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A Tool for Optimizing Simulated Discrete Variable Stochastic Systems: SIMICOM

Young Hae Lee*
F. Azadivar**

Abstract

A heuristic algorithm (SIMICOM) has been designed and tested for optimizing simulated stochastic systems whose performances are functions of several discrete decision variables. The approach adopted utilizes an integer complex method coupled with techniques of establishing confidence intervals for the system's responses. It can handle a general class of optimization problems that could be constrained or unconstrained. In constrained cases, the constraints could either be explicit analytical functions of decision variables or be expressed as other responses of the simulation model. In addition to obtain a reasonably accurate solution, the economic aspect of obtaining the solution has also been taken into consideration.

1. Introduction

Simulation is often used for evaluation of systems for given decision policies. In some applications the outcomes of various policies are compared through multiple comparisons or design of experiments employing computer simulation as the means of experimentation. However, relatively fewer attempts have been made to use simulation as a means of optimization. If a decision policy is defined as a set of values for several decision variables of the system, it is easy to see that simulation can be efficiently used as a means of optimization of such a system. In other words, simulation response can be used as an objective function of an optimization problem. To clarify this, consider the following example.

A multiuser computer system under interactive operating environments in which each user may input different classes of commands such as edit, compile, logon, logoff and several file manipulation

* Dept. of Industrial Engineering, Hanyang University
** Dept. of Industrial & Systems Engineering, Univ. of Illinois at Chicago

commands. Each class of command is characterized by its distribution of input-message length, CPU processing time, output-message length, and think times following each output-message. The operation of such a computer system for a given number of processors, terminals, and disk drives can be modeled through a computer simulation to minimize the system's response time (to maximize the throughput) within the available budget.

In optimizing the system such as above, one may be interested in finding the optimum values for the controllable variables such that the total operation of the system in terms of a given measure of effectiveness is optimized. In order to optimize such simulated systems a systematic procedure in the form of an algorithm is needed; it must be capable of interacting with the simulation model and obtaining the optimal values for the decision variables.

Most of the algorithms developed in the literature can only be applied to systems whose decision variables are represented by continuous variables (e.g., SAMOPT by Azadivar [1] and Response Surface Methodology [3], [4], [7], [21]). In some cases for dealing with the discrete variable simulation-optimization problem, rounding off of the continuous optimum was used [4], [23], which can lead to a point which may or may not represent the real discrete optimum [8].

The algorithm discussed in this paper deals with the optimization of stochastic simulation models whose control variables are discrete.

2. Statement of the Problem

It is known that the result of the evaluation of the response function of a simulated system for a given set of values for the decision variables is just one realization of a stochastic process. Let Z(X) denote the random variable representing the response of the simulation model for a set of values for the decision variables represented by vector X. Also let H(z/X) be the cumulative probability distribution function for the random variable Z such that

$$H(z/X) = P[Z(X) \leq z] \tag{2.1}$$

Obviously characteristics of H are functions of X and the structure and stochastic behavior of the simulation model. The expected value of Z(X) can be expressed as

$$E[Z/X] = \int_{-\infty}^{\infty} z dH(z/X) \tag{2.2}$$

E[Z/X] is called the conditional expected value of Z for given X. Now if a function Y(X) exists such that

$$Y(X) = E[Z/X] \quad \text{for all } X \tag{2.3}$$

then Y(X) is called the theoretical regression function of $\overline{Z(X)}$.

For stochastic functions, optimization often means the optimization of their expected value. In other words, those values of the decision variables for which the expected value of the response is optimized are of interest.

The problem under study could be formulated in its general form as follows:

$$\overline{\text{Min}}\ (\overline{\text{Max}}) \qquad Y(X) = E[\overline{Z(X)}]$$

$$\text{Subject to} \qquad g_j(X) \begin{matrix} \leq \\ = \\ \geq \end{matrix} c_j, \qquad j = 1,2,\ldots,m \tag{2.4}$$

where

X is a vector consisting of n discrete valued decision variables,

Z(X) is the random variable corresponding to the observation of the simulated systems,

Y(X) is the unknown theoretical regression function of Z(X) and

$g_j(X)$ is a set of m constraints on X .

In order for the algorithm to work, it must employ an optimum seeking search method that can converge to the optimum of Y(X) by making observations on Z. In order to apply the proposed algorithm the following requirements should be met:

i) The theoretical regression function Y(X) is a real-valued function.

ii) There exists a finite constant M such that

$$\mathrm{Var}[Z(X)] \leq M \text{ for all } X$$

iii) Elements of X are discrete valued variables.

3. Development of the Algorithm

Among the optimization procedures available, the simplex method [22] and the complex method (constrained-simplex) [6] seem to have better potentials for dealing with the discrete optimization problems through simulation. The reasons are a) starting from a point far away, the complex search approaches rapidly to the optimum [25], b) it can be modified relatively easily from its continuous version to discrete optimization [2], c) its constrained version is available so that it can be applied to discrete optimization problems with all types of constraints and d) it does not need an analytical expression of the objective function. Consequently this method has been used as a basis for development of the algorithm in this paper.

The complex method of Box [6] has been modified by Beveridge and Schechter [2] for discrete optimization. The following difficulties may occur when using the modified complex method of Beveridge and Schechter for discrete optimization problems.

a) The method may converge to a nonoptimal point on or near a resolution valley as illustrated in [8].

b) The search may become stranded if the centroid of the remaining vertices of the complex is sufficiently close to the point to be rejected, in which case the new vertex coincides with the originally rejected vertex. This particular difficulty often arises when the method attempts to move along a ridge or a constraint and the complex becomes very flat and long, or the point is inside the remaining vertices.

c) A similar stranding of the search may occur if the projected point is rejected and the retracted point coincides either with the first projected point or the point which was originally rejected. This last difficulty arises when there is no better point in the projected direction.

3.1 Modifications of Integer Complex Method

In order to prevent the search from becoming stranded because of the difficulties shown above the method of regeneration of search is proposed by Glankwahmdee et al. [8].

As reported in [20] and [24] the complex method is affected considerably by the scale and orientation chosen for the first complex. With a stochastic function the optimum of which is known we had a

similar experience. That is, when we chose the points in the initial complex near the boundry of the feasible region, sometimes the procedure did not converge to the optimum. To overcome this situation in this paper the nonrandom method rather than the random method of setting the initial complex i adopted.

Nonrandom Selection of the Initial Complex

Using an initial feasible point that does not lie on any constraint bound, a set of 2n+1 points can be generated as the initial complex by following a procedure similar to the one in [20]. But employing 2n+1 vertices in the initial complex usually requires too many evaluations of the simulation model before it converges to the optimum. To utilize the allowable simulation runs more economically this nonrandom method was modified and only n+1 points were included in the initial complex. These points are located by using the uniform search as follows.

First, a central point of the feasible region which satisfies the bound constraints, is selected. The coordinates of this point can be obtained as follows:

$$x_i = <(c_i - a_i) / 2>$$

where c_i and a_i are upper and lower bounds on variable x_i, respectively. The notation $<z>$ represents the nearest integer value to z.

Then the range of each variable is divided into two equal portions resulting in a total of 2^n equal regions. The centers of the regions including the central point of the feasible region are evaluated until n+1 points necessary to the initial complex are selected (See Figure 1).

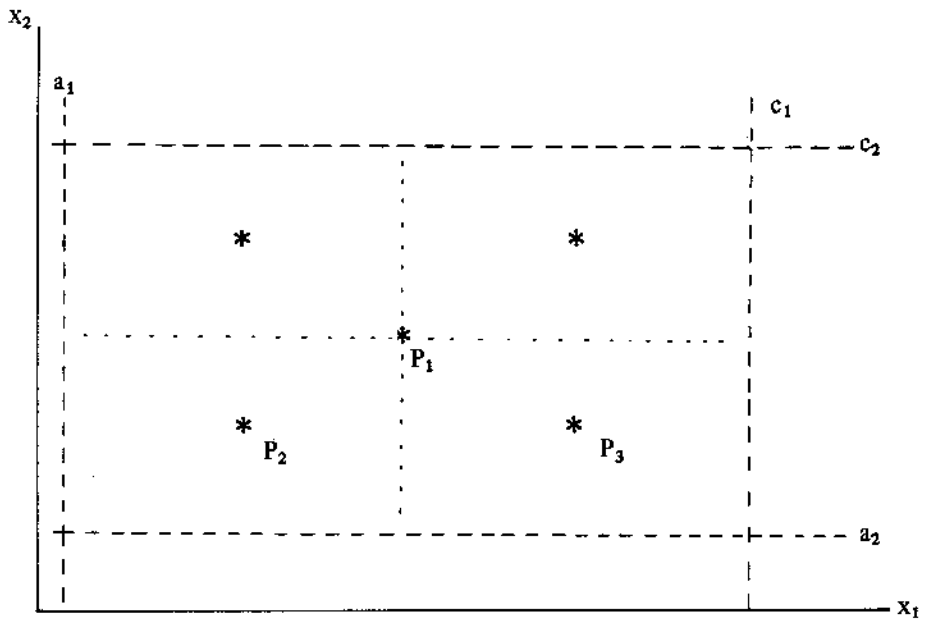

Figure 1. Nonrandom Selection of n+1 Points for Initial Complex

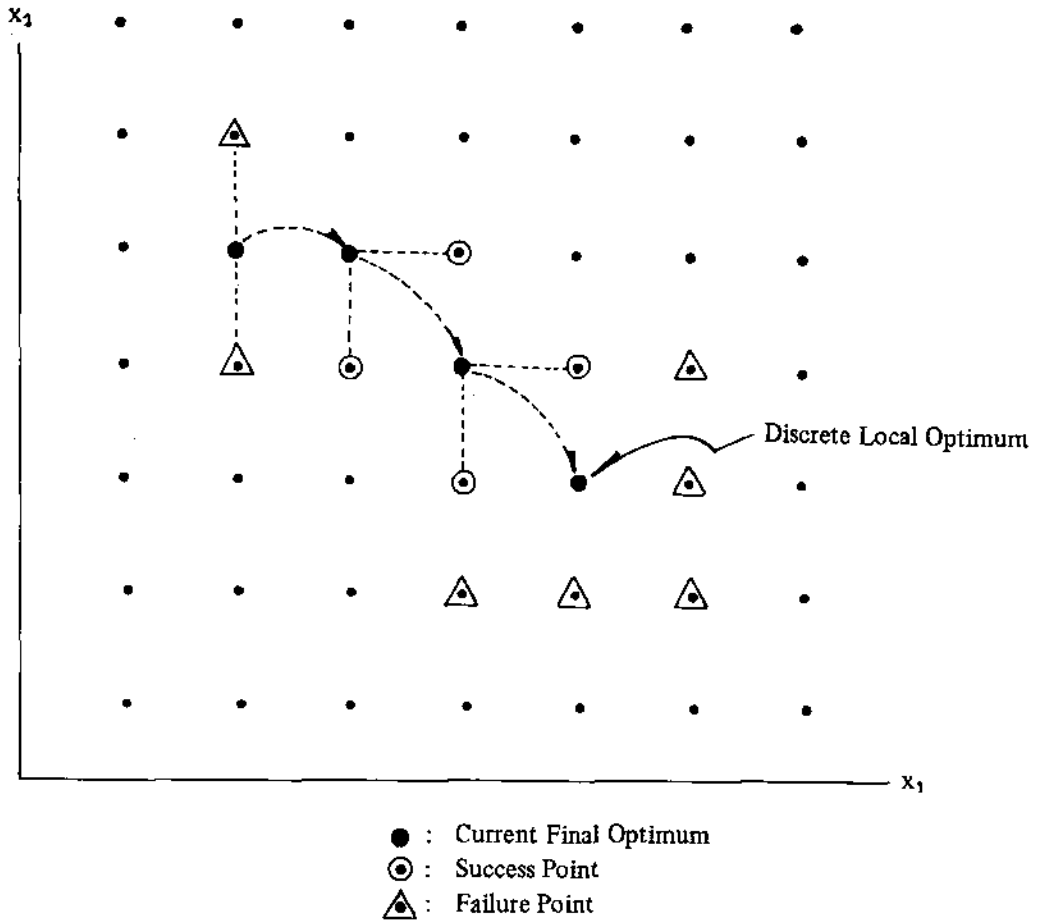

Figure 2. Searching Around the Final Optimum

Searching Around the Final Optimum

An option is provided to perform an additional search around the final optimum for the purpose of fine tuning. The proposed procedure is as follows (See Figure 2):

1) Let $P_O = (d_1, d_2, ..., d_j, ..., d_n)$ be the final optimum as obtained by the complex search.
2) Denote P_k, Q_k and S such that

$$P_k = (d_1, d_2, ..., d_k+1, ..., d_n)$$
$$Q_k = (d_1, d_2, ..., d_k-1, ..., d_n)$$
$$S = (s_1, s_2, ..., s_k, ..., s_n)$$

where S is a gradient vector whose components are +1, −1 or 0.

3) Let k = 1
4) Evaluate P_k. If P_k is a better point than P_O, then let $s_k = +1$ and go to step 6. Otherwise go to step 5.

5) Evaluate Q_k. If Q_k is a better point than P_o, then let $s_k = -1$, otherwise let $s_k = 0$. Go to step 6.
6) If k = n, go to step 7. Otherwise let k = k+1 and go to step 4.
7) If all components of S are equal to 0, then go to step 9. Otherwise evaluate point R such that

$$R = P_o + S$$

where the i-th component of $R = d_i + s_i$.
8) Select the best point among evaluated feasible points as the new final optimum. Go to step 3.
9) Evaluate the remaining feasible points in the unit neighborhood of P_o. If P_o is the discrete local optimum, STOP. Otherwise, select the best point and go to step 3.

3.2 Proposed Algorithm

The final version of the modified complex search algorithm for discrete optimization problems using simulation (called SIMICOM, SIMulation-optimization by Integer COmplex Method) is as follows:

1) Construct the initial complex consisting of n+1 vertices according to the modified nonrandom method.
2) Arrange all the vertices in the order of improving mean response,
$V(1), V(2), V(3), \ldots\ldots, V(K); \quad K = n+1$
and designate VR as a vertex with the least favorable mean response.
3) The centroid of the complex consisting of all vertices except VR is defined as

$$VM = \{ vm_i, i = 1,2,\ldots,n \}$$

$$vm_i = [\sum_{k=1}^{k} v_{k,i} - vr_i]/(K-1), \quad i = 1,2,\ldots,n$$

where $v_{k,i}$ is an i-th element of k-th vector point and vr_i is the i-th element of VR.
Let S be a vector pointing from the rejected vertex towards the centroid VM. Components of S are

$$s_i = vm_i - vr_i, \qquad i = 1,2,\ldots,n$$

A new vertex $VP = \{ vp_i, i = 1,2,\ldots,n \}$ can be defined as

$$vp_i = vr_i + < \delta * s_i/\Delta x_i > * \Delta x_i, \qquad i = 1,2,\ldots,n$$

where δ is the reflection coefficient and Δx_i is the shortest equal distance between two discrete points on a line parallel to the x_i axis. If VP violates a bound constraint on any variable, the corresponding coordinate is set equal to the violate constraint bound.

4) Replace V(1) by VP and compare the mean response at VP, Y(VP), to the mean responses at all other vertices of the complex. Two possible results are
   a) Y(VP) is not the least favorite vertex of the complex. In this case VP is acceptable; return to step 2.
   b) Y(VP) is the least favorite point of the complex. In this case reject VP and locate a new VP by retracting back toward VR one-half the distance to VR. Apply the retraction step, even if this point should coincide with another vertex of the complex. However, if VP coincides with VR without locating a better point, go to step 5. Otherwise restart step 4.

5) Restore VR and select the next worst point of the complex, designate this point as VR, and return to step 3.
6) The search terminates when:
   a) The complex collapses to one vertex. This point is then chosen as the optimum.
   b) V(K) is selected in step 5 and no better point can be located. In this case the best point of the complex is identified as the optimum.
7) (Option) Search around the final optimum to find a more accurate optimum.

The evaluation of the performance on several test problems showed that the choice of $\delta = 2$ produced good results [22].

3.3 Constrained Problem

Consider the problem of minimizing a system response f(X) from the simulation model subject to a set of constraints as follows:

$$\text{Min} \quad f(X)$$

$$\text{subject to} \quad a_i \le x_i \le c_i \quad , \; i = 1,2,...,n \tag{3.1}$$

$$g_j(X) \le b_j \quad , \; j = 1,2,...,m \tag{3.2}$$

$$h_k(X) \le d_k \quad , \; k = 1,2,...,p \tag{3.3}$$

where X is the vector of x_i's, $i = 1,2,...,n$. The constraints, $a_i \le x_i \le c_i$, $i = 1,2,...,n$ in (3.1) are the upper and lower bounds on each variable. These bounds arise from prior knowledge of the system, equipment limitations, and specifications on the product or process. The constraints $g_j(X)$, $j = 1,....,m$ in (3.2) are explicitly known deterministic functions in terms of the independent variables of X. The constraints $h_k(X)$ in (3.3) are implicitly known stochastic functions or other responses from the system that must be evaluated via computer simulation.

Due to the stochastic nature of $h_k(X)$, the above representation of constraints for $h_k(X)$ is not mathematically correct, because the left hand sides are random variables while the right hand sides are deterministic values. These constraints can better be stated in conjunction with a probability assigned to the possibility of their violation.

This can be done by expressing them as

$$\text{Min} \quad f(X)$$

$$\text{subject to} \quad a_i \le x_i \le c_i \quad , \; i = 1,2,...,n$$

$$g_j(X) \le b_j \quad , \; j = 1,2,...,m$$

$$P\,[h_k(X) \le d_k] \ge 1 - \beta_k \quad , \; k = 1,2,...,p \tag{3.4}$$

where β_k $(0 < \beta_k < 1)$ is the maximum probability of violating constraint k, $k = 1,2,....,p$.

To deal with this type of stochastic constraint which in stochastic programming is called chance-constraints, two different approaches, quantile approach [26], [10] and characteristic function approach [9], have been suggested in the literature. In this research the concept of quantile approach was adopted.

The stochastic constraints in (3.4) can be written as either

$$HU_k(X) \leq d_k \quad \text{for} \quad P\,[h_k(X) \leq d_k] \geq 1 - \beta_k \tag{3.5}$$

or

$$HL_k(X) \geq d_k \quad \text{for} \quad P\,[h_k(X) \geq d_k] \geq 1 - \beta_k \tag{3.6}$$

where $HU_k(X)$ and $HL_k(X)$ are the upper and lower limits, respectively, on the response $h_k(X)$ with $2\beta_k$ confidence level.

As shown above, there may exist three different kinds of constraints: bound, explicit and implicit. For the proposed SIMICOM algorithm to work for the constrained problems the following should be taken into account.

Selection of the Initial Complex

To construct the initial complex, 2^n+1 alternative points obtained from 2^n subregions plus the central point of the feasible region are checked against all explicit constraints to eliminate those which are infeasible. Only the remaining points are evaluated via simulation to select n+1 points for the initial

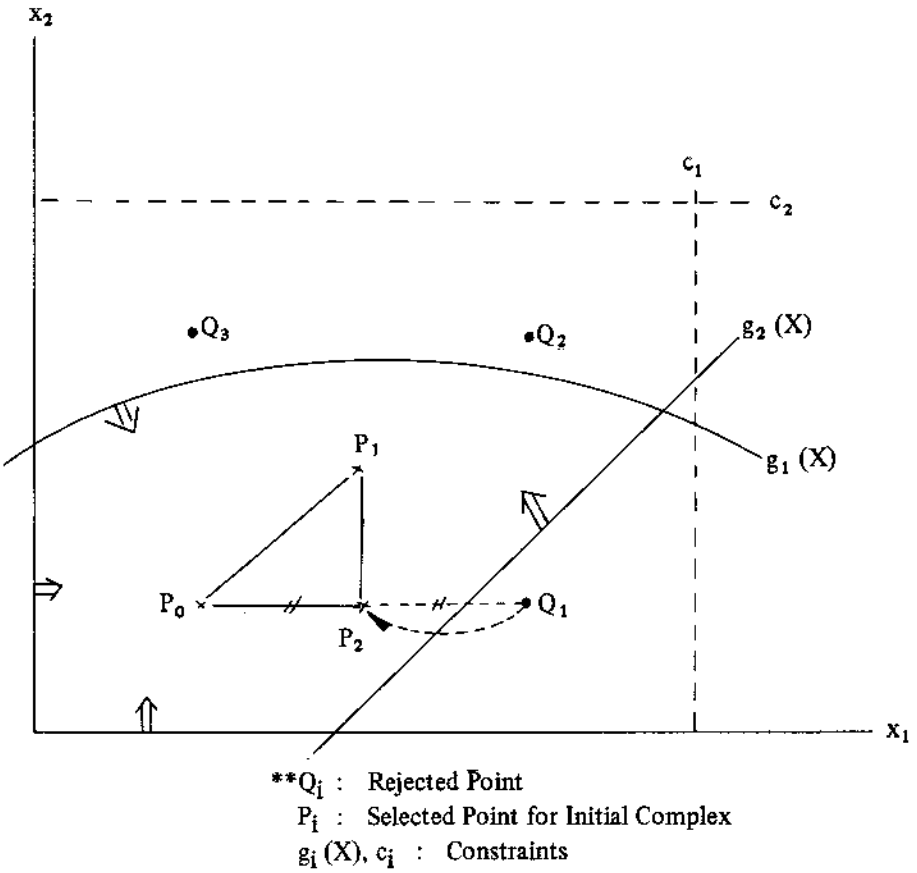

Figure 3. Selection of the Remaining Points for the Initial Complex in Constrained Problem

complex. When the selected points are less than n+1 points necessary for constructing the initial complex with the above procedure, the remaining points are selected according to the following procedure (See Figure 3).

i) Let $P_o = (d_{o1}, d_{o2},...,d_{oj}, ...,d_{on})$ be the best among p selected points and $Q_i = (q_{i1}, q_{i2},...,q_{ij}, ...,q_{in})$ be the i-th rejected point in the process of constructing the initial complex.

ii) Let k = 1.

iii) Let $P_k = <(P_o + Q_k)/2>$
where the j-th coordinate of P_k is $<(d_{oj} + q_{kj})/2>$.
Evaluate all explict and implicit constraints at P_k. If all are satisfied, select that point. Otherwise, move one-half distance to P_o such that

$$\text{new } P_k = <(P_o + \text{old } P_k)/2>$$

Repeat this process until P_k is feasible.

iv) If k = n+1−p, then stop. Otherwise, let k = k+1 and go to step (iii).

Similarly, in the reflection step of integer complex algorithm, if the new VP violates any explicit or implicit constraint, it is repeatedly replaced by a new point located one-half the distance to the centroid of the remaining n points, VM, until a feasible new point is found. In the retraction step the similar procedure is applied until an acceptable point is obtained.

4. Comparison of Alternative Stochastic Systems

The suggested algorithm is based on taking the next step according to the result of comparing the responses of alternative systems in the previous step. Since the objective function, being the response of the simulation model, is often a stochastic function of decision variables, comparing its mean values based on one observation at each alternative is often not conclusive. Such comparisons may result in the selection of a wrong alternative or a wrong direction for the next step. Sometimes even the average of several observations is not sufficient to offset the random characteristics of the response.

Under certain conditions it is possible to select between two alternatives (points) at a high level of confidence. Suppose that in addition to the mean response at each point, confidence intervals on the mean are also evaluated around the mean at a given level. Obviously the range of these intervals will be narrower for longer simulation runs. Let the lower and upper confidence limits on the response of the system at point X at β confidence level be represented by ZL(X) and ZU(X). Now if after comparing the responses at two points it is found that $ZU(X_1) < ZL(X_2)$ we can be almost sure (with a certain probability) that point X_1 is better than point X_2. If this conclusion is made based on a relatively short simulation run, there will be no need to continue running the model for any longer for the unfavorable point. However, if such a conclusion cannot be reached, running the model for a longer period that results in narrower confidence intervals may provide a better chance for such a conclusion.

In the development of the proposed algorithm for evaluating the upper and lower limits mentioned above, a sequential procedure is adopted. According to this procedure, initial, terminal and incremental run lengths are specified by the user. For each point, first the model is run for the initial run length. If a conclusive decision can be made based on this run length, the run is not continued any longer. However, if the result is inconclusive, the run is incremented by the specified incremental run length and the result is evaluated again. This process continues until either a conclusive result is obtained or the run length reaches its maximum allowable value. In the latter case only the means of the responses are compared.

5. Construction of Confidence Intervals

The batch means method for constructing the confidence intervals on the mean responses of simulation models is well described in [11], [13]. Let $Z_j(m)$ (j = 1,2,...,k) be the sample mean of the m observations in the j-th batch and let $\bar{Z}(k,m)$ be the grand sample mean of k batches. Then we can use the following to construct an approximate $100(1-\beta)\%$ confidence interval (c.i.) for μ;

$$\bar{Z}(k,m) \pm t_{k-1,\ 1-\beta/2} \sqrt{\hat{\sigma}^2 [\bar{Z}(k,m)]} \tag{5.1}$$

where $t_{k-1,\ 1-\beta/2}$ is the $1-\beta/2$ point for a t distribution with k-1 degrees of freedom and $\hat{\sigma}^2 [\bar{Z}(k,m)]$ is the estimate of variance of $\bar{Z}(k,m)$.

The problem with the current procedure using the batch means method is that one is almost never sure that the number of observations collected has been sufficiently large. To alleviate this problem to a certain extent a modified procedure is suggested below.

In using the classical formula to construct a c.i. there are three potential sources of error [12];

1) bias in $\hat{\sigma}^2 [\bar{Z}(k,m)]$ when m is too small for $Z_j(m)$'s to be uncorrelated,

2) nonnormality of $Z_j(m)$'s, and

3) the fact that the sequence z_i is not, in practice, covariance stationary.

For simple queueing models (e.g., M/M/1) Law [11] found that the bias in the estimated variance of the grand mean was the most serious source of error and that nonnormality was not a problem for k approximately 20 or more.

In procedure based on the batch means method, the batch size (m) is determined by changing the number of batches (k) such that $Z_j(m)$'s are approximately uncorrelated. In the procedure that is adopted here, k = 20 is used. After estimating batch means from the data, if it is found that these batch means are approximately uncorrelated, the classical formula (5.1) is used to generate c.i.. If not, the confidence intervals are estimated from :

$$\bar{Z}(k,m) \pm \lambda^{1/2} (\alpha_1, \alpha_2)\ t_{k-1,\ 1-\beta/2} \sqrt{\hat{\sigma}^2 [\bar{Z}(k,m)]} \tag{5.2}$$

where $\lambda(\alpha_1, \alpha_2)$ is a modification factor as suggested in [27] to compensate for the bias in the variance of the grand mean and α_1, α_2 are the coefficients in a second order autoregressive model, AR(2), ($y(t) = \alpha_1 y(t-1) + \alpha_2 y(t-2) + \epsilon(t)$) that is fitted to the data from the simulation.

In order to check whether the resulted batch means are correlated, the lag 1 autocorrelation coefficient is estimated by the jackknifed estimator because it will be less biased than the usual estimator [13], [19].

There are two different approaches for estimating the coefficients of a second order autoregressive model, AR(2), Maximum Likelihood Function Method [5] and Recursive Identification Method [17]. Among them the Recursive Identification Method has been shown to be easier to implement, comparatively simple and more accurate than the Maximum Likelihood Function Method. There are several versions of the Recursive Identification Method; in this paper the recursive least squares (RLS) approach was used because this is one of the most widely used methods which is also robust and easily implemented [17].

The procedures for estimating a modification factor depends on the nature of the characteristic equation of the underlying autoregressive process [27], [15].

6. Conclusions

In this paper a heuristic algorithm (SIMICOM) for optimization of discrete variable stochastic systems which are modeled through computer simulation has been developed.

The results from the applications showed that the SIMICOM is a very effective tool for optimizing discrete variable stochastic systems through simulation. For instance, in the robotic manufacturing system only 0.73% of all the feasible points were evaluated. Furthermore, because of the use of a sequential procedure, a considerable amount of computer time was saved by running highly suboptimal points for shorter periods of time. In some cases in average up to 36.7% of run lengths were saved [14], [15], [16].

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