$$(K_X - \lambda_1 I) K_1 = 0 \Rightarrow K_1 = \begin{pmatrix} 1 \sqrt{2} \\ 1 \sqrt{2} \end{pmatrix}^T$$

$$(K_X - \lambda_2 I) K_2 = 0 \Rightarrow K_2 = \begin{pmatrix} 1 \sqrt{2} \\ 1 \sqrt{2} \end{pmatrix}^T$$

Then the $U$ matrix whose columns are the unit eigenvectors is:

$$U = \begin{pmatrix} 1 \sqrt{2} & 1 \sqrt{2} \\ 1 \sqrt{2} & 1 \sqrt{2} \end{pmatrix}$$

Now the weight matrix ($D$) is simply the transpose of the $U$ matrix, i.e., :

$$D = \begin{pmatrix} 1 \sqrt{2} & 1 \sqrt{2} \\ 1 \sqrt{2} & 1 \sqrt{2} \end{pmatrix}$$

and the weights are $W_1 = \sqrt{2}$ and $W_2 = 0$. Also we have:

$$\sum_{i=1}^{k=2} W_i = \sqrt{2} + 0 = \sqrt{2}$$

and:

$$\sum_{i=1}^{k=2} W_i \bar{X}_i = (\sqrt{2}) (2) + (0) (4) = 2\sqrt{2}$$

Knowing that $Z_{a/2} = 1.96$ for $\alpha = 0.05$, then the 95% confidence interval on $\mu$ is:

$$Pr\left[\frac{2\sqrt{2} - (\sqrt{6}) (1.96)}{\sqrt{2}} < \mu < \frac{2\sqrt{2} + (\sqrt{6}) (1.96)}{\sqrt{2}}\right] = 1 - 0.05 = 0.95$$

which gives:

$$P[-1.39 < \mu < 5.39] = 0.95$$

Note that the variance-covariance matrix associated with the transformed random vector $Y = D\bar{X}$ will be in the following form:

$$K_Y = DK_X D^T = \begin{pmatrix} 1 \sqrt{2} & -1 \sqrt{2} \\ 1 \sqrt{2} & 1 \sqrt{2} \end{pmatrix} \begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} 1 \sqrt{2} \\ 1 \sqrt{2} \end{pmatrix} = \begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}$$

which, as expected, is a diagonal matrix. In other words, the random vector $\bar{X}$ with correlated components was converted through the above linear transformation to a random vector $Y$ with uncorrelated components. Also note that the eigenvalues are obtained along the diagonal of the $K_Y$ matrix.

**REFERENCE**


667-678.


