1981 Winter Simulation Conference Proceedings
T.I. Ören, C.M. Delfosse, C.M. Shub (Eds.)

COMPLEX SEARCH AND SECOND-ORDER RESPONSE SURFACE ANALYSIS

William E. Biles, Ph.D., P.E.
Professor and Chairman
Industrial Engineering Department
Louisiana State University
Baton Rouge, LA 70803

ABSTRACT

This paper describes a two-phase approach to systems optimization via computer simulation experimentation. In the first phase, Box's Complex Search is employed to search from some initial set of simulation trials $X_1, \ldots, X_K$ to an estimated optimum solution X*. Then a second-order response surface is fitted to these K points, or to some subset thereof, and analyzed through classical optimization procedures to gain yet another estimate X**. If y(X*) and y(X**) are sufficiently close, and X* and X** are close together, then the superior solution can be chosen. If either y(X*) is not close to y(X**), or X* is not close to X**, additional simulation trials in the neighborhood of X* and X** should be conducted to seek improved solutions.

1. INTRODUCTION

This paper describes a two-phase approach to system optimization via simulation experimentation. The proposed procedure adapts Complex Search, a computational search technique developed by M. J. Box (1965) for constrained optimization, to the simulation realm by coupling it with second-order response surface methodology. The resultant technique enables the simulationist to begin exploring from a current "solution" X^0 and move to a more promising region through a sequence of one-at-a-time simulation trials. Once the search begins to "envelop" a prospective optimum multiple regression techniques are employed to fit an estimating equation which can be analyzed mathematically to predict an optimum. The predicted optimum can then be evaluated through more simulation trials for confirmation.

2. THE COMPLEX METHOD

Consider the problem of maximizing (or minimizing) some system response y_0 subject to controls on a set of independent variables x_i, i = 1,..., n. That is,

$$\max\ (\min)\ y_0 = g_0(x_i,\ i = 1, \ldots, n) \qquad (1)$$

subject to

$$a_i \leq x_i \leq c_i\ , \qquad i=1,\ldots, n \qquad (2)$$

Suppose there are m other system responses which also depend on these same controls, so that

$$y_j = g_j(x_i, i=1,\ldots,n) \begin{Bmatrix} \leq \\ = \\ \geq \end{Bmatrix} d_j\ , \quad j=1,\ldots, m \qquad (3)$$

The functional relationships

$$y_j = g_j(X)\ , \quad j = 0, 1, \ldots, m \qquad (4)$$

are unknown and information about them must be evaluated experimentally, in this case via computer simulation.

The Complex Method of M. J. Box (1965) is initiated by randomly placing $2n \geq N \geq n+1$ experimental trials within the *a priori* experimental region established by the bounds in (2). These bounds arise from prior knowledge of the system, from equipment limitations, and from specifications on the product or process. Once procedure for generating a simulation trial is to use a uniformly-distributed random number generator U(0,1) in the following manner:

$$x_{\ell i} = a_i + u_{\ell i}(c_i - a_i)\ ;\ i=1,\ldots,n;\ \ell=1,\ldots,N \qquad (5)$$

Having generated the n coordinates of the ℓ-th simulation trial, the simulation is conducted and the m responses $y_{\ell j}$, j = 0, 1,...,m, are recorded. If a given response is found to violate one or more of the implicit constraints given by (3), the trial is "discarded" and a replacement simulation trial generated. When N feasible simulation trials have been generated, the sequential search phase of the Complex Search procedure is initiated.

The objective of the sequential search phase is to employ several simulation trials to envelop the model optimum. This phase evolves as follows:

1. The simulation trial yielding the worst value of the objective response y_0 is identified. This trial is denoted X^W and is selected for elimination from the "complex".

2. The centroid X^c of the remaining N-1 search points is found by the relation

$$X^c = \frac{1}{N-1} \sum_{\ell=1}^{N-1} X^{\ell} \quad \ell \neq w \tag{6}$$

3. The direction to the new search point is thus established by

$$S = X^c - X^W \tag{7}$$

4. The new search point is found by

$$X^{W'} = X^c + \alpha S \tag{8}$$

where $0 \leq \alpha \leq 1$. Values of α near 1 are preferred early in the search, but should be reduced to perhaps $0.4 \leq \alpha \leq 0.6$ as the search begins to envelop the optimum. Of course, if $\alpha > 1$ the "complex" expands in n-space, while for $\alpha < 1$ the "complex" is contracting as it moves nearer the optimum. This procedure is illustrated in Figure 1.

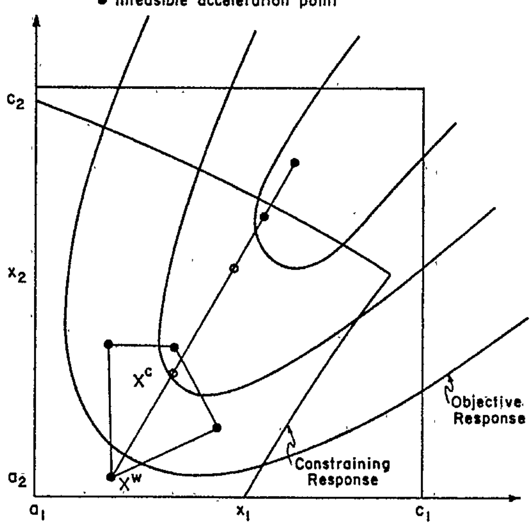

Figure 1. Complex Search

3. RESPONSE SURFACE FITTING

When the search has produced at least $K \geq (n+1)(n+2)/2$ simulation trials within an appropriately small region of interest, multiple regression procedures are employed to fit m+1 second-order response surface models of the form

$$y_k = b_{0,k} + \sum_{i=1}^{n} b_{ik} x_i + \sum_{i=1}^{n} b_{ii,k} x_i^2 + \sum_{i=1}^{n-1} \sum_{i+1}^{n} b_{ij,k} x_i x_j \quad k=0, 1, \ldots, m \tag{9}$$

An analysis of regression variance is performed for each response y_k to test whether the second-order surface adequately fits the set of K "design points". If all m+1 surfaces are found to adequately fit the search points, mathematical programming techniques are employed to seek a predicted optimum solution (X*,Y*). Box's Complex Search can be used in a purely computational mode to effect this optimization.

If one or more of the response surfaces is found inadequate in the analysis of variance, the simulation search can continue or the simulationist can simply place one or more additional simulation trials at "vacant" locations in the experimental region. It should be noted that search points that had been discarded during the sequential search phase of simulation experimentation, either because they violated an implicit constraint (3) or because they simply failed to produce an improved set of responses as compared to the current X^W, can be used in the response surface fitting stage of optimization.

4. APPLICATION OF THE METHODOLOGY TO AN INVENTORY SYSTEM

Ignall (1972) described the application of experimental design to the optimization of computer simulation responses. He employed as a simulation test model a discrete-event simulation of a stochastic inventory system in which mean daily demand and order lead time are random variables with known probability density (mass) functions. The two controllable variables were

x_1 = reorder point (ROP)

x_2 = economic order quantity (EOQ)

the lone simulation response was

y = mean daily cost, $

which was the sum of carrying, setup and shortage costs. The optimization problem was

$$\text{minimize} \quad y = g(x_1, x_2) \tag{10}$$

$$\text{subject to} \quad -5 \leq x_1 \leq 90 \tag{11}$$

$$50 \leq x_2 \leq 250 \tag{12}$$

Ignall found as a solution y = \$76 at x_1 = 45 and x_2 = 175 units, for a given set of values for the several constants in the model.

The manner in which this simulation test model is utilized for this paper does not involve an actual simulation program. Rather, the 20 x 9 response table is used as a graphical simulator. This response table is shown in Figure 2. For a given y, AVERAGE DAILY COST

x_2, EOQ

x_1, ROP	50	75	100	125	150	175	200	225	250
-5	312	221	168	143	123	118	107	104	100
0	288	202	155	130	112	109	101	97	96
5	267	185	143	120	105	101	96	82	92
10	249	170	132	110	99	97	91	88	88
15	232	159	125	105	95	91	89	88	87
20	215	147	117	97	90	87	86	83	85
25	198	136	109	92	85	83	84	81	84
30	180	124	100	88	80	80	81	79	83
35	167	117	93	85	78	78	79	80	83
40	160	111	91	84	77	77	79	79	82
45	154	107	90	81	78	76	79	81	83
50	145	102	87	80	77	77	79	81	83
55	142	101	86	79	78	79	80	82	85
60	138	100	86	79	79	79	80	85	87
65	135	99	85	79	80	80	81	85	88
70	134	100	86	81	81	81	83	87	90
75	134	101	88	83	83	84	85	89	93
80	135	101	89	85	84	86	87	90	95
85	134	103	91	87	86	88	88	92	97
90	135	105	93	88	88	89	91	95	99

Figure 2. Response Surface for a Stochastic Inventory Model

Optimization Method	Starting Seed	Estimated Solution x_1	x_2	y	Number of Trials
Complex Search	12471 21437	50 43	177 245	\$76.20 81.00	13 14
First-Order Factorial Design	17332	70	125	79.00	40
First-Order Simplex Design	17332	42	159	76.78	41
Second-Order Central Composite	35188	53	183	70.32* 79.00†	9
Second-Order Complex Design	14271	41	163	76.78** 77.52*	14

*(Predicted) **(Search) †(Actual)

Notes: (1) Known Solution $x_1 = 45$ $x_2 = 175$ $y = \$76.00$

(2) CPU times less than 5 sec. per optimization run on an IBM 370/168 computer.

(3) Complex search terminated because 2n = 4 search points were conducted without an improved solution.

Table 1. Summary of Simulation/Optimization Results for the Stochastic Inventory Model

(x_1, x_2), an interpolation is performed in this response table to find y.

This minimizing problem is first transformed to a maximizing problem by changing the sign of the mean daily cost, y, so that (10) becomes

$$\text{maximize} \quad -y = -g(x_1, x_2) \qquad (13)$$

while (11) and (12) remain unchanged.

The optimal solution obtained after fourteen experimental complex search points in the first phase is

$$x_1 = 41 \text{ units}, \; x_2 = 163 \text{ units}, \; y = \$76.78 \qquad (14)$$

The estimated response surface function after regression analysis is

$$y = 291.61 - 2.703\, x_1 - 1.656\, x_2 + 0.01463\, x_1^2 + 0.003611\, x_2^2 + 0.006590\, x_1 x_2 \qquad (15)$$

The optimal solution for the regression model (15) is found to be

$$x_1 = 51 \text{ units}, \; x_2 = 182 \text{ units}, \; y = \$71.24 \qquad (16)$$

A final simulation trial at ($x_1 = 51$, $x_2 = 182$) yields

$$x_1 = 51 \text{ units}, \; x_2 = 182 \text{ units}, \; y = \$77.52 \qquad (17)$$

which is not better than (14). Solution (14) is therefore selected as an optimal solution. Table 1 compares the performance of the two-phase Complex Search with that of several other response surface procedures.

5. APPLICATION OF THE METHODOLOGY TO A "TANK DUEL" SIMULATION MODEL

In describing the application of multiple response surface methods in computer simulation, Montgomery and Bettencourt (1977) employed a stochastic simulation model of a tank duel. The model simulates brief fire engagements between two armored vehicles. A stationary defending vehicle (Blue Tank) fires first at a fully-exposed attacking vehicle (Red Tank). The engagement ends when a kill occurs or a pre-determined time limit of 120 seconds expires.

The input variables to the tank duel model are presented in detail in Montgomery and Bettencourt. But for purposes of evaluating the technique described in this paper, the following independent variables x_i and response variables y_j are chosen:

x_1 = mean time to fire first round for the Blue crew (sec.),

x_2 = mean time between rounds (sec.),

y_1 = probability of Blue victory,

y_2 = expected number of rounds fired by the Blue tank.

The objective of the search is to find the optimal solution that Blue Tank has a maximal probability to win during the engagement. Two cases are formed by assigning different sets of restrictions to the model. In the first case the mean time to fire the first round for Blue crew is restricted from 8 to 30 seconds and the mean time between firing rounds is between 5 and 30 seconds. In the second case, the mean number of rounds carried by

Blue Tank is limited to 2 in addition to those restrictions in the first case. The results from the two-phase Complex Search method are as follows.

Case 1

The optimization problems were framed as those of constrained optimization. The first case is formulated as follows

$$\text{maximize} \quad y_1 = g_1(x_1, x_2) \quad (18)$$

$$8 \leq x_1 \leq 30 \quad (19)$$

$$5 \leq x_2 \leq 30 \quad (20)$$

The optimal solution after fifteen simulation trials in the experimental complex search phase is

$$x_1 = 8.599,\ x_2 = 5.6592,$$
$$y_1 = 0.7060, \quad y_2 = 2.5484 \quad (21)$$

and the estimated response surface functions are

$$y_1 = 0.9135 - 0.01241\ x_1 + 0.02120\ x_2 + 0.000032\ x_1^2 + 0.000249\ x_2^2 + 0.000161\ x_1x_2 \quad (22)$$

$$y_2 = 3.5437 - 0.05301\ x_1 - 0.1179\ x_2 + 0.000210\ x_1^2 + 0.001632\ x_2^2 + 0.000973\ x_1x_2 \quad (23)$$

and the F-values are 15635 and 3530 for (22) and (23) respectively, which are by far greater than the required minimal value.

The optimal solution for (23) is found to be

$$x_1 = 8.0360,\ x_2 = 5.0558,$$
$$y_1 = 0.7219,\ y_2 = 2.616 \quad (24)$$

A simulation trial on this point (x_1 = 8.0360, x_2 = 5.0558) gives the responses

$$x_1 = 8.0360,\ x_2 = 5.0558,$$
$$y_1 = 0.7236,\ y_2 = 2.6436 \quad (25)$$

which is better than (21), and is taken as the estimated optimal solution. Table 2 summarizes the results obtained by this technique and those by three other approaches to optimizing the problem for this case.

Case 2

In the second case the problem is formulated as that of the first case except that the constraint

$$y_2 \leq 2 \quad (26)$$

is added as the third constraint function.

The obtained optimal solution after fifteen simulation trials of the first phase is

$$x_1 = 13.5151,\ x_2 = 11.2764$$
$$y_1 = 0.5673, \quad y_2 = 1.8650 \quad (27)$$

and the regression response surface functions are

$$y_1 = 0.8980 - 0.0122\ x_1 - 0.1970\ x_2 + 0.000040\ x_1^2 + 0.000222\ x_2^2 + 0.000139\ x_1x_2 \quad (28)$$

$$y_2 = 3.365866 - 0.048945\ x_1 - 0.1031\ x_2 - 0.000222\ x_2^2 + 0.000139\ x_1x_2$$

The F-values are 14877 and 3048, respectively, which are large enough.

The computational complex search finds the point

$$x_1 = 8.1750,\ x_2 = 12.2108,$$
$$y_1 = 0.6074,\ y_2 = 1.9999 \quad (30)$$

as the optimal solution for the regression functions (28) and (29). This point is then applied to the simulation model and yields the responses

$$x_1 = 8.1750,\ x_2 = 12.2108,$$
$$y_1 = 0.6054,\ y_2 = 1.9908 \quad (31)$$

which surpasses (27) and is taken as the estimated optimal solution. The results of this methodology and three other approaches to this case are shown in Table 3.

Optimization Method	Estimated Solution x_1	x_2	y_1	y_2	Number of Trials
Complex Search	8.5860	5.006	0.7187	2.6243	21
Second-Order Central Composite	8.0000	5.0000	0.7194	2.5783*	9
Second-Order Simplex Design	8.0000	5.0000	0.7194	2.5798*	7
Second-Order Complex Search	8.5990 8.0360	5.660 5.0558	0.706 0.7219	2.548** 2.616*	15

*(Predicted) **(Search)

Notes: (1) Known optimum at x_1 = 8.0 sec., x_2 = 5.0 sec., y_1 = 0.724, y_2 = 2.644 rds.
(2) CPU times less than 5 sec. per optimization run on an IBM 370/168 computer.
(3) Complex Search was terminated because 2n = 4 search points were evaluated without obtaining an improved solution.

Table 2. Summary of Simulation/Optimization Results for the Tank Duel Model Case 1.

Optimization	Estimated Solution x_1	x_2	y_1	y_2	Number of Trials
Complex Search	12.9	10.1	0.59	1.97	20
First-Order Simplex Design	8.2	12.4	0.60	1.97	55
Second-Order Central Composite	8.0	12.5	0.61	2.00	9
Second-Order Complex Search	13.5 8.2	11.3 12.2	0.57 0.61	1.86** 1.99*	15

*(Predicted) **(Search)

Notes: (1) Known optimum at x_1 = 8.2 sec., x_2 = 12.5 sec., y_1 = 0.61, y_2 = 2 rds.
(2) CPU times less than 5 sec. per optimization run on an IBM 370/168 computer.
(3) Complex search was terminated because 2n = 4 search points were evaluated without obtaining an improved solution.

Table 3. Summary of Simulation/Optimization Results for the Tank Duel Model Case 2

REFERENCES

Biles, W.E., and J.J. Swain (1980), Optimization and Industrial Experimentation, Wiley-Interscience, New York, 368 p.

Biles, W.E., and J.J. Swain (1979), Mathematical Programming and the Optimization of Computer Simulations, In: Mathematical Programming Study II - Engineering Optimization, M. Avriel and R.S. Dembo (ED.), pp. 189-207.

Biles, W.E., and M.L. Lee (1978), A Comparison of Second-Order Response Surface Methods for Optimizing Computer Simulations, 1978 Fall ORSA/TIMS National Meeting, Los Angeles, 28 p.

Box, M.J. (1965), A New Method of Constrained Optimization and a Comparison with Other Methods, Computer Journal, Vol. 8, No. 1, pp. 42-52.

Ignall, E.J. (1972), On Experimental Designs for Computer Simulation Experiments, Management Science, Vol. 18, No. 7, pp. 384-388.

Montgomery, D.C., and W.M. Bettencourt (1977), Multiple Response Surface Methods in Computer Simulation, Simulation, Vol. 29, No. 4, pp. 113-121.