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THE USE OF SECOND ORDER RESPONSE SURFACE DESIGNS

IN DIGITAL SIMULATION

A THESIS

Presented to

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IN DIGITAL SIMULATION

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SUMMARY

This study presents the topic of the use of second order response surface designs and their applications to digital simulation. In particular, it examines methods to determine the combination of factor levels at which the response variable is optimized. Specifically, the questions considered are associated with problems of experimental design in simulation, where the experimenter's objective is to optimize some appropriate response of the system under study.

The research surveys the field of response surface methodology, with emphasis on the use of second order experimental designs and optimization techniques. Several second order experimental designs are constructed and applied to various known response surfaces which typically might be generated by a digital computer simulation model.

The results are analyzed from two points of view; first, comparison by design and second, comparison by surface. Conclusions are then drawn in such a manner as to apply them to constructing designs in general or designs for specific surfaces. When comparing results, the class of orthogonal equiradial designs demonstrates the best performance in all average situations. The best achievement on ridge surfaces was obtained by the use of uniform precision and minimum bias central composite designs. Irregular, asymmetric surfaces are best explored using the minimum bias central composite design. Finally, the concept of rotatability was presented and its importance demonstrated.

CHAPTER I

INTRODUCTION

1.1 Experimental Optimization

In recent years experimental optimization techniques have found wide application in a variety of situations. These techniques may be applied to situations in which one is interested in determining the levels to which independent variables or factors are adjusted to optimize some response, say y, associated with a system. This relationship may be described mathematically as

$$y = \phi(x_1, x_2, \ldots, x_k) + \varepsilon \tag{1.1}$$

where x_i is the i^{th} factor in the observation and the residual ε measures the associated experimental error. In the experimental design literature, the function ϕ is called a <u>response surface</u>. If the mathematical form of ϕ is known, the function fully describes the response surface in the area of interest. In most cases, however, the form of ϕ is unknown and usually extremely complicated. Then it is assumed that the function may be reasonably approximated by a low order polynomial in the variables x_i within the experimental region of interest.

If there is little curvature in the true surface, then one may use as the approximating function a first order polynomial, say

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \varepsilon \ . \tag{1.2}$$

If significant curvature in $\emptyset$ is present the experimenter may turn to the second order polynomial model

$$y = \beta_0 + \sum_i \beta_i x_i + \sum_i \beta_{ii} x_i^2 + \sum_{\substack{i \ j \\ i<j}}\sum \beta_{ij} x_i x_j + \varepsilon \ . \tag{1.3}$$

The experimenter may, due to lack of fit of the second order model, resort to cubic or even higher order models. The Taylor Series expansion provides the rationale for the polynomial approximation of $\emptyset$. For example, the first order model is developed from the first order Taylor Series expansion about $x_1 = x_2 = \dots = x_k = 0$

$$\emptyset = \emptyset_{\underline{x}=\underline{0}} + \left(\frac{\partial f}{\partial x_1}\right)_{\underline{x}=\underline{0}} x_1 + \left(\frac{\partial f}{\partial x_2}\right)_{\underline{x}=\underline{0}} x_2 + \dots + \left(\frac{\partial f}{\partial x_k}\right)_{\underline{x}=\underline{0}} x_k \ , \tag{1.4}^*$$

where the β_i are the appropriate derivatives.

Fitting the approximating polynomial (i.e. estimating the coefficients) is usually accomplished by least squares, which uses as an estimate of $\underline{\beta}$ a vector $\hat{\underline{\beta}}$ which results in a minimum value for the sum of the squares of the deviations

$$L = \sum_{i=1}^{N} \varepsilon_i^2 = \underline{\varepsilon}'\underline{\varepsilon} \ . \tag{1.5}$$

---

*Matrices will be denoted by upper case underlined letters. Column vectors will be denoted by lower case underlined letters. The transpose of a matrix or vector is denoted by a prime (').

It is well known that the model of equation (1.1) can be written in the form

$$\underline{y} = \underline{X\beta} + \underline{\varepsilon} , \tag{1.6}$$

or

$$\underline{y} - \underline{X\beta} = \underline{\varepsilon} . \tag{1.7}$$

Substituting equation (1.7) into equation (1.5) and expanding gives

$$L = \underline{y}'\underline{y} - 2\underline{\hat{\beta}}'\underline{X}'\underline{y} + \underline{\hat{\beta}}'\underline{X}'\underline{X\hat{\beta}} . \tag{1.8}$$

Now taking the partial derivative of L with respect to $\underline{\hat{\beta}}$

$$\frac{\partial L}{\partial \underline{\hat{\beta}}} = -2\underline{X}'\underline{y} + 2(\underline{X}'\underline{X})\underline{\hat{\beta}} , \tag{1.9}$$

and then setting the partial derivative equal to zero and solving for $\underline{\hat{\beta}}$ yields

$$\underline{\hat{\beta}} = (\underline{X}'\underline{X})^{-1}\underline{X}'\underline{y} \tag{1.10}$$

Of course, the usual assumptions of multiple linear regression regarding $\underline{\varepsilon}$ must hold, that is $E(\underline{\varepsilon}) = \underline{0}$ and $Var(\underline{\varepsilon}) = \sigma^2\underline{I}_N$.

It is now possible to estimate each of the model parameters and obtain a fitted equation for the response surface. From this fitted surface the experimenter may obtain estimates of the optimum levels for the independent variables and predicted experimental responses. Also, one may test various hypotheses about the parameters in the model of equation (1.6). This is discussed extensively in Graybill (17).

1.2 Digital Simulation

Digital simulation is a numerical technique for conducting experiments on certain types of mathematical models describing the behavior of a system (or its components) on a digital computer over extended periods of real time (10). The behavior of a system in turn, is described by a collection of entities which act and interact together toward the accomplishment of some logical end.

Before one can simulate a given system, a representative model of that system must be constructed. This is the major difference between an actual experiment and an experiment involving simulation of a system. Given a model of the system, Hunter and Naylor (18) have shown that a computer simulation experiment usually requires that the analyst give special attention to the following four activities:

1. Formulation of a Computer Program. The formulation of a computer program for the purpose of conducting computer simulation experiments requires that some consideration be given to the following: flow charts, computer program, error checking, data input and starting conditions, data generation, and output reports.

2. Validation. The model must be validated by comparing simulated

data with actual and historical data. If the model proves inadequate, then changes must be made in the variables, parameter estimates, and structure of the model.

3. Experimental Design. Two different types of experimental objectives can be defined: (a) to find the combination of factor levels at which the response variable is optimized and (b) to explain the relationship between the response variable and the controllable factors in the experiment. The type of experimental design employed will depend on the objectives.

4. Analysis of Simulated Data. The analysis of data generated by a computer model consists of the collection and processing of the simulated data, computation of meaningful statistics, and interpretation of the results. The analysis includes the use of such techniques as regression analysis and analysis of variance.

This investigation is concerned primarily with step 3(a) of this procedure. Specifically, the questions considered here are associated with problems of experimental design in simulation, where the experimenter's objective is to optimize some appropriate response of the system under study.

Experimental optimization techniques and their use in conjunction with digital computer simulation models have been discussed by many authors. The basic optimization technique employed most often is the method of steepest ascent, or some other closely related technique, such as the sequential simplex (27), the one-factor-at-a-time method (16), or stochastic approximation (19). These are usually called first order techniques, since they require the experimenter to assume that a first order model is adequate to explain the response. Examples of the use of first order optimization techniques in conjunction with digital computer simulation may be found in the texts of Schmitt and Taylor (25) and Meier, Newell, and Pazer (21), also articles by Meier (20), Montgomery, Talavage, and Mullen (22), Dickey and Montgomery (14), Baasel (2), Carpenter and Sweeny (12), Duer (15), and Naylor and Burdick (10).

Few authors have discussed the use of higher order approximating polynomials and associated optimization techniques with computed simulation models to improve the estimate of the optimum obtained by a method such as steepest ascent. Burdick and Naylor (11), Sasser (24), and Brooks (8) have stressed the need for a survey discussing the relationship of experimental design techniques to simulation. As these techniques have been widely and successfully employed in a variety of other experimental settings, it would seem that some account of their application to simulation be given.

1.3 Objectives

The primary objectives of this thesis are:

1. To investigate the use and properties of second order experimental designs.

2. To investigate and analyze the effectiveness and efficiency of designs from this class through simulation modeling.

3. To demonstrate these applications to simulation experiments by examining the relationship between experimental design techniques and the design of computer simulation experiments.

4. To draw conclusions regarding types of designs presented.

The above objectives will be accomplished by first surveying the field of response surface methodology, and in particular, the use of second order experimental designs and optimization techniques. Several second order experimental designs will be constructed so that valid comparisons can be presented. The experimental designs will then be applied to various known response surfaces which typically might be generated by a digital computer simulation model, the results analyzed, and conclusions drawn. The techniques of experimental design, as they apply to computer simulation, will be reviewed throughout the presentation.

1.4 Assumptions

The following assumptions are made:

1. With the extensive literature and experimentation concerning search techniques and first order experimentation, it is assumed that the simulation investigation has already encountered a near optimal region in which a "lack of fit" situation exists. Therefore emphasis will be placed on the investigation of the second order situation.

2. A representative cross section of frequently employed experimental designs will be used. This will include a factorial design, two rotatable central composite designs, a minimum bias design, and two equiradial designs.

CHAPTER II

RESPONSE SURFACE METHODOLOGY

2.1 General

The underlying goal of response surface methodology is the determination of the optimum operating conditions for a system. Basically we encounter two distinct situations in examining a response surface: (1) the actual optimum is unknown or remote from the current experimental region, and (2) the actual optimum is within or close to the experimental region. As a result, a response surface study usually proceeds in two phases, the first being a sequential procedure which leads one to a near optimal region, and the second being a simultaneous procedure to more precisely estimate the optimum and describe the nature of the fitted surface.

2.2 Phase I

Experimenters are quite hesitant about designing elaborate simultaneous experiments unless they are sure that the optimum lies either in or near the region under consideration. Because of this, an experimenter should be acquainted with procedures for searching a large region for a near optimal response. Probably the most widely used optimum seeking procedure is the method of steepest ascent (7). It is a method by which one moves in a sequential manner along a path of increasing response.

The procedure begins by fitting a first order polynomial

$$\hat{y} = b_0 + b_1x_1 + b_2x_2 + \ldots + b_kx_k \tag{2.1}$$

to approximate the response surface $\emptyset$ in some restricted region in the vicinity of the starting point. The path of steepest ascent is defined as that direction which maximizes y on the surface of a hypersphere of a given radius. That is, the experimenter must maximize y subject to the constraint that the x_i's are on a hypersphere of radius R. Coding the variables, i.e. assuming the center of the design to be the origin (0,0,...,0), the problem becomes one of finding the values of x_i which maximize

$$\hat{y} = b_0 + \sum_{i=1}^{k} b_ix_i \tag{2.2}$$

subject to

$$\sum_{i=1}^{k} x_i^{\,2} = R^2 \ . \tag{2.3}$$

Lagrange multipliers are used to maximize the function

$$Q(x_1,x_2, \ldots, x_k) = b_0 + \sum_{i=1}^{k} b_ix_i - \lambda(\sum_{i=1}^{k} x_i^{\,2} - R^2) \ . \tag{2.4}$$

Taking partial derivatives, one obtains

$$\frac{\partial Q}{\partial x_i} = b_i - 2\lambda x_i \tag{2.5}$$

and

$$\frac{\partial Q}{\partial \lambda} = -\ (\sum_{i=1}^{k} x_i^{\,2} - R^2) \ . \tag{2.6}$$

Now setting $\frac{\partial Q}{\partial x_i} = 0$ results in

$$x_i = \frac{b_i}{2\lambda} \qquad (i=1,2, \ldots, k) \tag{2.7}$$

At this point the experimenter can either choose a value for λ or choose an arbitrary change in one of the x_i's and from it compute λ, hence, defining the coordinates of the remaining k-1 variables along the path of steepest ascent. Points along the path of steepest ascent are then computed and experimentation continues until one of two possibilities occurs:

(1) The coefficients b_i become small and the linear equation still fits. This result implies that a plateau has been reached.

(2) Curvature becomes evident as the result of a lack of fit test. For one to obtain more information about the location of the optimum in these situations, second order designs must be constructed.

A word of caution should be given concerning the importance of the appropriate choice of levels used in this phase. If the levels of a factor are too close, the results of each subsequent experiment may seem negligible. Consequently, one may have to conduct far too many experiments in moving along the path of steepest ascent. Likewise, if the levels are too far away, too much curvature may be present early in experimentation and one may be forced to a higher order design when it is not necessary. Further discussion of this problem will be presented in Chapter III. An excellent example of correction for errors in the choice of levels for this phase can be found in Cochran and Cox (13) on page 362.

The method of steepest ascent is probably the most often used optimum seeking procedure. Examples of its use are found in Box and Wilson (7) page 18, Cochran and Cox (13) page 357, and Myers (23) page 90. Its all-around reliability is demonstrated by Brooks (8) in his comparison of maximum-seeking methods. Other first order methods used to a lesser degree are Bulher, Shah, and Kempthorne's method of parallel tangents (9), Friedman and Savage's one-factor-at-a-time procedure (16), Anderson's random test point selection (1), a single large factorial (8), Schmitt and Taylor's quadratic approximation (26), and Spendley, Hext, and Himsworth's sequential simplex (27).

2.3 Phase II

As a result of experience, previous experimentation, prior knowledge of the system, or phase I experimentation, the experimenter will at some point in time arrive in the general vicinity of the optimum. A more elaborate analysis must be conducted to obtain an improved estimate of the optimum. A major portion of this analysis is the design of the experiment.

Let the unknown parameters in the second order model equation (1.3) be estimated by least squares, resulting in the fitted second order response surface

$$\hat{y}_u = b_0 + \sum_i b_i x_{iu} + \sum_i b_{ii} x_{iu}^2 + \sum_{\substack{i \; j \\ i<j}} \sum b_{ij} x_{iu} x_{ju} + \varepsilon_u \qquad (2.8)$$

where $u = 1,2, \ldots, N$ and y_u represents the N observations in an experiment. Of interest here is the fact that, in order to estimate the regression coefficients in a model of this type, there must be at least three different levels for each variable x_{iu}.

Assuming an arbitrary choice of design and using the fitted response surface (equation (2.8)), the experimenter wishes to choose $x_1, x_2, \ldots, x_k$ so as to optimize $\hat{y}_u$. In matrix notation, the second order polynomial is written

$$\hat{y} = b_0 + \underline{x}'\underline{b} + \underline{x}'\underline{Bx} \tag{2.9}$$

where

$$x' = [x_1, x_2, \ldots, x_k]$$
$$b' = [b_1, b_2, \ldots, b_k]$$

and

$$\underline{B} = \begin{bmatrix} b_{11} & b_{12}/2 & \cdots & b_{1k}/2 \\ & b_{22} & \cdots & b_{2k}/2 \\ & & \ddots & \vdots \\ & & & b_{kk} \end{bmatrix}$$

In equation (2.9) $\underline{x}'\underline{b}$ contains the first order terms $(\sum_i b_i x_i)$ as indicated in equation (2.8). $\underline{x}'\underline{Bx}$ contains both pure $(\sum_i b_{ii} x_i^2)$ and mixed $(\sum_i \sum_j b_{ij} x_i x_j)$ quadratic coefficients. Differentiating equation (2.9) with respect to $x_1, x_2, \ldots, x_k$ will provide the stationary point. It follows that

$$\frac{\partial \hat{y}}{\partial \underline{x}} = \underline{b} + 2\underline{Bx} \tag{2.10}$$

Setting equation (2.10) equal to zero and solving for $\underline{x}$ yields the stationary point

$$\underline{x}_0 = -\ 1/2B^{-1}\underline{b} \tag{2.11}$$

At this point one can easily predict the response at $\underline{x}_0$ by substituting equation (2.11) into equation (2.9)

$$\begin{aligned} \hat{y}_0 &= b_0 + \underline{x}_0'\underline{b} + \underline{x}_0'\underline{Bx}_0 && (2.12) \\ &= b_0 + (-1/2\underline{B}^{-1}\underline{b})' + (-1/2\underline{B}^{-1}\underline{b})'\underline{B}(-1/2\underline{B}^{-1}\underline{b}) \\ &= b_0 - 1/2\underline{b}'\underline{B}^{-1}\underline{b} + 1/4\underline{b}'\underline{B}^{-1}\underline{BB}^{-1}\underline{b} \\ &= b_0 - 1/2\underline{b}'\underline{B}^{-1}\underline{b} + 1/4\underline{b}'\underline{B}^{-1}\underline{b} \\ &= b_0 + 1/2\underline{x}_0'\underline{b} && (2.13) \end{aligned}$$

One sees that the stationary point can be either a maximum, minimum, or saddle point. To determine the nature of this point the experimenter may perform a canonical analysis, which is a method of not only determining the nature of the stationary point but certain general properties of the response surface.

The canonical analysis consists of a translation of coordinates from the original origin to the stationary point and then a rotation of the coordinates to correspond to the principal axes of the contour system. A new set of axes $\underline{z}$ is defined at the stationary point as

$$\underline{z} = \underline{x} - \underline{x}_0 \tag{2.14}$$

Substituting this into equation (2.9) one may redefine the response in terms of the new variable $\underline{z}$. It follows that

$$\begin{aligned} \hat{y} &= b_0 + (\underline{z}+\underline{x}_0)'\underline{b} + (\underline{z}+\underline{x}_0)'\underline{B}(\underline{z}+\underline{x}_0) \qquad (2.15) \\ &= b_0 + \underline{x}_0'\underline{b} + \underline{x}_0'\underline{Bx}_0 + \underline{z}'\underline{b} + \underline{z}'\underline{Bz} + \underline{x}_0'\underline{Bz} + \underline{z}'\underline{Bx}_0 \end{aligned}$$

Recognizing that the first three terms are $\hat{y}_0$ (equation (2.12)

$$\begin{aligned} \hat{y} &= \hat{y}_0 + 2\underline{z}'\underline{Bx}_0 + \underline{z}'\underline{Bz} + \underline{z}'\underline{b} \\ &= y_0 + \underline{z}'[\underline{b} + 2\underline{Bx}_0] + \underline{z}'\underline{Bz} \ . \end{aligned}$$

Substituting equation (2.11) for $\underline{x}_0$

$$\hat{y} = \hat{y}_0 + \underline{z}'\underline{Bz} \tag{2.16}$$

Thus equation (2.16) is the response at any point in the system in terms of the new set of variables $\underline{z}$. The second part of the canonical analysis rotates equation (2.16) to a new set of axes, say $\underline{w}$ corresponding to the principal axes of the contour system. The final form, which is called the canonical form, is

$$y = y_0 + \lambda_1 w_1{}^2 + \lambda_2 w_2{}^2 + \ldots + \lambda_k w_k{}^2 \tag{2.17}$$

where $\hat{y}_0$ is the estimated response from equation (2.13), w_i are the new translated and rotated axes, and the λ_i are constants which indicate the nature of the stationary point and the response surface.

It is well known that any real symmetric matrix, say $\underline{B}$, can be orthogonally transformed to a diagonal matrix, say $\underline{Q} = \underline{M}'\underline{BM}$. Here $\underline{M}$ is the orthogonal transformation matrix of $\underline{w}$ to $\underline{z}$ or

$$\underline{z} = \underline{Mw} \tag{2.18}$$

Thus

$$\begin{aligned} \underline{z}'\underline{Bz} &= \underline{w}'\underline{M}'\underline{BMw} \\ &= \sum_{i=1}^{k} \lambda_i w_i^2 \end{aligned} \tag{2.19}$$

Thus one may write

$$\underline{M}'\underline{BM} = \begin{bmatrix} \lambda_1 & & & & \\ & \lambda_2 & & 0 & \\ & & \cdot & & \\ & 0 & & \cdot & \\ & & & & \lambda_k \end{bmatrix} \tag{2.20}$$

where the λ_i's are the latent roots or eigenvalues of the matrix B. The eigenvalues determine the nature of the stationary point and the response surface. Several situations may be encountered:

(1) All λ_i are negative. This implies that the fitted surface is a maximum at the stationary point within the experimental region.

(2) All λ_i are positive. This implies that the fitted surface is a minimum at the stationary point within the experimental region.

(3) All λ_i are negative or all λ_i are positive and the stationary

point lies outside the region of experimentation. Polynomials are not trustworthy when extrapolated. In other words, inferences about results outside the area of experimentation are quite unreliable. Therefore, the experimenter can only continue investigating in the direction of the expected maximum or minimum in a cautious manner.

(4) Some λ_i are negative and some positive. This implies that the experimenter has found a saddle point.

(5) All λ_i are negative with magnitudes greatly different. For example, consider two variables where λ_1 is large and λ_2 close to zero. The situation is illustrated below.

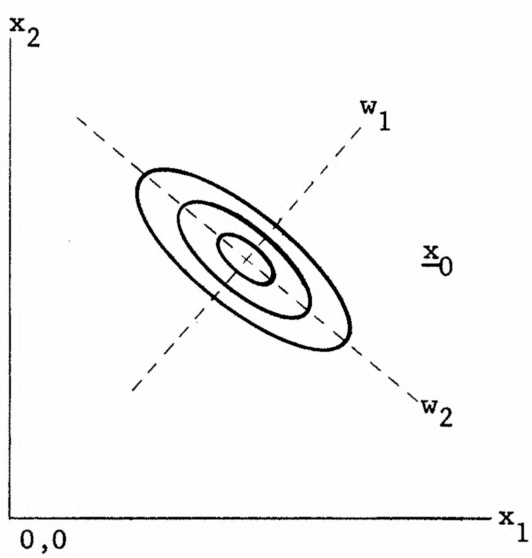


Figure 1. Illustration of Canonical Form in Two Variables (Maximum elongated along w_2 axis)

From situation (1) the experimenter knows that a maximum already exists, but from the difference in the λ_i he can determine the shape of the response surface in the experimental region. The λ_i tell him that the response is more sensitive along the w_1 axis than along the w_2 axis. The result is a ridge system along the w_2 axis.

2.4 Designs for the Second Order Model

2.4.1 General

Each independent variable x_i must take on at least three different levels to estimate the regression coefficients of a second order polynomial. This thesis attempts to investigate the efficiency and effectiveness of designs that fall in this class. There are numerous designs in this class, and only a representative cross section of them, including some of the more popular designs in use today, will be investigated.

If a polynomial relationship is to be investigated, an important part of the experiment is the choice of design matrix. The matrix

$$\underline{D} = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{k1} \\ x_{12} & x_{22} & \cdots & x_{k2} \\ \cdots & \cdots & \cdots & \cdots \\ x_{1n} & x_{2n} & \cdots & x_{kn} \end{bmatrix} \qquad (2.21)$$

indicates the combinations of levels chosen, and it is defined as the design matrix. Each row $(x_{1i}, x_{2i}, \ldots, x_{ki})$ represents one experimental run.

In what follows it becomes convenient to invoke the scaling convention

$$\sum_{u=1}^{N} x_{iu}^{2} = N \qquad (i=1,2, \ldots,k) \tag{2.22}$$

and

$$\sum_{u=1}^{N} x_{iu} = 0 \qquad (i=1,2, \ldots,k) \tag{2.23}$$

One could easily obtain a scaled design if the natural variables do not conform to this convention. Letting ξ_{iu} be the natural variable, the corresponding coded value would be

$$x_{iu} = \frac{\xi_{iu} - \bar{\xi}_i}{S_i} , \tag{2.24}$$

where $\bar{\xi}_i = \frac{1}{N} \sum_{u=1}^{N} \xi_i$;

and

$$S_i = \sqrt{\frac{\sum_{u=1}^{N} (\xi_{iu} - \bar{\xi}_i)^2}{N}} .$$

2.4.2 3^k Factorial Designs

As three different levels are required for x_{iu}, one immediately considers the use of the 3^k factorial design. Here the three levels of x are easily coded -1,0,1, and the second order polynomial may be fit very easily. One major disadvantage of this design is that, for a large number of independent variables, the experiment becomes too large. Box and Wilson (7) show that the 3^k factorial design provides estimates of quadratic coefficients having variances eight times greater than those for interaction coefficients. Geometrically, the design is shown in Figure 2 for the case k=2.

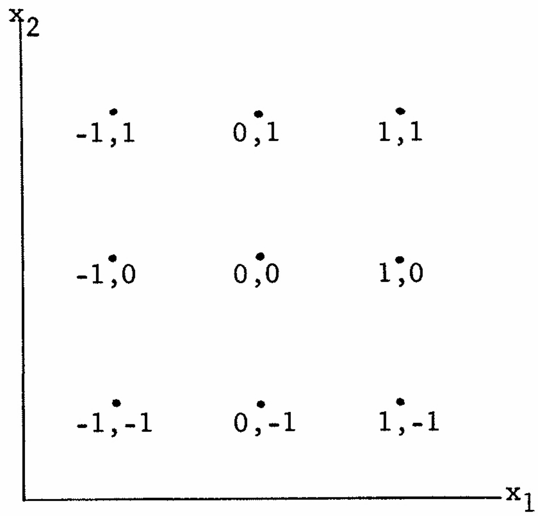


Figure 2. 3^2 Factorial Design

The 3^2 factorial design matrix is given by

$$\underline{D} = \begin{array}{c} \begin{array}{cc} x_1 & \quad x_2 \end{array} \\ \begin{bmatrix} -1 & -1 \\ -1 & 0 \\ -1 & 1 \\ 0 & -1 \\ 0 & 0 \\ 0 & 1 \\ 1 & -1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \end{array} \tag{2.25}$$

2.4.3 Central Composition Designs

2.4.3.1 General. Box and Wilson (7) developed this class of designs as alternatives to the 3^k factorial. Basically, the central composite design is a 2^k factorial augmented by at least one center point and 2k axial points. The design in two variables is shown in Figure 3.

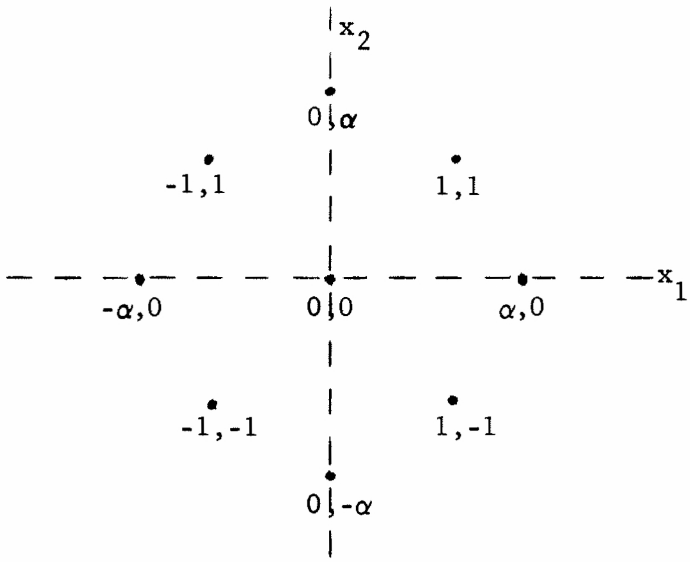


Figure 3. Central Composite Design

The design matrix for two variables, and considering only one center point is given by

$$\underline{D} = \begin{array}{c} \begin{array}{cc} x_1 & x_2 \end{array} \\ \left[\begin{array}{cc} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \\ \hdashline 0 & 0 \\ \hdashline -\alpha & 0 \\ \alpha & 0 \\ 0 & -\alpha \\ 0 & \alpha \end{array}\right] \end{array} \tag{2.26}$$

This design is widely used, as it may be derived easily from the 2^k. The method of steepest ascent often uses the 2^k design to estimate the parameters in the first order model. When lack-of-fit of the first order model becomes significant, all that is required to complete the central composite design is the addition of 2k axial points plus center points.

2.4.3.2 Rotatability. A very important property, one which will be used extensively in Chapter III, is that or rotatability. A design for which the variance of $\hat{y}$ is a function of distance from the design origin only and not direction is said to be rotatable. In other words, all points equidistant from the center of the experimental design have a common variance. Thus the variance contours for a rotatable design are circles or spheres centered at the origin.

2.4.3.3 Design Moments. An important concept that aids in developing concepts of rotatability and other properties is the design moment. Design moments are the elements of the moment matrix of the design, which is defined as $N^{-1}\underline{X}'\underline{X}$ where N is the total number of runs specified by the design. For example, the moment matrix of a second order design is given by

$$N^{-1}\underline{X}'\underline{X} = \begin{array}{c} \begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\ \begin{bmatrix} [1] & [1] & [2] & [11] & [22] & [12] \\ & [11] & [12] & [111] & [122] & [112] \\ & & [22] & [112] & [222] & [122] \\ & & & [1111] & [1122] & [1112] \\ & & & & [2222] & [1222] \\ & & & & & [1122] \end{bmatrix} \end{array} \qquad (2.27)$$

where

$$[i] = 1/N \sum_u x_{iu}$$

$$[ij] = 1/N \sum_u x_{iu} x_{ju}$$

$$[iiii] = 1/N \sum_u x_{iu}{}^4$$

$$[iiij] = 1/N \sum_u x_{iu}{}^3\ x_{ju}$$

$$[iijj] = 1/N \sum_u x_{iu}{}^2\ x_{ju}{}^2 \text{ , etc.}$$

The quantities [i], [ij], [iiij], and [iijj] are called first, second, third, and fourth order design moments. The elements of the moment matrix can be easily verified by obtaining the sums of squares and products of the appropriate $\underline{X}'\underline{X}$ matrix. The inverse of the moment matrix is called the precision matrix and contains elements which are related to the variances and covariances of the model coefficients.

Box and Hunter (6) show that a necessary and sufficient condition for a d^{th} order design to be rotatable is that the moments of order $\delta(\delta = 1,\ldots,2d)$ be of the form

$$N^{-1} \sum_{u=1}^{N} x_{1u}^{\delta 1}, x_{2u}^{\delta 2}, \ldots, x_{ku}^{\delta k} = \frac{\lambda_\delta \Pi_{i=1}^{k} \left(\delta_i \right)!}{2^{\delta/2} \Pi_{i=1}^{k} \left(\frac{\delta_i}{2} \right)!} \tag{2.28}$$

for all δ_i even, and

$$N^{-1} \sum_{u=1}^{N} x_{1u}^{\delta 1}, x_{2u}^{\delta 2}, \ldots, x_{ku}^{\delta k} = 0 \tag{2.29}$$

for ~~all~~ any δ_i odd. Here $\delta = \sum_{i=1}^{k} \delta_i$ and λ_δ is a quantity which is a function of δ. An excellent derivation of the above results can be found in Appendix A of Myers (23).

One may now construct a moment matrix for a second order rotatable design. Examining (2.27) it is obvious that [1] has δ_i odd. Therefore [1] = 0. [11], however, has a δ_i even and, therefore, $\delta = \sum_{i=1}^{k} \delta_i = 2$. From this $[11] = \frac{\lambda_2(2)!\ (0)!}{2(1)!\ (0)!} = \lambda_2$. [1111] represents an even δ_i where $\delta = 4$ and $[1111] = \frac{\lambda_4(4)!\ (0)!}{2^2(2)!\ (0)!} = 3\lambda_4$. The resulting moment matrix for a second order rotatable design is given by

$$N^{-1}(\underline{X}'\underline{X}) = \begin{array}{c} \begin{matrix} \cdot & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & \lambda_2 & \lambda_2 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_2 & 0 & 0 & 0 \\ \lambda_2 & 0 & 0 & 3\lambda_4 & \lambda_4 & 0 \\ \lambda_2 & 0 & 0 & \lambda_4 & 3\lambda_4 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_4 \end{bmatrix} \end{array} \tag{2.30}$$

Two key characteristics of this matrix are:

(i) All moments with at least one δ_i odd are zero

(ii) The ratio of the fourth pure moment to the fourth mixed moment is always 3.

Thus, if the moments of a second order design meet conditions (i) and (ii), the design is rotatable. Notice that, by definition $[iijj] = \lambda_4$. This gives the experimenter a great deal of flexibility in constructing designs, as λ_4 can be conveniently altered without affecting rotatability. This admits further properties of the central composite class of designs.

2.4.3.4 Rotatable Central Composite Designs. The previous section has shown that flexibility exists in choosing rotatable designs. One may find the value of α to make any central composite design rotatable. From inspection of the general form of $\underline{X}'\underline{X}$ one sees that, for a central composite design, all odd moments are zero, and also

$$\frac{[iiii]}{[iijj]} = 3 = \frac{\sum_{u=1}^{k} x_{iu}^4}{\sum_{u=1}^{k} x_{iu}^2 x_{ju}^2}$$

Letting F be the number of factorial points in a central composite design and referring to the general moment matrix, one sees that $\sum_{u=1}^{k} x_{iu}^4 = F + 2\alpha^4$ and that $\sum_{u=1}^{k} x_{iu}^2 x_{ju}^2 = F$. Therefore, $\frac{F + 2\alpha^4}{F}$ must equal 3 or

$$\alpha = (F)^{1/4} \tag{2.31}$$

Thus, α is completely independent of the number of center points. One may alter the value of λ_4 by adding or deleting center points without affecting rotatability.

At this point it is necessary to digress somewhat to gain insight on how changes in the value of λ_4, the mixed fourth moment [iijj], affect the properties of the fitted response surface for a rotatable design.

From the earlier discussion on the precision matrix, and considering the precision of $\hat{y}$, one can see that

$$\frac{N \operatorname{Var} \hat{y}}{\sigma^2} = \frac{N}{\sigma^2} \operatorname{Var} b_0 + \sum_{i=1}^{k} x_i^2 \operatorname{Var} b_i + \sum_{i=1}^{k} x_i^4 \operatorname{Var} b_{ii} \tag{2.32}$$

$$+ \sum_{\substack{i \; j \\ i<j}}\sum x_i^2 x_j^2 \operatorname{Var} b_{ij} + 2 \sum_{i=1}^{k} x_i^2 \operatorname{Cov}(b_0, b_{ii})$$

$$+ 2 \sum_{\substack{i \; j \\ i<j}}\sum x_i^2 x_j^2 \operatorname{Cov}(b_{ii}, b_{jj})$$

Myers (23) shows that the elements of the precision matrix (inverted moment matrix (equation (2.27))) are

$$\frac{N \operatorname{Var} b_0}{\sigma^2} = 2 \lambda_4^2 (k+2) A \tag{2.33}$$

where $A = \{2\lambda_4[(k+2)\lambda_4 - k]\}^{-1}$

$$\frac{N \operatorname{Var} (b_i)}{\sigma^2} = 1 \tag{2.34}$$

$$\frac{N \operatorname{Var} (b_{ii})}{\sigma^2} = [(k+1)\lambda_4 - (k-1)]A \tag{2.35}$$

$$\frac{N \operatorname{Var} (b_{ij})}{\sigma^2} = \frac{1}{\lambda_4} \qquad (i \neq j) \tag{2.36}$$

$$\frac{N\ \mathrm{Cov}\ (b_0, b_{ii})}{\sigma^2} = 2\lambda_4 A \tag{2.37}$$

$$\frac{N\ \mathrm{Cov}\ (b_{ii}, b_{ij})}{\sigma^2} = (1-\lambda_4)A \qquad (i \neq j) \tag{2.38}$$

All other elements are zero.

Two interesting observations can be made at this point.

(i) Examining equation (2.38) one sees that, if $\lambda_4 = 1$, Cov $(b_{ii}, b_{jj}) = 0$ and an orthogonal design results. So it is possible to construct a central composite design which is both rotatable and orthogonal.

(ii) If $\underline{X}'\underline{X}$ is singular, its determinant is zero; further, an A of infinity yields infinite variances and covariances and a useless design.

Now defining ρ as the distance from some point $(x_1, x_2, \ldots, x_k)$ to the center of the design, and since $\rho^4 = \sum_{i=1}^{k} x_i^4 + 2 \sum_{\substack{i \\ i<j}} \sum_{j} x_i^2 x_j^2$, one can apply the results of equations (2.33) through (2.38) to equation (2.32) to yield

$$\frac{N\ \mathrm{Var}\ \hat{y}}{\sigma^2} = A\ \{2\lambda_4^2(k+2) + 2\rho^2\lambda_4(\lambda_4-1)(k+2) + \rho^4[(k+1)\lambda_4 - (k-1)]\} \tag{2.39}$$

This equation will now be the basis to select from the class of rotatable second order designs that give desirable values of λ_4. Plotting $\sigma^2[N\ \mathrm{Var}\ \hat{y}]^{-1}$ for k=2 variables against ρ indicates, as shown in Figure 4, that basically the "best" precision is obtained at $\rho = 1$.

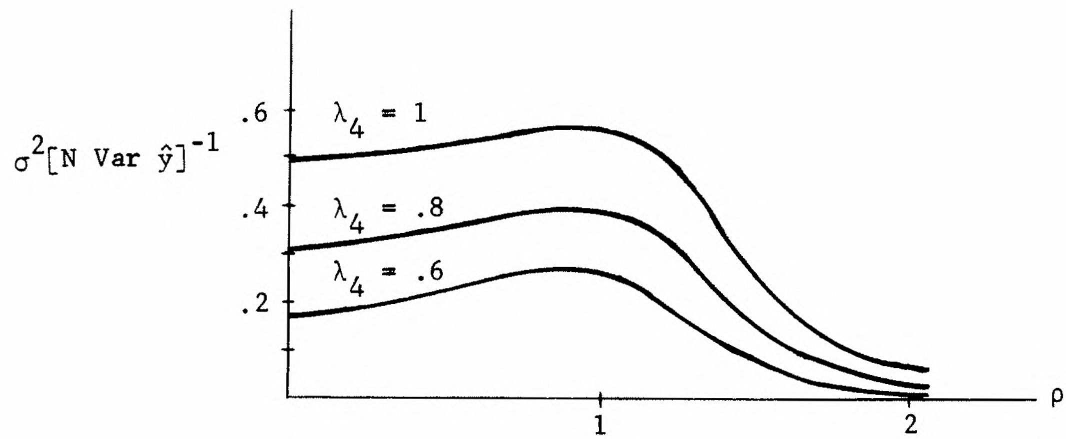


Figure 4. Design Precision Versus ρ

Notice also that small values of λ_4 lead to poor precision, especially near the design center. Also, large values of λ_4 lead to good precision near the center of the design whereas the precision drops off rapidly when $\rho > 1$. However, large values of λ_4 lead to heavy biasing of the regression coefficients if the surface happens to be greater than second order.

Box and Hunter (6) proposed a solution to this dilemma. They defined the uniform precision design to have a value of λ_4 such that the precision on $\hat{y}$ at the center ($\rho = 0$) is equal to the precision at $\rho = 1$. In other words

$$[N \text{ Var } \hat{y}]^{-1}_{\rho=0} = [N \text{ Var } \hat{y}]^{-1}_{\rho=1}$$

They based their design on the hypothesis that, in the region $\rho < 1$, there should be equal importance so far as estimation of response is concerned. Table 1 presents the values of λ_4 found by setting the variance function for $\rho = 1$ and then substituting for k.

Table 1. Values of λ_4 for Second Order Rotatable Designs Which Result in Uniform Precision

k	2	3	4	5
λ_4	.7844	.8385	.8704	.8918

In the specific case of the rotatable central composite design, one can achieve uniform precision by varying the number of center points. One may express λ_4 as a function of N, the total sample size, and F, the number of points in the factorial. Because of the scaling convention, each column in the design matrix must be multiplied by g, where

$$g = \sqrt{\frac{N}{F + 2\alpha^2}} \tag{2.40}$$

Now taking the fourth pure design moment and recalling that $\alpha = F^{1/4}$

$$[iiii] = \frac{Fg^4 + 2\alpha^4 g^4}{N} \tag{2.41}$$

After some algebra this reduces to

$$[iiii] = \frac{3N}{F + 4F^{1/2} + 4} \tag{2.42}$$

Now to complete the rotatability requirement

$$[iijj] = \lambda_4 = 1/3[iiii]$$

and

$$\lambda_4 = \frac{N}{F + 4F^{1/2} + 4} \qquad (2.43)$$

The property of rotatability is completely independent of λ_4. Table 2, created by Box and Hunter (6), serves to summarize the results of this section.

Table 2. Uniform Precision and Orthogonal Rotatable Central Composite Designs

k	2	3	4	5
F	4	8	16	32
n_a(axial points)	4	6	8	10
n_2 (UP)	5	6	7	10
n_2 (ORTH)	8	9	12	17
N(UP)	13	20	31	52
N (ORTH)	16	23	36	59
α	1.414	1.682	2.000	2.378
λ_4(UP)	0.81	0.86	0.86	0.89
λ_4 (ORTH)	1.00	0.99	1.00	1.01

2.4.3.5 Other Second Order Rotatable Designs for Small Values of k. The class of equiradial designs (designs at which all points are equidistant from the origin) offers practical alternatives to the central composite design for certain problems. This investigation will consider one of them, the hexagon.

A hexagon would have $n_1 = 6$ equally spaced points on a circle of radius ρ, augmented by n_2 center points. Meyers (23) shows that one may start by placing the first design point at an angle θ with the x_1 axis. The general form of the design matrix then becomes for $k = 2$

$$\underline{D} = \{\overset{x_1}{\rho\cos[\theta + (2\pi u)/n_1]},\ \overset{x_2}{\rho\sin[\theta + (2\pi u)/n_1]}\} \qquad (u=0,1,2,\ldots,n_1-1) \tag{2.44}$$

which leads to

$$\underline{D} = \begin{array}{cc} x_1 & x_2 \\ \end{array} \left[\begin{array}{ll} \rho\cos\theta & \rho\sin\theta \\ \rho\cos(\theta+\pi/3) & \rho\sin(\theta+\pi/3) \\ \rho\cos(\theta+2\pi/3) & \rho\sin(\theta+2\pi/3) \\ \rho\cos(\theta+\pi) & \rho\sin(\theta+\pi) \\ \rho\cos(\theta+4\pi/3) & \rho\sin(\theta+4\pi/3) \\ \rho\cos(\theta+5\pi/3) & \rho\sin(\theta+5\pi/3) \\ \cdots\cdots\cdots & \cdots\cdots\cdots \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{array}\right] \tag{2.45}$$

and the design is as shown in Figure 5. This design is rotatable as it satisfies the necessary and sufficient conditions stated previously. Other properties, such as uniform precision and orthogonality, are also applicable here.

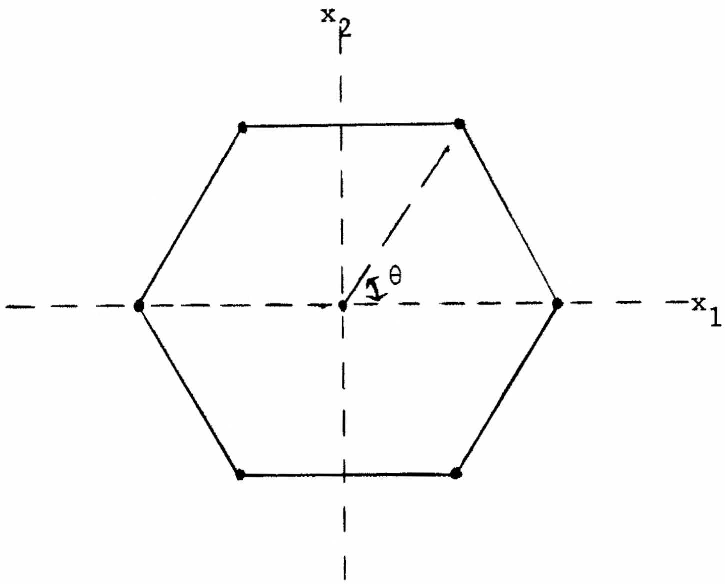


Figure 5. Hexagon Design

An expression for λ_4 can be obtained which again is independent of the factors affecting rotatability. In general

$$\lambda_4 = \frac{n_2 + n_1}{2n_1} \tag{2.46}$$

Therefore, if one chooses a specific equiradial design, he can change λ_4 easily by varying the number of center points. Table 3 gives information concerning some equiradial designs. It is obtained in the same manner as the data of Table 2. Many other equiradial designs are possible and such shapes as octagons, tetrahedrons, dodecahedrons, and icosohedrons are all feasible. Likewise, Box and Hunter (6) have also shown that interesting possibilities exist for certain combinations of equiradial rotatable designs.

Table 3. Orthogonal and Uniform Precision Equiradial Designs in Two Variables

n_1	5	6	7
n_2 ORTH)	5	6	7
n_2 (UP)	3	3	4
λ_4 (ORTH)	1.0	1.0	1.0
λ_4 (UP)	0.8	0.75	0.786

2.4.3.6 Other Criteria for Choosing Response Surface Designs. So far consideration has only been given to the variance of an estimated response $\hat{y}$, while the bias of $\hat{y}$ due to the inadequate representation of the polynomial has been almost ignored. It would seem desirable for a design to be chosen that would simultaneously consider both the variance of the predictor $\hat{y}$ and the bias of the regression coefficients. Box and Draper (3,4,5) proposed a solution to this problem by suggesting that a reasonable design would be one that minimized

$$J = \frac{N}{\sigma^2} \frac{\int_R E[\hat{y}(\underline{x}) - g(\underline{x})]^2 \, d\underline{x}}{\int_R d\underline{x}} \tag{2.47}$$

where $y(\underline{x})$ represents the fitted model and $g(\underline{x})$ the true model. It may be shown that

$$J = \frac{NK}{\sigma^2} \left\{ \int_R E[\hat{y} - E(\hat{y})]^2 \, d\underline{x} + \int_R [E(\hat{y}) - g]^2 \, d\underline{x} \right\} \tag{2.48}$$

where $K = \frac{1}{\int_R d\underline{x}}$. The first quantity on the right hand side of equation (2.48) is the variance averaged over the region R and the second quantity is the square of the bias averaged over the region R. Alternately, one may write

$$J = V + B \tag{2.49}$$

where V is the average variance of $\hat{y}$, and B is the average squared bias of $\hat{y}$.

Box and Draper suggested that some possible objectives would be to choose a design matrix that would

(i) minimize $J = V + B$

(ii) minimize V

(iii) minimize B.

It may be shown that it is impossible to minimize $J = V + B$. Thus one must consider (ii) and (iii). Myers (23) shows that, for the first order model

$$J = \left\{1 + \frac{1}{3[11]}\right\} + \frac{N\beta_{11}^2}{\sigma^2}\left\{([11] - 1/3)^2 + 4/45\right\} \tag{2.50}$$

Here the second moment occurs in both V and B and thus the value of [11] which minimizes J depends on the quadratic coefficient β_{11}. Therefore, with no prior knowledge of β_{11}, $J = V + B$ cannot be minimized. Now from equation (2.50) one sees that

(i) If bias is expected to be negligible in comparison to error variance resulting in a small value for $\frac{N\beta_{11}^2}{\sigma^2}$, one should minimize V by making [11] as large as possible. This is accomplished by spreading the design points out as far as practically possible. Unfortunately, if β_{11} is not zero, a large value of [11] results in a heavy bias contribution. Thus, to use a large second moment, one must be sure that the system is of order d with no order d+1 contribution.

(ii) If one is to consider minimizing bias in $\hat{y}$, the second term or B should be minimized. From equation (2.50) the required second moment is [11] = 1/3. Box and Draper show that the best experimental approach is to choose the design which protects against bias, or an all-bias design, and to use this design unless bias is <u>very</u> unlikely. In fact, they show that only if V, the variance contribution, is greater than six times B, the bias contribution, is there any apparent significant increase in J over the minimum value used for the all-bias design.

A central composite design will be used which is from the class of all-bias designs. The design will resemble equation (2.26).

CHAPTER III

EXPERIMENTAL DEVELOPMENT: SURFACE AND DESIGNS

3.1 The Work of Brooks in Comparing Maximum-Seeking Methods

Brooks, in his doctoral dissertation and a later article (8), conducted a simulation study to compare the performance of various first order experimental optimization methods. He constructed four two-variable surfaces, each with a well-defined maximum. Each surface was chosen to describe and represent functions that are suspected to occur often in practice. Their contours will be presented later.

Factorial designs, one-factor-at-a-time procedures, methods of steepest ascent, and random experimentation were compared for seeking maxima by trying versions of these techniques in several two-factor situations, with and without experimental error. The factorial method is characterized by the use of a single factorial design, either fractional, complete, or replicated. The one-factor-at-a-time procedure may be regarded as the exploration of the response surface by optimizing the response for one of the k factors while holding the remaining $k-1$ constant. This process is repeated until all factors have been tried at least once with no further improvement in response. In the method of steepest ascent, the course of experimentation is directed by the sequentially determined estimates of the gradient direction. In the random method, trials are made at randomly selected points in the factor space.

For each surface investigated, nine different starting positions were tried. Two series of experiments were run, the first in which 16 trials were allotted to locate the optimum and the second in which 30 were allotted.

The performance of each method was judged by the true response $\phi(x_1,x_2)$ at the (near) optimum values of x_1 and x_2 as found by each method. He concluded that:

1. The all-around reliability of the method of steepest ascent was suggested.

2. The factorial method is inferior to sequential methods.

3. Random methods are clearly the worst for a small number of factors. For a very large number of factors, random methods may be of some benefit.

4. The univariate method performed in an average manner. Brooks terminated his study at this point and did not investigate further the region around the stationary point. His results were good, but could have been better had he carried out a phase II investigation. Further, a more accurate description of the nature of the surface would have been given. Two examples of the improvements achieved through phase II investigation are shown in Appendix A.

3.2 The Response Surfaces

The four surfaces of Brooks will be used in this study. The experimental region of each surface contains a single maximum $y = 1$ at $x_1 = 1$ and $x_2 = 1$. Figures 6(a) through 6(d) show the three contour lines

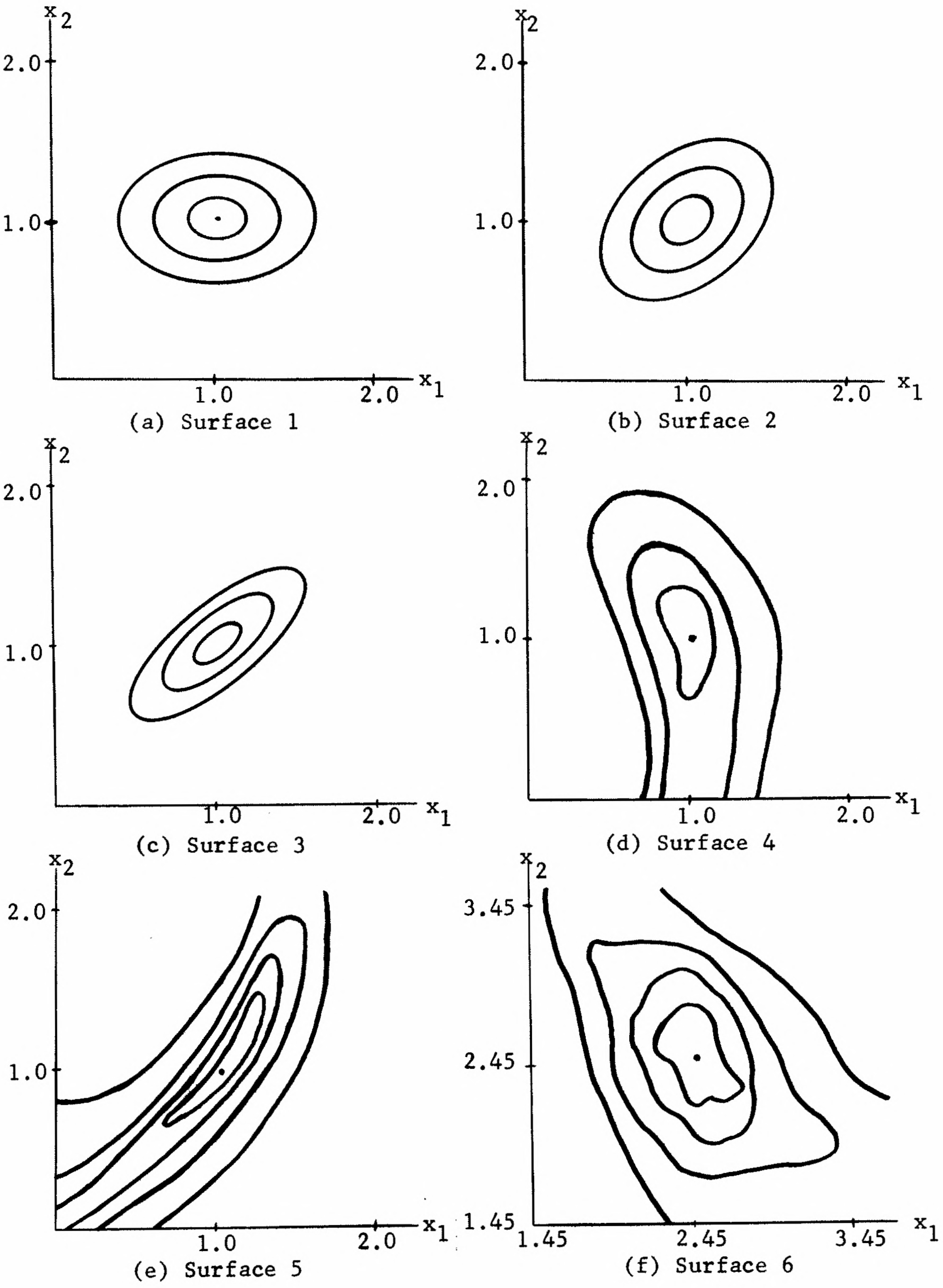


Figure 6. Response Surfaces

$y = 0.25$, 0.50, and 0.75 for these surfaces. In addition to these four surfaces, two others were considered, the first being a modification of Rosenbrock's curved valley and the second, a surface developed from an inverse polynomial function. Rosenbrock's curved valley has been modified so that a maximum of $y = 0$ is achieved at $x_1 = 1$ and $x_2 = 1$. Figure 6(e) shows the contour lines $y = -8, -4, -1$, and -0.5. Figure 6(f), developed from an inverse polynomial function, shows the contour lines $y = 4.15$, 4.05, 3.85, and 3.75. The surface has a maximum response of $y = 4.173749909$ at $x_1 = 2.4475$ and $x_2 = 3.8875$.

3.2.1 Surface 1

$y = (0.5 + 0.5x_1)^4 x_2^4 \exp[2 - (0.5 + 0.5x_1)^4 - x_2^4] + \varepsilon$. In this response surface the relative effect of one factor is independent of the level of the other factor.

3.2.2 Surface 2

$y = (0.3 + 0.4x_1 + 0.3x_2)^4(0.8 - 0.6x_1 + 0.8x_2)^4 \exp[2 - (0.3 + 0.4x_1 + 0.3x_2)^4 - (0.8 - 0.6x_1 + 0.8x_2)^4] + \varepsilon$. This response surface is the same as Surface 1 rotated approximately 37 degrees, as would occur if x_1 and x_2 were not independent.

3.2.3 Surface 3

$y = x_1^2 \exp[1 - x_1^2 - 20.25(x_1 - x_2)^2] + \varepsilon$. This response surface is a sharp narrow ridge with large flat areas of low response.

3.2.4 Surface 4

$y = (0.3x_1^2 + 0.7x_2^2)^3 \exp[1 - 0.6(x_1 - x_2)^2 - (0.3x_1^2 + 0.7x_2^2)^3] + \varepsilon$. This response surface is a relatively flat curvilinear ridge.

3.2.5 Surface 5

$y = -[100(x_2 - x_1^2)^2 + (1 - x_1)^2 + \epsilon]$. This response is a fairly steep curved ridge.

3.2.6 Surface 6

$y = [(x_1x_2)/(.9 + .066x_1 - .001x_2 - .01x_1^2 + .03x_2^2 + .005x_1x_2 + .01x_1^2x_2 - .017x_1x_2^2 + .013x_1^2x_2^2)] + \epsilon$. This response surface is a low, bumpy, irregular surface.

3.3 Comparisons Between Designs

Any second order design can be systematically compared with another second order design on the basis of the precision with which the designs allow estimates of the model coefficients. For such comparisons to be valid, the two designs must be scaled so that their "spreads" are equal, the measure of spread being $\sum_u x_{iu}^2/N$, the pure second moment of the design.

As an example, the design matrix of the 3^2 factorial is

$$\underline{D} = \begin{array}{cc} x_1 & x_2 \end{array} \atop \begin{bmatrix} -1 & -1 \\ -1 & 0 \\ -1 & 1 \\ 0 & -1 \\ 0 & 0 \\ 0 & 1 \\ 1 & -1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \tag{3.1}$$

It can be seen that, for this design, $\sum_u x_{iu}^2/N = 2/3$. Now referring to equation (2.26) and Table 2, the scaled design matrix for an orthogonal, rotatable central composite design should be

$$\underline{D} = \begin{array}{cc} x_1 & x_2 \\ \left[\begin{array}{cc} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \\ \cdots & \cdots \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \cdots & \cdots \\ -1.414 & 0 \\ 1.414 & 0 \\ 0 & -1.414 \\ 0 & 1.414 \end{array}\right] \end{array} \tag{3.2}$$

In this case $\sum_u x_{iu}^2/N = 1/2$, which is not equal to the second pure moment of the 3^2 factorial design. If both designs were subsequently used to analyze a specific response surface, invalid comparisons would result. Therefore, it is necessary to rescale the elements of the design matrix for the orthogonal central composite design so that $\sum_u x_{iu}^2/N = 2/3$. The moment $\sum_u x_{iu}^2/N = 2/3$ will be used as a standard for all designs. This results in a new design matrix

$$
\underline{D} = \begin{array}{c} \begin{array}{cc} x_1 & \qquad\qquad x_2 \end{array} \\ \left[\begin{array}{cc} -1.15 & -1.15 \\ -1.15 & 1.15 \\ 1.15 & -1.15 \\ 1.15 & 1.15 \\ \hdashline 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \hdashline -1.63 & 0 \\ 1.63 & 0 \\ 0 & -1.63 \\ 0 & 1.63 \end{array}\right] \end{array} \tag{3.3}
$$

The design matrix for the uniform precision central composite design is

$$
\underline{D} = \begin{array}{c} \begin{array}{cc} x_1 & \qquad\qquad x_2 \end{array} \\ \left[\begin{array}{cc} -1.04 & -1.04 \\ -1.04 & 1.04 \\ 1.04 & -1.04 \\ 1.04 & 1.04 \\ \hdashline 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \hdashline -1.47 & 0 \\ 1.47 & 0 \\ 0 & -1.47 \\ 0 & 1.47 \end{array}\right] \end{array} \tag{3.4}
$$

The design matrix for the minimum bias design is

$$\underline{D} = \begin{array}{cc} x_1 & x_2 \\ \left[\begin{array}{cc} -.99 & -.99 \\ -.99 & .99 \\ .99 & -.99 \\ .99 & .99 \\ \cdots & \cdots \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \cdots & \cdots \\ -1.40 & 0 \\ 1.40 & 0 \\ 0 & -1.40 \\ 0 & 1.40 \end{array}\right] \end{array} \qquad (3.5)$$

The design matrix for the orthogonal hexagonal design is

$$\underline{D} = \begin{array}{cc} x_1 & x_2 \\ \left[\begin{array}{cc} 1.56 & 0 \\ .78 & 1.35 \\ -.78 & 1.35 \\ -1.56 & 0 \\ -.78 & -1.35 \\ .78 & -1.35 \\ \cdots & \cdots \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{array}\right] \end{array} \qquad (3.6)$$

The design matrix for the uniform precision hexagonal design is

$$\begin{array}{cc} x_1 & x_2 \end{array}$$

$$\underline{D} = \begin{bmatrix} 1.41 & 0 \\ .71 & 1.22 \\ -.71 & 1.22 \\ -1.41 & 0 \\ -.71 & -1.22 \\ .71 & -1.22 \\ \hdashline 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{3.7}$$

In applying these designs to the six surfaces, the coding

$$x_i(\text{surface}) = \frac{x_i(\text{design})}{5}$$

is used, and the origin of the design ($\underline{x} = \underline{0}$ on the design matrix) may be any arbitrary point on the surface.

The second design parameter considered in this study is ρ, the distance from the true optimum to the design center. For response surfaces 3 and 5, $\rho = 1.1$ and, for the remaining surfaces, $\rho = 1.18$. Every design examined on each surface has a constant ρ. It is important to note that, for all designs, ρ is chosen to insure that the optimal factor combination lies within the limits of the respective design.

3.4 The Computer Program

Because of the many similar subroutines, the complete computer program listing will not be presented. Appendix B contains a listing of the main program and one of the six major experimental design subroutines. A general flow chart is depicted in Figure 7. Basically, the computer pro-

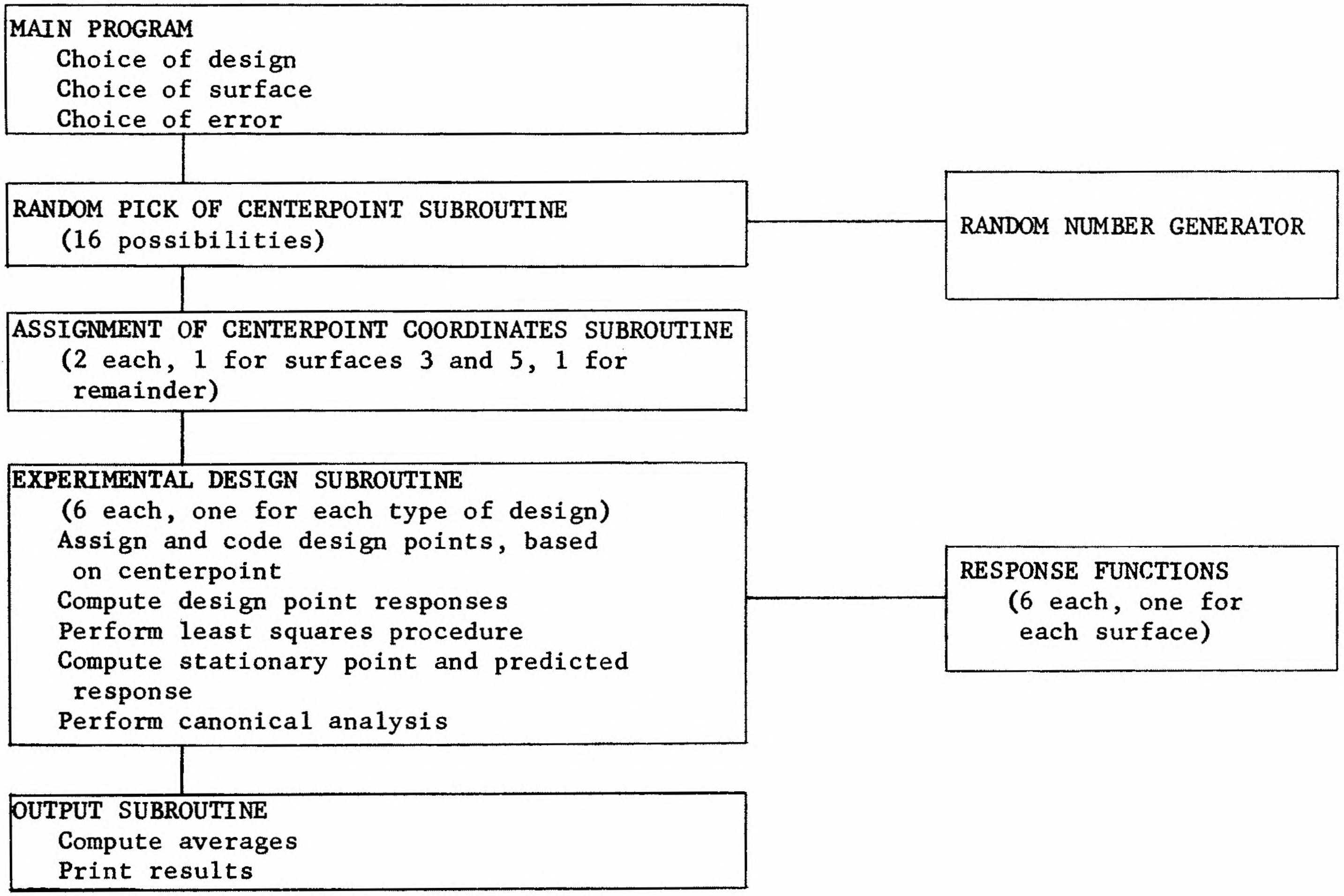


Figure 7. Generalized Flow Chart of Computer Program

gram consisted of a main program, seven functions, and ten subroutines.

3.4.1 Main Program

This segment of the program serves to drive the experiment and input necessary data. Three main variables are varied per run; the surface, the design, and the magnitude of the error. The other input data consist of a table of normal deviates used to compute the error term of the response functions.

3.4.2 Random Choice of Center Point and Assignment of Center Point Coordinate Subroutines

Recall the earlier discussion of ρ, the distance from the true optimum to the design center point. If one is to agree with the first assumption discussed in the introduction, which was that the experimenter has already encountered a near optimal region in which a "lack of fit" situation exists, some method must be used to provide a starting point or a design center. The method utilized in this study was to choose a value of ρ, circumscribe an arc of radius ρ around the known optimum, and randomly assign starting points along this arc. Sixteen possible starting points were chosen per arc. In order to choose a value for ρ, an average was taken of the near optimal responses using the method of steepest ascent. This average was then transformed into an average linear deviation of the predicted optimum from the true optimum. In other words, taking Surface 1 as an example, it is assumed that, on the average, the method of steepest ascent will get the experimenter within .18 scaled units of the optimum.

3.4.3 Response Functions

This is a set of six functions, one for each surface described. In addition, it was decided to vary the standard deviation of the experimental error from 0.00 to 0.15. The relatively high values of the error standard deviation were employed because digital computer simulations often exhibit considerable random variation in their output statistics.

3.4.4 Experimental Design Subroutines

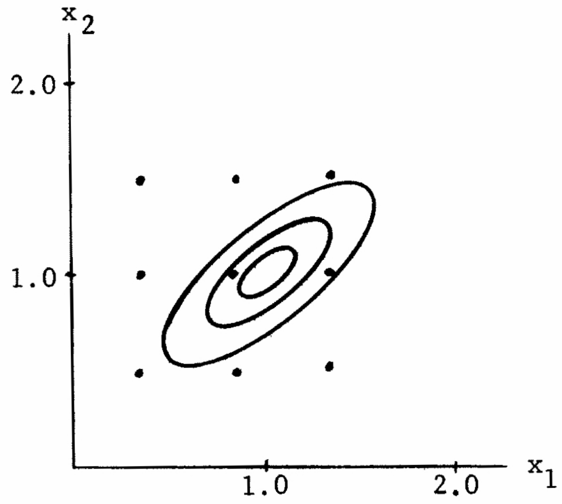
This is a set of six subroutines designed to investigate each experimental design on all surfaces. As shown in the flow chart, it assigns and codes design points, computes responses, performs least squares estimation, computes the stationary point and predicted response, and performs a canonical analysis thirty times for each design on each surface varying the error standard deviation from 0.00 to 0.15 in steps of 0.03.

3.4.5 Output Subroutine

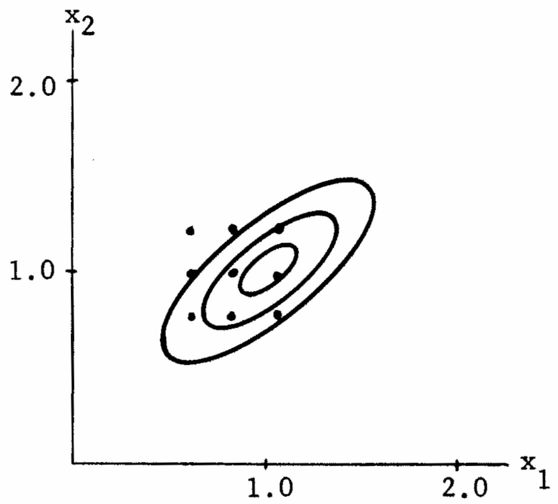
This section takes the results of the previous experimental designs, stores them, computes averages, and prints the results.

3.5 Problems Encountered

This discussion would not be complete without briefly discussing a major potential problem area encountered when using response surface techniques. It was observed that the choice of levels used in phase I investigation was important. This problem is also present in phase II investigation in the choice of "spread," or second moment of the design. The nature of the problem can best be demonstrated by an example. Consider two 3^2 factorial designs superimposed on the same surface (Surface 3), shown in Figure 8.



(a) Distance between design points = .5 units



(b) Distance between design points = .2 units

Figure 8. 3^2 Factorial Design with Varying Spread

Obviously, different results will occur for each design.

The stationary point $\underline{x}_0$ will probably be quite different for each design. This problem was avoided in this study as only designs having the same second moment were compared. However, this is a major problem area when working with these techniques in practice. The best solution to this issue is experience with the model under study so far as the choice of scale of variables is concerned. The surfaces discussed in this investigation are artificial. For example, the first four were constructed to cover 2 units on the x_1 and x_2 axes, to vary the response from 0 to 1, and to have a maximum at $x_1 = 1$, $x_2 = 1$. The factors and response have no physical meaning, they are merely numbers. In practical situations one would be dealing with such variables as time, temperature, distance, etc. Thus, the variables and response have physical significance to the experimenter, and the choice of an appropriate scale of measurement is simplified.

CHAPTER IV

EXPERIMENTAL RESULTS

4.1 Measures of Effectiveness

This investigation utilizes two measures of effectiveness of a second order experimental design. In comparing maximum-seeking methods, Brooks (8) proposed that the measure of effectiveness of an optimization method in any given situation be the magnitude of the response at the estimate of the optimal factor combination that resulted from applying that particular method. In this study this will be a comparison of the respective responses achieved for each combination of surface/design/error, on the basis of the average "response achievement" of each method. Defining y_0 as the achieved response and y_* as the true response, then the response achievement, say R, is

$$R = \frac{y_0}{y_*} \tag{4.1}$$

The second criteria used will be the linear distance from the stationary point (the predicted optimum levels for the independent variables) to the true optimum levels of the independent variables. Defining x_{i0} as the stationary point, x_{i*} as the true optimal factor combination, and L as the distance, then

$$L = (x_{10} - x_{1*})^2 + (x_{20} - x_{2*})^2 \tag{4.2}$$

when k = 2.

In examining the experimental results, each measure will be analyzed from two points of view; first, comparison by design and second, comparison by surface. Thus, one will be able to observe the conclusions and apply them to constructing designs in general or designs for specific surfaces.

4.2 Experimental Results by Design

In this section, the results obtained will be described on a design basis. The objectives of this section will be to give insight to the experimenter in choosing an efficient second order experimental design irregardless of surface.

Table 4 shows the average response achievement by design for all surfaces (R).

Table 5 shows the average distances from the optimal factor combinations to the predicted factor combinations by design for all surfaces (L). For each design and error standard deviation thirty replications were performed on each surface. The design center was 0.18 units from the optimal factor combination for all surfaces, except for Surfaces 3 and 5, where it was 0.11.

4.2.1 3^2 Factorial Design

Figure 2 describes the geometric configuration for this design. In the design matrix used on each surface (equation (2.21)) the scaled value of "1" is equal to "0.2" surface units.

Because it was the simplest design tested, the 3^2 factorial was chosen as the standard with regard to the second moment [ii] (see section

Table 4. Average Response Achievements (R) and Standard Errors (S) by Design for All Surfaces

Design	$\sigma\varepsilon$	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2 Factorial	R	.9489	.8772	.8057	.7677	.7357	.7051	.8067
	S	.0576	.0659	.0916	.1107	.1259	.1262	.0963
Orthogonal CCD	R	.9792	.9228	.9043	.8694	.8191	.7451	.8733
	S	.0406	.0901	.0815	.0648	.0656	.0971	.0733
Uniform Precision CCD	R	.9692	.9572	.9089	.8660	.8185	.7949	.8858
	S	.0194	.0181	.0489	.0718	.1003	.1055	.0607
Minimum Bias CCD	R	.9755	.9580	.9335	.8769	.8347	.7943	.8955
	S	.0234	.0349	.0191	.0309	.0449	.0572	.0351
Orthogonal Hexagon	R	.9814	.9744	.9394	.9092	.8627	.8229	.9150
	S	.0214	.0197	.0432	.0496	.0471	.0316	.0354
Uniform Precision Hexagon	R	.9762	.9310	.8585	.7890	.7448	.6699	.8282
	S	.0226	.0507	.0248	.0640	.0944	.0776	.0557

Note: All designs except 3^2 are rotatable.

Table 5. Average Distance Achievements (L) and Standard Errors (S) by Design for All Surfaces

Design	$\sigma\epsilon$	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2 Factorial	L	.0290	.1024	.1082	.1169	.1873	.2108	.1258
	S	.0345	.1436	.0529	.1228	.2531	.2456	.1421
Orthogonal CCD	L	.0105	.0343	.0517	.0828	.1128	.1065	.0664
	S	.0079	.0435	.0502	.0828	.1128	.1065	.0664
Uniform Precision CCD	L	.0319	.0404	.0613	.0778	.0935	.1186	.0706
	S	.0159	.0185	.0523	.0569	.0764	.0796	.0499
Minimum Bias CCD	L	.0151	.0368	.0290	.0467	.0909	.0982	.0450
	S	.0146	.0391	.0330	.0512	.0729	.0559	.0445
Orthogonal Hexagon	L	.0153	.0226	.0537	.0589	.0697	.0901	.0517
	S	.0129	.0178	.0696	.0752	.0295	.0621	.0445
Uniform Precision Hexagon	L	.0194	.0239	.0558	.0912	.1243	.1819	.0828
	S	.0158	.0172	.0272	.0588	.0809	.1075	.0512

Note: All designs except 3^2 are rotatable.

3.4). In other words, the 3^2 factorial design was used with values of -1,0,+1, the second moment recorded, and then all other designs subsequently rescaled to adhere to this convention.

As a whole, the 3^2 factorial design showed achievement averages lower than all other designs. An exception will be found in the discussion of Surface 5 (see section 4.3.5). Average distance from the true optimal level of factor combinations turned out to be higher than all other designs. Standard errors for this design were also generally larger.

An interesting point to be made here is that, for two independent variables, the 3^2 factorial design is equivalent to a 2^2 design augmented by four axial points, a distance of "1" from the design center and one center point. By definition this is a central composite design with $\alpha = 1$. (Recall that in section 2.4.3.4, equation (2.27) required that $\alpha = F^{1/4}$. Applying this $\alpha = 4^{1/4} = \sqrt{2}$, so here the design is not rotatable.) Therefore the 3^2 factorial design is the same as a nonrotatable central composite design. This fact will become important later when commenting on the effect and desirability of the property of rotatability.

4.2.2 Central Composite Designs (Orthogonal, Uniform Precision, and Minimum Bias)

Figure 3 describes the design point configuration for these designs. In the design matrices, equations (3.3), (3.4), and (3.5), the ± 1 factors and α had to be scaled accordingly in order that the second pure moment $[ii] = 2/3$. The difference between these designs and the 3^2 factorial is that design points were added at the center to achieve orthogonality, uniform precision, or minimum bias.

As a class, the central composite designs showed a good average achievement with the minimum bias design giving the best average in all but the "no-error" case. The next best design was the uniform precision which was better than the orthogonal in all but two error cases. The orthogonal design generally revealed the lowest averages except in the case of "no-error" where it performed best.

The average distance measure of effectiveness demonstrated about the same results. Overall, the minimum bias design showed the smallest distance except for the orthogonal design with no error which again gave the best results of the entire class. In this case, the orthogonal design performed a little better in lower error situations and the uniform precision a little better in higher error situations

4.2.3 Hexagon Designs (Orthogonal and Uniform Precision)

Figure 5 describes the design configuration for these designs. Again the design matrices (equations (3.6) and (3.7)) had to be scaled to the second pure moment standard. A big difference between these designs and those of the central composite class is that the hexagon designs attempt to investigate the same situation, but they use fewer design points. For orthogonality, the hexagon design requires 11 total points compared to 16 for the central composite design. For uniform precision the ratio is 9 to 13. This could be an important economic criterion if the performance of the hexagon design is acceptable.

The two hexagon designs, on the average, performed similarly to the central composite designs when examining their average response achievement. Considered individually, the orthogonal design had much higher averages than the uniform precision design. The orthogonal design provided very good results for all values of experimental error, but the uniform precision design, after starting out well with little or no error, began to drop off significantly. The same comments can be made for the average distance criterion. The significant increase in distance from the optimum can be observed as the error increases.

4.2.4 Comparison of Results for All Designs

Overall, one cannot help but be impressed with the performance of the Orthogonal Hexagon Design. The results of its achievements are better in all average situations than any other design examined. The minimum bias design also performed quite well. The 3^2 factorial design and the uniform precision hexagon design, in situations of large experimental error, were definitely poorer in performances than the other designs.

4.3 Experimental Results by Surface

In this section each design will be investigated on each surface to determine its effectiveness. The objective of the section will be to give insight to the experimenter in choosing an efficient second order experimental design when he has a priori knowledge of the shape of the surface.

4.3.1 Surface 1

Figure 6(a) describes this surface as a symmetric surface on which the relative effect of one factor is independent of the level of the other factor. Table 6 shows the average response achievements for each design.

This being a simple, symmetric (along the x_1,x_2 axes) surface, it would seem almost intuitive that all designs would perform well. This is

Table 6. Surface 1 Average Response Achievement (R)

Design $\sigma\varepsilon$	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2 Factorial	.9752	.9129	.8003	.7635	.7557	.7451	.8255
Orthogonal CCD	.9948	.9913	.9755	.9168	.8345	.7492	.9104
Uniform Precision CCD	.9717	.9647	.9284	.8744	.7903	.7524	.8803
Minimum Bias CCD	.9887	.9768	.9462	.8564	.8201	.7701	.8931
Orthogonal Hexagon	.9939	.9879	.9765	.9557	.9140	.8574	.9476
Uniform Precision Hexagon	.9892	.9628	.8648	.7447	.6249	.5683	.7725

true for all cases except the 3^2 factorial and the uniform precision whose response achievements drop significantly as the experimental error increases. The orthogonal hexagonal design reveals the best average achievement in all error situations. It is followed by the orthogonal central composite design and the minimum bias design.

Figure 9 depicts the distance of the estimated optimal factor combination from the true optimal factor combination for surface 1. The smallest distances overall come from the orthogonal hexagonal, orthogonal central composite, and minimum bias designs respectively which agree with the results of the first measure of effectiveness.

4.3.2 Surface 2

Figure 6(b) describes this surface as a rotated Surface 1. Table 7

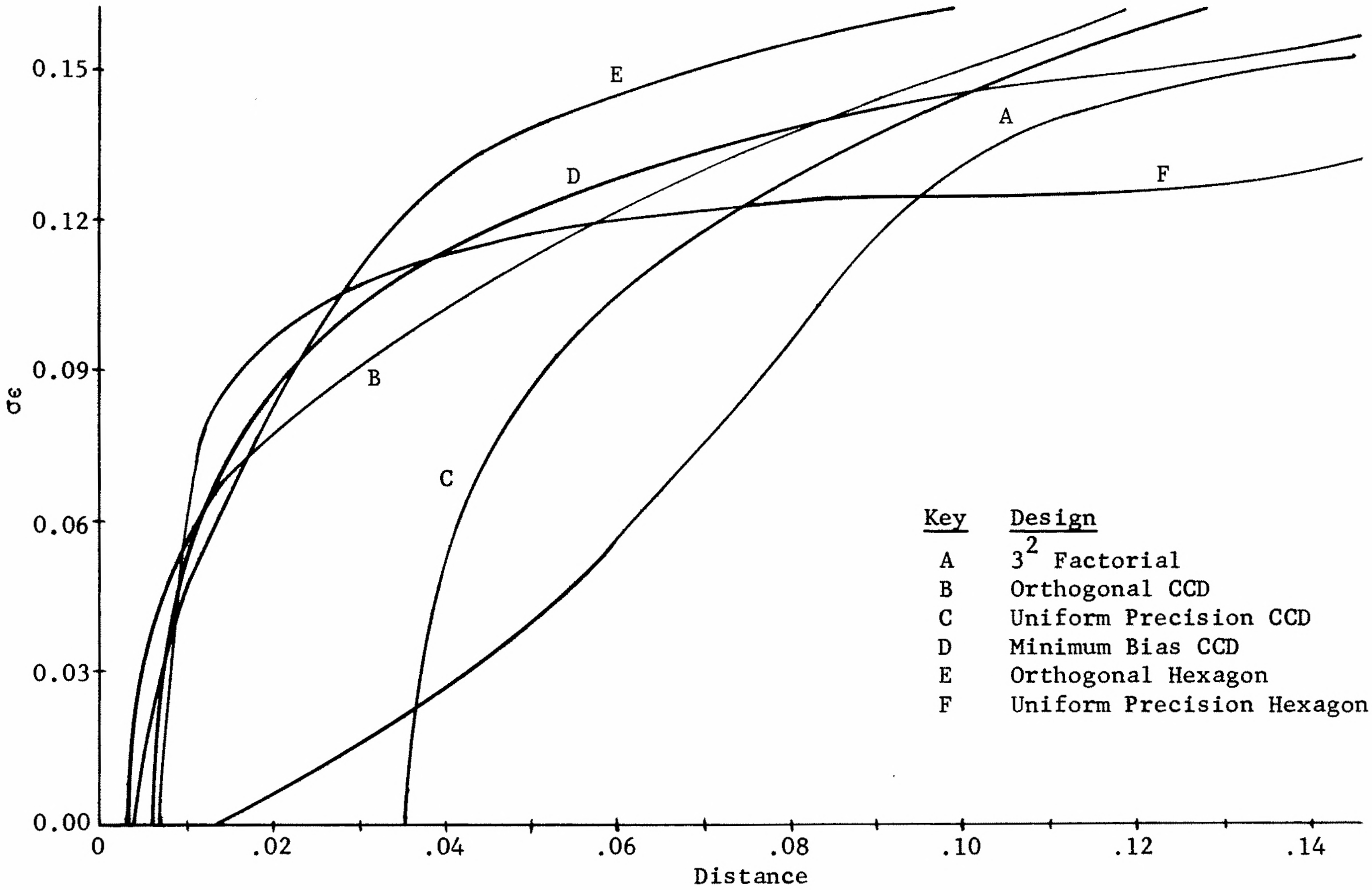


Figure 9. Surface 1 Distance from True Optimum (L)

shows the average response achievements for each design.

Table 7. Surface 2 Average Response Achievement (R)

Design $\sigma\epsilon$	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2Factorial	.9781	.9312	.8163	.7296	.7008	.6642	.8034
Orthogonal CCD	.9947	.9885	.9675	.9005	.7875	.6520	.8818
Uniform Precision CCD	.9577	.9487	.8861	.8484	.7703	.7462	.8596
Minimum Bias CCD	.9878	.9752	.9395	.8623	.8022	.7475	.8858
Orthogonal Hexagon	.9919	.9861	.9729	.9464	.8855	.8406	.9372
Uniform Precision Hexagon	.9870	.9583	.8441	.7277	.6808	.6126	.8018

As Surface 2 is similar to Surface 1 except for rotation; one would expect results to be similar to the results achieved in Surface 1 experiments, especially for the rotatable designs. Obviously, as observed in the above table this is so. The only appreciable difference occurs in the 3^2 factorial design which, as shown earlier, is the same as a nonrotatable central composite design. Similar results are demonstrated by the second measure of effectiveness as shown in Figure 10.

4.3.3 Surface 3

Figure 6(c) depicts this surface as a sharp narrow ridge. A lack-of-fit test on the quadratic polynomial indicated a cubic or higher order

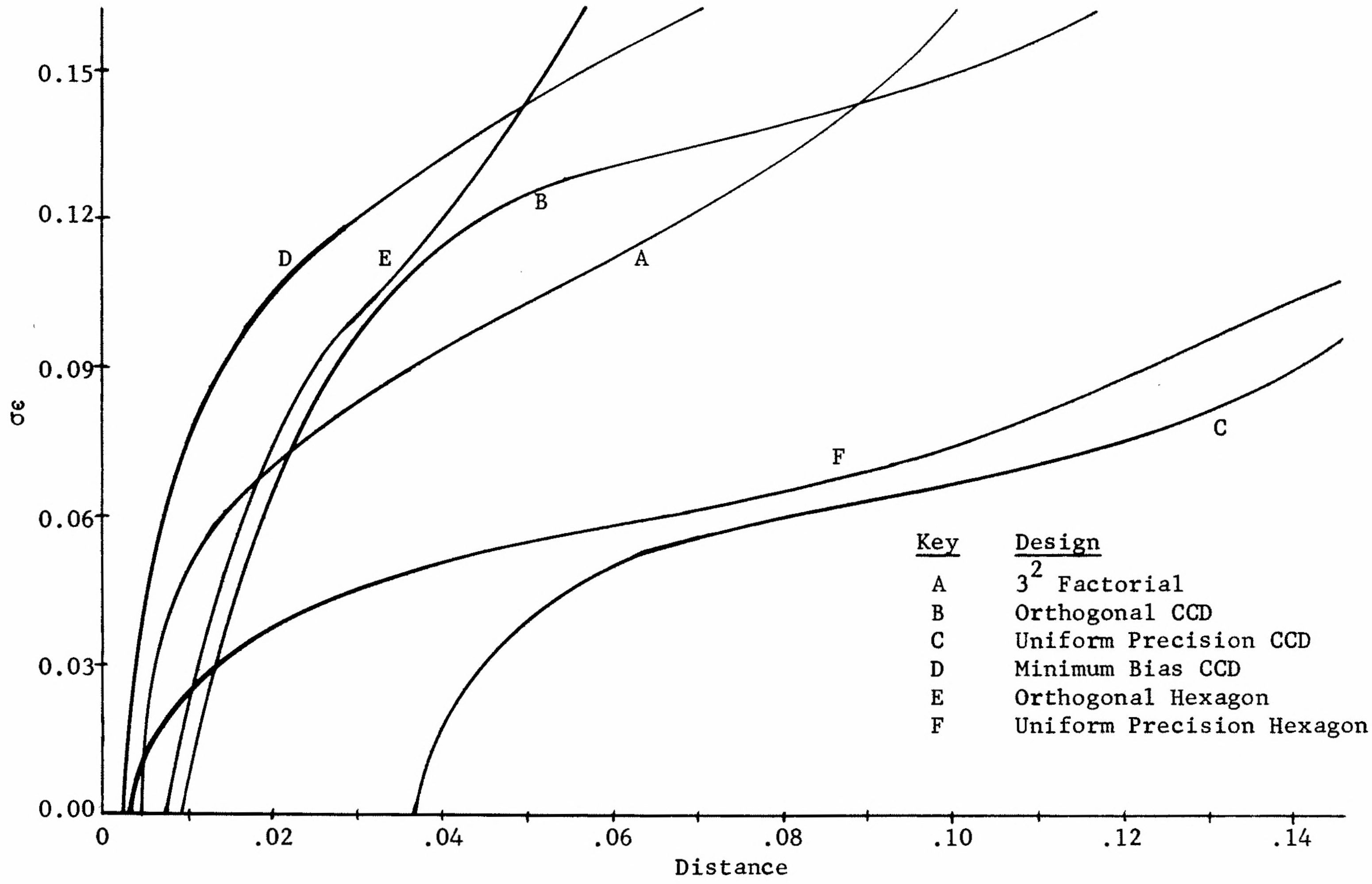


Figure 10. Surface 2 Distance from True Optimum (L)

surface. Table 8 shows the average response achievements for each design.

Table 8. Surface 3 Average Response Achievement (R)

Design $\quad\sigma_\epsilon$	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2 Factorial	.9443	.8879	.8797	.8764	.8405	.7812	.8683
Orthogonal CCD	.9261	.9205	.9199	.9183	.9171	.8822	.9140
Uniform Precision CCD	.9588	.9554	.9527	.9482	.9427	.9116	.9449
Minimum Bias CCD	.9529	.9458	.9376	.9254	.9139	.8927	.9281
Orthogonal Hexagon	.9473	.9424	.9311	.8962	.8532	.8137	.8973
Uniform Precision Hexagon	.9580	.9467	.8831	.8425	.8059	.7512	.8646

Even before examining the data computed in this experiment, one would suspect that the minimum bias design would perform well because of the lack-of-fit of the quadratic polynomial. The results of the Surface 3 experiments demonstrate this, but also show that the uniform precision central composite design is somewhat better in all error standard deviations. It is interesting to note that both orthogonal designs do not perform as well as they had on the earlier surfaces.

Figure 11 depicts the distance of the estimated optimal factor combination from the true optimal factor combination for Surface 3. Again the minimum bias design performs well, as would be expected from the above discussion. The orthogonal central composite design, however, achieves

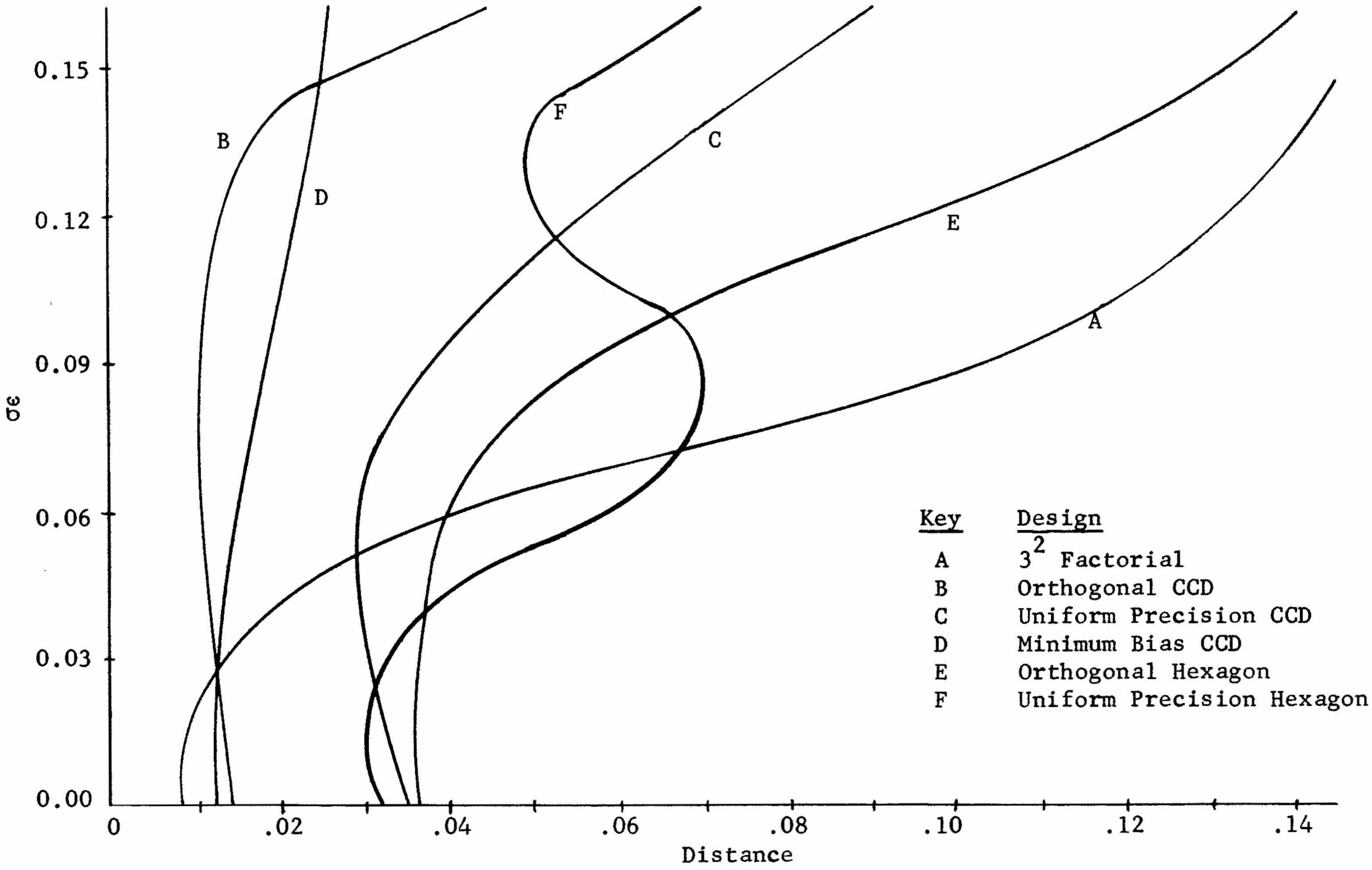


Figure 11. Surface 3 Distance from True Optimum (L)

even better results which is in direct contrast to the lower percentage achievement attained under the first measure of effectiveness. Likewise, after yielding good results under the first measure of effectiveness, the uniform precision central composite design does not do as well with regard to distance, although the results should not be considered bad.

4.3.4 Surface 4

Figure 6(d) is a relatively flat curvilinear ridge with a gradual slope and gentle curvature. Again the orthogonal hexagon design performs best in all situations (Table 9). The entire class of central composite designs also indicates good results with the orthogonal being the best.

Table 9. Surface 4 Average Response Achievement (R)

Design σ_ϵ	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2 Factorial	.8472	.8244	.7337	.7606	.7406	.6965	.7672
Orthogonal CCD	.9804	.9613	.9084	.8648	.8190	.7521	.8810
Uniform Precision CCD	.9602	.9539	.8607	.8551	.8364	.8206	.8812
Minimum Bias CCD	.9482	.9024	.8999	.8507	.8175	.7917	.8684
Orthogonal Hexagon	.9741	.9679	.9469	.9163	.8724	.8287	.9177
Uniform Precision Hexagon	.9467	.8412	.8231	.7583	.7515	.6874	.8014

Examining Figure 12, similar situations arise as for Surface 3. To begin with, the orthogonal hexagon design achieves by far the best

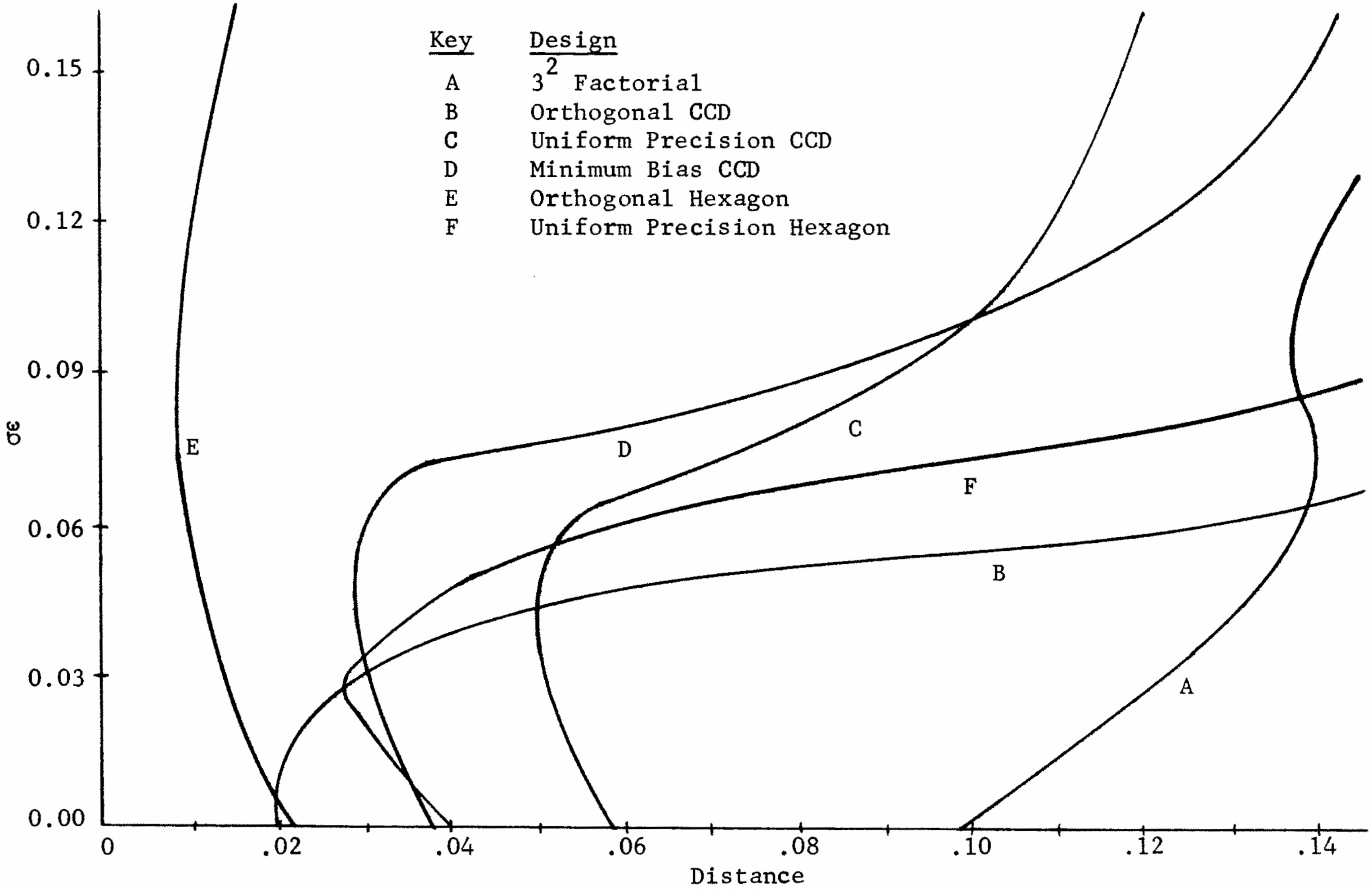


Figure 12. Surface 4 Distance from True Optimum (L)

results. This agrees with the first measure of effectiveness. The remaining designs, except for the 3^2 factorial, start out fairly well; but, as error increases, they tend to develop large distances between estimated and true optimal factor combinations.

4.3.5 Surface 5

This is a modification of Rosenbrock's curved valley. This surface (Figure 6(e)) is a steep curving ridge with much more prominent features than Surface 3. Table 10 shows the average response achievement for each design.

Table 10. Surface 5 Average Response Achievement (R)

Design \ $\sigma\epsilon$	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2 Factorial	.9992	.9992	.9991	.9990	.9989	.9867	.9970
Orthogonal CCD	.9056	.8871	.8895	.8895	.8883	.8863	.8911
Uniform Precision CCD	.9991	.9991	.9990	.9990	.9990	.9989	.9990
Minimum Bias CCD	.9448	.8886	.7164	.0090	.0000	.0000	.4265
Orthogonal Hexagon	.2970	.0000	.0000	.0000	.0000	.0000	.0495
Uniform Precision Hexagon	.6695	.5195	.2593	.0000	.0000	.0000	.2414

The uniform precision central composite and 3^2 factorial designs do extremely well for all error standard deviations. The orthogonal central composite design likewise offers good results. All other designs do very poorly in analyzing the surface. This phenomenon is difficult to explain completely, although it is probably related to the steepness and excessive curvature of the ridge. The distance measure of effectiveness (Figure 13) demonstrates similar results.

4.3.6 Surface 6

This is the surface described in Figure 6(f). It was developed from an inverse polynomial and presents a "bumpy," irregular, asymmetric surface. Table 11 shows the average response achievement for each design.

Table 11. Surface 6 Average Response Achievement (R)

Design $\sigma\epsilon$	0.0	0.3	0.6	0.9	0.12	0.15	Average
3^2 Factorial	.9998	.8296	.7988	.7088	.6411	.6386	.7695
Orthogonal CCD	.9999	.7524	.7503	.7468	.7373	.6902	.7795
Uniform Precision CCD	.9975	.9632	.9166	.8041	.7527	.7439	.8630
Minimum Bias CCD	1.0000	.9897	.9441	.8898	.8200	.7696	.9022
Orthogonal Hexagon	.9999	.9875	.8698	.8313	.7883	.7741	.8752
Uniform Precision Hexagon	.9999	.9462	.8773	.8719	.8607	.7299	.8810

Both the 3^2 factorial and the orthogonal central composite designs show a rapid decrease in response when error is introduced. The remain-

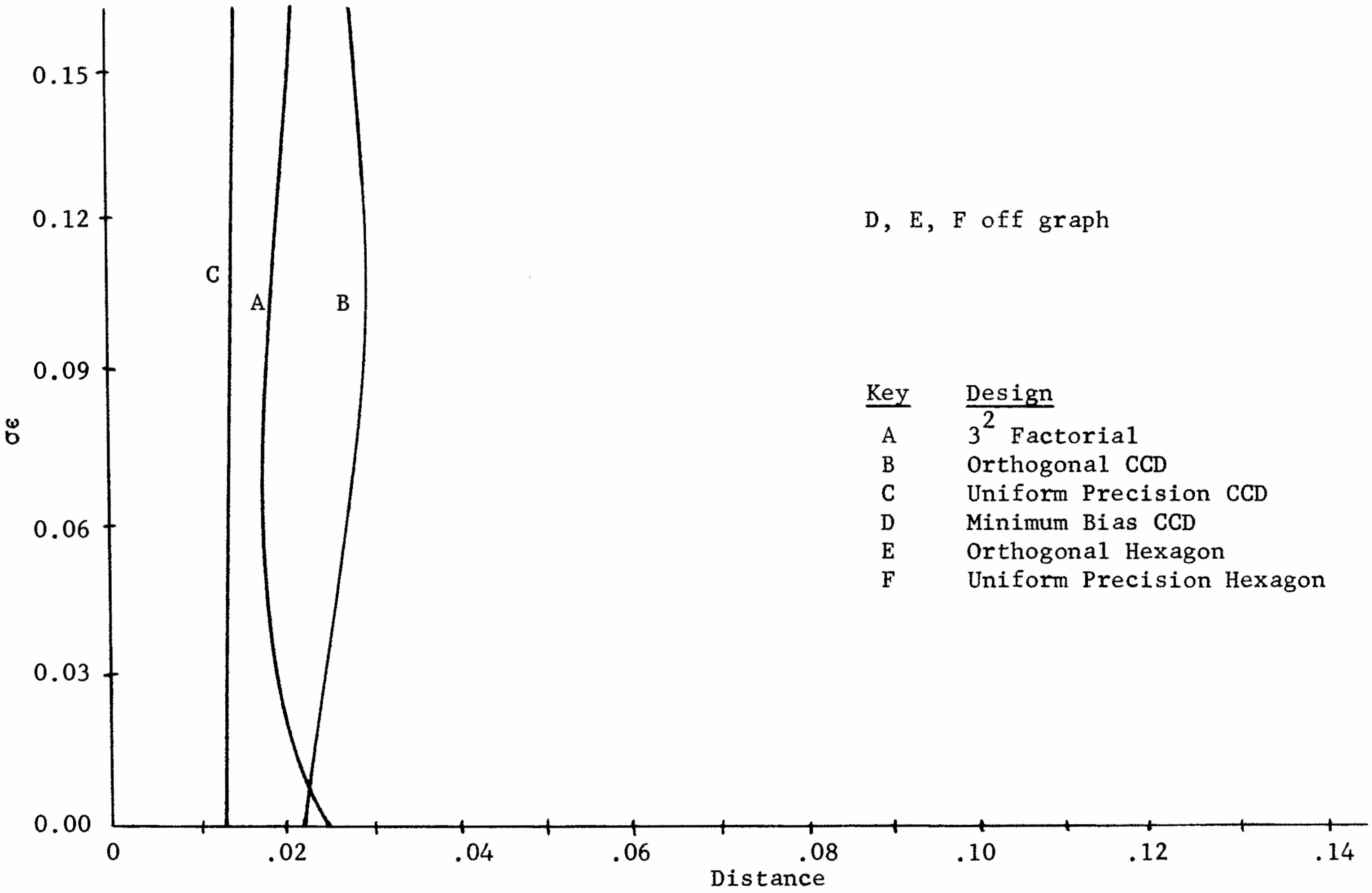


Figure 13. Surface 5 Distance from True Optimum (L)

ing designs do well with the minimum bias central composite design presenting the best results.

Figure 14 depicts the results of the second measure of effectiveness. Here, the same four designs do well again, with the uniform precision hexagon design yielding the smallest distance between the predicted and true optimum of the factors.

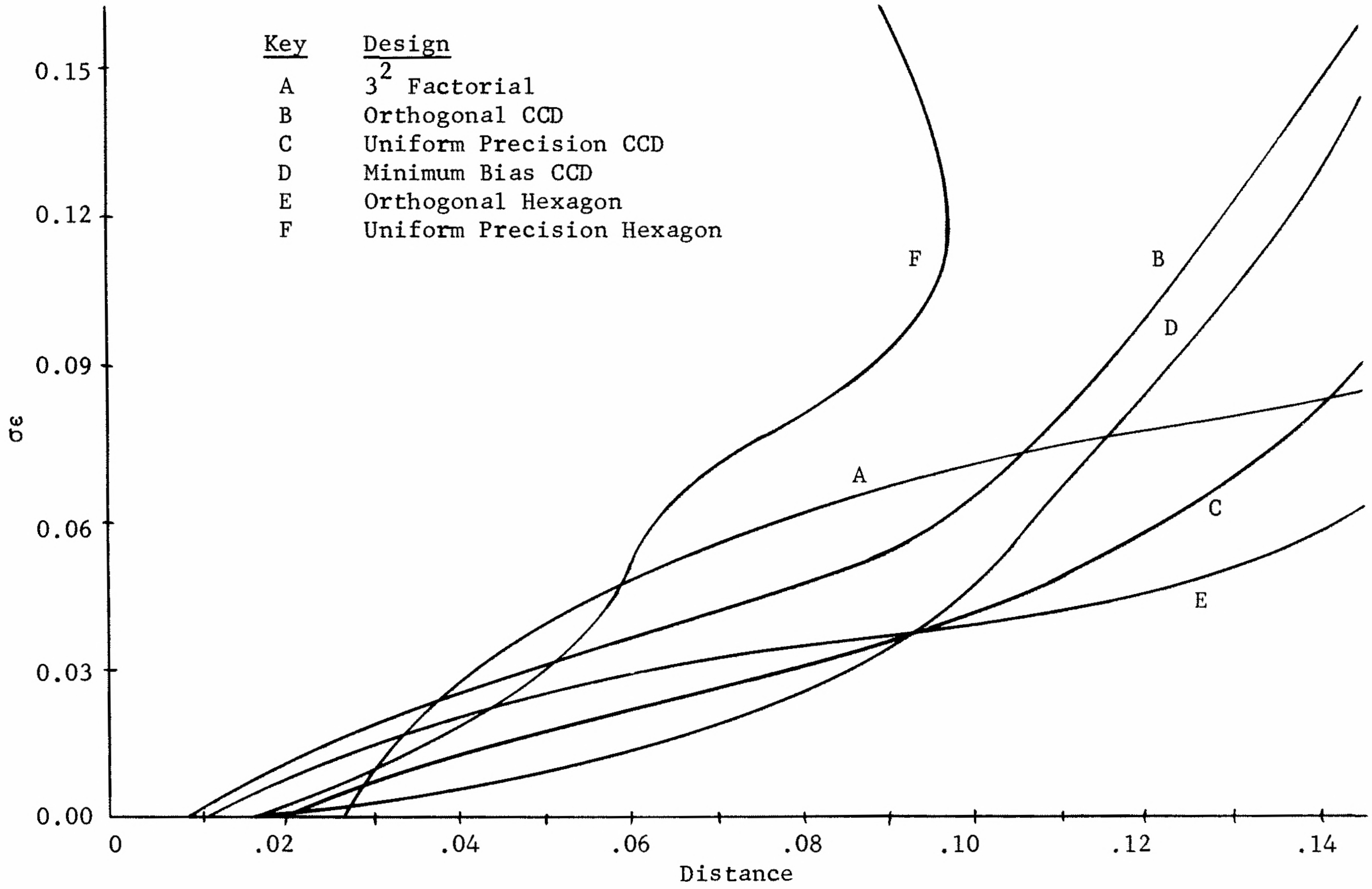


Figure 14. Surface 6 Distance from True Optimum (L)

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

The conclusions derived from this study are the following:

1. A survey of the literature revealed a definite need for an investigation of the utility of second order experimental design techniques to digital simulation.

2. The concept of rotatability is an important factor in experimental design. This is evident in comparing the achievements of the 3^2 factorial design, which is also a non-rotatable central composite design, to the achievements of the class of rotatable central composite designs.

3. Design "spread," or choice of second moment, can be a potentially dangerous problem and lead to erroneous conclusions if the experiment is not properly designed. The only solution is experience with the model under study and a thorough knowledge so far as the choice of scale of the variables is concerned.

4. When comparing results for all designs, the orthogonal hexagon design shows better performance in all average situations than any other design. Close in performance was the minimum bias design followed by the remaining central composite designs. The 3^2 factorial design, as well as the uniform precision hexagon design were definitely poorer in performance than the other designs.

5. When comparing results of experimental designs by surface,

the orthogonal hexagon and orthogonal central composite designs provide the best performance on gently sloping surfaces with little curvature. The best achievement on ridge surfaces was obtained by the use of uniform precision central composite designs, followed by the minimum bias central composite design. Irregular, asymmetric surfaces are best explored using the minimum bias central composite design.

5.2 Recommendations for Further Study

The relationship of experimental design techniques and simulation offers many areas of potential research. The following is a brief outline of recommendations for further research in this area.

1. An investigation of experimental optimization and its relationship to simulation with three or more variables and cubic and higher order surfaces.

2. The results of this study warrant a further investigation of the class of rotatable equiradial designs as well as the possibilities of combinations of equiradial designs.

3. Further investigation of the minimum bias criteria and its use with equiradial, rotatable designs.

APPENDICES

APPENDIX A

EXAMPLES OF THE USE OF SECOND ORDER DESIGNS

Situation 1

An experimenter has arrived at a near optimal region while exploring Surface 1 by the method of steepest ascent. His optimal factor combination is $x_1 = .94$ and $x_2 = 1.00$ which in turn give a response of .9929. A lack-of-fit test tells him that a first order model is no longer adequate.

Solution

In Chapter III it was shown that the rotatable, orthogonal, hexagon second order design would perform well in a Surface 1 type response region. Letting 1 in the design be equivalent to .07 on the surface and using the optimal factor combination as the design center, the following design matrix is constructed.

$$\begin{array}{cc} x_1 & x_2 \end{array}$$
$$\underline{D} = \begin{bmatrix} 1 & 0 \\ 0.5 & 0.75 \\ -0.5 & 0.75 \\ -1 & 0 \\ -0.5 & -0.75 \\ 0.5 & -0.75 \\ \cdots & \cdots \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

The $\underline{X'X}$ matrix is

$$\underline{X'X} = \begin{bmatrix} 12.0000 & .0000 & .0000 & 3.0000 & 2.9999 & .0000 \\ & 3.0000 & .0000 & .0000 & .0000 & .0000 \\ & & 2.9999 & .0000 & .0000 & .0000 \\ & & & 2.2500 & .7499 & .0000 \\ & & & .7499 & 2.2497 & .0000 \\ & & & & & .7499 \end{bmatrix}$$

This leads to the fitted equation

$$y = .9929 + .0161x_1 - .00069x_2 - .0093x_1^2 - .0383x_2^2 + 0.0000x_1x_2 \ ,$$

the stationary point is

$$x_{1*} = 1.00059$$

$$x_{2*} = .999367 \ ,$$

and the response at the stationary point

$$y \approx .9999961 \ .$$

The computed eigenvalues are -.0001075 and -.002611, which indicate a maximum response and a surface slightly elongated along the x_1 axis.

The distance from the predicted optimal factor combination to the true optimal factor combination is 0.000865. This compares to 0.06 achieved by the method of steepest ascent. Likewise, the optimum response was increased by 0.0070961.

Situation 2

An experimenter has arrived at a near optimal point while exploring Surface 3 by the method of steepest ascent. His optimal factor combination is $x_1 = .95$ and $x_2 = .95$ which give a response of .9949. A lack-of-fit test tells him that a first order model is no longer adequate.

Solution

In Chapter III it was shown that both the uniform precision central composite (rotatable) and the minimum bias central composite would achieve consistent good results in a Surface 3 type situation.

Minimum Bias Central Composite Design

Letting 1 in the design be equivalent to .06 on the surface and using the optimal factor combination as the design center, the following design matrix is constructed.

$$\underline{D} = \begin{array}{cc} x_1 & x_2 \end{array} \\ \left[\begin{array}{rr} -.996 & -.996 \\ -.996 & .996 \\ .996 & -.996 \\ .996 & .996 \\ \hline -1.408 & 0 \\ 1.408 & 0 \\ 0 & -1.408 \\ 0 & 1.408 \\ \hline 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{array}\right]$$

The $\underline{X}'\underline{X}$ matrix is

$$\underline{X}'\underline{X} = \begin{bmatrix} 15.0000 & .0000 & .0000 & 7.9329 & 7.9329 & .0000 \\ & 7.9329 & .0000 & .0000 & .0000 & .0000 \\ & & 7.9329 & .0000 & .0000 & .0000 \\ & & & 11.7967 & 3.9364 & .0000 \\ & & & 3.9364 & 11.7967 & .0000 \\ & & & & & 3.9364 \end{bmatrix}$$

This leads to the fitted equation

$$y = .9929 + .0179x_1 + .000791x_2 - .07127x_1^2 - .06479x_2^2 + .1259x_1x_2 ,$$

the stationary point is

$$x_{1*} = .984235$$

$$x_{2*} = .983620 ,$$

and the response at the stationary point

$$\hat{y} = .99949.$$

The computed eigenvalues are -.0001997 and -.07630 which signify a maximum response and an elongated ridge along an axis through the design center origin at an angle of approximately 45°.

The distance from the predicted optimal factor combination to the true optimal factor combination is 0.02273. This compares to 0.0708 achieved by the method of steepest ascent. Likewise, the optimum response was increased by 0.00459.

Uniform Precision Central Composite Design

Letting 1 in the design be equivalent to .055 on the surface and using the optimal factor combination as the design center, the following design matrix is constructed.

$$
\begin{array}{cc}
 & \begin{array}{cc} x_1 & x_2 \end{array} \\
\underline{D} = & \left[\begin{array}{cc}
-1 & -1 \\
-1 & 1 \\
1 & -1 \\
1 & 1 \\
\cdots & \cdots \\
-1.414 & 0 \\
1.414 & 0 \\
0 & -1.414 \\
0 & 1.414 \\
\cdots & \cdots \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0
\end{array}\right]
\end{array}
$$

The $\underline{X}'\underline{X}$ matrix is

$$
\underline{X}'\underline{X} = \left[\begin{array}{cccccc}
13.0000 & .0000 & .0000 & 7.9999 & 7.9999 & .0000 \\
 & 7.9999 & .0000 & .0000 & .0000 & .0000 \\
 & & 7.9999 & .0000 & .0000 & .0000 \\
 & & & 12.0000 & 4.0000 & .0000 \\
 & & & 4.0000 & 12.0000 & .0000 \\
 & & & & & 4.0000
\end{array}\right]
$$

This leads to the fitted equation

$$
y = .9949 + .01005x_1 + .00060x_2 - .06122x_1^2 - .05572x_2^2 + .1074x_1x_2 \ ,
$$

the stationary point is

$$x_{1*} = .980859$$

$$x_{2*} = .980036 \ ,$$

and the response at the stationary point

$\hat{y} = .999249.$

The computed eigenvalues are -0.0002128 and -0.08909 which signify a maximum response and an elongated ridge along an axis that goes out from the design center origin at an angle of approximately 45°.

The distance from the predicted optimal factor combination to the true optimal factor combination is 0.028233. This compares to 0.0708 achieved by the method of steepest ascent. Likewise, the optimum response was increased by 0.00435.

APPENDIX B

COMPUTER PROGRAM LISTING

```
      DIMENSION PT(100)
      DIMENSION R(16)
      DIMENSION ERR(50,10)
      COMMON/BLOKA/ERR,ER,L,K
      COMMON/BLOKC/SURF
      COMMON/BLOKD/IPO
      INTEGER SURF
      INTEGER YY
      READ(5,498) ((ERR(I,J),I=1,50),J=1,10)
498   FORMAT(10F6.3)
1     WRITE(6,700)
700   FORMAT(//2X,'ENTER NEW INPUT DATA',//)
      READ(5,710,END=9999) IDES,SURF,ER
710   FORMAT(2I1,F6.3)
      RN=.0
      IPO=0
      IX=19427
      L=1
      K=1
      GO TO (20,22,23,24,25,26),IDES
20    WRITE(6,499) ER,SURF
499   FORMAT(/-8X,'THREE K DESIGN (ERROR=',F5.2,') - SURFACE',I3,/8X,40(
     11H-))
      GO TO 30
22    WRITE(6,501) ER,SURF
501   FORMAT(//8X,'ORTHOGONAL CCD DESIGN (ROTATABLE) (ERROR=',F5.2,') -
     1SURFACE',I3,/8X,60(1H-))
      GO TO 30
23    WRITE(6,502) ER,SURF
502   FORMAT(//4X,'UNIFORM PRECISION CCD DESIGN (ROTATABLE) (ERROR=',F5.
     12,') - SURFACE',I3,/4X,67(1H-))
      GO TO 30
24    WRITE(6,503) ER,SURF
503   FORMAT(//8X,'MODERN DESIGN (CCD ROTATABLE) (ERROR=',F.2,') - SURF
     1ACE',I3,/8X,56(1H-))
      GO TO 30
25    WRITE(6,504) ER,SURF
504   FORMAT(//3X,'HEXAGONAL DESIGN (ORTHOGONAL - ROTATABLE) (ERROR=',F5
     1.2,') - SURFACE',I3,/3X,68(1H-))
      GO TO 30
26    WRITE(6,505) ER,SURF
505   FORMAT(//3X,'HEXAGONAL DESIGN (UNIF. PREC. - ROTATABLE) (ERROR=',F
     15.2,') - SURFACE',I3,/3X,69(1H-))
      GO TO 30
30    DO 11 J=1,30
      CALL RANDU(IX,RN)
      X=RN
      PT(J)=XX(X)
      YY=IFIX(PT(J))
      IF(SURF.EQ.3.OR.SURF.EQ.5) GO TO 31
      IF(SURF.EQ.6) GO TO 33
      CALL CNTRPT(YY,S,T)
      GO TO 32
31    CALL CNTR(YY,S,T)
      GO TO 32
33    CALL CPT(YY,S,T)
32    CONTINUE
      GO TO (40,42,43,44,45,46),IDES
40    CALL THKAY(S,T,R)
      GO TO 10
42    CALL ORCCD(S,T,R)
      GO TO 10
43    CALL UPCCD(S,T,R)
      GO TO 10
44    CALL MODCCD(S,T,R)
      GO TO 10
45    CALL HEXOR(S,T,R)
      GO TO 10
46    CALL HEXUP(S,T,R)
      GO TO 10
10    CONTINUE
11    CONTINUE
      CALL OUTPUT
      GO TO 1
9999  END
```

```
      SUBROUTINE ORCCD(S, T, R)
      DIMENSION R(16)
      DIMENSION Y(16),XY(6),BETA(6)
      DIMENSION LITL(20), V(2)
      DIMENSION B(20,20),A(20,20),C(20,20),D(20,20)
      DIMENSION DIAG(2),OFFD(2),E(2),TEMP1(20),TEMP2(20)
      DIMENSION XOX(1)
      DIMENSION BB(2,2),BL(2),BIN(2,2),XO(2),LIT(10),XI(2),XOI(1,2)
      DIMENSION SPC(2),SPU(2)
      DIMENSION ADR1(30),ADR2(30),ADX(30),ADY(30),ADZ(30)
      DIMENSION ASP1(30),ASP2(30),AYHAT(30),ARESP(30),AE1(30),AE2(30)
      COMMON/BLOKB/ASP1,ASP2,AYHAT,ARESP,AE1,AE2,ADR1,ADR2,ADX,ADY,ADZ
      COMMON/BLOKC/SURF
      COMMON/BLOKD/IFO
      INTEGER SURF
      SS=S
      TT=T
      I=1
      GO TO (1,2,3,4,5,6), SURF
1     S1=S-.23094
      T1=T-.23094
      R(I)=RESP1(S1,T1)
      I=2
      T1=T+.23094
      R(I)=RESP1(S1,T1)
      I=3
      S1=S+.23094
      T1=T-.23094
      R(I)=RESP1(S1,T1)
      I=4
      T1=T+.23094
      R(I)=RESP1(S1,T1)
      I=5
      T1=T+.3266
      R(I)=RESP1(S,T1)
      I=6
      T1=T-.3266
      R(I)=RESP1(S,T1)
      I=7
      S1=S+.3266
      R(I)=RESP1(S1,T)
      I=8
      S1=S-.3266
      R(I)=RESP1(S1,T)
      DO 123 I=9,16
      R(I)=RESP1(S,T)
123   CONTINUE
      GO TO 59
2     S1=S-.23094
      T1=T-.23094
      R(I)=RESP2(S1,T1)
      I=2
      T1=T+.23094
      R(I)=RESP2(S1,T1)
      I=3
      S1=S+.23094
      T1=T-.23094
      R(I)=RESP2(S1,T1)
      I=4
      T1=T+.23094
      R(I)=RESP2(S1,T1)
      I=5
      T1=T+.3266
      R(I)=RESP2(S,T1)
      I=6
      T1=T-.3266
      R(I)=RESP2(S,T1)
      I=7
      S1=S+.3266
      R(I)=RESP2(S1,T)
      I=8
      S1=S-.3266
      R(I)=RESP2(S1,T)
      DO 124 I=9,16
      R(I)=RESP2(S,T)
124   CONTINUE
      GO TO 59
3     S1=S-.23094
      T1=T-.23094
      R(I)=RESP3(S1,T1)
      I=2
      T1=T+.23094
      R(I)=RESP3(S1,T1)
      I=3
      S1=S+.23094
      T1=T-.23094
      R(I)=RESP3(S1,T1)
      I=4
      T1=T+.23094
      R(I)=RESP3(S1,T1)
      I=5
      T1=T+.3266
      R(I)=RESP3(S,T1)
      I=6
      T1=T-.3266
      R(I)=RESP3(S,T1)
      I=7
      S1=S+.3266
      R(I)=RESP3(S1,T)
      I=8
```

```
      S1=S-.3266
      R(I)=RESP3(S1,T)
      DO 125 I=9,16
      R(I)=RESP3(S,T)
125   CONTINUE
      GO TO 59
4     S1=S-.23094
      T1=T-.23094
      R(I)=RESP4(S1,T1)
      I=2
      T1=T+.23094
      R(I)=RESP4(S1,T1)
      I=3
      S1=S+.23094
      T1=T-.23094
      R(I)=RESP4(S1,T1)
      I=4
      T1=T+.23094
      R(I)=RESP4(S1,T1)
      I=5
      T1=T+.3266
      R(I)=RESP4(S,T1)
      I=6
      T1=T-.3266
      R(I)=RESP4(S,T1)
      I=7
      S1=S+.3266
      R(I)=RESP4(S1,T)
      I=8
      S1=S-.3266
      R(I)=RESP4(S1,T)
      DO 126 I=9,16
      R(I)=RESP4(S,T)
126   CONTINUE
      GO TO 59
5     S1=S-.23094
      T1=T-.23094
      R(I)=RESP5(S1,T1)
      I=2
      T1=T+.23094
      R(I)=RESP5(S1,T1)
      I=3
      S1=S+.23094
      T1=T-.23094
      R(I)=RESP5(S1,T1)
      I=4
      T1=T+.23094
      R(I)=RESP5(S1,T1)
      I=5
      T1=T+.3266
      R(I)=RESP5(S,T1)
      I=6
      T1=T-.3266
      R(I)=RESP5(S,T1)
      I=7
      S1=S+.3266
      R(I)=RESP5(S1,T)
      I=8
      S1=S-.3266
      R(I)=RESP5(S1,T)
      DO 127 I=9,16
      R(I)=RESP5(S,T)
127   CONTINUE
      GO TO 59
6     S1=S-.23094
      T1=T-.23094
      R(I)=RESP6(S1,T1)
      I=2
      T1=T+.23094
      R(I)=RESP6(S1,T1)
      I=3
      S1=S+.23094
      T1=T-.23094
      R(I)=RESP6(S1,T1)
      I=4
      T1=T+.23094
      R(I)=RESP6(S1,T1)
      I=5
      T1=T+.3266
      R(I)=RESP6(S,T1)
      I=6
      T1=T-.3266
      R(I)=RESP6(S,T1)
      I=7
      S1=S+.3266
      R(I)=RESP6(S1,T)
      I=8
      S1=S-.3266
      R(I)=RESP6(S1,T)
      DO 128 I=9,16
      R(I)=RESP6(S,T)
128   CONTINUE
      GO TO 59
59    DO 10 J=1,16
10    B(J,1)=1
      DO 11 J=1,2
11    B(J,2)=-1.15470
      DO 12 J=3,4
12    B(J,2)=1.15470
      DO 13 J=5,6
```

```
13    B(J,2)=0.0
      B(7,2)=1.63299
      B(8,2)=-1.63299
      DO 14 J=9,16
14    B(J,2)=0.0
      DO 15 J=1,3,2
15    B(J,3)=-1.15470
      DO 16 J=2,4,2
16    B(J,3)=1.15470
      B(5,3)=1.63299
      B(6,3)=-1.63299
      DO 17 J=7,16
17    B(J,3)=0.0
      DO 18 J=1,4
18    B(J,4)=1.33333
      B(5,4)=0.0
      B(6,4)=0.0
      B(7,4)=2.66666
      B(8,4)=2.66666
      DO 19 J=9,16
19    B(J,4)=0.0
      DO 20 J=1,4
20    B(J,5)=1.33333
      B(5,5)=2.66666
      B(6,5)=2.66666
      DO 21 J=7,16
21    B(J,5)=0.0
      B(1,6)=1.33333
      B(2,6)=-1.33333
      B(3,6)=-1.33333
      B(4,6)=1.33333
      DO 23 J=5,16
23    B(J,6)=0.0
      DO 28 I=1,16
      DO 28 J=1,6
28    A(J,I)=B(I,J)
      CALL MXMLT(A,B,C,6,16,6,20,20)
      DO 34 I=1,6
      DO 34 J=1,16
      IF(ABS(C(I,J)).LT..1) GO TO 33
      GO TO 34
33    C(I,J)=0.0
34    CONTINUE
      DO 25 I=1,16
25    Y(I)=R(I)
      CALL MXMLT(A,Y,XY,6,16,1,20,16)
      DO 32 I=1,6
      IF (ABS(XY(I)).LT..001) GO TO 35
      GO TO 32
35    XY(I)=0.0
32    CONTINUE
      V(1)=3.
      DO 30 I=1,6
      DO 30 J=1,16
30    D(I,J)=C(I,J)
      CALL GJR(D,20,20,6,6,$60,LITL,V)
      CALL MXMLT(D,XY,BETA,6,6,1,20,6)
      DO 40 I=1,6
      IF (ABS(BETA(I)).LT..001) GO TO 41
      GO TO 40
41    BETA(I)=0.0
40    CONTINUE
      BB(1,1)=BETA(4)
      BB(2,2)=BETA(5)
      BB(1,2)=(BETA(6))/2
      BB(2,1)=BB(1,2)
      DO 31 I=1,2
      DO 31 J=1,2
31    BIN(I,J)=BB(I,J)
      V(1)=3.
      CALL GJR(BIN,2,2,2,2,$60,LIT,V)
      BL(1)=BETA(2)
      BL(2)=BETA(3)
      CALL MXMLT(BIN,BL,XI,2,2,1,2,2)
      XO(1)=-((XI(1)/2)
      XO(2)=-((XI(2))/2)
      XOI(1,1)=XO(1)
      XOI(1,2)=XO(2)
      DO 42 I=1,2
42    SPC(I)=XO(I)*.2
      SPU(1)=SS+SPC(1)
      SPU(2)=TT+SPC(2)
      IPO=IPO+1
      ASP1(IPO)=SPU(1)
      ASP2(IPO)=SPU(2)
      CALL MXMLT(XOI,BL,XOX,1,2,1,1,2)
      YHATO=BETA(1)+(XOX(1)/2)
      AYHAT(IPO)=YHATO
      GO TO (61,62,63,64,65,54),SURF
61    RESP=RESP1(SPU(1),SPU(2))
      GO TO 69
62    RESP=RESP2(SPU(1),SPU(2))
      GO TO 69
63    RESP=RESP3(SPU(1),SPU(2))
      GO TO 69
64    RESP=RESP4(SPU(1),SPU(2))
      GO TO 69
65    RESP=RESP5(SPU(1),SPU(2))
      GO TO 69
54    RESP=RESP6(SPU(1),SPU(2))
```

```
      GO TO 69
   69 ARESP(IPO)=RESP
      CALL TRIDMX(2,2,BB,DIAG,OFFD)
      CALL EIGVAL(2,E,DIAG,OFFD,TEMP1,TEMP2)
      AE1(IPO)=E(1)
      AE2(IPO)=E(2)
      IF(SURF.EQ.5) GO TO 66
      IF(SURF.EQ.6) GO TO 56
      DR1=1.0-YHATO
      DX=1.0-SPU(1)
      DY=1.0-SPU(2)
      DR2=1.0-RESP
      GO TO 67
   66 DR1=0.0-YHATO
      DX=1.0-SPU(1)
      DY=1.0-SPU(2)
      DR2=0.0-RESP
      GO TO 67
   56 DR1=4.17374909-YHATO
      DX=2.4475-SPU(1)
      DY=3.8875-SPU(2)
      DR2=4.17374909-RESP
   67 CONTINUE
      ADR1(IPO)=DR1
      ADR2(IPO)=DR2
      ADX(IPO)=DX
      ADY(IPO)=DY
      DZ=SQRT(DX**2+DY**2)
      ADZ(IPO)=DZ
      RETURN
   60 STOP
      END
```

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