Proceedings of the 1999 Winter Simulation Conference
P. A. Farrington, H. B. Nembhard, D. T. Sturrock, and G. W. Evans, eds.

SIMULATION OPTIMIZATION METHODOLOGIES

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ABSTRACT

Simulation models can be used as the objective function and/or constraint functions in optimizing stochastic complex systems. This tutorial is not meant to be an exhaustive literature search on simulation optimization techniques. It does not concentrate on explaining well-known general optimization and mathematical programming techniques either. Its emphasis is mostly on issues that are specific to simulation optimization. Even though a lot of effort has been spent to provide a reasonable overview of the field, still there are methods and techniques that have not been covered and valuable works that may not have been mentioned.

1 INTRODUCTION

Computer simulation is a powerful tool in evaluating complex systems. These evaluations are usually in the from of responses to "what if" questions. Practical questions, however, are often of "how to" nature. "What if" questions demand answers on certain performance measures for a given set of values for the decision variables of the system. "How to" questions, on the other hand, seek optimum values for the decision variables of the system so that a given response or a vector of responses are maximized or minimized. These decision variables could be quantitative variables such as the number of machines needed for a given manufacturing line, the inventory level at a warehouse or the duration of a traffic light in an intersection. They could, however, be some non-quantitative characteristics of the system such as the type of machines to purchase, the production routing procedure, or the layout of an office space.

Comprehensive reviews of literature on Simulation optimization have been provided by Glynn (1986), Meketon (1987), Jacobson and Schruben (1989), Safizadeh (1990) and Andradottir (1998). In this tutorial these citations will not all be repeated. Instead, issues that make simulation optimization distinct from generic optimization procedures will be addressed, various classifications of these problems will be presented and solution procedures suggested in the literature and applied in practice will be explored.

2 SPECIFIC ISSUES

Using simulation as an aid for optimization presents several specific challenges. Some of these issues are those involved in optimization of any complex and highly nonlinear function. Others are more specifically related to the special nature of simulation modeling. Simply stated, a simulation optimization problem is an optimization problem where the objective function (objective functions, in case of a multi-criteria problem) and/or some constraints, are responses that can only be evaluated by computer simulation. As such, these functions are only implicit functions of decision parameters of the system. In addition, these functions are often stochastic in nature as well. With these characteristics in mind, the major issues to address when comparing them to generic non-linear programming problems are as follows:

- There does not exist an analytical expression of the objective function or the constraints. This eliminates the possibility of differentiation or exact calculation of local gradients.
- The objective function(s) and constraints are stochastic functions of the deterministic decision variables. This presents a major problem in estimation of even approximate local derivatives. Furthermore, this works against even using complete enumeration because based on just one observation at each point the best decision point cannot be determined.
- Computer simulation programs are much more expensive to run than evaluating analytical functions. This makes the efficiency of the optimization algorithms more crucial.

- Most practitioners use some kind of simulation language for modeling their systems. Optimization, on the other hand, requires using some other kind of programming language that differs from one practitioner to the next. Interfacing simulation models with generic optimization routines is not always a simple task. This is especially true for newer higher level user friendly simulation languages.

There are, however, advantages in using simulation in optimization that can be exploited. In particular:

- Complexity of the system being modeled does not significantly affect the performance of the optimization process.
- For stochastic systems, the variance of the response is controllable by various output analysis techniques.
- Where structural optimization of systems are considered, simulation provides an advantage that is often not possible in classical optimization procedures. Here, by employing appropriate techniques, the objective function or constraints can be changed from one iteration to another to reflect alternative designs for the system.

We will address the effect of each of these issues on each particular situation in the following sections.

3 GENERAL FORMULATION

The formulation of simulation optimization problems is often done for maximization or minimization of the expected value of the objective function of the system. This, however, does not have to be the case. Operation of a system might be considered optimal if the risk of exceeding a certain threshold is minimized. On other situations, one might be interested in minimizing the dispersion of the response rather than its expected value. Here, we limit ourselves to optimization of the expected values.

Another pertinent issue in formulating simulation optimization problems is the treatment of stochastic constraints. These constraints, like the objective functions are sometimes functions of deterministic decision variables and are supposed to define a deterministic feasible region. For instance, the goal in a resource allocation problem may be to minimize the lead time subject to a limited in-process inventory. The lead time and in-process inventories could be stochastic responses of a simulation model. One could try to come up with the optimum values of the decision variables such that the expected value of the lead time is minimized. However, stating that the optimization should be done such that the expected value of the in-process inventories not to exceed a certain threshold may not be the right approach. Inventories are physical entities and require physical space. Even if their expected values are within accepted limits, their actual values may exceed the physical space constraints. In practice, many decision makers prefer to deal with their constraints as the risk of violation of a particular constraint rather than being within a certain range for the expected value of the feasible region.

Then two alternative ways of formulating the general simulation optimization problem are:

$$\text{Maximize(Minimize)} \quad \mathbf{f}(\mathbf{X}) = E[\mathbf{z}(\mathbf{X})]$$

$$\text{Subject to:} \quad \mathbf{g}(\mathbf{X}) = E[\mathbf{r}(\mathbf{X})] < \mathbf{0} \tag{1}$$

$$\text{and} \quad \mathbf{h}(\mathbf{X}) < \mathbf{0}$$

where $\mathbf{z}$ and $\mathbf{r}$ are random vectors representing several responses of the simulation model for a given $\mathbf{X}$, a p-dimensional vector of decision variables of the system. $\mathbf{f}$ and $\mathbf{g}$ are the unknown expected values of these vectors (their theoretical regression functions) that can only be estimated by noisy observations on $\mathbf{z}$ and $\mathbf{r}$. $\mathbf{h}$ is a vector of deterministic constraints on the decision variables.

The alternative formulation is:

$$\text{Maximize(Minimize)} \; \mathbf{f}(\mathbf{X}) = E[\mathbf{z}(\mathbf{X})]$$

$$\text{Subject to:} \quad \mathbf{P}\{\mathbf{g}(\mathbf{X}) < \mathbf{0}\} > \mathbf{1} - \boldsymbol{\alpha} \tag{2}$$

$$\text{and} \quad \mathbf{h}(\mathbf{X}) < \mathbf{0}$$

where $\mathbf{P}$ is the vector of probabilities of violation of constraints and $\boldsymbol{\alpha}$ is the vector of risks of these violations the decision maker is prepared to accept. This formulation yields itself well to simulation analysis because the constraints can easily be transformed into a manageable form as follows:

$$UCL_{1-\alpha j}\, g_j(\mathbf{X}) < 0 \tag{3}$$

where $UCL_{1-\alpha j}$ indicates the upper confidence limit calculated for the response g_j at $1-\alpha_j$ level. This form of constraint can be easily used to check whether a decision point is feasible, because one can use available means of estimating confidence intervals for a given $\mathbf{X}$.

4 PROBLEM CLASSIFICATION

There are several ways simulation optimization problems can be classified. Each class can be considered as a special case of the above general formulation. If $\mathbf{f}(\mathbf{X})$ is a one-dimensional vector, the problem is reduced to a single objective optimization while in its general form it is a multiple objective problem. If elements of $\mathbf{X}$ are continuous variables the problem is often easier to solve by available stochastic search methods. If they are discrete but still quantitative, the problem will be closer to those addressed by integer programming techniques. If **X** represents a vector of qualitative decision policies, optimization becomes more difficult because of the lack of available analytical tools to treat this type of problems. In addition, for such problems there will be a need for automatic generation of simulation models according to a systematic process. here, we refer to those problems as non-parametric optimization problems.

In following sections we will cover available solution procedures for various classes of these problems. First, procedures applied to single objective problems with continuous or discrete quantitative decision variables subject to deterministic or stochastic constraints will be discussed. Multiple objective problems will be addressed next. Finally, a discussion on non-parametric optimization problems will be presented. In each case, the issues pertaining specifically to simulation will be explored.

5 SINGLE OBJECTIVE PROBLEMS

Some popular approaches to solving these problems are:

- Gradient based search methods
- Stochastic approximation methods
- Sample path optimization
- Response surface methods
- Heuristic search methods

5.1 Gradient Based Search Methods

These methods attempt to take advantage of the vast amount of literature available on search methods developed for non-linear programming problems. The major contribution of practitioners in simulation optimization to this field has been the various methods of efficient estimation of gradients. Two major factors in determining the success of these methods are the reliability and the efficiency. Reliability is important because simulation responses are stochastic and a large error in gradient estimation may result in a movement in an entirely wrong direction. The efficiency is a major factor because simulation experiments are expensive and it is desirable to estimate gradients with minimum number of function evaluations. The gradient estimation methods often employed in simulation optimization are as follows:

5.1.1 Finite Difference Estimation

This is the crudest method of estimating the gradient. Partial derivatives of f(**X**) in this case are estimated by:

$$\delta z/\delta X_i=[z(X_1,..,X_i+\Delta X_i,..,X_p)-z(X_1,..,X_p)]/\Delta X_I \qquad (4)$$

As a result, to estimate the gradient at each point at least p+1 evaluations of the simulation model will be required. Furthermore, to obtain a more reliable estimate of the derivatives there may be a need for multiple observations for each derivative.

The distinction between using this technique for a more defined objective function compared to a response of a simulation model is that the responses here are stochastic in nature. Since observations are only a noisy estimation of the objective function, it is quite likely that one estimate of the gradient point the search to an entirely wrong direction.

5.1.2 Infinitesimal Perturbation Analysis (IPA)

Perturbation analysis, when applied properly and to models that satisfy certain conditions estimates all gradients of the objective function from a single simulation experiment. Since its introduction to simulation field a significant volume of work on this topic has been reported in the literature. A sample of these works can be found in Ho (1984), Ho et al (1983), Ho et al (1984), and Suri (1983). A complete discussion of all issues in IPA has been published in a book by Ho and Cao (1991).

The main principle behind perturbation analysis is that if a decision parameter of a system is perturbed by an infinitesimal amount, the sensitivity of the response of the system to that parameter can be estimated by tracing its pattern of propagation through the system. This will be a function of the fraction of the propagations that die before having a significant effect on the response of interest. The fact that all derivatives can be derived from the same simulation run, represents a significant advantage to IPA in terms of the efficiency. However, some restrictive conditions have to be satisfied for IPA to be applicable. For instance, if as a result of perturbation of a given parameter, the sequence of events that govern the behavior of the system changes, the results obtained by perturbation analysis may not be reliable. Considering the complex nature of most simulation models this condition may not be satisfied most of the time. Heidelburger (1986) presents a study of deficiencies of IPA in estimating the gradients. There are also reports that additional work done in this area in recent years may alleviate some of the problems in its application to simulation optimization.

One difficulty with application of IPA to simulation optimization problems is that the modeler has to have a thorough knowledge of the simulation model and in some situations must have built it from scratch to be able to add additional tracking capabilities that are needed by IPA. Most practitioners build their simulation models using some kind of simulation language. With the advance of object oriented simulation methodology and languages, it will become even more difficult to build these additional tracking capabilities into a reusable simulation model.

5.1.3 Frequency Domain Analysis

Frequency domain analysis in estimating the sensitivity and gradients of the responses of simulation models was suggested by Schruben and Cogliano (1981). Additional work on the subject has been reported by Jacobson (1988) and Jacobson and Schruben (1988). The gradients are estimated by analyzing the power spectrum of the simulation output function which is affected by inducing specific sinusoidal oscillations to the input parameters. In a recent work, Jacobson and Schruben (1991) have used this in applying the Newton's method to simulation optimization. The frequency domain analysis suffers from the same difficulty as IPA because of the complexity of incorporating it with independently built simulation models. Besides, it may not be possible to induce sinusoidal oscillations to some input parameters of interest.

5.1.4 Likelihood Ratio Estimators

Glynn (1987) presents an overview of Likelihood Ratio Estimators and their potential use in simulation optimization. Two algorithms are discussed by which the gradient of a simulation response function with respect to its parameters can be estimated. Rubenstein (1989) suggests a variation of this method and shows how it can be used in estimation of Hessians and higher level gradients to be incorporated in the Newton's method.

Once the method of estimating the gradients is decided upon, one of the available search techniques can be employed to search for the optimum. For a work using Quasi-Newton's method refer to Safizadeh (1992).

5.2 Stochastic Approximation Methods (SAM)

Stochastic approximation methods refer to a family of recursive procedures that approach to the minimum or maximum of the theoretical regression function of a stochastic response surface using noisy observations made on the function. These are based on the original work by Robbins and Monro (1951) and Kiefer and Wolfowitz (1952). The original recursive formula is given for a single variable function and is stated as:

$$X_{n+1}=X_n+(a_n/2c_n)[f(X_n+c_n)-f(X_n-c_n)] \quad (5)$$

where a_n and c_n are two series of real numbers that satisfy the following conditions:

$$\Sigma a_n<\infty,\ \mathrm{Lim}_{n\to\infty}(c_n)=0,\ \text{and}\ \mathrm{Lim}_{n\to\infty}(a_n/c_n)^2<\infty \quad (6)$$

It has been proven that as n approaches infinity X_n approaches to a solution such that the theoretical regression function of the stochastic response is maximized or minimized. This proof has been extended to multi-dimensional decision variables as well.

A neat characteristic of the stochastic approximation method when applied to simulation optimization is that the optimum of the expected value of the response could be reached using noisy observations. The difficulty is that a large number of iterations of the recursive formula will be required to obtain the optimum. Besides, for multi-dimensional decision vectors, p+1 observations will be needed for each iteration. Glynn (1986) has provided estimates of speed of convergence for some variations of this method. The other difficulty with these methods is the incorporation of the constraints into the optimization.

An earlier work applying stochastic approximation method to simulation optimization is reported by Azadivar and Talavage (1980). In this work an automatic optimum seeking algorithm was developed that could be interfaced with any independently built simulation model. This algorithm also applies to problems with decision variables constrained by a set of linear deterministic constraints.

5.3 Response Surface Methodology (RSM)

Response surface methodology is the procedure of fitting a series of regression models to the responses of the simulation model evaluated at several points and trying to optimize the resulting regression function. The process usually starts with first order regression function and after reaching the vicinity of the optimum, higher degree regression functions are utilized. Among the earlier works in application of RSM to simulation optimization are those of Biles (1974) and Smith (1976). Additional work has been reported by Daugherty and Turnquist (1980), and Wilson (1987). Smith developed an automatic optimum seeking program based on RSM that could be interfaced with independently built simulation models. This program was developed for both constrained and unconstrained problems. Compared to many gradient based methods, RSM is a relatively efficient method of simulation optimization in terms of the number of simulation experiments needed. However, Azadivar and Talavage (1980) show that for complex functions with sharp ridges and flat valleys it does not provide good answers.

5.4 Sample Path Optimization

In these methods, the deterministic optimization techniques are applied to a sample path observed on the simulation model. The expected value of the objective function is estimated by the average of a large number of observations at each point. Some descriptions of these methods sited in the literature and conditions for these to be effective are given by Chen and Schmeiser (1994), Shapiro (1996), and Gurken, Ozge, and Robinson (1994). The problem with this method with respect to simulation optimization is the large number of system evaluations involved.

5.5 Heuristic Methods

There are two heuristic methods that have shown promise in application of simulation optimization. These are Box's (1965) Complex Search method and Simulated Annealing.

5.5.1 Complex Search

Complex search is an extension of Nelder and Mead's (1965) Simplex search that has been modified for constrained problems. The search starts with evaluation of points in a simplex consisting of p+1 vertices in the feasible region. It proceeds by continuously dropping the worst point from among the points in the simplex and adding a new point determined by the reflection of this point through the centroid of the remaining vertices.

The major issue in applying this procedure to simulation models is the determination of the worst point. Since the responses are stochastic, an apparently worst point may actually be one of the better points and dropping it may take the search away from the optimum region.

Azadivar and Lee (1988) developed a program based on Complex Search that automatically applies this process to any given simulation model. The decision variables of these models can be constrained by deterministic as well as stochastic constraints that may be responses of the same or other simulation models. In order to avoid making a wrong decision regarding the worst point the values of the responses at vertices are compared statistically. If the result of the multiple comparison is conclusive and shows that one point is significantly worse than others, it is dropped. Otherwise additional simulation runs are made to reduce the variance and the comparison is repeated.

Huphery and Wilson (1998) report on a revised simplex search that they believe resolves several of shortcomings of regular simplex search methods such as sensitivity to starting values and premature termination.

5.5.2 Simulated Annealing

A description of this procedure is presented by Eglese (1990). Simulated annealing is a gradient search method that attempts to achieve a global optimum. In order not to be trapped in a locally optimum region, this procedure sometimes accepts movements in directions other than steepest ascend or descend. The acceptance of an uphill rather that a downhill direction is controlled by a sequence of random variables with a controlled probability. Alrefaei and Andradottir (1995) present a variation of simulated annealing in which they keep the cooling temperature fixed and show that under mild condition it almost surely converges to the global optimum.

6 MULTI-CRITERIA OPTIMIZATION

In addition to the common difficulties with all other multi-criteria optimization problems, multi-criteria simulation optimization possesses its own complexities, which are mostly due to the stochastic nature of the response functions. Most of the works done in this area are slight modifications of the techniques used in operations research for generic multi-objective optimization. Some of these approaches are:

- Using one of the responses as the primary response to be optimized subject to certain levels of achievement on the other objective functions. Biles (1975,1977) uses this approach in conjunction with a version of Box's complex method and alternatively with a variation of gradient and gradient projection method.
- Variations of goal programming approach as those reported by Biles and Swain (1980), Clayton et al (1982), and Rees et al (1985).
- Multi-attribute value function methods such as the one used by Mollaghasemi et al (1991)

Teleb and Azadivar (1992) exploit the stochastic nature of the responses to the advantage of optimization. They use the Complex search method but suggest an alternative way of comparing the responses at vertices. For each point in the complex they calculate a probability that the response vector belongs to the random vector representing the best value for all objective functions. The point with the lowest probability is dropped and its reflection with respect to the centroid of the rest of the points is added to the simplex.

7 ON-PARAMETRIC OPTIMIZATION

Many industrial, service, and other complex systems that are modeled by computer simulation need to be optimized in terms of their structural designs and operational policies. For instance, instead of the optimum number of machines in a workstation, one might be interested in the way workstations are arranged on the factory floor. Or, instead of the level of in-process inventory at each station, the problem of interest could be the routing policies for finished parts coming out of each station. Mathematical programming techniques are not usually applicable in these situations. In order to address these problems, each function evaluation requires a new configuration of the simulation model. This is equivalent to changing the objective function in each iteration. Furthermore, since decision variables are not quantitative, regular hill climbing, infinitesimal perturbation analysis, and stochastic approximation methods are not quite applicable. To deal with these problems an automatic model generation and a new optimization procedure have to be developed.

The most common approaches to solving these problems have been complete enumeration or random sampling. Complete enumeration is possible only if the number of configurations for the system is small. However, even for a modest problem such as a production system with only 4 stations, 3 product types, 3 routing policies for each station and 4 different maintenance policies, 144 different simulation models might need to be built for a complete enumeration.

The next best thing to complete enumeration is to evaluate a random sample of system configurations and select the best using some type of selection and comparison analysis. Random sampling is still among the best alternatives when the number of feasible configurations is too large. Various rules could be used to select the random sample of cases from all possible alternatives. However, often one has to select all the candidate alternatives at the same time. The “wait and see” approach common in regular quantitative optimization problems cannot be implemented here.

In “wait and see” random search one takes a small sample and based on the information obtained from this sample additional points are selected more intelligently than if all the points were selected at once. Gradient search and simplex methods are examples of this philosophy where the next point to consider is selected by a move in a geometrically defined n-dimensional decision variables space. In non-parametric optimization, however, the solution space cannot be defined geometrically. There is no increasing or decreasing direction for the value a decision variable can assume.

Genetic algorithms (GA) have recently emerged as a powerful approach for solving these problems. In genetic algorithms, the search can be guided systematically from one sample to the next without the need to define the decision variables space geometrically.

GAs are computer imitation of a simplified and idealized evolution. DNA is represented as a string where each position in the string may take on one of a finite sets of values. The fitness of the organism is determined by a fitness function; the function decodes the string and returns a real scalar value. The more desirable the value (larger for maximization and smaller for minimization problems) more fit the individual. A group of strings taken together forms a population.

The transition from one population to the next is achieved by performing GA operators of crossover and mutation among the individual members of the population. With crossover operation, the strings representing two individual members of the population are broken and certain portions of the strings are exchanged between the two strings thus creating two new strings. In mutation, a certain position in a string is selected at random and with a predetermined probability the value of the variable represented by that position is changed. After crossovers and mutation a new population is selected from among the existing and the new members of the previous population. Davis, (1991) and Goldberg, (1989) present comprehensive descriptions of the concepts and techniques in genetic algorithms.

The final step from the biological to the systems realm is made by linking a string to a system. To accomplish this, two steps need to be taken. First, a mechanism needs to be developed through which systems could be represented by a string containing places for assigning critical design parameters of the system. Second, the information contained in a string needs to be automatically translated into a simulation model for the system.

Azadivar and Tompkins (1999) developed a procedure that utilizes GA in design and optimization of flexible manufacturing systems. This process involves a genetic algorithm linked with an automated simulation model generator, which interact with each other. It also contains an input data collection where users can provide data on the structure of the system.

8 CONCLUSIONS AND RECOMMENDATIONS

The choice of the procedure to employ in simulation optimization depends on the analyst and the problem to be solved. However, we believe the modeler is often not a good mathematician and the mathematician is not necessarily a good simulation modeler. When it comes time to model a complex system a team of experts will work on developing a valid simulation model. These models are usually rather complex and do not yield themselves to the type of tracking needed in perturbation analysis and frequency domain analysis. Until a significant progress is made in these areas, practitioners will treat their simulation models as black boxes. Instruction from the optimization routines should be such that they can directly interface with these black boxes and operate on them in an input output mode without putting too much demand on the modelers to modify them for each iteration.

We recommend, parallel to additional efforts spent on advancing theoretical concepts such as IPA and frequency domain analysis, researchers work on making simulation optimization procedures more suitable to be interfaced with independently built models. We believe intelligent frameworks to perform these interfaces will make this task more feasible.

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