CONSTRAINED SEQUENTIAL-BLOCK SEARCH IN SIMULATION EXPERIMENTATION

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Abstract

This paper describes the application of sequential-block search techniques to simulation experimentation with constrained systems. Two basically different approaches are examined. One approach combines designed experiments, multiple regression, and mathematical optimization to predict a constrained optimum solution, which is then checked by further experimentation in the region of the predicted solution. A second approach employs a sequential optimum-seeking technique, such as gradient search or sequential simplex search, modified to accommodate constraints. These techniques are illustrated with a simple inventory system modeled with the GASP-II simulation language. A comparison of the effectiveness of these approaches is presented.

INTRODUCTION

The objective of simulation experimentation is to determine the optimum response y^* of some function of unknown form

$$y = F(X), \qquad (1)$$

where y is some measure of system effectiveness and X is an n-dimensional vector of input variables, x_i, i = 1, ..., n. Simulation experimentation consists of controlling the levels of the input variables X at several distinct sets of values, observing the simulated response y at each X, and eventually selecting X^* so as to yield the most beneficial response y^*.

Most realistic systems require consideration of several system responses, y_j, j = 0, 1, ..., m. The most expedient approach to multiple-response simulation experimentation is that of constrained optimization. In this approach, one response, y_o, is designated a primary or objective response. The remaining responses y_j, $j = 1, \ldots, m$ become restrictions or constraints by placing specifications on their performance. The mathematical statement of this problem is as follows:

Maximize (or minimize) $y_o = F(X)$ (2)

subject

$$a_i \le x_i \le c_i, \quad i = 1, \ldots, n \qquad (3)$$

$$y_j = G_j(X) \le (\text{or} \ge)\ d_j, \quad j = 1, \ldots, m \qquad (4)$$

where

- X = n-dimensional vector of input variables, x_i, $i = 1, \ldots, n$;
- x_i = value of the ith input variable;
- a_i = lower bound on the ith input variable;
- c_i = upper bound on the ith input variable;
- F = objective function, of unknown form;
- y_o = objective response variable;
- y_j = jth response variable;
- G_j = jth constraint function, often of unknown form;
- d_j = specification on the performance of the jth system response y_j;
- n = number of input variables in the simulation model;
- m = number of secondary system responses.

Although much has been done to develop improved techniques for simulation experimentation, scant attention has been given to the constrained optimization problem. This paper examines two basically different approaches to simulation experimentation with constrained systems. One approach combines designed experiments, regression, and mathematical programming in a procedure for predicting a constrained optimal solution. This paper compares central composite and simplex lattice designs for their effectiveness in predicting an optimal solution. A second approach utilizes search techniques in seeking a constrained optimal solution. This paper compares gradient search with two direct methods, sectional search (one-at-a-time method) and accelerated sequential simplex search.

EXAMPLE PROBLEM

The problem used to compare these various techniques is a simple (R, r, T) inventory system. In this problem, a retail outlet sells a particular item for \$65. The wholesale cost of this item is \$40. There is an inventory carrying charge of \$0.20 per dollar-year. If a customer demands a unit when it is not in stock, he will purchase it at a competing retail outlet. The outlet under study assigns a loss of \$20 to each such lost sale. The inventory position (units in stock plus those on order) is reviewed every T time periods. If inventory position P is less than or equal to the reorder point r, an order is placed for R-P units. The cost of each review is \$2 and the cost of placing an order is \$3. The demand for the item is Poisson-distributed with a mean of five units per week. The procurement lead time is Erlang-distributed according to the relation

$$f_x(x) = \begin{cases} \dfrac{\mu}{(k-1)!}(\mu x)^{k-1} e^{-\mu x} & x > 0 \\ 0 & \text{otherwise} \end{cases} \qquad (5)$$

with u equal to 2 and k equal to 6.

The retail outlet wishes to maximize profits from retailing this item, but it must operate within the following conditions:

1. The stock-on-hand cannot exceed 60 units due to space limitations;
2. Only one review can be performed on any given day, and a review is required by management policy at least once every three months;
3. The manager wishes to have the average weekly lost sales not exceed 0.2 units.

This leads to the following constrained optimization problem:

$$\text{Maximize } y_o = \$25\, y_1 - \$20\, y_2 - \$0.15344\, y_3 - \$3\, y_4 - \$2/x_3 \quad (6)$$

subject to

$$\begin{aligned} 0 \le x_1 &\le 60 \\ 0 \le x_2 &\le 60 \\ x_1 &\ge x_2 \quad (7) \\ 0.2 \le x_3 &\le 13.0 \\ y_2 &\le 0.2 \end{aligned}$$

where

y_o = average weekly profit, \$;

y_1 = average weekly sales, units;

y_2 = average weekly lost sales, units;

y_3 = average stock-on-hand per week; units;

y_4 = average weekly orders;

x_1 = inventory position, R, units;

x_2 = reorder point, r, units;

x_3 = review period, T, weeks

This problem assumes a five-day week. Note the discrete nature of the independent variables. If x_3 is considered on a daily basis, all three independent variables x_i, i = 1, 2, 3 are discrete. Note also that the objective response function is expressed in terms of four response variables. Hence, there are five response variables which must be observed experimentally.

The simulation model for this problem is written in FORTRAN using the GASP-II simulation language [13]. The simulator used in this study consists of a MAIN program, an EVNTS subroutine, and four events subroutines DMAND, PEREV, RECPT, and ENDSM. These components provide the following functions:

1. MAIN
   a. Initializes model variables.
   b. Turns control over to GASP executive.
2. Subroutine EVNTS
   a. Transfers control to the appropriate event subroutine.
3. Subroutine DMAND
   a. Creates next demand in accordance with the Poisson-distributed arrival rate.
   b. Tests stock level. The variable SALES is incremented by one if STOCK > 0 and SLOST is incremented by one if STOCK=0.
   c. Collects statistics on STOCK if a sale is made.
4. Subroutine PEREV
   a. Checks inventory position P against reorder point r. If P ≤ r, the receipt of R-P units is scheduled in accordance with the Erlang-distributed procurement lead time.
   b. Increments number of orders ORD by one if an order is placed.
   c. Restores inventory position P to level R if an order is placed.
5. Subroutine ENDSM
   a. Terminates simulation.

b. Computes weekly averages for the following quantities:

   1.) Stock, y_3,

   2.) Orders placed, y_4,

   3.) Sales, y_1;

   4.) Lost sales, y_2;

   5.) Profit, y_0;

A six-year or 312-week period of operation is examined for all experiments in this study.

DESIGNED EXPERIMENTS

Considerable attention has been given to using designed experiments in simulation experimentation. Burdick and Naylor [4], Hunter and Naylor [7], Mihram [9], and Schmidt and Taylor [14] provide excellent treatments of this subject. Most of these works suggest the use of a sequence of first-order experiments in moving toward an optimum, switching to a second-order design in the vicinity of the optimum. Montgomery and Evans [10] have evaluated several second-order designs for experimenting with simulation models.

This paper examines the use of two second-order designs for simulation experimentation, (1) a central composite design by Box [3] and (2) a simplex lattice design. The basic procedure used for this study is as follows:

1. A designed experiment consisting of a predetermined set of design points is performed with the GASP-II simulation model of the (R, r, T) inventory system. Each of the responses y_k, $k=0, 1, \ldots, m$ is observed and recorded.
2. A multiple linear regression program is used to fit quadratic models of the form

$$y_k = b_0 + \sum_{i=1}^{n} b_i x_i + \sum_{i=1}^{n} b_{ii} x^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} b_{ij} x_i x_j \qquad (8)$$

   for each of the m+1 responses [8].
3. The fitted equations are used to formulate a constrained optimization problem as expressed by equations (2) - (4), which is solved using a computerized constrained pattern search procedure [11] based on the Hooke and Jeeves search method [6].

Central Composite Design

The central composite design for a system of three independent variables is shown in coded form in Table I. Table II gives the actual values of x_1, x_2, and x_3 for the present problem. Observe that the radial points in the design are not exactly equal to the α values specified by the central composite design, due to the discrete nature of x_i, $i = 1, 2, 3$. The values y_0 and y_2 are also given in Table II. The center point is thrice replicated to provide an estimate of lack-of-fit error. The central composite design provides $(2^n + 2n + 1)$ points, compared to the $[(n+1)(n+2)/2]$ coefficients in the quadratic model given by (8). For larger problems, the number of points in the central composite design considerably exceeds the number required by the quadratic model.

Simplex Lattice Design

A design that is very economical for use with quadratic models is the $\{n, 2\}$ simplex lattice design. Myers [12] describes the use of simplex designs for first-order experiments. Figure 1 shows two and three-dimensional first-order simplex designs. The $\{n, 2\}$ simplex lattice design follows directly from the first-order simplex design by placing a point at the mid-point of each edge of the simplex, as illustrated in Figure 2. This provides exactly the [(n+1) (n+2)/2] design points needed for estimating the quadratic model. A center point can be placed at the centroid of this system and replicated to provide a test of error due to lack of fit. Table III gives the design points and responses for a simplex lattice design for the (R, r, T) inventory problem.

Comparison of the Two Designs

To provide a comparison of the two designs, the data from Tables II and III were employed in a "canned" multiple regression package to fit quadratic equations of the form given by (8). The resulting equations were then used in formulating the constrained optimization problem which was solved using the "canned" pattern search. The results of these studies were as follows:

	Central Composite	Simplex Lattice
X	(60, 45, 12)	(49, 37, 9)
Profit (predicted)	$124.25	$122.43
Profit (actual)	118.52	121.49
Lost Sales (predicted)	0.011	0.036
Lost Sales (actual)	0.035	0.0

Hence, the simplex lattice design performs slightly better than the central composite design in this problem. The main advantages of the simplex lattice design, however, are those which contribute to its relative economy:

1. It uses exactly the [(n+1) (n+2)/2] points needed to estimate the quadratic model.

2. It develops directly from a first-order design.

3. It contains smaller simplices (refer to Figure 2) which can be used to form a simplex lattice design in a sub-space of the experimental region around a predicted solution simply by performing the experiments corresponding to the edge mid-points for the simplex sub-space.

Disadvantages of the simplex lattice design are as follows:

1. It does not possess optimal statistical properties, such as minimum bias and minimum variance. Furthermore, no attention has yet been given to describing the mathematical properties of the design.

2. The orientation of the simplex in the factor space is left to the judgement of the experimenter. (The vertices of the design given in Table III closely approximate an orthogonal first-order simplex design given by Myers [12]).

SEARCH METHODS

An alternative to employing designed experiments in simulation experimentation is to use a search technique. These fall into one of two basic categories, (1) gradient methods and (2) direct methods. They can be made completely automatic by having a "canned" program compute the succession of observations in the search, or they can be made adaptive by having the experimenter examine the results after each block of experiments and plan the next block. The latter approach is likely to make more efficient use of computer time and is the scheme developed in this paper. A gradient search procedure is compared with two direct search methods, sectional (one-at-a-time) search and accelerated sequential simplex search. Each of these methods has the feature that experimentation proceeds in a sequence of blocks, allowing the experimenter to exercise his judgement as experimentation progresses.

Gradient Search

Gradient search is initiated by placing a set of experiments around a base point X_o to estimate the gradient. For a system of n variables, n+1 experiments must be employed in estimating the gradient, as given by the following expression:

$$\begin{aligned} &X_o \\ &X_1 = X_o + \Delta x_1 \\ &\vdots \qquad\quad \vdots \\ &X_n = X_o + \Delta x_n \end{aligned} \qquad (9)$$

After observing the n+1 responses $y_o, y_1, \ldots, y_n$, the experimenter can compute the gradient direction as

$$m_j = B_j / \left[\sum_{i=1}^{n} B_i^2 \right]^{\frac{1}{2}} \qquad j = 1, \ldots, n \qquad (10)$$

where

$$B_j = \frac{\Delta y_j}{\Delta x_j} \qquad (11)$$

Δy_j is the change in the response y caused by the incremental change Δx_j, with all other variables held at the X_o level.

Having determined the gradient direction, the next block of experiments is performed at uniform intervals along this direction. For constrained systems, the bounds given by (3) will limit the step in the gradient direction. This combination of a gradient-determining block and a step-determining block is repeated until an acceptable solution is found. Beveridge and Schechter [1] give an excellent presentation of this topic.

Table IV presents the results of a gradient search approach to the example (R, r, T) inventory problem. The requirement for discrete values of x_i, i = 1, 2, 3 somewhat complicated the selection of experiments in the step-determining blocks, so that in effect only a "near-gradient" direction could be followed. Nevertheless, gradient search is seen to be adequately effective as a simulation search technique. The search was terminated after block 8, because the indicated gradient direction would have caused constraint violation.

In Table IV, blocks 1, 3, 4, 6, and 8 are gradient-determining blocks. Blocks 2, 5, and 7 are step-determining blocks. In block 2, the best point along the gradient direction was (60, 20, 30). The gradient from this point, however, as computed from the results from in block 3, would have violated the upper bound on the variable x_1. Therefore, the decision was made to evaluate the gradient from the next best point in block 2, (40, 20, 34), which produced the results in block 4. This episode points out one of the difficulties in sequential-block experimentation, that subjective judgements must often enter the experiment selection process.

Sectional Search

Perhaps the simplest direct search method is that in which only one variable at a time is changed. By keeping n - 1 of the n variables fixed at some level, the remaining variable can be altered over its range. This process is repeated until an optimal solution is found.

Table V gives the results of a sectional search applied to the example inventory problem. Four experiments are used in each block, except in block 2 where the fourth experiment would have duplicated an experiment from block 1. In block 2, X_2 was varied from 18 to 36, since it could not exceed X_1, which was maintained at 40. In block 3, X_1 was varied from 38 to 56, since it could not fall below the value of X_2 at 36. In block 4, X_3 was varied from 4 to 16, since higher values had been shown in block 1 to be less profitable. The search was halted in block 6, since none of the experiments in the block produced results superior to the solutions observed in blocks 4 and 5.

Accelerated Sequential Simplex Search

A technique that appears promising for simulation experimentation is the accelerated sequential simplex search method [2], which is based on the sequential simplex method of Spendley, Hext, and Himsworth [15]. Instead of moving along one point at a time, however, this new technique employs a simplex of n+1 points in each successive block. The direction of movement is that from the worst point in the simplex through the centroid of the n remaining points. If the same direction is maintained in successive blocks, the movement accelerates in accordance with the following relations:

$$X_k' = X_k + 2h(X_c - X_w), \quad k = 0, 1, \ldots n \qquad (12)$$

where

X_k' = kth vertex in the next simplex,

X_k = kth vertex in the current simplex,

h = no. successive blocks in which the same direction is maintained,

X_w = point yielding worst response y,

$$X_c = [\sum_{j \in S} X_j]/n, \qquad (13)$$

where S is the set of all points in the simplex other than X_w.

Figure 3 shows the progress of the standard sequential simplex search technique for a simple two-dimensional problem. Figure 4 shows the progress of the accelerated method for the same problem. Table VI presents the results from employing accelerated sequential simplex search with the (R, r, T) inventory problem. The worst point in each simplex is noted with an asterisk. The search was halted after block 6 because the indicated direction of movement to a seventh block was toward a region that had already been examined in block 5. Moreover, the maximum profit in block 6 was less than 0.6 percent higher than that in block 5.

Comparison of Search Methods

Of the three search methods examined here, the accelerated sequential simplex procedure yielded the best solution to the example (R, r, T) inventory problem. With respect to search efficiency, the simplex and sectional search procedures each required six sequential blocks, compared to eight blocks for the gradient procedure. The results are conditioned, however, on the somewhat arbitrary criteria which were used to stop the search.

The initial experiments by each procedure produced solutions that violated the lost sales constraint; however, moves that gave improved values of the objective response y_0 also reduced the extent of lost sales constraint violation. This outcome is not surprising, considering the relatively high cost of a lost sale. This is not the most realistic situation one could encounter, however, and the example problem is defective in that regard.

To summarize the procedures to apply in the face of constraints, the foremost rule is to initiate the search in the interior of the feasible region. The three search methods could then operate in the following ways:

1. In gradient search, select as a point along the gradient direction that point which yields the maximum value of the objective response y_0 without violating a constraint. The gradient-determining block would then be performed to establish the best direction from that point.

2. In sectional search, consider only those experimental points in each block which do not violate constraints, selecting that point which maximizes the objective response.

3. In accelerated sequential simplex search:

   a. If, for a simplex derived by letting $h \geq 2$, constraint violation occurs, set $h = 1$ and compute the next simplex.

   b. If, for a simplex derived by letting $h=1$, constraint violation occurs, select a point other than the worst point as X_W. Recompute a new simplex with $h = 1$.

   c. If rules a and b fail to yield a solution satisfying all constraints, curtail the search and adopt the best observed point as a solution.

It should be stressed that none of these methods produce a globally optimal solution. They are effective, however, in producing a very worthwhile solution.

CONCLUSIONS

This paper has discussed the use of sequential-block search techniques in simulation experimentation with constrained systems. Two basically different procedures have been examined, each of which is effective in locating an acceptable constrained solution. None of the techniques examined here assure a globally optimal solution, however.

Of the two second-order experimental designs studied, the simplex lattice design offers both economy and search effectiveness in simulation experimentation. There is much to be learned about this design, however, and additional research in both its theoretical and practical aspects is necessary. The approach of performing a designed experiment, fitting first or second-order response models, and applying a mathematical programming procedure in seeking a constrained optimal solution is definitely worthwhile for simulation experimentation.

Gradient or direct search is another practical and effective approach to constrained systems simulation experimentation. This approach is especially useful for complex systems, where the experimenter desires to exercise his own judgement after each block of experimentation. A technique that appears to be very promising for sequential-block experimentation is accelerated sequential simplex search. This technique retains the advantages of the standard sequential simplex search technique, including an effective direction-determining mechanism, and adds the capability for acceleration in a direction that consistently proves favorable. There is a definite need, however, to evaluate this technique for problems of dimension greater than three. Additional evaluation of movements near binding constraints is also necessary.

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Table I

Coded Design Points for the Central Composite Design

Design Point	x_1	x_2	x_3
1	-1	-1	-1
2	-1	-1	1
3	-1	1	-1
4	-1	1	1
5	1	-1	-1
6	1	-1	1
7	1	1	-1
8	1	1	1
9	$-\alpha$	0	0
10	α	0	0
11	0	$-\alpha$	0
12	0	α	0
13	0	0	$-\alpha$
14	0	0	α
15	0	0	0

Note: For $n = 3$, $\alpha = 1.216$

TABLE II

DESIGN POINTS FOR CENTRAL COMPOSITE DESIGN FOR EXAMPLE PROBLEM

Design Point	R x_1	r x_2	T x_3	Profit y_o	Lost Sales y_2	Seed
1	46	36	2	$117.27	0.0	5461
2	46	36	18	118.35	0.11	5461
3	46	44	2	116.81	0.0	5461
4	46	44	18	118.31	0.11	5461
5	54	36	2	117.54	0.02	5461
6	54	36	18	112.68	0.23	5461
7	54	44	2	119.78	0.0	5461
8	54	44	18	122.31	0.01	5461
9	45	40	10	121.90	0.01	5461
10	55	40	10	122.88	0.01	5461
11	50	35	10	121.80	0.04	5461
12	50	45	10	121.43	0.0	5461
13	50	40	1	114.86	0.0	5461
14	50	40	19	125.50	0.02	5461
15	50	40	10	119.88	0.0	5461
16	50	40	10	125.84	0.02	1971
17	50	40	10	119.53	0.01	8433

TABLE III

DESIGN POINTS FOR SIMPLEX LATTICE DESIGN FOR EXAMPLE PROBLEM

Design Point	R x_1	r x_2	T x_3	Profit y_o	Lost Sales y_2	Seed
1	50	46	2	$116.93	0.0	5461
2	40	36	18	110.58	0.30	5461
3	50	26	2	115.78	0.11	5461
4	60	36	18	117.98	0.11	5461
5	45	41	10	120.35	0.01	5461
6	50	36	2	118.76	0.0	5461
7	55	41	10	119.36	0.0	5461
8	45	31	10	117.82	0.13	5461
9	50	36	18	118.24	0.10	5461
10	55	31	10	118.27	0.05	5461
11	50	36	10	121.73	0.02	5461
12	50	36	10	125.42	0.06	1971
13	50	36	10	121.10	0.08	8433

TABLE IV

GRADIENT SEARCH APPLIED TO (R, r, T) INVENTORY PROBLEM

Block	R x_1	r x_2	T x_3	Profit y_o	Lost Sales y_2
1	30	20	36	$50.37	1.72
	33	20	36	59.99	1.51
	30	23	36	50.37	1.72
	30	20	39	48.39	1.72
2	35	20	35	65.69	1.37
	40	20	34	81.67	0.98
	45	20	33	61.32	1.47
	50	20	32	65.75	1.37
	55	20	31	76.08	1.12
	60	20	30	91.01	0.74
3	57	20	30	85.17	0.93
	60	23	30	92.26	0.75
	60	20	27	87.88	0.82
4	43	20	34	80.32	1.01
	40	23	34	83.55	0.92
	40	20	31	85.43	0.90
5	38	23	28	74.40	1.18
	36	26	22	91.54	0.77
	34	29	16	104.74	0.44
	32	32	10	111.98	0.25
6	35	32	10	116.39	0.15
	32	29	10	105.27	0.40
	32	32	7	118.18	0.20
7	34	33	7	120.94	0.13
	36	34	4	122.70	0.01
	38	35	1	112.94	0.0
8	39	34	4	120.82	0.04
	36	31	4	119.86	0.06
	36	34	7	121.62	0.08

TABLE V

SECTIONAL SEARCH APPLIED TO (R, r, T) INVENTORY PROBLEM

Block		R x_1	r x_2	T x_3	Profit y_o	Lost Sales y_2
	*	40	30	10	$119.95	0.058
1		40	30	25	95.18	0.72
		40	30	40	69.40	1.30
		40	30	55	49.94	1.70
		40	18	10	85.74	0.92
2		40	24	10	102.90	0.48
	*	40	36	10	120.38	0.022
		38	36	10	119.26	0.067
3		44	36	10	120.67	0.0
	*	50	36	10	121.73	0.022
		56	36	10	119.71	0.039
		50	36	4	120.19	0.019
4		50	36	8	122.38	0.035
	*	50	36	12	122.87	0.058
		50	36	16	119.60	0.074
		50	34	12	117.28	0.12
5		50	38	12	121.94	0.006
	*	50	40	12	122.87	0.019
		50	42	12	121.73	0.010
		46	40	12	121.71	.003
6		48	40	12	122.81	0.016
		52	40	12	121.93	0.0
		54	40	12	118.93	0.055

Note: * denotes best value of X

TABLE VI

ACCELERATED SEQUENTIAL SIMPLEX SEARCH WITH (R, r, T) INVENTORY PROBLEM

Block		R x_1	r x_2	T x_3	Profit y_o	Lost Sales y_2
	*	30	20	35	$ 48.74	1.75
1		34	21	36	62.95	1.44
		31	24	36	53.77	1.65
		31	21	39	51.63	1.65
		34	24	39	60.50	1.45
2		38	25	40	67.25	1.32
		35	28	40	57.98	1.54
	*	35	25	43	48.92	1.79
		35	25	32	68.76	1.32
3		39	26	33	87.27	0.84
		36	29	33	79.14	1.02
	*	36	26	36	68.73	1.31
		38	28	19	106.31	0.46
4		42	29	20	105.46	0.44
		39	32	20	107.72	0.42
	*	39	29	23	104.12	0.46
	*	41	31	2	118.82	0.055
5		45	32	3	119.28	0.016
		42	35	3	120.27	0.0
		42	32	6	123.94	0.039
		45	35	6	124.64	0.045
6		49	36	7	122.49	0.0
		46	39	7	120.90	0.0
	*	46	36	10	120.34	0.003

Note: * denotes worst point, X_w

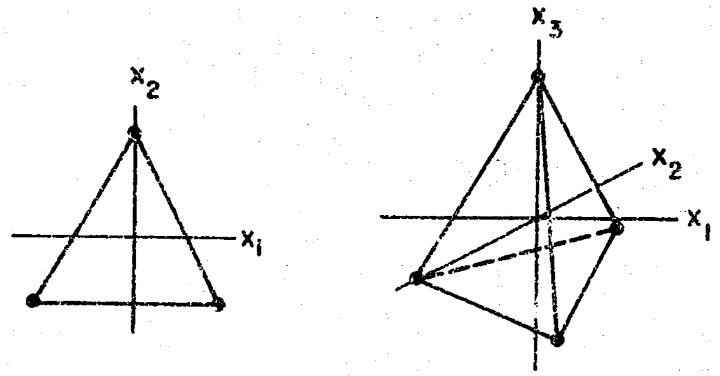

Figure 1
First-Order Simplex Designs

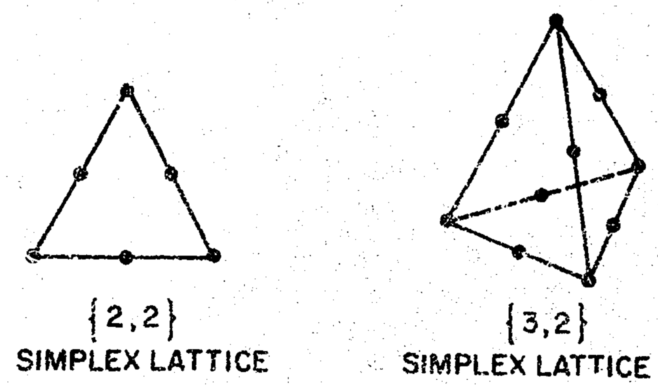

Figure 2
Second-Order Simplex Designs

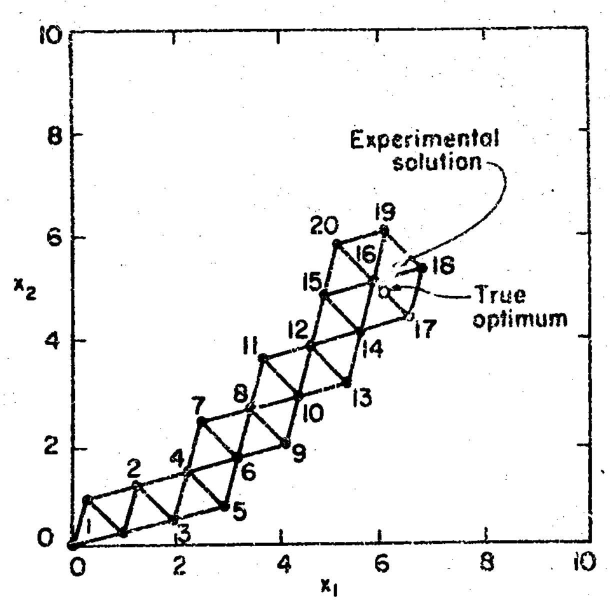

Figure 3
Sequential Simplex Search

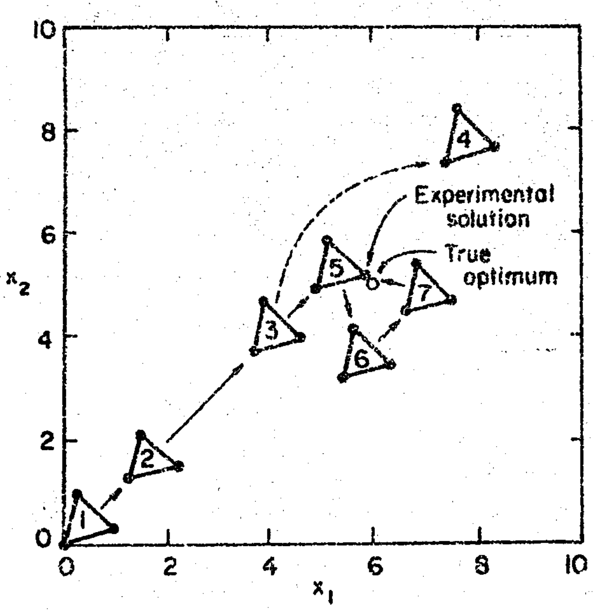

Figure 4
Accelerated Sequential Simplex Search