AN EFFICIENT PROCEDURE FOR LOCATING THE OPTIMAL SIMULAR RESPONSE

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Summary

This paper indicates the applicability of statistical procedures, known as response surface methodology, to the design and analysis of experiments performed with a stochastic simulation model. Fundamental simplex-sum designs are displayed explicitly and inferences therefrom are interpreted in terms suitable to the optimisation of the simular response function.

Introductory Remarks

The specification of the environmental conditions for a simulation model and the subsequent observation of the model's behaviour may be termed an encounter with the model (or, a simular encounter). By means of alternative specifications for the model's environmental conditions (as reflected in the input data of a computerized simulation), one may experiment with the model in an endeavour to achieve either of two goals:

(a) to ascertain the relative importance of alternative policies, of dissimilar environmental conditions, or of differing parametric specifications as they affect the simular response at some point, T, in simular time; or,

(b) to determine that combination of policies, environmental conditions, or parametric specifications which will provide, according to some criterion, the optimal simular response at the end of T simular time units.

For the purposes of this paper, we shall denote the simular response at the end of T simular time units by Y(T), an univariate quantity which is characteristically represented by the status of some system attribute whenever the simular clockworks arrives at time T. Furthermore, we shall presume that the class of simulation models of interest is the stochastic category, requiring along with its input (environmental) specifications one or more random number seeds for each encounter. The simular response becomes then a random variable

$$Y(T) = Y(x_1, x_2, \ldots, x_p; s) ,$$

where $x_1, x_2, \ldots, x_p$ denote p environmental conditions other than the seed s. Quite generally, one may write

$$Y(x_1, x_2, \ldots, x_p; s) = f(x_1, x_2, \ldots, x_p) + \varepsilon(s),$$

where f is also a function of unknown form, and where $\varepsilon(s)$ is a random variable of mean zero and of variance σ^2, regardless of the environmental specification $(x_1, x_2, \ldots, x_p)$. Thus the stochastic simular response becomes representable as

$$Y(T) = f(x_1, x_2, \ldots, x_p) + \varepsilon(s) ,$$

a random variable of variance σ^2 and with expectation:

$$E[Y(T)] = f(x_1, x_2, \ldots, x_p) ,$$

denominated the simular response function. The function, when plotted in terms of the p environmental conditions, may be considered a hyper-surface, herein referred to as the simular response surface.

Presuming that the stochastic simulation model has been properly verified (i.e., the model and its component modules have been checked in order to assure that each responds in accordance with its intended, programmed structure) and has been adequately validated (i.e., the model has been compared with the known behaviour of the simulated system), the analyst should be in a position to commence systematic experimentation with the model. This experimentation shall be in consonance with one of the aforementioned purposes and shall require, since the model is presumed to be of the stochastic variety, the use of appropriate statistical techniques.

If the purpose of the experimentation is to ascertain the relative significance of alternative environmental specifications, the analyst shall likely employ either the technique of the analysis of variance or its close associate, regression methodology. These procedures permit one to vary simultaneously, yet in a scientifically organised fashion, a number of input variables so as to estimate the marginal simular response attributable to each altered environmental condition. For the application of these statistical procedures, the reader is referred to the review paper of J. S. Hunter and T. H. Naylor (1970) or to the monograph of A. Huitson (1966).

The concern of this paper shall be the second of the aforementioned analytical goals of simular experimentation; viz., the determination of the environmental specifications (i.e., input conditions) under which the simular response function attains its optimal value. Without significantly restricting generality, one may presume that the locus $(x_1, x_2, \ldots, x_p)$ at which $f(x_1, x_2, \ldots, x_p)$ attains its maximal value is sought. This search shall necessarily be conducted by defining successive encounters with the simulation model until such time as the desired locus can be reasonably well affixed. Underlying the motivation for the search is, of course, the anticipation that the optimal simular environmental specifications, when translated into terms of the operating conditions for the simulated system and when implemented there, shall provide a nearly optimal system performance as well.

The Simular Response Surface

The simular response function $f(x_1, x_2, \ldots, x_p)$ is then the mean value of the simular response, a random variable dependent upon the specification of p pertinent environmental conditions. These input conditions, or factors as they are termed, may be of one of two types:
(a) qualitative - those environmental conditions which are usually best considered as variates which assume at most a finite number of values; and
(b) quantitative - those environmental conditions whose assignable values may be deemed to constitute a continuum of real numbers.
Qualitative factors are typified by policy specifications, such as an input parameter whose values denote whether a queuing discipline shall be FIFO (First In, First Out) or LIFO (Last In, First Out), whereas quantitative factors are exemplified by a fluid flow rate which is deemed variable between successive model encounters.

The determination of the relative effects of qualitative factors upon the simular response is ideally suited to the factorial experimental designs, whereas the assessment of the relative significance of alterations in quantitative factors is in reality amenable to analysis by means of regression techniques. It is the latter type of factors which shall be of interest in this paper.

Indeed, one may presume that the initial analyses of encounters with the simulation model have provided an adequate understanding of the effects of the pertinent qualitative factors, so that all p of the factors remaining as independent variables in the simular response function, $f(x_1, x_2, \ldots, x_p)$, may be assumed to be of the quantitative type. If the simular response function can be assumed to be a continuous and well-behaved function of these quantitative variables, then one may represent the function as a Taylor series about some particular environmental condition,

$$\vec{x}_0 = (x_{1,0}, x_{2,0}, \ldots, x_{p,0}) .$$

This representation then becomes

$$f(x_1, x_2, \ldots, x_p) = f(\vec{x}_0) + \sum_{k=1}^{p} f_k(\vec{x}_0) \cdot (x_k - x_{k,0}) +$$

$$+ \tfrac{1}{2} \sum_{k=1}^{p} \sum_{\ell=1}^{p} f_{k\ell}(\vec{x}_0) \cdot (x_k - x_{k,0}) \cdot (x_\ell - x_{\ell,0}) + \ldots,$$

where $f_k(\vec{x}_0)$ denotes the first partial derivative, evaluated at $\vec{x}_0$, of f with respect to x_k, and where $f_{k\ell}(\vec{x}_0)$ is the second partial derivative, evaluated at $\vec{x}_0$, of f with respect to x_k and x_ℓ, ℓ, k = 1, 2, ..., p.

The selection of the particular vector, $\vec{x}_0$, of environmental specifications is somewhat arbitrary, though the choice shall presumably reflect one's a priori, subjective speculations regarding the location of the optimal simular response; alternatively, in the absence of such speculations, one may select $\vec{x}_0$ as that vector of input conditions which corresponds to the simulated system's standard operating conditions. For reasons which shall become apparent momentarily, the vector

$$\vec{x}_0 = (x_{1,0}, x_{2,0}, \ldots, x_{p,0})$$

shall be referred to as the initial search center.

The subsequent discussion shall be considerably simplified if, without loss of generality, one translates the p quantitative factors, $x_1, x_2, \ldots, x_p$, according to the transformations:

$$z_k = (x_k - x_{k,0}) / S_k ,$$

where S_k is an appropriate scale factor for the k^{th} variate, $k = 1, 2, \ldots, p$. In terms of the vector $(z_1, z_2, \ldots, z_p)$, termed the search vector or vector of search variates, the Taylor series representation for the simular response function becomes:

$$f^*(z_1, z_2, \ldots, z_p) = \beta_0 + \sum_{k=1}^{p} \beta_k z_k + \sum_{k=1}^{p} \sum_{\ell=k}^{p} \beta_{k\ell} z_k z_\ell + \ldots, \qquad (1)$$

where

$\beta_0 = f(\vec{x}_0)$,

$\beta_k = S_k f_k(\vec{x}_0)$, $\quad k = 1, 2, \ldots, p$,

$\beta_{k\ell} = S_k S_\ell f_{k\ell}(\vec{x}_0)$, $\quad 1 \le k < \ell = 2, 3, \ldots, p$,

$\beta_{kk} = S_k^2 f_{kk}(\vec{x}_0)/2$, $\quad k = \ell = 1, 2, \ldots, p$,

et cetera.

Ideally, the scale factors (S_k) are to be selected so that unit changes in the resulting search variates (z_k) would provide essentially the same marginal simular responses. But, since this knowledge is presumably of the very nature of that being sought by the experimentation itself, the analyst shall need to select these scale factors with some care. One approach is to select each S_k as that change (in units appropriate to the original quantitative factor x_k) which requires a unit cost to implement in the system being simulated; in this manner, unit changes in the search variates correspond to equivalent marginal costs for their corresponding implementation in the simulated system.

Once the search variates have been defined, the experimental/analytical task of locating the optimal simular response may be begun. The search procedure may be summarised as a two-phased operation:
(a) an initial search phase, during which the behaviour of the simular response function is approximated by p-dimensional hyperplanes, the phase terminating whenever an approximating plane is found devoid of any significant tilt; and,
(b) an intensive search phase, during which the nature of the simular response function is revealed by the estimation of approximating surfaces of higher degree, so that the locus of the optimal response may be more accurately situated.
This search procedure is conducted in terms of the search variates, z_k, but, once located, the situs of the optimal simular response may be unravelled and presented in terms of the original environmental conditions by means of the inverse translations,

$$x_k = x_{k,0} + S_k z_k, \quad k = 1, 2, \ldots, p. \tag{2}$$

The general procedure for exploring the simular response surface in a p-dimensional search space is somewhat constrained by the difficulties of pictorially representing a general hypersurface in more than two dimensions. Thus, the remainder of this paper shall be constituted by an explanation of a useful response surface methodology, applicable (without an attendant loss of generality) to the search for the location of the optimal simular response whenever the simular response surface may be deemed functionally dependent upon only two quantitative factors, x_1 and x_2. Alternatively, the simular response surface may be considered a function of the two search variates, z_1 and z_2: $f^*(z_1, z_2)$. A representative selection of four types of such response surfaces is presented in Figure 1.

The varieties of such response surfaces are of course boundless. Those depicted are representative of the types of response surfaces which shall likely be encountered by the analyst who searches for the maximal simular response. An alternative presentation for the simular response surface is the two-dimensional plot of its isohypses, or contour lines, each of which connects the locations (x_1, x_2) at which the response surface assumes a constant altitude.

Figure 2 depicts contours for the four types of response surfaces displayed in the preceding figure; viz.,
(a) a unique maximum;
(b) a ridge of maxima;
(c) a rising ridge; and,
(d) a minimax.
The reader should note that, in the first two cases, (a) and (b), the maximal simular response is extant, though in the second situation (b) there exists a number of environmental specifications (x_1, x_2) at which the maximal response is attained. The loci of these maxima may be referred to as a stationary ridge.

A second type of ridge is depicted in the third contour, graph (c). Here, no search procedure shall be capable of locating the maximal simular response, yet, if the nature of the rising ridge could be ascertained, environmental conditions could be rapidly altered so as to improve the simular response.

In the last graph (d), a minimax (or "saddle-point") exists. If one were to search in the x_2-direction along a line passing vertically through the contour labels (1 and 3), he would declare that a maximal response, somewhat less than 4, would exist. If a similar search were conducted in the x_2-direction, yet a few x_1-units to the right or left, an inevitable conclusion would be derived that the maximal response be, say, 4, 6, or 8, depending upon the x_1-situs of the search. Of course, were a search to be conducted along some fixed x_2-value, one would likely discover an apparent minimal (but no maximal) simular response. Hence, the term minimax is applied, as the "saddle point" constitutes either a minimum or a maximum, dependent upon the direction from which it is approached along the surface. Because of the possibility of such contingencies, it is wise to conduct the search simultaneously in the several quantitative variables, rather than by altering one variable at a time.

The Initial Search, or Isolation, Phase

As a function of two search variates, z_1 and z_2, the simular response surface may be written

$$f^*(z_1, z_2) = \beta_0 + (\beta_1 z_1 + \beta_2 z_2) + (\beta_{11} z_1^2 + \beta_{12} z_1 z_2 + \beta_{22} z_2^2) + \ldots \tag{3}$$

where β_0 represents the height of the surface at $z_1 = z_2 = 0$ (i.e., at the initial search center), β_k represents the slope of the surface at the search center in the direction x_k, $\beta_{k\ell}$ represents the second derivative of the surface at the search center with respect to x_k and x_ℓ, $1 \le k \le \ell = 1, 2, \ldots, p$; et cetera. One may presume that, in a sufficiently small neighborhood of the search center, the simular response function can be represented by the planar approximation,

$$f^*(z_1, z_2) \cong \beta_0 + \beta_1 z_1 + \beta_2 z_2 = f_1^*(z_1, z_2), \tag{4}$$

for (z_1, z_2) within, say, the unit circle or square centered at the origin.

By means of this proximate representation, the simular responses themselves become

$$Y(T) = \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \epsilon(s) ,$$

where $\epsilon(s)$ now represents a random variable whose distribution is affected by errors of two types:
(a) the inadequacy of the planar approximation, $f_1^*(z_1, z_2)$, as a functional representation for the simular response function; and,
(b) the intrinsic variability inherent in the structure of a stochastic simulation model.
Nonetheless, it has become accepted procedure to assume that the random variable $\epsilon(s)$ has mean zero and variance σ^2 throughout the area immediate to the search center. (Cf: O. L. Davies (1954).)

Furthermore, if a set of N search vectors, $(z_1, z_2)_j$, $j = 1, 2, \ldots, N$, is defined within the search area immediately surrounding the search center, and if a set of N corresponding encounters are specified by the environmental conditions corresponding to these search vectors and by an independently and non-repetitiously selected random number seed, then the resulting simular responses,

$$Y_j = f_1^*(z_1, z_2)_j + \epsilon(s_j) ,$$

shall constitute a normal random sample if one assumes that the error terms, $\epsilon(s_j)$, are normally and independently distributed random variables, $j = 1, 2, \ldots, N$. If the search vectors, $(z_1, z_2)_j$, are distinct points in the search area, then each Y_j shall have its own mean, $f_1^*(z_1, z_2)_j$, though their common variance shall be σ^2.

Ideally, one should seek to specify as many search vectors (z_1, z_2) as possible, thereby affixing the alignment of the planar approximation, $\beta_0 + \beta_1 z_1 + \beta_2 z_2$, as accurately as possible. Yet, since the planar representation is at best approximate, and since each selected search vector implies the organisation of a separate encounter with the model, one is frequently required to resort to the selection of as few search vectors as are adequate to estimate the three coefficients: β_0, β_1, and β_2.

The selection of the necessary search vectors for such a purpose is termed an <u>experimental design</u>, the selected vectors of which may be referred to alternatively as the <u>design points.</u> Adequate for the purpose of estimating the three coefficients, then, is a set of three design points, provided that the three points are not collinear in the search area.

An experimental design of some virtue for the estimation of the three coefficients, β_0, β_1, and β_2, is the equilateral triangular design, which permits the analyst to select as the three design points the vertices of any equilateral triangle which is inscribed in the unit circle centered at the search center. Two possible orientations of such a design are depicted in Figure 3. Once the three design points have been selected, the corresponding environmental specifications may be determined, in accordance with Equation (2), and employed together with independently selected seeds in order to specify the input conditions for three successive encounters with the simulation model.

If the design points employed are $(0, 1)$, $(-\sqrt{3}/2, -1/2)$, and $(+\sqrt{3}/2, -1/2)$, the vertices of Figure 3 marked by crosses (X), the resulting simular responses, Y_1, Y_2, and Y_3, respectively, may be employed in order to obtain the unbiassed least-squares estimates:

$$\tilde{\beta}_0 = (Y_1 + Y_2 + Y_3)/3 ,$$

$$\tilde{\beta}_1 = (-Y_2 + Y_3)/\sqrt{3} , \qquad (5)$$

and

$$\tilde{\beta}_2 = (2Y_1 - Y_2 - Y_3)/3 .$$

With these three estimates, the planar approximation to the simular response function may itself be estimated at any point (z_1, z_2) in the search area by

$$\tilde{y} = \tilde{\beta}_0 + \tilde{\beta}_1 z_1 + \tilde{\beta}_2 z_2 . \qquad (6)$$

The contours of this estimated simular response may then be plotted by solving for loci (z_1, z_2) such that

$$\tilde{y} = \tilde{\beta}_0 + \tilde{\beta}_1 z_1 + \tilde{\beta}_2 z_2 = c \text{ (constant)} ,$$

for selected constants, c. (An initial and convenient selection for such a constant might be $\tilde{\beta}_0$; others may be selected from computationally convenient values near this initial constant.) A typical set of contour lines for the estimated planar approximation is displayed in Figure 4.

One may note from these contours that the apparently optimal direction in which to move in order to locate a new search center shall be in a direction perpendicular to the contour lines. Movement in this direction is the equivalent of movement, in the z_1 and z_2 directions, proportionate to $\tilde{\beta}_1$ and $\tilde{\beta}_2$, respectively, so that the subsequent search center may be located at search vector $(k\tilde{\beta}_1, k\tilde{\beta}_2)$, for some constant k, chosen so that the new search center be situated not too far outside the present search area; the motivation for such a recommendation may become more apparent when one considers that the current estimates, $\tilde{y}$, of the simular response surface are based merely on a planar approximation.

About the newly located search center, which may be relabelled (0, 0) in terms of newly defined search variates, another equilateral triangular design may be defined and a triplet (Y_1, Y_2, and Y_3) of simular responses subsequently recorded. The resulting estimated slopes, $\tilde{\beta}_1$ and $\tilde{\beta}_2$ may again be used to move the search to another center. Such a procedure should continue until the estimated slopes are no longer significantly different from zero, at which point one may presume that a stationary point has been located at or near the most recently employed search center.

The determination of the significance of the magnitudes of $\tilde{\beta}_1$ and $\tilde{\beta}_2$ must, since they are transformations (Cf: Equations (5)) of random variables and therefore random variables themselves, depend upon knowledge of the intrinsic variability of the simular responses, as measured usually by the error variance, σ^2. Unfortunately, unless a priori information has been acquired regarding the magnitude of σ^2, no information is available from the recorded responses about any particular search center. (The reader may verify that the estimated simular response,

$$\tilde{y} = \tilde{\beta}_0 + \tilde{\beta}_1 z_1 + \tilde{\beta}_2 z_2 ,$$

passes directly through the three loci $((z_1, z_2)_j, Y_j)$, $j = 1, 2$, and 3, so that no measure of the lack of fit for the planar approximation is available.)

The situation may be somewhat rectified by the addition of a fourth design point to any one of the equilateral triangular designs. By situating this design point at the particular search center (0, 0) and by denoting the resulting simular response there by Y_4, the least-squares estimates of β_1 and β_2 remain unchanged, whereas the estimate of β_0 becomes

$$\tilde{\beta}_0 = (Y_1 + Y_2 + Y_3 + Y_4)/4. \tag{7}$$

Under the assumptions of the normality and independence of the distributions of the four error terms, an unbiassed estimate of the error variance becomes

$$\tilde{\sigma}^2 = (Y_1 + Y_2 + Y_3 - 3Y_4)^2/12 , \tag{8}$$

a statistic which is independently distributed of $\tilde{\beta}_1$ and $\tilde{\beta}_2$. One may show (See G. A. Mihram (1971).) that an appropriate test of a null hypothesis of the form,

$$H_0: \beta_k = 0 ,$$

results from the computation of the respective test statistics

$$T_k = 3(\tilde{\beta}_k)^2 \;/\; 2(\tilde{\sigma}^2), \quad k = 1 \text{ or } 2, \tag{9}$$

and comparison of each with the cumulative distribution function for a Snedecor's variate of one and one degrees of freedom. The null hypothesis is rejected whenever the computed statistic, T_k, is improbably large with respect to this F distribution; otherwise, the magnitude of $\tilde{\beta}_k$ cannot be assumed to be significantly different from zero.

The reader may note that the proposed estimate of the error variance is actually a measure of the inability of the estimated plane,

$$\tilde{y} = \tilde{\beta}_0 + \tilde{\beta}_1 z_1 + \tilde{\beta}_2 z_2 ,$$

to pass exactly through the four points in Euclidean three-dimensional space; indeed,

$$\tilde{\sigma}^2 = \sum_{j=1}^{4} (\tilde{y}_j - Y_j)^2 ,$$

the sum of the squared deviations of the observed responses Y_j at $(z_1, z_2)_j$ from the estimated responses, $\tilde{y}_j$, at the same loci. One must conclude then that $\tilde{\sigma}^2$ represents a measure of the lack of fit of the planar surface to the four points and is therefore not a true measure of the intrinsic variability in the simular responses. Nonetheless, its use in the suggested F-tests for determining the significance of the magnitudes of $\tilde{\beta}_1$ and $\tilde{\beta}_2$ is widespread.

Thus, the movement from search center to search center continues until such time as both $\tilde{\beta}_1$ and $\tilde{\beta}_2$, the estimated planar slopes, become insignificantly different from zero. This insignificance is measured with respect to the most recent estimate of the error variance σ^2. As a matter of fact, one need not repeatedly employ the central design point in other than the initial equilateral triangular design, for a valid estimate of σ^2 is assumed valid throughout the search region. Of course, greater accuracy in the estimation of σ^2 may be obtained if the error variance estimates, $\tilde{\sigma}^2$, as they may arise in successive equilateral triangular designs, are pooled together. In this case, however, the degrees of freedom for Snedecor's F test must be altered accordingly, the details of which may be found in Huitson (1966).

The Intensive Search, or Local Exploration, Phase

Once both estimated slopes, $\tilde{\beta}_1$ and $\tilde{\beta}_2$, are no longer significantly different from zero, the analyst may tentatively entertain the notion that the most recently employed search center is in the proximity of a stationary point on the simular response surface. Indeed, at such a stationary point, the actual slopes β_1 and β_2 would be null.

In order to develop further insight into the nature of the simular response function at this search center, one may next attempt further experimentation in the immediate search area. This experimentation should be designed to estimate an approximation to the simular response surface more accurate than the planar representation; for this purpose, the quadratic approximation,

$$f_2^*(z_1, z_2) = \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \beta_{11} z_1^2 + \beta_{12} z_1 z_2 + \beta_{22} z_2^2 , \tag{10}$$

for the simular response surface may be employed. Assuming that the simular responses in the immediate neighborhood of the most recent search center may be denoted as

$$Y(T) = f_2^*(z_1, z_2) + \varepsilon(s),$$

where again $\varepsilon(s)$ is an error random variable of mean zero and variance σ^2 representative of variations due both to the inadequacy of the quadratic approximation and to the intrinsic stochasticity of the model, then one seeks an efficient experimental design which will permit:
(a) the facile and unbiassed estimation of the coefficients,

$$\vec{\beta} = (\beta_0, \beta_1, \beta_2, \beta_{11}, \beta_{12}, \beta_{22});$$

(b) accurate estimation (in terms of low statistical variance), both of the coefficients and of the quadratic approximating surface.

Minimally, such a design should require six different environmental conditions and, hence, six encounters with the simulation model. Ideally suited for this purpose, it would appear superficially, should be an hexagonal design, for the design could be readily achieved by the superimposition of an inverted equilateral triangular design atop the most recently employed triangular design with center at the most recently employed search center, as depicted in Figure 3. In this manner, only three additional simulation encounters would need be defined, those corresponding to the loci marked by naughts (0) in the figure. The description of the resulting simular responses, their loci in terms of the search variates, and their respective expectations are presented in the first six rows of Table I.

Despite the apparent optimality of the hexagonal design, it suffers from one minor defect; viz., the least-squares estimates of the coefficients $\vec{\beta}$ are linearly dependent random variables and therefore are not unbiassed for the individual parameters. The statistician would say that the estimators have confounded the coefficients to be estimated. Nonetheless, this defect is indeed minor and may be readily overcome by the definition of a seventh simulation encounter at the current search center itself. The corresponding response, Y_7, and it properties are delineated in the last row of Table I.

As a matter of fact, the analyst may well have already recorded a simular response at the search center during the most recent stage of the initial search phase, in which instance only the three additional responses, those above the vertices of the superimposed equilateral triangular design, need be recorded. As a result of recording the total of the seven simular responses, one may estimate unbiassedly the six coefficients by means of the following linear combinations:

$$\tilde{\beta}_0 = Y_7 ,$$

$$\tilde{\beta}_1 = \sqrt{3}\,(-Y_2 + Y_3 - Y_5 + Y_6)/6,$$

$$\tilde{\beta}_2 = (2Y_1 - Y_2 - Y_3 - 2Y_4 + Y_5 + Y_6)/6 ,$$

$$\tilde{\beta}_{11} = (-Y_1 + 2Y_2 + 2Y_3 - Y_4 + 2Y_5 + 2Y_6 - 6Y_7)/6 ,$$

$$\tilde{\beta}_{12} = \sqrt{3}\,(Y_2 - Y_3 - Y_5 + Y_6)/3 , \tag{11}$$

and

$$\tilde{\beta}_{22} = (Y_1 + Y_4 - 2Y_7)/2 .$$

Since the estimates are those of the least-square procedure, the assumptions of the nullity of the means of the seven error terms, their homogeneity of variance, and their mutual lack of correlation imply that, among all unbiassed estimates of the elements of $\vec{\beta}$ which are linear combinations of the seven recorded responses, the preceding estimators have the least variance. (Cf: Gauss-Markov theorem, as discussed by Graybill (1961).) Thus, in a certain sense, the accuracy of the estimators is assured.

In the neighborhood of the search center, the simular response function may be estimated at any point (z_1, z_2) by

$$\tilde{y} = \tilde{\beta}_0 + \tilde{\beta}_1 z_1 + \tilde{\beta}_2 z_2 + \tilde{\beta}_{11} z_1^2 + \tilde{\beta}_{12} z_1 z_2 + \tilde{\beta}_{22} z_2^2 , \tag{12}$$

itself a random variable having expectation $f_2^*(z_1, z_2)$ and variance which may be computed as

$$\mathrm{Var}(\tilde{y}) = \sigma^2[6 - 10(z_1^2 + z_2^2) + 9(z_1^2 + z_2^2)^2]/6. \tag{13}$$

Of primary import is the plotting of the isohypses of the estimated quadratic approximation to the response surface, accomplished by plotting loci (z_1, z_2) for which $\tilde{y} = c$, constants chosen at the discretion of the analyst. (Again an initial choice of $c = \tilde{\beta}_0$ is recommended, the subsequent constants being selected for computational convenience and pictorial appeal.) The transformation of the quadratic form, $\tilde{y}$, to its canonical form before plotting the contours, as discussed in the book edited by Davies (1954), is also recommended.

The resulting contours for the quadratic shall be of one of four types, corresponding to the four types of surfaces depicted in Figures 1 and 2; viz.,

(a)	<u>concentric ellipses</u>	- a single maximum;
(b)	<u>parallel lines</u>	- a stationary ridge of maxima;
(c)	<u>parabolae</u>	- a rising ridge;
(d)	<u>hyperbolae</u>	- a minimax .

Depending upon the category of the isohypses, subsequent search may be undertaken in the respective cases by:
(a) defining another augmented hexagonal design at the center of the ellipses, so as to reconfirm its position as the locus of the maximum;
(b) defining equilateral triangular designs along the apparent stationary ridge of maxima so as to explore further the possibility that a stationary ridge truly

exists;

(c) defining equilateral triangular or hexagonal designs at an appropriate point along the apparent rising ridge so as to verify that such a ridge indeed exists on the simular response surface itself; and

(d) defining equilateral triangular designs in both directions away from the apparent minimax location and toward apparent optimal increase, thus exploring the possibility of a bimodal simular response surface.

In each instance, the subsequent exploration of the simular response surface may be conducted in accordance with the aforementioned design and analysis procedures.

Conclusions

This paper presents a fundamental approach to the search for a description of the simular response surface, defined as the locus of the expectations of the simular responses, random variables each of which derives from a particular environmental specification $\vec{x}$ for a stochastic simulation model. The paper has dwelt upon the exploration of such a surface by means of the simplex experimental designs of the equilateral triangular and hexagonal varieties, which are quite adequate for estimating planar and quadratic approximations to the simular response surface as a function of two environmental conditions.

In the likely event that one's simular experimentation should involve examinations of more than two factors, these designs admittedly shall not be adequate for the purpose; however, they do depict the fundamental phases in the search for optimal simular environmental conditions, and are readily extended to simplex designs in three or more dimensions (Cf: G. E. P. Box and D. W. Behnken (1960)).

These experimental techniques have been fruitfully applied to industrial processes wherein the process' operating conditions are readily controllable, as reported by G. E. P. Box and J. S. Hunter (1958). They shall prove equally applicable to the study of the behaviour of stochastic simulation models, for the environmental conditions of such models are quite easily controlled by means of alternative input data descriptions. The assignment of independently and non-repetitiously selected random number seeds for the successive encounters during the simular experimentation assures the necessary randomness for the application of these designs and their subsequent analyses.

Of particular interest is the quite sequential decision process which is implicit in these search procedures. One would prefer to know whether the recommended simplex procedures are the optimal approach to this experimental technique; i.e., could alternative techniques or search procedures locate optima, ridges, or saddle points with less effort or fewer simular encounters? Which decision variables, such as the size of the equilateral triangles (or other simplex designs, such as squares, or regular pentagons and hexagons) or the size of the step to be taken in the movement between successive search centers, affect the quality of the search most critically? The answers to these queries pose interesting research problems, the answers to which may prove to be best answered via Monte Carlo sampling techniques, though some analytical results are available in the paper of Brooks and Mickey (1961).

Acknowledgement

The author gratefully acknowledges the support of the National Science Foundation, under whose grant number GK-5289 this paper was prepared.

References

1. Box, G. E. P. and D. W. Behnken (1960), "Simplex-Sum Designs: A Class of Second Order Rotatable Designs Derivable from Those of First Order", Annals of Mathematical Statistics, 31, 838-864.

2. Box, G. E. P. and J. S. Hunter (1958), "Experimental Designs for the Exploration and Exploitation of Response Surfaces", pp. 138-190 of Experimental Designs in Industry, edited by Victor Chew, published by John Wiley and Sons, New York.

3. Brooks, S. H. and M. R. Mickey (1961), "Optimum Estimation of Gradient Directions in Steepest Ascent Experiments", Biometrics, 17, 48-56.

4. Davies, O. L. (1954), Design and Analysis of Industrial Experiments, Hafner Publishing Company, London.

5. Graybill, F. A. (1961), An Introduction to Linear Statistical Models, McGraw-Hill Books, New York

6. Huitson, A. (1966), The Analysis of Variance, Hafner Publishing Company, London.

7. Hunter, J. S. and T. H. Naylor (1970), "Experimental Designs for Computer Simulation Experiments", Management Science, A16, 422-434.

8. Mihram, G. A. (1971), Simulation: Its Statistical Foundations, Academic Press, New York.

TABLE I

Loci and Expectations of Simular Responses,

Hexagonal Design

Response	Loci	Expectation					
		β_0	β_1	β_2	β_{11}	β_{20}	β_{12}
Y_1	(0, 1)	1	0	1	0	1	0
Y_2	$(-\sqrt{3}/2, -1/2)$	1	$-\sqrt{3}/2$	$-1/2$	3/4	1/4	$+\sqrt{3}/4$
Y_3	$(+\sqrt{3}/2, -1/2)$	1	$+\sqrt{3}/2$	$-1/2$	3/4	1/4	$-\sqrt{3}/4$
Y_4	(0, -1)	1	0	-1	0	+1	0
Y_5	$(-\sqrt{3}/2, +1/2)$	1	$-\sqrt{3}/2$	$+1/2$	3/4	1/4	$-\sqrt{3}/4$
Y_6	$(+\sqrt{3}/2, +1/2)$	1	$+\sqrt{3}/2$	$+1/2$	3/4	1/4	$+\sqrt{3}/4$
Y_7	(0, 0)	1	0	0	0	0	0

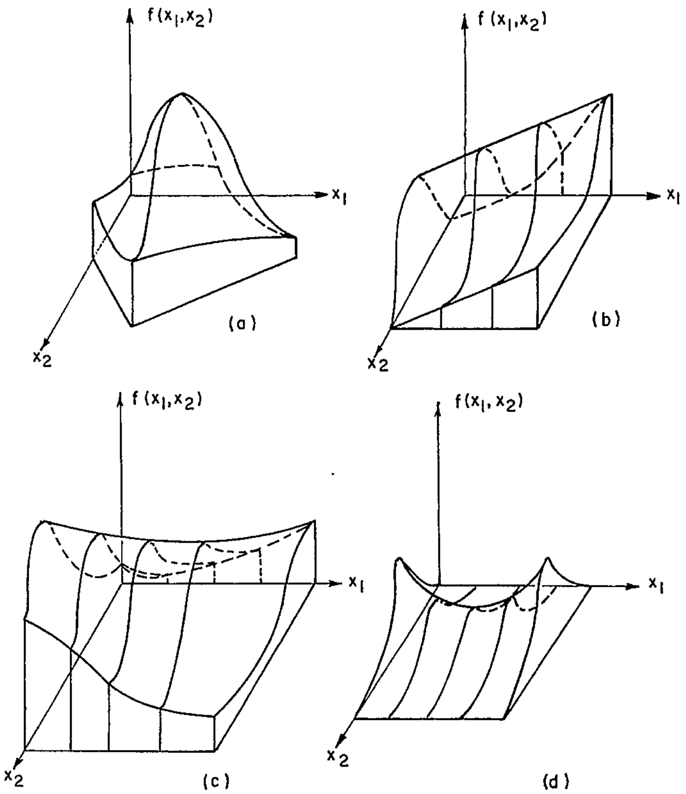

FIGURE 1. EXEMPLARY SIMULAR RESPONSE FUNCTIONS

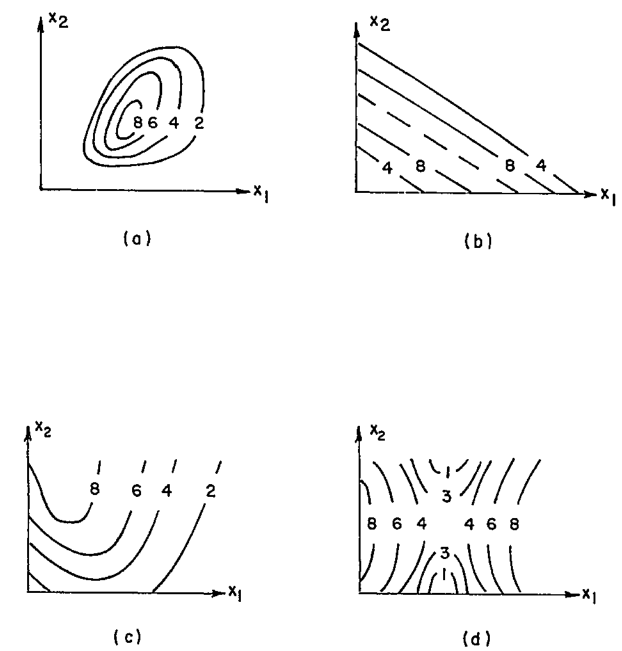

FIGURE 2. ISOHYPSES OF TYPICAL SIMULAR RESPONSE SURFACES

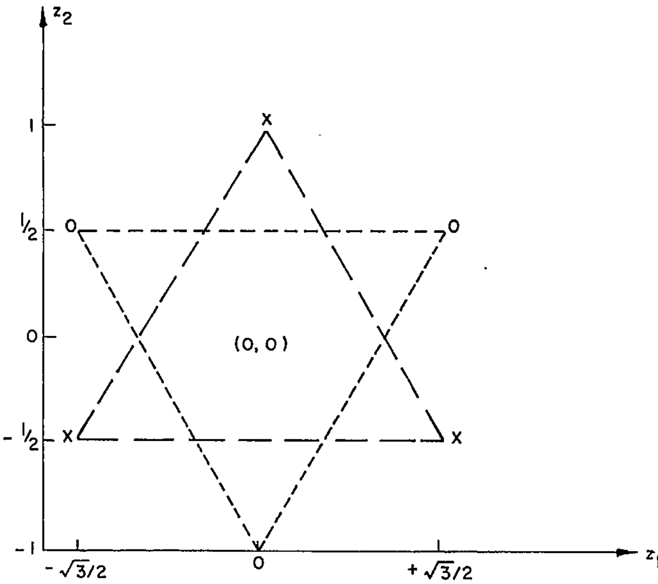

FIGURE 3. SUPERIMPOSED EQUILATERAL TRIANGULAR DESIGNS (THE HEXAGONAL DESIGN)

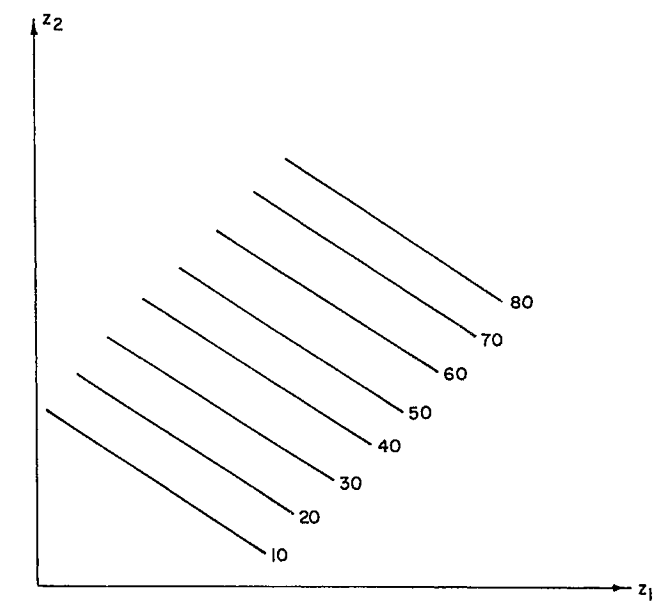

FIGURE 4. CONTOURS OF THE ESTIMATED RESPONSE $\tilde{y}=\tilde{\beta}_0+\tilde{\beta}_1 z_1+\tilde{\beta}_2 z_2$