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An Efficient Method of Estimating Confidence Intervals for Use in Simulation-Optimization

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Abstract

In many applications of simulation-optimization, when comparing two or more alternatives, it is crucial to be able to estimate the confidence intervals on the outputs of interest with a reasonable level of accuracy. This accuracy has often been tested by the closeness of the coverage of the estimated confidence interval to the intended coverage. In this paper two variations to the Batch-Means Method of estimating the confidence intervals are presented and their performances are compared with the original method. The results indicate that the Batch Means Method modified by factors obtained by a second order autoregressive method is superior to the original and the one modified based on factors obtained from autocorrelation analysis.

1. Introduction

Let $\{X_i, i \geq 1\}$ be a stochastic process resulted from a simulation output analysis with a steady-state mean, μ. That is:

$$\mu = \lim_{n \to \infty} \sum_{i=1}^{n} E[X_i]/n = \lim_{n \to \infty} E[\sum_{i=1}^{n} X_i/n] \qquad (1)$$

Consider the problem of estimating the confidence interval for the steady-state mean, μ where there is enough time such that n observations for the system response can be obtained from the running of the simulation model. In most cases, nonstationarity and autocorrelation in output data from simulation make the correct estimation of confidence intervals difficult. Therefore, the classical method which assumes that data are from independent and identically distributed

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populations cannot be applied directly.

Two most often used methods, Replication Method and Batch Means Method were compared with each other by Law [6] in terms of the coverages and half lengths of confidence intervals. In that experiment, it was concluded that the Batch Means Method performed better than the Replication Method.

In the Batch Means Method in general, after making a large number of observations ($n=m\times x$) they are divided into k batches, each with length of m, such that the batch means are approximately independent. Then confidence intervals are estimated based on these batch means. The problem in this method is that when there exist autocorrelations between batch means, coverage becomes smaller than the theoretical value. To overcome this problem, the simulation model must be run for much longer periods to provide enough data for constructing more accurate confidence intervals. However, in simulation-optimization problems [1,2,3] and in simulation of complex manufacturing systems [13] a large number of simulation runs are required. Thus very long simulation runs may not be feasible. Therefore, the autocorrelations between batch means may not be eliminated.

In this paper two possible modifications to Batch Means Methods are proposed for overcoming these situations. These are based on the second order autoregressive method and the autocorrelation method based on time series analysis. The results of these methods are then compared to those of the original Batch Means Method.

The remainder of the paper is organized as follows. In section 2, the details of these modified methods are described. In section 3, the results of the coverages obtained by testing the methods on an M/ M/ 1 queuing system are presented and compared to each other. Section 4 presents summary and conclusions.

2. Modified Batch Means Methods

In the classical Batch Means Method n simulation output data $x_1, x_2, \cdots, x_n$ Equation are divided into k batches of size m and the mean of the output parameter is estimated by

$$Z(k,m) = \sum_{i=1}^{k} Y_i(m) / k \tag{2}$$

where $Y_i(m)$ is the mean of the k-th batch. If $s^2(k,m)$ is the sample variance for $Y_i(m)$ and $\sigma^2[Z(k,m)]$ is the unbiased estimator for variance of $Z(k,m)$,

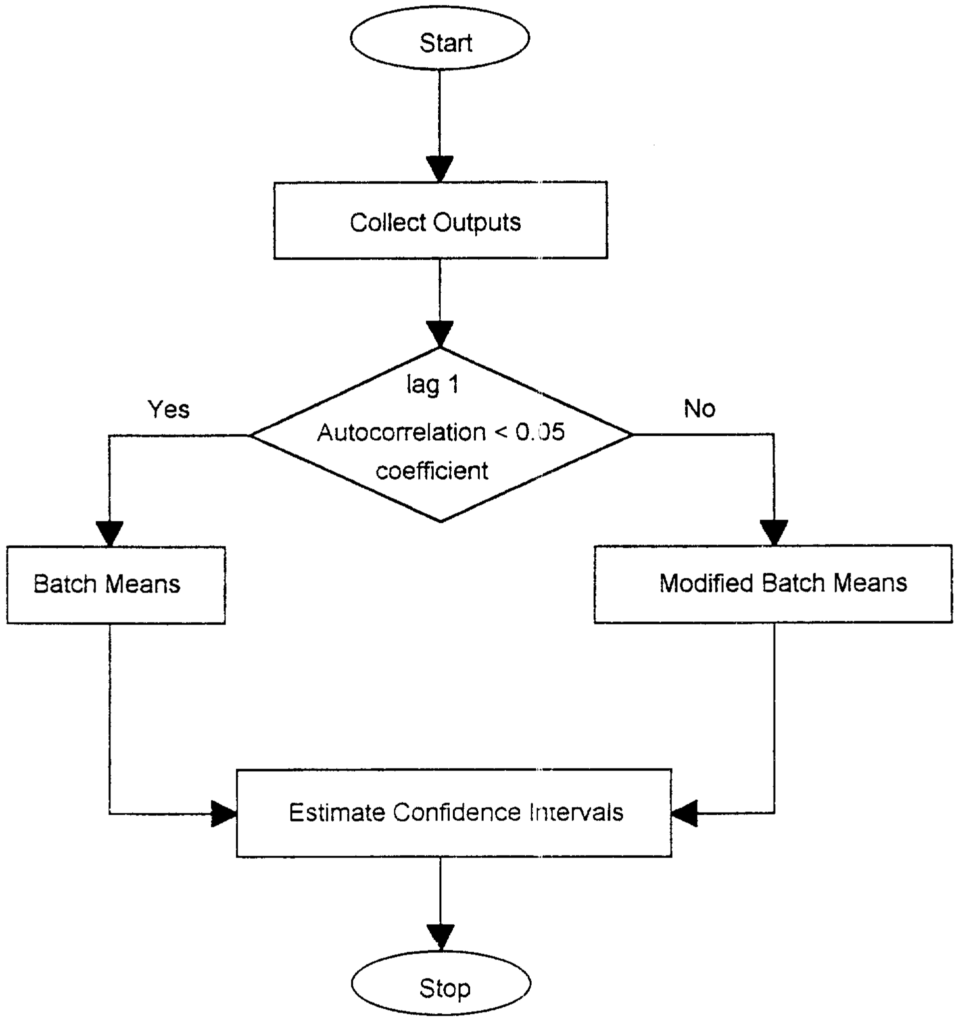
$$s^2(k,m) = \frac{\sum_{i=1}^{k} [Y_i(m) - Z(k,m)]^2}{(k-1)} .$$

$$\sigma[Z(k,m)] = \frac{s^2(k,m)}{k} = \sum_{i=1}^{k} \frac{[Y_i(m) - Z(k,m)]^2}{k(k-1)} . \qquad (3)$$

$100(1-\alpha)\%$ confidence interval for μ can be expressed as

$$Z(k,m) \pm t^{k-1}_{1-\alpha/2} \cdot \sqrt{\alpha^2[Z(k,m)]} \qquad (4)$$

where $t^{k-1}_{1-\alpha/2}$ is $1-\alpha/2$ level of t distribution with $k-1$ degrees of freedom.



[Figure 1] Flow Chart of Confidence Intervals by Modified Batch Means

According to Law [6] in this estimation there may exist the following sources of error:

(1) Bias in variance of $\sigma^2[Z(k,m)]$ if m is not large enough to eliminate the correlations between batch means,

(2) Nonnormality of $Y_i(m)$'s,

(3) Violation of the assumption of covariance stationarity of the process.

Law [7] pointed out that in estimating the confidence interval for an M/ M/ 1 queuing system with Batch Means Method the bias in variance of $\sigma^2[Z(k,m)]$ is the most serious source of error, while nonormality does not pose a significant problem when k is greater than 20.

In the modified methods suggested here, the confidence intervals obtained by the original Batch Means Method are modified by factors obtained by one of the statistical analyses suggested below. In each of these cases, first the batch means are checked for independence. This is done by estimating lag 1 autocorrelation coefficient $\rho_1(m)$.

$$\hat{\rho}_1(k,m) = \frac{\sum_{i=1}^{k-1}[Y_i(m)-Z(k,m)]\,[Y_{i+1}(m)-Z(k,m)]}{\sum_{i=1}^{k}[Y_i(m)-Z(k,m)]^2} \tag{5}$$

It must be pointed out that for estimating lag 1 autocorrelation coefficient $\rho_1(m)$, Jackknife estimator $\tilde{\rho}_1(k,m)$ could be used which in general has smaller bias than $\hat{\rho}_1(m)$[9].

$$\tilde{\rho}_1(k,m) = 2\hat{\rho}_1(k,m) - \frac{\hat{\rho}_1^1(k/2,m)+\hat{\rho}_1^2(k/2,m)}{2} \tag{6}$$

where $\hat{\rho}_1^1(k/2,m)$ is an estimator for $\rho_1(m)$ using the first half and $\hat{\rho}_1^2(k/2,m)$, the second half of k batches.

After checking the correlations between batch means, if there exists no correlation, the classical formula in equation (4) can be used. Otherwise one of the modified Batch Means Method which will be explained in the following sections could be employed. This procedure is summarized in Figure 1.

2.1 Second Order Autoregressive Method

Let us assume that the batch means based on the observed simulation data are correlated but can appropriately fit an AR(2) model. In this case, the confidence interval calculated by (4) can be modified as follows.

$$Z(k,m) \pm \sqrt{\lambda(\alpha_1, \alpha_2)} \cdot t^{k-1}_{1-\alpha/2} \cdot \sqrt{\sigma^2[Z(k,m)]} \tag{7}$$

where $\lambda(\alpha_1, \alpha_2)$ is a modification factor which has been shown to reduce the bias of estimation of $\sigma^2[Z(k,m)]$ and α_1, α_2 are coefficients of AR(2) model such that

$$x_t = \alpha_1 x_{t-1} + \alpha_2 x_{t-2} + \zeta_t$$

This modification was originally developed for calculating the limits for quality control charts in the presence of data correlation [10].

To estimate α_1 and α_2 we use the Recursive Least Squares Method [8]. For this purposes, AR(2) model is expressed as follows:

$$x_t = -c_1 x_{t-1} - c_2 x_{t-2} + v_t \tag{8}$$

where $c_1 = -\alpha_1$, $c_2 = -\alpha_2$ *and* $v_t = \zeta_t$. Using state variables, these coefficients can be expressed as follows:

$$C_t^T = [c_1, c_2] \text{ and } F_t^T = [-x_{t-1}, -x_{t-2}]$$

where C_t^T and R_t^T are transposes of C_t and R_t, respectively. If coefficients are constant, the following expressions hold:

$$C_{t+1} = C_t = C.$$

Thus

$$x_t = C^T R_t + v_t.$$

To estimate C_1 and C_2 the following recursive algorithm can be used:

$$C_t = C_{t-1} + L_t [x_t - C_{t-1}^T R_t]$$

$$L_t = \frac{P_{t-1} R_t}{1 + R_t^T P_{t-1} R_t}$$

$$P_t = P_{t-1} - L_t^T P_{t-1}$$

where L_t is a (2×1) matrix and P_t is a (2×2) matrix. Initial conditions for this recursive algorithm is set to be as:

$$C_2 = [0, 0]^T$$

$$P_2 = \begin{bmatrix} d & 0 \\ 0 & d \end{bmatrix}$$

$$R_3 = [-x_2, -x_1]^T$$

where 50 is recommended as an appropriately large value for d.

To estimate modification factor, $\lambda(\alpha_1, \alpha_2)$ the characteristic equation of AR(2) can be used as follows [12]:

$$\Phi(B) = 1 - \alpha_1 B - \alpha_2 B^2 = 0$$

or

$$\Phi(B) = (1 - G_1 B)(1 - G_2 B) = 0 \qquad (9)$$

where

$$G_1 = (\alpha_1 + \sqrt{\alpha_1^2 + 4\alpha_2}) / 2$$

$$G_2 = (\alpha_2 - \sqrt{\alpha_1^2 + 4\alpha_2}) / 2.$$

If G_1^{-1}, G_2^{-1} are solutions to the characteristic equation in (9) and $f(G_1, G_2) = \lambda(\alpha_1, \alpha_2)$ depending on values of G_1^{-1}, G_2^{-1}, there could exist three different cases for $f(G_1, G_2)$ as follows [10]:

(1) G_1^{-1}, G_2^{-1} have different real values ($\alpha_1^2 + 4\alpha_2 > 0$):

$$f(G_1, G_2) = P - Q$$

where $P = \{G_1(1 - G_2^2)\} / \{(G_1 - G_2)(1 + G_1 G_2)\} \times \Phi(G_1)$

$Q = \{G_2(1 - G_1^2)\} / \{(G_1 - G_2)(1 + G_1 G_2)\} \times \Phi(G_2)$

and $\Phi(G) = [(1 + G) / (1 - G)] - [(2G/k)\{(1 - G^k) / (1 - G)^2\}]$

(k: number of batches)

(2) $G_1^{\,1}$, $G_2^{\,1}$ have the same values ($\alpha_1^2+4\alpha_2=0$):

$$f(G_1, G_2) = K_1(G) - K_2(G) \times T$$

where $K_1(G) = (1+G)/(1-G)$

$K_2(G) = (2G/k)\{(1-G^k)/(1-G)^2\}$

$T = 1 + \{(1+G)^2(1-G^k) - k(1-G^2)(1+G^k)\}/\{(1+G^2)(1-G^k)\}$

(3) $G_1^{\,1}$, $G_2^{\,1}$ have imaginary values ($\alpha_1^2+4\alpha_2<0$):

$$f(G_1, G_2) = P/Q + \{2d/k\} \times \{R/S\}$$

where $P = 1 - d^4 + 2d(1-d^2)\cos\omega$

$Q = (1+d^2)(1+d^2-2d\cos\omega)$

$R = R_1 + R_2$

$R_1 = 2d(1+d^2)\sin\omega - (1+d^4)\sin 2w - d^{k+4}\sin(k-2)\omega$

$R_2 = 2d^{k-3}\sin(k-1)\omega - 2d^{k+1}\sin(k-1)\omega + d^k\sin(k+2)\omega$

$S = (1+d^2)(1+d^2-2d\cos\omega)^2\sin\omega$

where $d = -\alpha_2$, $\cos\omega = \alpha_1/2d$

$\sin\omega = \sqrt{-\alpha_1^2-4\alpha_2}\,/\,2d$

$\tan\omega = \sqrt{-\alpha_1^2-4\alpha_2}\,/\,\alpha_1$

$\omega = \tan^{-1}[\sqrt{-\alpha_1^2-4\alpha_2}\,/\,\alpha_1]$

2.2 Autocorrelation Method

When the output data is correlated $s^2(k,m)$ is a biased estimator of the variance of $Y_i(m)$. The expected value of $s^2(k,m)$ can be expressed as follows [7,11]:

$$E[s^2(k,m)] = \sigma^2\{1 - 2\sum_{j=1}^{k-1}(1-j/k)\rho_j/(k-1)\} \qquad (10)$$

where ρ_j is lag j autocorrelation coefficient. The variance for grand sample mean $Z(k,m)$ can then be expressed as follows:

$$\sigma^2[Z(k,m)] = \sigma^2 \frac{1 + 2\sum_{j=1}^{k-1}(1 - j/k)\rho_j}{k} \tag{11}$$

From equation (10) and (11) the expected value of the estimator for variance of grand sample mean $Z(k,m)$ can be expressed as follows:

$$\begin{aligned} E\{\hat{\sigma}^2[Z(k,m)]\} &= E[s^2(k,m)/k] \\ &= \frac{\sigma^2}{k} \cdot \left[1 - 2\sum_{j=1}^{k-1}\frac{(1 - j/k)\rho_j}{k-1}\right] \\ &= \frac{\sigma^2}{k(k-1)} \cdot \left[k - 1 - 2\sum_{j=1}^{k-1}(1 - j/k)\rho_j\right] \\ &= \frac{[k - a(k,m)]}{k(k-1)} \cdot \sigma^2 \\ &= \frac{k/a(k,m) - 1}{k-1} \cdot \sigma^2 \cdot \frac{a(k,m)}{k} \\ &= \frac{[k/a(k,m) - 1]}{k-1} \cdot \sigma^2[Z(k,m)] \\ &= b(k,m) \cdot \sigma^2[Z(k,m)] \end{aligned} \tag{12}$$

where $a(k,m) = 1 + 2\sum_{j=1}^{k-1}(1 - j/k)\rho_j$

$b(k,m) = \dfrac{[k/a(k,m) - 1]}{k-1}$.

From equation (12)

$$\begin{aligned} \hat{\sigma}^2[Z(k,m)] &= \frac{s^2(k,m)}{k} \cdot \frac{1}{b(k,m)} \\ &= \frac{\sum_{j=1}^{k}[Y_j(m) - Z(k,m)]^2}{k(k-1)} \cdot \frac{1}{b(k,m)} \end{aligned} \tag{13}$$

Lag j autocorrelation coefficient can be estimated by the following equation :

$$\rho_j = \frac{C_j}{s^2(k,m)} \tag{14}$$

where

$$C_j = \frac{\sum_{i=1}^{k-j}[Y_i(m) - Z(k,m)]\,[Y_{i+j}(m) - Z(k,m)]}{k-j}$$

In the Autocorrelation Method which considers correlations between the means, the formula for calculating $100(1-\alpha)\%$ confidence interval for μ is the same as one in equation (4) except that equation (13) is used to estimate $\sigma^2[Z(k,m)]$.

When data are positively autocorrelated, the value of a(k,m) is greater than 1 while b(k,m) is less than 1. Thus the calculated variance becomes larger than the value obtained without considering correlation and thereby, the confidence interval becomes wider. That is, if data are positively autocorrelated, the actual value of variance is larger than the one estimated by using $s^2(k, m)/k$.

The only problem with this method is that the accuracy of estimation of correlation coefficients is decreased when k is very small or lag j is relatively large compared to k.

3. Comparison of Methods

To compare the Modified Batch Means Method based on the second order autoregressive method and the autocorrelation method developed in section 2 with the original Batch Means Method, a large number of experiments were conducted on an M/M/1 queuing system with various values of traffic intensity. As traffic intensity increases, so does the correlation between observed output data. In these experiments, random numbers $\{U_i, i \geq 1\}$ were generated based on the Linear Congruential Method using the following formula [7]:

$$X_i = (5^{15} X_{i-1} + 1) \bmod 35846594356784$$
$$U_i = X_i / 35846594356784 \qquad (15)$$

where X_0 was given.

Let D_i be the waiting time for the i-th customer which excludes service time and assumes that the system starts empty and idle, i. e. $D_1=0$. To estimate mean waiting time w_g at steady-state data for $\{D_i, i \geq 1\}$ are obtained through simulation experiments. Theoretically, the true means are 1.633, 3.2, and 8.1 for traffic intensities of $\rho=0.7$, 0.8 and 0.9 respectively. Run lengths, n=320,640,1280 and 2560 and number of batches, k=5, 10, 20 and 40 were used. For each combination of values for n and k, 200 different runs were conducted and 90% confidence intervals for each case were estimated using the three different methods, i.e. , original Batch Means Method (BM), Modified Batch Means Method based on the second order autoregressive method (AR) and the autocorrelation method (AC). Coverages were also estimated by calculating the percentage of intervals that actually included the true mean. The detailed results for coverages and half lengths of confidence intervals are shown in Table 1 through 3 for each value of ρ. Figures 2 through 5 show coverage vs. number of batches, k for $\rho=0.7$, 0.8, and 0.9 and n=1280 and 2560. In Figure 6 coverage vs. ρ with n=2560 and k=20 is plotted.

From these results the following conclusions can be drawn. In general the results follow the same pattern as reported in [6]. With increased n, coverages improved and larger batch sizes provide better coverages. However, a significant difference is observed in the performance of the Batch Means Method modified by the second order autoregressive model. In all cases, this modification shows a marked improvement in the coverage.

Comparing the performance of the classical Batch Means Method with the Batch Means Method modified by autocorrelation, Figures 2 to 6, doses not indicate that a significant difference for coverages exists. The reason for this might be that the corrections by this modification might have been offset by the errors in estimating the correlation factors.

Figure 6 shows another interesting result. According to this figure the coverages by all three methods improve as the traffic intensity and consequently the correlation among data increases. This improvement is more pronounced for the classical Batch Means Method and the Batch Means Method modified by autocorrelation factors. This indicates that in these two cases as correlation within the data increases, the effect of modification factors is more than the errors induced by their estimation. However, a more important conclusion is that the Batch Means Method modified by the second order autoregressive model is less sensitive to the level of dependence in the output data compared to the other two methods.

Finally, Tables 2, 3 and 4 show that the confidence intervals are wider for higher levels of coverages. This is understandable because the number of observations have been kept the same for all three methods. The choice of which alternative to choose should be obvious, because one would prefer a wider confidence interval with a coverage closer to the intended theoretical value to a narrower interval erroneously claiming a reasonable coverage.

〈Table 1〉 Coverages and Half Lengths for 90% Confidence Intervals for an M/ M/ 1 with ρ=0.9

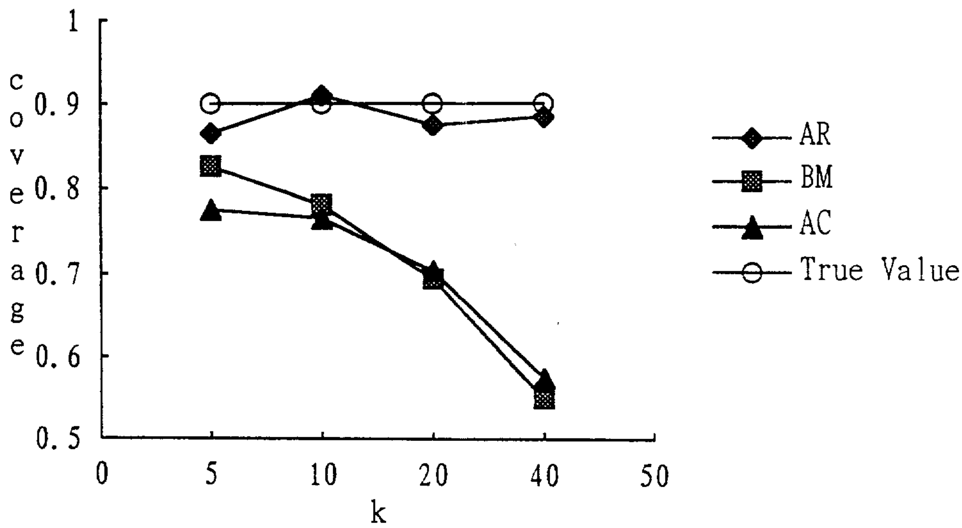
n \ k		5		10		20		40	
		C	H.L	C	H.L	C	H.L	C	H.L
320	BM	0.460	3.080	0.340	2.096	0.280	1.488	0.200	1.059
	AR	0.520	3.808	0.505	3.479	0.540	3.796	0.530	3.764
	AC	0.395	2.694	0.320	2.151	0.290	1.581	0.200	1.110
640	BM	0.585	3.346	0.510	2.481	0.430	1.812	0.310	1.303
	AR	0.720	4.616	0.685	4.372	0.745	4.744	0.740	4.912
	AC	0.550	2.359	0.500	2.498	0.430	1.882	0.310	1.358
1280	BM	0.825	2.665	0.780	2.206	0.695	1.829	0.310	1.358
	AR	0.865	3.700	0.910	4.582	0.875	4.995	0.885	4.604
	AC	0.775	2.343	0.765	2.141	0.705	1.851	0.575	1.399
2560	BM	0.860	1.909	0.885	1.789	0.835	1.595	0.780	1.342
	AR	0.925	2.981	0.890	3.843	0.965	4.300	0.960	3.854
	AC	0.825	1.695	0.880	1.706	0.840	1.580	0.790	1.353

〈Table 2〉 Coverages and Half Lengths for 90% Confidence Intervals for an M/ M/ 1 with ρ=0.8

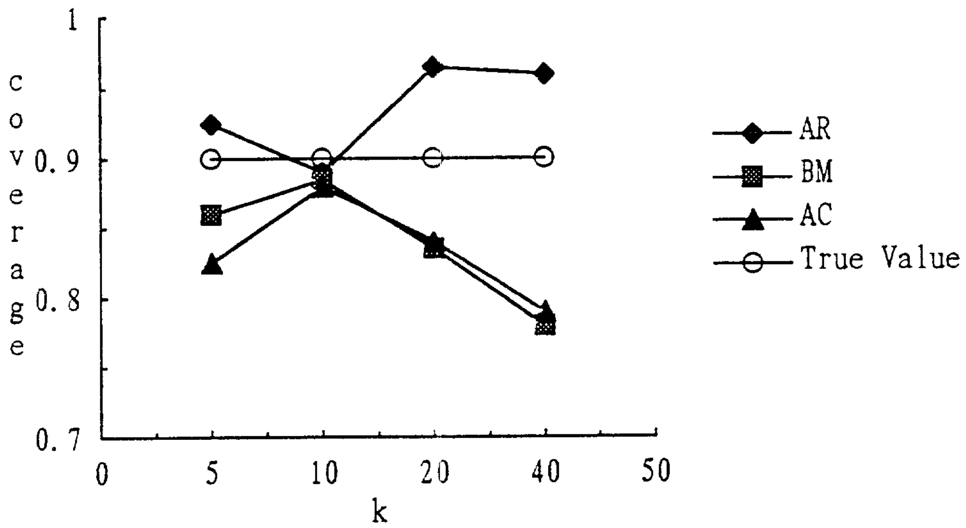
n \ k		5		10		20		40	
		C	H.L	C	H.L	C	H.L	C	H.L
320	BM	0.475	1.304	0.415	1.002	0.295	0.760	0.210	0.564
	AR	0.580	1.708	0.585	1.730	0.590	1.874	0.620	1.875
	AC	0.420	1.156	0.405	1.001	0.310	0.786	0.225	0.582
640	BM	0.252	1.310	0.505	1.095	0.430	0.860	0.380	0.652
	AR	0.635	1.703	0.700	1.854	0.730	2.194	0.700	2.143
	AC	0.490	1.151	0.515	1.082	0.430	0.874	0.385	0.671
1280	BM	0.890	1.077	0.830	0.950	0.710	0.832	0.495	0.650
	AR	0.915	1.488	0.905	1.999	0.915	1.880	0.920	1.765
	AC	0.800	0.940	0.800	0.921	0.710	0.832	0.515	0.657
2560	BM	0.520	0.640	0.545	0.616	0.520	0.593	0.450	0.533
	AR	0.750	0.946	0.835	1.316	0.910	1.380	0.910	1.208
	AC	0.460	0.573	0.470	0.590	0.485	0.586	0.450	0.534

〈Table 3〉 Coverages and Half Lengths for 90% Confidence Intervals for an M/ M/ 1 with $\rho=0.7$

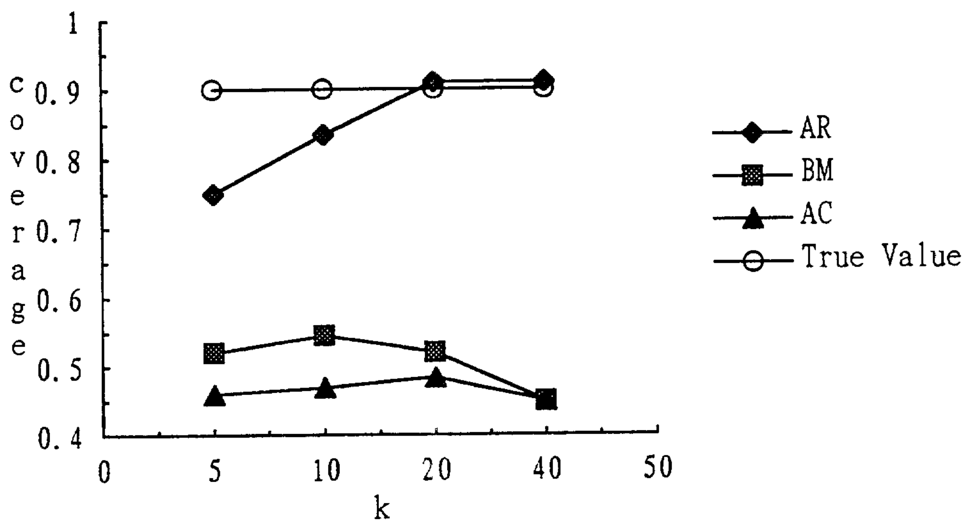
n \ k		5		10		20		40	
		C	H.L	C	H.L	C	H.L	C	H.L
320	BM	0.630	0.619	0.560	0.526	0.500	0.429	0.400	0.335
	AR	0.790	0.838	0.745	0.910	0.815	0.956	0.810	0.948
	AC	0.595	0.551	0.560	0.518	0.495	0.433	0.400	0.342
640	BM	0.685	0.507	0.640	0.426	0.575	0.379	0.525	0.317
	AR	0.860	0.691	0.810	0.802	0.920	0.092	0.905	0.832
	AC	0.635	0.448	0.630	0.420	0.580	0.382	0.530	0.321
1280	BM	0.540	0.282	0.450	0.255	0.450	0.234	0.425	0.218
	AR	0.820	0.430	0.780	0.550	0.865	0.658	0.795	0.469
	AC	0.460	0.247	0.435	0.245	0.450	0.233	0.430	0.210
2560	BM	0.230	0.143	0.265	0.167	0.265	0.163	0.250	0.156
	AR	0.320	0.215	0.805	0.398	0.845	0.468	0.720	0.473
	AC	0.205	0.129	0.260	0.160	0.255	0.160	0.250	0.153



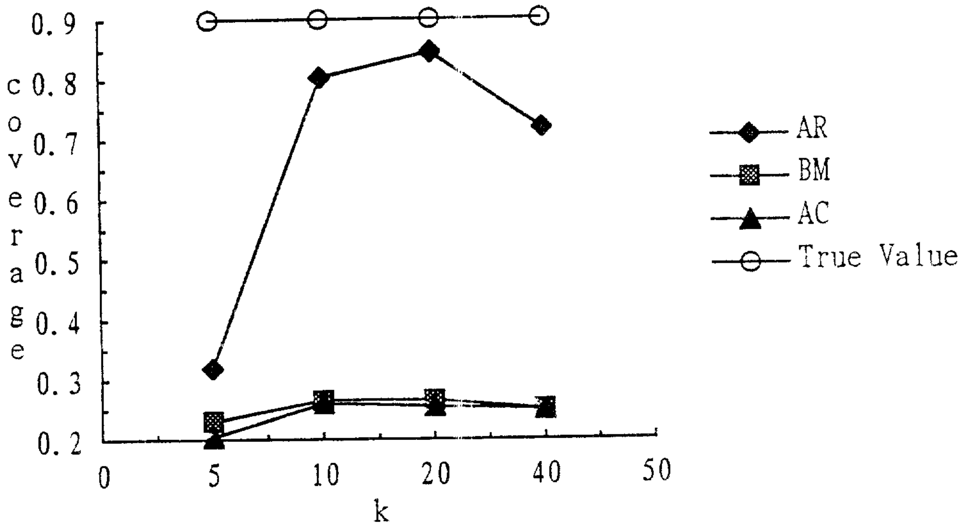
[Figure 2] Coverage of Estimated Confidence Intervals When $\rho=0.9$, n=1280



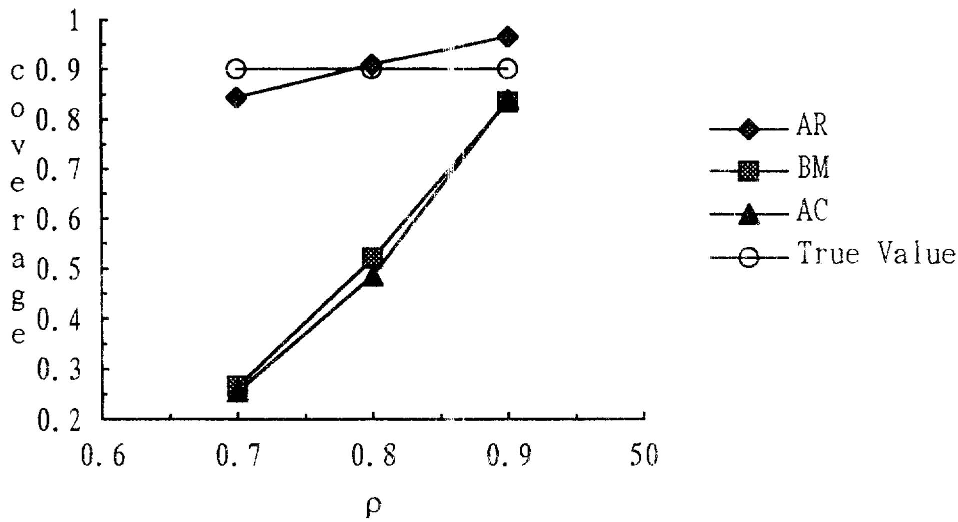
[Figure 3] Coverage of Estimated Confidence Intervals When ρ=0.9, n=2560



[Figure 4] Coverage of Estimated Confidence Intervals When ρ=0.8, n=2560



[Figure 5] Coverage of Estimated Confidence Intervals When ρ=0.7, n=2560



[Figure 6] Coverage vs. Various Values of ρ When n=2560, k=20

4. Conclusions

In this paper the performances of the Batch Means Method of estimating the confidence intervals on the output of simulation experiments and two modifications to this method were evaluated based on tests on an M/M/1 queuing system. One modified method modifies the confidence intervals based on the autocorrelation factors estimated from data. The other method modifies the confidence intervals based on coefficients of a second order autoregressive model fitted to the data.

The results indicate that autoregressive modification performed consistently better than the original Batch Means Method and the one modified by autocorrelation factors. The difference between the other two methods was insignificant. Also, it was shown that the performance of all methods improves as the autocorrelation within the output data increases while second order autoregressive model is less sensitive to this variation than the other two methods.

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