Simulation

OPTIMIZATION OF SIMULATION MODELS USING THE BOX-COMPLEX AND THE MODIFIED BOX-COMPLEX ALGORITHMS

by

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Presented at WAEA meetings, Lincoln, Nebraska, July 19-21, 1981.

ABSTRACT

Optimizing simulation models may require the use of a nonlinear direct search method such as the Box-Complex algorithm. The Box-Complex has been found to be inefficient in some cases in deriving optimal solutions for simulation models. This paper presents results from a modification of the Box-Complex designed to derive more efficiently optimal solutions. The potential efficiency of the Modified Box-Complex is illustrated by using it to solve two problems on which the Box-Complex had been found to be inefficient. The Modified Box-Complex may offer considerable savings in computer time and cost for some problems.

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In recent years, much of the firm level analysis in agricultural economics has concentrated on the complex interactions among forces endogenous and exogenous to the firm using systems analysis. Depending on the nature of the problem being analyzed, researchers have either simulated the economic phenomenon a number of times to present an array of results or attempted to "optimize" the results for one or more of the key decision variables in the model. Introduction of time and risk have often greatly complicated the optimization process.

Optimization procedures for simulation models may be classified into two broad categories: response surface methodology and direct search techniques. In response surface procedures, uncontrolled random variation with the simulation model is ignored and the response surface is defined in (k + 1) dimension, where k is the number of controllable variables (Smith). Response surface methodology (RSM) is often a combination of experimental design, statistical techniques, and regression analysis. RSM may be described as a sequential adaptive procedure for locating improved solutions. First and second order differential equations are estimated to approximate the simulation response surface and derivatives are taken and solved to locate the optimum point.

In direct search techniques, sometimes called "hill climbing methods", the path toward the optimum is derived by evaluating the objective function at several points rather than calculating derivatives. Because the direct search techniques do not employ derivatives, they can be applied to objective functions which are continuous but not differentiable.[1]

Optimal control theory has been used in a number of studies in general economics (Arrow; Chow; Dorfman) and in agricultural economics (Richardson, et al.; Trapp; Zaveleta, et al.; Conrad) to optimize models built to simulate economic systems of various types. In many agricultural economics studies, the Box-Complex has been used to derive optimal solutions to simulation models (Richardson, et al., Trapp, and Harris and Mapp). The Box-Complex is a nonlinear direct search procedure which incorporates constraints on the decision variable. Other direct search techniques, such as the Hooke-Jeeves pattern search, Rosenbrock's method of rotating coordinates, the simplex method by Spendley, Hext, and Himsworth, and the flexible polyhedral search by Nelder and Mead, have been used to optimize simulation model results. However, the above four direct search procedures are for unconstrained models. The unconstrained Nelder-Mead flexible polyhedral search is a modified simplex method as derived by Spendley, Hext, and Himsworth. Box modified the Nelder-Mead routine to incorporate constraints and called the program the Complex Method.

The Box-Complex procedure has been incorporated into many simulation models because the computer algorithm, as derived by Keuster and Mize, is easily adaptable to existing Fortran-based models. Response surface procedures are not as easily adapted to simulation models, and the Box-Complex, which can incorporate constraints on the decision variables and response values, is superior to the unconstrained direct search procedures.

BOX-COMPLEX ALGORITHM

The Box-Complex determines the maximum of a multivariable, nonlinear function subject to linear and/or nonlinear inequality constraints, and may be written as:

(1) Maximize: $F(x_1,x_2,\ldots,x_n)$

Subject to:

(2) $G_i \leq x_i \leq H_i$ where $i = 1,2,\ldots,m$

In the terminology of the Box-Complex, the decision variables are divided into implicit variables, such as x_{n+1}, x_{n+2}, ..., x_m and explicit variables such as $x_1,x_2,\ldots x_n$, where variables x_{n+1}, $x_{n+2},\ldots x_m$ are functions of x_1, $x_2,\ldots,x_n$.

In the Complex algorithm, $k \geq n+1$ points or vertices are used which must satisfy all imposed constraints. An initial feasible point is provided which satisfies the constraints. The other (k-1) points of the initial complex figure are derived from the following relationship:

(3) $$x_{ij} = G_i + r_{ij}(H_i - G_i) \qquad i = 1,2,\ldots,n \quad j = 1,2,\ldots,k-1$$

where r_{ij} are random numbers generated in the range from 0 to 1. This procedure generates points within a rectangle search region defined by constraint levels and no further scaling is required. After the initial points are derived, they are used to determine a value for the objective function. The points associated with the lowest objective function value are replaced by a point that is reflected across the centroid of the remaining points. If this reflected point, after being valued through the objective function, also becomes the lowest valued point of the remaining points, it is retracted one-half the distance to the centroid of the remaining points. The search for the optimum point continues in this fashion.

THE MODIFIED BOX-COMPLEX

As an increasing number of researchers have used the Box-Complex procedure to optimize simulation models, certain problems have arisen. The Box-Complex being used by many researchers does not incorporate all the routines of the Nelder-Mead flexible polyhedral search technique. The flexible polyhedral procedures of retraction, expansion, and reduction are not included in the Box-Complex algorithm. Therefore, the Box-Complex algorithm does not use all the information generated from the simulation model to maximize the simulated objective function. The implication of this omission is that the Box-Complex algorithm has considerable difficulty solving for an optimal value when a point repeats as the lowest functional value. When this occurs, the lowest valued functional point is moved one-half the distance to the centroid of the remaining points and a new iteration is begun. At the beginning of a new iteration, various functional values are evaluated and the stopping criteria is checked. If the response surface of the simulation model is relatively flat, the lowest valued point may be contracted repeatedly causing cycling to occur. Once cycling occurs, the program never checks the stopping criteria and the problem is not solved. The typical result is that cycling continues until the time parameter specified for the computer job is exhausted. Since it is difficult to predict when cycling will occur, this can be an expensive problem.

The Modified Box-Complex incorporates all the procedures of the flexible polyhedral search.[2] This procedure insures against the problem of cycling and uses all the information available from the simulation model in order to derive an optimal solution.

ANALYSIS

To illustrate the potential solution efficiency of the Modified Box-Complex algorithm, it was applied to a dynamic simulation model of grain sorghum plant growth for the Oklahoma Panhandle. The objective function is specified in terms of maximizing net returns to the irrigated grain sorghum producer. The model utilizes daily weather data (rainfall, maximum and minimum temperature and solar radiation) and determines the daily growth of the grain sorghum plant. The model also maintains a daily soil water balance which determines the amount of current soil water which is extractable from the soil profile.

In this analysis, the extractable soil water ratio (formed by dividing the current level of soil water by the maximum level of extractable soil water) is used to initiate irrigation applications. When the current extractable soil water ratio falls to 45 percent, leaf curl begins and plant stress is eminent.[3] Farm operators are assumed to observe leaf curl and to initiate an irrigation application. The grain sorghum plant is more susceptible to water stress during some stages of growth than others. For example, water stress early in the development of the plant does not affect final yield nearly as much as soil water stress during the grain filling stage. Thus, the critical level of extractable soil water differs for different stages of growth. The problem is formulated to derive the extractable soil water ratios for each of four stages of grain sorghum growth which maximize net returns to the irrigation producer. Formally, the problem is to:

(4) Maximize $NR = GR - CST1 - CIG$

(5) Subject to: $0 \leq P_i \leq 0.60, \quad i = 1,2,3,4$

where NR is net returns to the irrigated producer, GR is gross receipts, CST1 is nonirrigation costs, and CIG is irrigation costs. P_i is the extractable soil water ratio at which a three-inch irrigation application is initiated during each of the four growth stages and is constrained to be between 0 and 60 percent.

The Box-Complex and Modified Box-Complex were both used to solve this problem and solution efficiencies are compared.

RESULTS

Rather than using probabilistic weather data, the grain sorghum plant growth model utilizes actual daily weather data from the study area. Two years of actual data were selected at random to test the solution efficiencies of the different algorithms. These weather data were read into the model and an attempt was made to use each algorithm to determine the critical soil moisture ratio at which grain sorghum irrigations would be initiated during each stage of plant growth to maximize net returns in dollars per acre.

Results for the Box-Complex and Modified Box-Complex are presented in Table 1. The Box-Complex failed to determine optimal solutions in either of the two years. In the first year, the Box-Complex cycled for 278 iterations before the five minutes specified for completion of the job had expired. In the first year, the Modified Box-Complex executed in 0.85 minutes, determining optimum critical soil moisture ratios by growth stage in 19 iterations. Net returns per acre were $81.79.

Results for the second year were very similar. The Box-Complex algorithm cycled for 265 iterations and failed to derive an optimum solution before time expired for completion of the job. However, the Modified Box-Complex derived optimum soil moisture ratios in 12 iterations and determined net re-

TABLE 1. Optimum Extractable Soil Moisture Ratio by Stage of Grain Sorghum Development for the Box-Complex and Modified Box-Complex Algorithms.

Algorithm	Objective Function Value ($/acre)	- - Critical Soil Moisture Ratio - - Stage 1	Stage 2	Stage 3	Stage 4	Number of Iterations	Execution Time (minutes)
First year							
Box-Complex	a/	a/	a/	a/	a/	278	5.02
Modified Box-Complex	81.79	.24	.36	.34	.11	19	0.85
Second Year							
Box-Complex	a/	a/	a/	a/	a/	265	5.02
Modified Box-Complex	91.26	.08	.22	.24	.09	12	0.81

a/ Optimum values were not determined due to the cycling problem and the job terminated when the time parameter was exhausted.

turns per acre to be $91.26.

CONCLUDING COMMENT

The results presented in this paper represent fairly limited testing of one simulation model. A number of additional experiments have been conducted, including a test on the "Post Office problem" presented in the original article by Box and a test on one additional simulation model. In the other experiments, the results are not as dramatic as for the grain sorghum model simulated for this paper. However, in every case, the Modified Box-Complex achieved substantial solution efficiencies relative to the Box-Complex. It appears that the addition of the expansion, contraction, and reduction procedures of the Nelder-Mead flexible polyhedral search to the original Box-Complex results in a more efficient algorithm for deriving optimum solutions for certain simulation models. Additional experiments and an expanded description and documentation of the Modified Box-Complex are in progress.

FOOTNOTES

[1]Beveridge and Schechter give examples of discrete direct search techniques.

[2]A manuscript is in progress to describe in detail the different procedures of the Modified Box-Complex.

[3]The 45 percent value, which is termed the critical extractable soil moisture ratio, was obtained in conversations with Joe T. Ritchie, a Soils Specialist with the Blackland Conservation Research Center, USDA/ARS, Temple, Texas.

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