AN EVALUATION OF RESPONSE SURFACE DESIGNS FOR SIMULATION EXPERIMENTS AND THE ASSIGNMENT OF RANDOM NUMBERS TO EXPERIMENTAL POINTS

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER I

INTRODUCTION

This research will develop a methodology for assigning random numbers to the experimental points of response surface designs for increasing the efficiency of simulation results. The methodology will be based on the recent findings of Schruben and Margolin (52). The research will compare the efficiency of the recommended methodology with those of the rival methodologies. It will use an inventory simulation model to show and support the analytical findings. Additionally, it will present a new classification for response surface designs which could help simulation designers decide which design to use.

Response surface methodology consists of strategies and experimental designs used for exploring unknown surfaces or for determining the optimum conditions, i.e., the optimum levels of factors involved in an experiment. For example, in a chemical plant it is used to determine the level of such factors as temperature, concentration, etc., which will result in the highest yield or the lowest cost. The desirability of response surface methodology stems from the fact that it finds the optimum or discovers an unknown relationship with a limited number of observations.

The mathematical relationship between the factors and the response can be expressed as:

$$G = f(\xi_1, \xi_2, \xi_3, \ldots, \xi_k) \qquad (1.1)$$

where G is the response and $\xi_1, \xi_2, \ldots, \xi_k$ represents factors 1 through k, respectively. Although multiple responses are allowed, this study is limited to the single response case. Response surface methodology requires (1) the factors to be quantitative and (2) the response, G, be measured on a continuous scale.

Generally speaking, the form of the response function (1.1) is unknown and the experimenter approximates it by a polynomial of low order. To do so, he explores a small sub-region of the experimental region which enables him to move to another sub-region with a better set of responses. This process is continued until the sub-region containing the possible optimum is found and explored.

The first sub-region is almost always investigated through fitting a first order polynomial. Designs used for this purpose are called first order designs. Depending upon the obtained results, either the present sub-region will be explored by a second degree equation or a new sub-region will be examined by another first order design. A second order polynomial is employed when the optimum is suspected to be in the present region. Designs proposed for fitting a second degree polynomial are called second order designs. Second order designs should ideally be obtained by adding observations to the points of a first order design.

Box and Wilson (10), in 1951, investigated response surfaces in detail and recommended the optimal strategy and some useful designs for exploring them. The proposed strategy is called the steepest ascent (for maximization problems) or the steepest descent (for minimization problems) method. Although the technique was not new, its application to the purpose at hand was novel. Their work definitely laid the foun-

dation for many studies that have been carried out since then. All the subsequent work was mainly aimed at determining the most efficient designs for exploring response surfaces which meet certain assumptions (1) (6) (7) (9) (20) (21) (22) (23) (24) (37) (40) (41).

When a low order polynomial is fitted to a surface, there could be two sources of variation between the estimated and the true responses. One is due to sampling variation and the other is because of the inadequacy of the fitted equation to represent the true function. The first one is called variance error and the second one is called bias error. Consequently, some response surface designs have been derived to minimize variance alone, some to minimize bias alone, and the rest to minimize both variance and bias. Response surface methodology and its literature are discussed in Chapter II.

The objective of response surface methodology coincides with the objective of most simulation studies. Indeed, many simulations are designed to determine the values of some factors that will optimize a response function. Naylor et al. (48) define the purposes of simulation as the determination of the optimum combination of factors and the general investigation of the relationship between the response and the factors. However, it is surprising to find only a few simulation studies that utilize the concept and the methods of response surfaces.

Although the importance and the benefits of RSM to simulation have been emphasized in several papers, simulation designers have, in the past, been negligent about it (11) (13) (43). The unwillingness to use response surface methodology is perhaps due to three factors. First, response surface methodology was originally designed for physical processes and has yet to find its place in synthetically controlled

business experiments. Second, simple design proposals have been hidden behind complicated statistical proofs.

Third, in view of RSM's seeming complexity, simulators may have used an enumerative approach--changing values of the parameters one at a time until all possible combinations have been considered. Such as approach, however, is neither suitable to large-sized complex problems nor can be employed for finding a functional relationship.

Recently there has been a growing awareness among decision scientists of the importance of response surface methodology in simulation experiments. Brightman (11) has used design of marketing policies as an example to show the usefulness of response surface methodology to simulation experiments. He has argued that

> although from a historical viewpoint RSM has been applied primarily to Operations Management, its greatest value to decision scientists is its potential application to simulation studies. . . . Once a simulation model has been built and validated, RSM could be utilized to determine the best policy in an optimal fashion (p. 495).

Schruben and Margolin (53, p. 524), in discussing the random number assignment in simulation, write, "our basic development, however, applies to a wider class of experiments. This class includes response surface designs, whose true value for simulation has yet to be fully realized."

Successful application of response surface methodology to simulation requires efficiency in execution. Data generated by computer simulation experiments is costly. Thus, it is vital to obtain as much information as possible with the minimum possible sample size. In doing so, variance reduction techniques have been developed for increasing the efficiency of the desired estimators with a given sample size.

Naturally, the extra work involved for implementing these techniques should not exceed the benefits that will be accrued by the reduction in variance. Two of the most routinely used variance reduction techniques are (1) common random numbers and (2) antithetic random numbers method.

Random numbers are used in simulation for the random selection of observations from a given probability distribution. The common random numbers technique uses the same stream(s) of random numbers for each experimental point. The antithetic random numbers technique uses $\underline{R}$, a vector of random numbers, and $(\underline{1} - \underline{R})$ to generate each simulation response. These two techniques, which require no or little extra computer programming as compared to other variance reducing techniques, induce correlations between responses leading to increases in the efficiency of results.

The use of common random numbers has empirically been shown to cause positively correlated responses; the use of antithetic random numbers has led to negative correlation between responses (38). However, whether one can benefit from their joint application in the same simulation experiment has been controversial. While Kleijnen (38) and Fishman (27) have obtained pessimistic results, Schruben and Margolin's (52) work has proved to be very encouraging. These studies will be discussed in Chapter III.

Having assumed the induction of positive and negative correlation through utilization of common and antithetic random numbers, Schruben and Margolin (52) derived an optimal rule for assigning random numbers to the experimental designs that admit orthogonal blocking. Their result can be adopted for 2^n factorial designs and 2^{n-r} fractional

factorial designs. These designs have been strongly recommended for estimating linear effects in response surface methodology.

In summary, response surface methodology and its associated designs have not received as much attention as they deserve in simulation analysis. Applying response surface methodology to simulation studies substantially increases the strength of an already powerful technique. Although designs developed for exploring response surfaces are efficient, more efficiency might be obtained by using two variance reducing techniques, namely common random numbers and antithetic random numbers.

Study Objectives and Contributions

It is the first objective of this study to design a methodology for assigning random numbers (common, antithetic, and independent) to the design points to increase the efficiency of simulation results. The second objective is to create a presentation scheme for response surface designs to facilitate their application to simulation. Specifically, the study shall attempt to:

1. Examine the designs proposed for exploring response surfaces and provide the user with a summary of these proposals along with the conditions under which they should be used. This step should not be mistaken with a review of literature in this field. The objective is the clarification and reclassification of available designs for future applications. Over the last three decades, alternative criteria (minimizing bias, variance, or both) have been adopted for deriving the optimal designs for learning about the behavior of response functions. Regardless of the criterion selected, factorial and fractional

factorial designs have been mostly recommended by estimating first order effects. However, the optimal designs developed for estimating second order effects have been based on a number of assumptions and should not be used indiscriminately in different experiments. It is neither practical nor economical for a simulation designer to study all the formulated designs in order to find his appropriate design. Therefore, to encourage and facilitate the use of response surface designs there is a need for a study to probe the literature and present it in a complete and an understandable form.

2. Investigate the assignment of common and antithetic random numbers to the designs evaluated in (1) above. Since a blocking arrangement is possible in these designs, the study will examine the implication of applying Schruben and Margolin's assignment rule to them. This assignment rule is primarily useful when it is possible to plan the whole experiment at one time, which is not true for response surface problems. The sequential nature of response surface designs may make it difficult to come up with a general rule for assigning random numbers to the experimental points optimally. The difficulty arises due to the uncertainty in the number of steepest ascent iterations needed to reach to the near-stationary region. For example, an assignment rule which is optimal when the number of steepest ascent iterations required is two may have adverse effect on efficiency when the number of necessary iterations is different than two.

The analysis here is intended to offer an assignment rule that remains optimal regardless of the number of steepest ascent iterations required. In other words, attempts will, first, be made to divide observations into two orthogonal blocks for all the first order designs.

Since first order designs are, in general, factorial and fractional factorial designs, this will be an easy task. Second, when the search process indicates the necessity for fitting a second order polynomial, a methodology will be developed for generating two orthogonal blocks by adding observations to the two orthogonal blocks of the first order design. The optimality of this methodology cannot be evaluated analytically. However, empirical work is an alternate way of testing its validity.

3. Illustrate the application of response surface methodology to an inventory simulation problem. The last part of this research applies the analytical results to an inventory simulation case. An illustrative example will be discussed in detail. The example will provide an opportunity to appreciate the potentiality of response surface design in simulation experiments. In addition, it will furnish an empirical evaluation of the alternative random numbers assignment rules.

Scope and Boundaries

The scope and the boundaries set for this research are as follows: First, it is limited to maximization problems although minimization problems can be transferred to maximization problems simply by multiplying the response by a negative sign. In fact, the example discussed at the end of Chapter IV is a minimization problem. Second, to keep the analysis simple, the discussion (for the most part) will be restricted to two independent variables; however, the obtained results will be general and can be applied to problems with more than two independent variables as well. Third, the response function will be

limited to include second order terms at most. This will not create a great amount of bias in the results because a quadratic function has been shown (in most cases) to provide an adequate fit in the region close to the optimum. The adequacy of a quadratic function has actually been assumed in the literature of response surface methodology and not much discussion exists for cubic functions. Fourth, the study focuses only on the efficiencies that can be obtained when common and antithetic random numbers are assigned to the experimental points. While other variance reducing techniques might be more efficient, they are not as widely and commonly used. Last, it is assumed that correlation with desired signs can be generated by the use of common and antithetic random numbers. The validity of this assumption rests on the empirical findings and not on the mathematical proofs.

Organization of Chapters

Chapter II is devoted to discussion of response surface methodology and contains the proposed experimental designs in chronological order. Chapter III explains the two variance reduction techniques employed in this paper. It also discusses the joint application of common and antithetic random numbers plus the result of Schruben and Margolin's (52) work upon which part of this study is based. Chapter IV has three parts. In the first part, a framework is developed for presenting the proposed designs discussed in Chapter II. This framework is detailed enough to let users with different problems and objectives optimally select their designs. The second part of Chapter IV examines the application of Schruben and Margolin's random number assignment rule to

the designs summarized in the first part. The last part of Chapter IV applies the analytical results to an inventory simulation. Finally Chapter V closes the paper by stating the conclusions as well as implications for future research.

CHAPTER II

RESPONSE SURFACE METHODOLOGY

In this chapter, response surfaces are first defined. Then an efficient method for exploring them is described. Next, designs developed for experimenting with the response surfaces are explained. Finally, a summary of the discussion will be given.

The Concept of Response Surfaces

Response surfaces are usually used for two purposes. First, they might be used to determine the values of some factors that will optimize a response (or a set of responses). Second, they might be employed for learning about the mathematical relationship that exists between the factors and the responses. The discussion here is aimed at the optimization aspect of response surfaces, specifically at single response maximization problems (for example, a firm which maximizes its profits based on prices, advertising expenditures, etc.).

Let G denote the response and $\xi_1, \xi_2, \ldots, \xi_k$ represent factors 1 through k, respectively. Then a response function when the factors are quantitative and the response is measurable on a continuous scale can be expressed by:

$$G = f(\xi_1, \xi_2, \ldots, \xi_k) \tag{2.1}$$

In practice, the form of (2.1) is unknown and the experimenter approximates it by a polynomial of low order. Because of the

experimental error, G, the true response, is never observed and Y is used to indicate the observed response. For convenience, designers do not work with the real values of the factors, but with their standardized values. A standardized variable has its origin at the center of the design and its unit is set equal to the amount by which the factor is changed. Mathematically it is derived as follows:

$$x_{iu} = \frac{(\xi_{iu} - \bar{\xi}_i)}{S_i}, \tag{2.2}$$

where

$$S_i = \left(\sum_{u=1}^{N} \frac{(\xi_{iu} - \bar{\xi}_i)^2}{N} \right)^{1/2},$$

and where N represents the total number of observations. Therefore, for the x's, two relationships will be true:

$$\sum_{u=1}^{N} x_{iu} = 0 \quad \text{and} \quad \sum_{u=1}^{N} x_{iu}^2 = N. \tag{2.3}$$

A polynomial equation for two standardized variables is:

$$Y = \beta_o + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \beta_{111} x_1^3 + \ldots \tag{2.4}$$

Clearly, a better fit is obtained as terms of higher order are included. Each polynomial equation is naturally a regression function with x_1, x_2, x_1^2, x_2^2, x_{12}, etc., as the independent variables in the regression equation. In the polynomial equation, β_1 and β_2 measure the linear effects, β_{11} and β_{22} the quadratic effects, β_{12} the linear x linear interaction effects and so on. An investigator is normally able to identify, at least approximately, the region of factor space corresponding to factor combinations of his interest. This region is called the experimental region and the problem is to find the point(s) of the maximum response

in this region. Polynomials provide an approximate fit only within the experimental region and become untrustworthy when extrapolated.

When the number of factors is small (three or less), there are two convenient ways to visualize the relationship involved. One method is to graph the relationship directly to obtain the response surface. Figure 1 shows a response surface with two factors.

An alternative approach is drawing contour lines--lines of equal response on a graph whose coordinates represent the levels of the factors. Figure 2 illustrates some contour lines corresponding to the response surface in Figure 1. The first technique is useful when there are one or two factors while the second one can be used with as many as three factors.

To find the optimal values of the factors, the designer has to formulate a search strategy. Circumstances that influence his choice are:

(i) The magnitude of experimental error
(ii) The complexity of the response surface
(iii) Whether or not experiments may be conducted sequentially so that each set may be designed using the knowledge gained from the previous sets (10, p. 2).

Generally speaking, in response surface problems, the experimenter does not need to plan the whole experiment at one time and sets of trials are conducted sequentially allowing him to plan new trials based on the responses obtained in the previous ones.

For experiments with small experimental error, a small sub-region of the factor space may be explored with only a few experimental points by utilizing a polynomial of low order. This, plus the sequential nature of the experiments, make it possible for the investigator to specify the next region t be considered or to choose new points in the

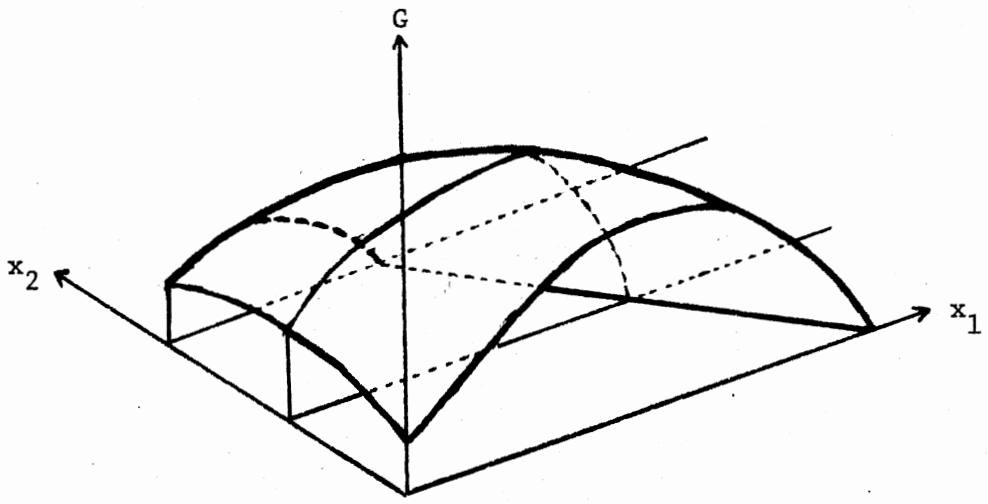
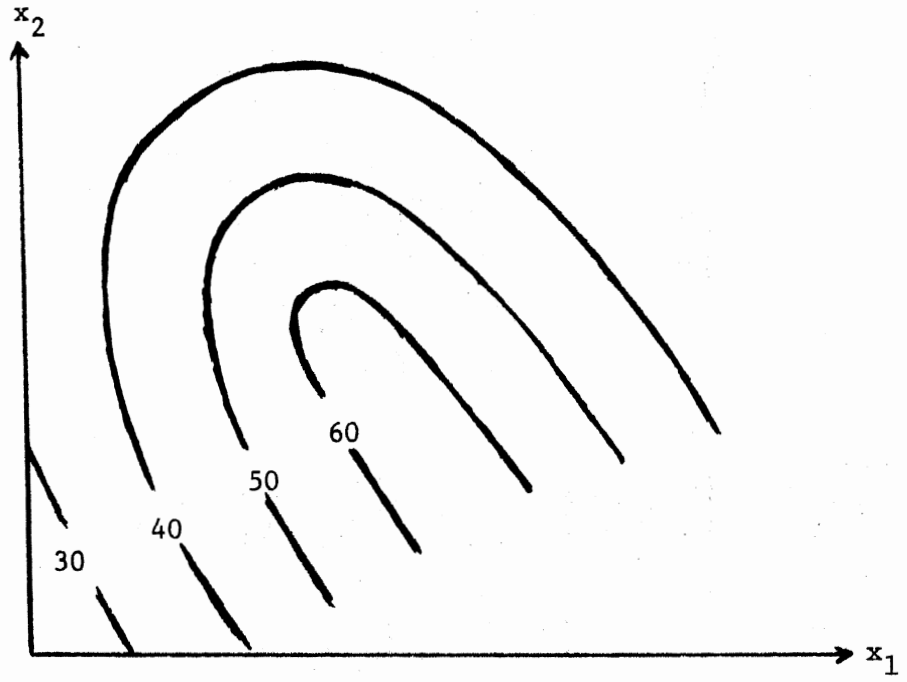


Figure 1. A Response Surface



Source: Davies (9, pp. 497-498).

Figure 2. Response Contour Lines Corresponding to the Response Surface of Figure 1

present region to be studied next. An efficient method of locating the optimum level of each factor was adopted from the field of nonlinear mathematics by Box and Wilson (10). This method, the steepest ascent method, is discussed below within the context of a situation involving two factors x_1 and x_2.

Steepest Ascent Method

The steepest ascent method consists of two distinct phases. In the first phase, due to the likely remoteness of the initial conditions from the maximum, the surface is approximated locally by a sloping plane. In doing so, the slopes, b_1 and b_2 of plane in direction of x_1 and x_2 are estimated. The relative magnitudes and signs of these slopes determine the direction of the greatest increase in responses called steepest ascent. Graphically this direction is perpendicular to the contour lines and shows the amount by which the factors must be varied for gaining the maximum increase in response. Using the steepest ascent direction, the search effort moves from the initial point to another point on the path of steepest ascent and new slopes will be calculated. A hypothetical steepest ascent path, $\overline{0I_1}$, is shown in Figure 3.

To move from the initial point to another, first, a new point along the steepest ascent path is selected. Then, the response for this point is measured to find out whether the predicted increase in response actually takes place. (The size of the jump that is made is very much subjective.) If the actual response is close to the predicted one, another point is tested along the same path. This process is continued until the actual response is substantially diferrent than the one

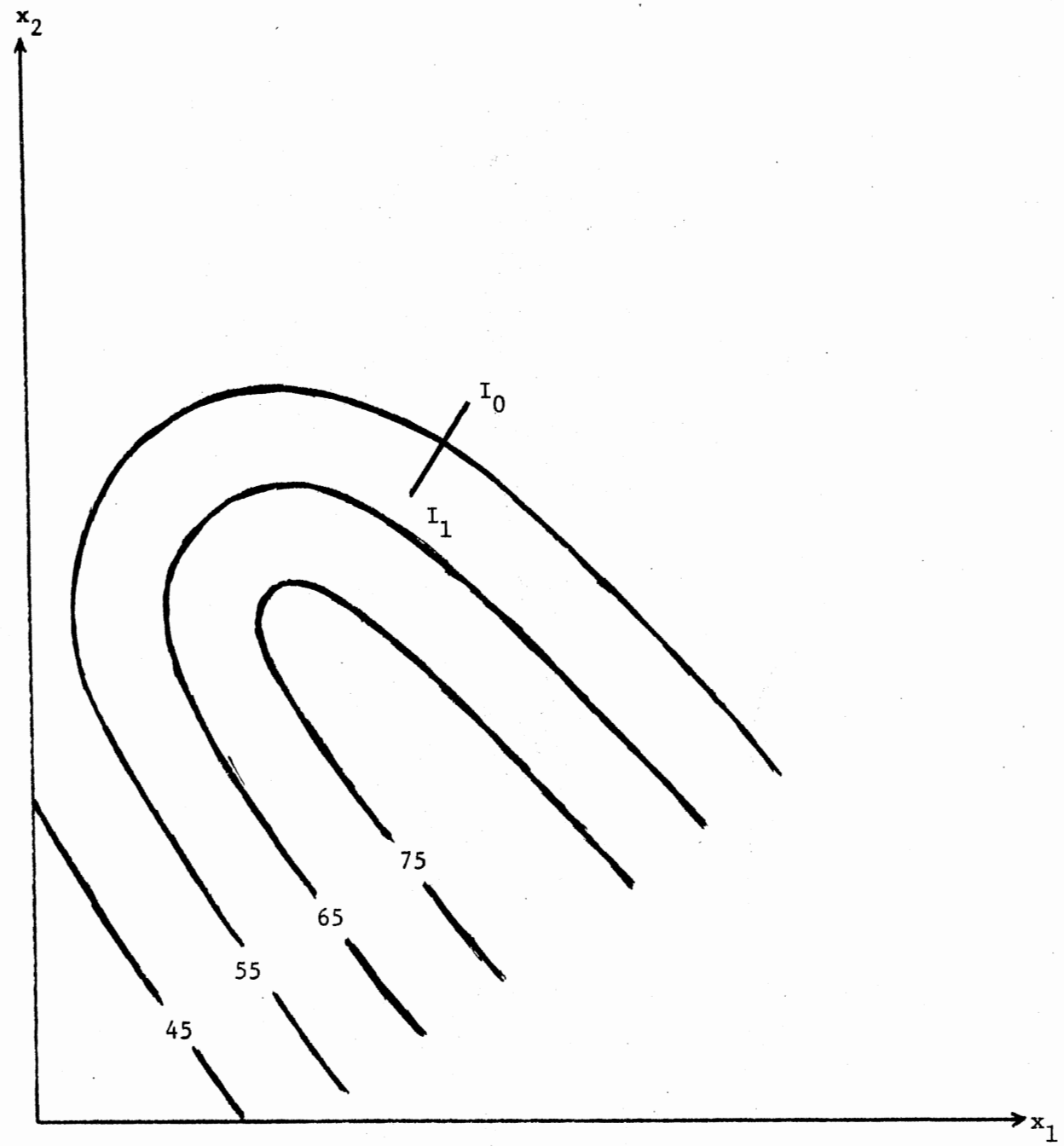


Figure 3. A Hypothetical Steepest Ascent Path, I_0I_1

predicted. At this point, another first degree polynomial is fitted and if the linear approximation turns out to be adequate, a new steepest ascent path is calculated.

This procedure will eventually lead to a region in which the surface can no longer be approximated by a plane and the quadratic coefficients become relatively more important. Therefore, the first phase by itself is usually inadequate to find the optimum, but will quickly direct the search process to a region close to the maximum. This region is called the near-stationary region and will be explored in the second phase.

The initial value and the unit adopted for a factor should be changed before exploring the next sub-region if its estimated linear effect is relatively small. A small linear effect could be caused by one of the following:

1. The factor does not influence the response.
2. The unit selected for this variable is relatively small.
3. The initial value of this factor is close to a conditional maximum.

Based on the new estimates, the cause will be determined and appropriate measures should be taken accordingly.

The objective of the second phase is to determine the nature of the near-stationary region and, if possible, the location of the maximum. This is done through performing a set of trials in the near-stationary region and fitting a polynomial of second degree to the surface in this region.

Being in the near-stationary region does not necessarily mean that the experimenter is in the neighborhood of a global maximum. That will

be the case only if the experimental region has one peak, otherwise convergence to a local maximum is possible. Steepest ascent method, therefore, leads to a stationary point which could be (1) a true maximum (Figure 4a), (2) a stationary ridge (Figure 4b), (3) a rising ridge (Figure 4c), or (4) a saddle point (Figure 4d).

While graphical presentation is helpful in examining a stationary point, it demands an enormous amount of work and is not useful when there are more than three factors in the experiment. Canonical analysis is a mathematical method developed for evaluating the stationary point. To construct the canonical function, the origin of the design is moved to the stationary point and the original coordinate axes are rotated until they correspond to the axes of the conics (the collection of curves which make up the contour surfaces). The signs and the magnitudes of the coefficients of the variables in the new coordinate system determine the type of maximum reached.

Discovering the nature of the near stationary-ridge is of great practical importance. For example, for a stationary ridge like that in Figure 4b there are multiple optimal solutions and from these alternatives the one that satisfies or optimizes some auxiliary condition should be selected.

The method discussed above does not explore the whole experimental region and is based on the premise that the maximum can be reached through a rising path. It is successful in a global sense only if the experimental region has one peak.

Before discussing the experimental designs prescribed for the two phases of the steepest ascent method a word about the importance of the scales of measurement for the variables is in order. As noted earlier,

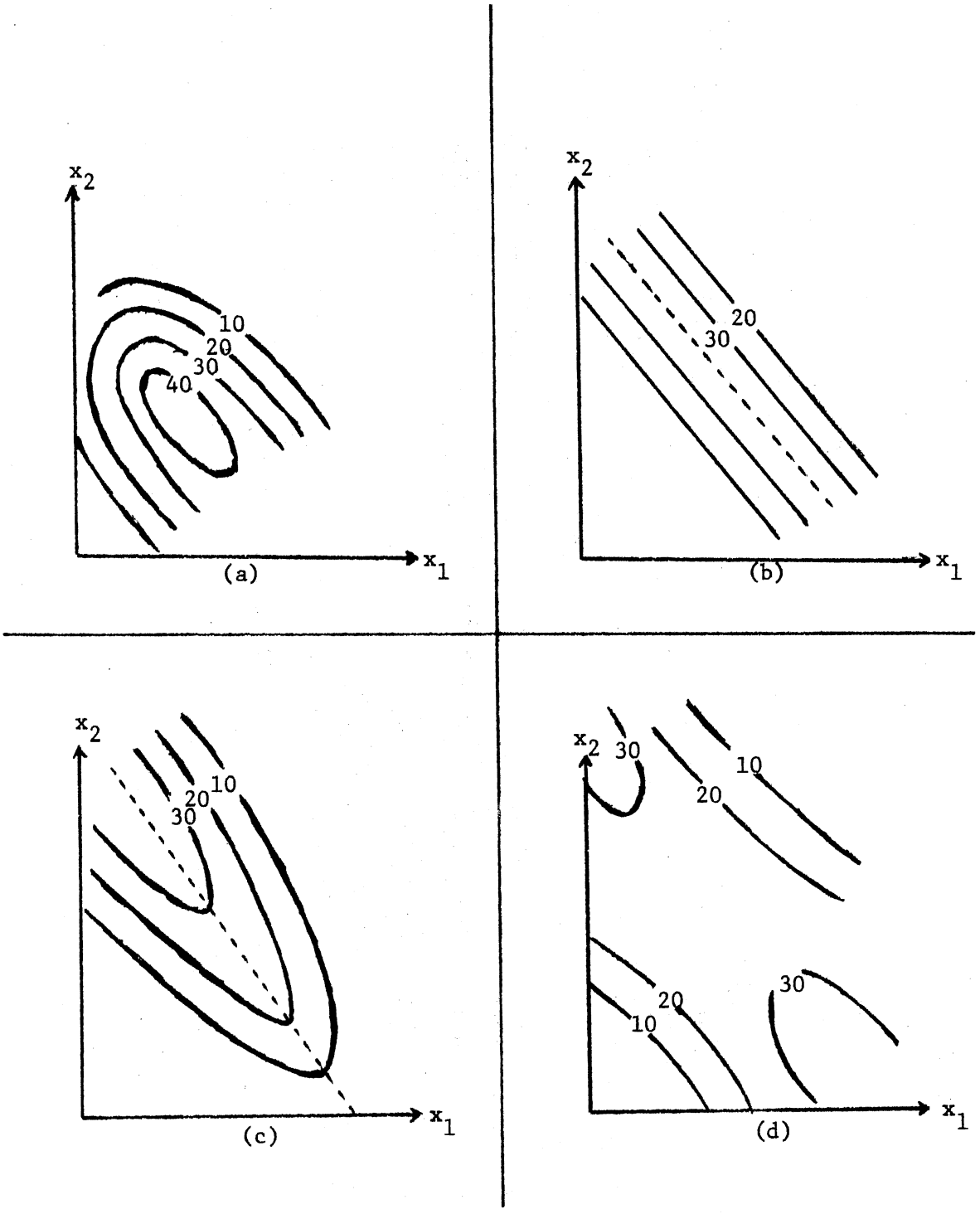


Figure 4. Contour Lines Corresponding to Four Possible Surfaces in a Near-Stationary Region

the direction of the steepest ascent is at right angles to the contour lines of equal responses. The slope of a contour line is itself a function of the relative scales of measurements for the two variables. There is no unique way of determining the relative scales of measurements but it is wise to select them such that the response function is symmetrical with respect to the factors (19).

A Review of Response Surfaces Experimental Designs

For any experiment, each combination of the levels of the factors represents one experimental point and the collection of such points used for employing the surface is called the experimental design. It is well realized that the random selection of experimental points may not only fail to provide accurate estimates of constants but might even furnish separate estimates of some coefficients. A well developed experimental design for estimating effects up to order d should meet the following requirements:

(a) The design should allow the approximating polynomial of order d (tentatively assumed to be representationally adequate) to be estimated with satisfactory accuracy within the region of interest.
(b) It should allow a check to be made on the representational accuracy of the assumed polynomial.
(c) It should not contain an excessively large number of points.
(d) It should lend itself to 'blocking'.
(e) It should form a nucleus from which a satisfactory design of order d+1 can be built in case the assumed degree of polynomial proves inadequate (9, p. 197).

A discussion of designs, in chronological order, is given below.

Factorial and Composite Designs

In 1951, Box and Wilson (10) initiated the development of experimental designs and method of analysis for fitting polynomials of first and second degree to the response surfaces. By applying first degree polynomials, one is able to calculate the first order effects by varying each of the factors at two levels. Box and Wilson set the levels of the factors at +1 and -1 and proposed complete and fractional two level factorial designs for estimating the linear coefficients. Cochran and Cox (16) have tabulated some useful first order designs as are shown in Table I.

TABLE I

SOME USEFUL FIRST ORDER DESIGNS

Number of Factors	Size of Experiment (units)	Fraction of a Full Factorial	Number of Degrees of Freedom "Lack of Fit"
3	8	1	4
4	8	1/2	3
5	8	1/4	2
5	16	1/2	10
6	8	1/8	1
6	16	1/4	9

Source: Cochran and Cox (16, p. 341).

The designs given in Table I provide some degrees of freedom for testing the adequacy of the linear model assuming that a measure of

experimental error variance is available.

To estimate the quadratic coefficients, each factor should take at least three values. Therefore, a natural tendency would be to use a complete or fractional three-level factorial design. But, when the number of factors is more than two, the number of observations required becomes excessively large. Further, the quadratic coefficients are estimated with a lower precision compared to the interaction coefficients (10).

To overcome these two problems, Box and Wilson (10) formulated composite designs. These designs are constructed by adding further treatment combinations to 2^k factorial or fractional factorial designs. Composite designs are classified into central and noncentral groups. In central composite designs there are (2k + 1) additional factor combinations tested at:

$(0, 0, \ldots, 0)$; $(-\alpha, 0, \ldots, 0)$; $(\alpha, 0, \ldots, 0)$; $(0, -\alpha, \ldots, 0)$;

$(0, \alpha, \ldots, 0)$; . . . $(0, 0, \ldots, -\alpha)$; $(0, 0, \ldots, \alpha)$.

Thus, the total number of experimental points is $(2^k + 2k + 1)$ which for $k \geq 4$ is smaller than 3^k.

Central designs are helpful when the result of the 2k factorial design suggests that the surface is curved and the center of the first experiment is close to a point of maximum. On the other hand, noncentral composite designs are used when the initial experiment indicates that a factor combination other than the center is close to the maximum. In noncentral composite designs, the number of treatment combinations added is k, one for each factor. The new level of each factor could be $1 + \alpha$ or $-1 - \alpha$ depending upon the possible location of the maximum. For example, in an experiment with three factors, if the point

of maximum is thought to be around (-1, -1, 1), then the extra treatment combinations are: $(-1-\alpha, -1, 1)$; $(-1, -1-\alpha, 1)$; $(-1, -1, 1+\alpha)$. Figure 5 shows central and noncentral composite designs for three factors.

In a subsequent paper, Box (2) examined the efficiency of coefficients in first order designs and concluded the following: assuming that the linear approximation is adequate, the most efficient first order designs of size N are obtained by having k mutually orthogonal column vectors each with N elements and orthogonal to U, the column vector of unit elements.[1] While the variance and covariances of the coefficients remain constant for orthogonal rotation of designs, the magnitude and the arrangement of possible biases will be different. Therefore, it is feasible to rotate the proposed designs until the biases are as small as possible. But, unless the experimenter has some prior knowledge of the response function, he would not be able to select the optimum design--the one with minimum bias.

DeBaun (20) expanded the idea of central composite designs by incorporating blocking effect into the analysis. Referring to our previous discussion of central composite designs, DeBaun derived a value for α that makes the added factor combinations form a block orthogonal to the one formed by the factorial or fractional factorial designs used in the first phase of the experiment.

Rotatable Designs

Box and Hunter's (9) work, in 1957, resulted in the development of

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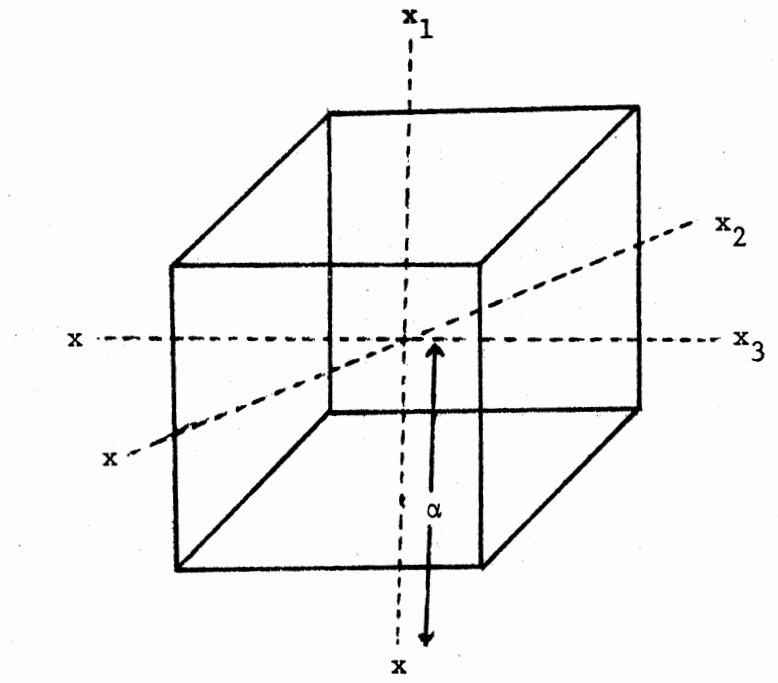
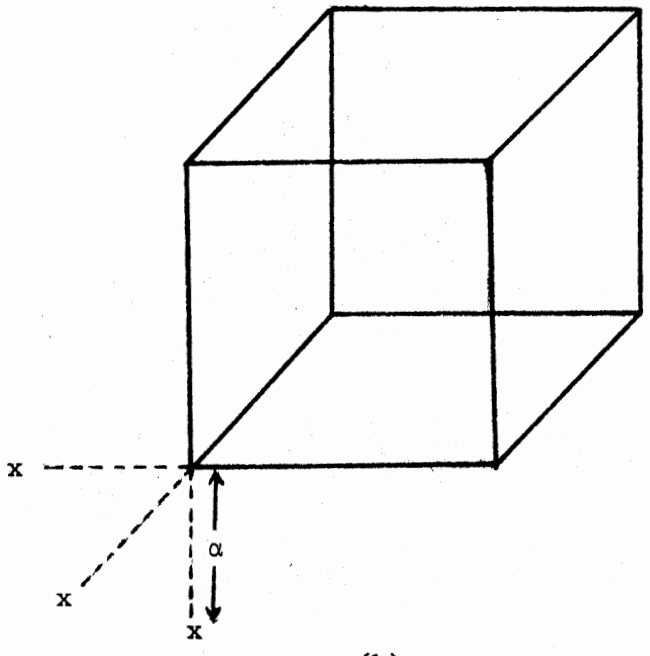
[1] Fortunately, factorial and fractional factorial designs proposed by Box and Wilson meet these requirements.



(a)



(b)

Figure 5. Central Composite Design (a) and Non-Central Composite Design (b)

rotatable designs. They argued that the previous attempts to find the best designs for fitting the model $\underline{G} = \underline{X\beta}$ to a surface was interpreted as selecting a design that would allow the coefficients to be separately estimated with the smallest variance.[2] In other words, the X'X matrix should be diagonal, implying orthogonal designs. While construction of first order orthogonal designs is an easy task, it poses some difficulties for second order designs since some of the independent variables become correlated, e.g., x_i^2 and x_j^2. This correlation is due to the standardized values of the variables, i.e., +1 and -1. But this problem can be resolved by redefining the independent variables in terms of the orthogonal polynomials. However, it is not clear that the second order orthogonal designs obtained this way are optimal for at least two reasons.

First, second order orthogonal designs may cause large biases in the estimated coefficients. Secondly, the quadratic coefficient β_{ii} measures the curvature of the surface in the direction of the ith coordinate axis. Orthogonal polynomials indicate the precision with which the curvature is determined in a given direction of the coordinates axes. However, the curvature may be measured with less precision in some other direction, possibly of equal importance to the designer. Based on these reasonings, Box and Hunter (9) formulated rotatable designs as are described below.

Let z, a k x 1 vector, represent an experimental point and $\hat{Y}_z$ denote the response estimated at this point. Also, assume that $\hat{Y}_z$ is obtained from a polynomial equation that was fitted by the method of

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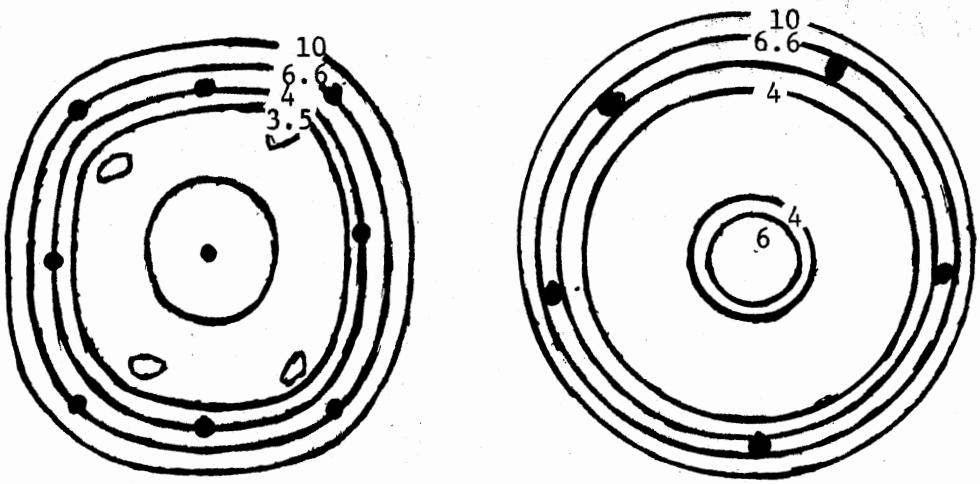
[2] $\underline{G}$ is an N x 1 column vector, $\underline{\beta}$ is a k x 1 column vector, and $\underline{X}$ is an N x k matrix.

least squares to N observations of an experimental design. Then, the variance of $\hat{Y}_z$ is a function of z and σ_E^2, the experimental error, and will certainly decrease if N is increased. Thus, the quantity $V(z) = NV(\hat{Y}_z)$ is called the variance function and is defined as the standardized measure of the accuracy with which a design estimates the response at point z. Figure 6 shows three variance functions for two dimensional designs.

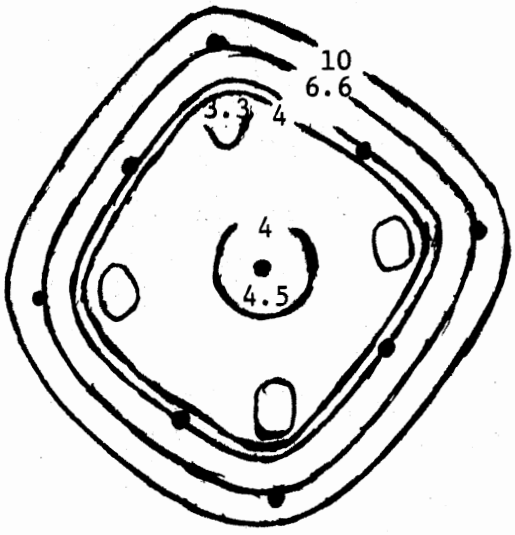
If there is no prior knowledge about the orientation of the surface, Box and Hunter (9) propose designs with variance functions like that of the pentagonal design shown in Figure 6(b). In other words, experiments would be designed such that the response is estimated with a constant variance for all the points equidistant from the origin of the design. A formal definition of rotatable designs is given by the authors:

> In general, for any k-dimensional design, if the variance of response estimated by the fitted polynomial is a function only of
>
> $$P^2 = \sum_{i=1}^{k} x_i^2$$
>
> so that the variance contours in the space of variables are circles, spheres, or hyperspheres centered at the origin, the design will be said to have a spherical variance function V(P). An arrangement of points giving such a variance function will be called a rotatable design (p. 205).

The conditions derived for first order rotatable designs coincide with the ones obtained for designs with smallest variance, i.e., X'X should be an identity matrix. To build second order rotatable designs, one should set all the odd moments at 0, second moments at 1, and exercise his option on the value of the fourth moment. For example, one value of the fourth moment makes the design rotatable as well as



(a) 3^2 Factorial Design (b) Pentagonal Design



(c) Composite Design

Source: Box and Hunter (9, p. 205).

Figure 6. Three Variance Contours for Two Dimensional Designs

orthogonal while another value of it makes the variance for the points on a circle with radius 1 equal to the variance for the points at the center. Box and Hunter (9) concluded their analysis by showing the formation of orthogonal blocking arrangements for rotatable designs.

A number of procedures have been proposed for constructing second order and third order rotatable designs. Central composite designs are capable of forming second order rotatable designs when the value of α is selected appropriately. Balanced incomplete block designs offer a method for building second and third order rotatable designs. Equiradial sets provide an alternative technique for building second and third order rotatable designs. Finally, second order rotatable designs may be formed by using first order designs.

Design Criterion of Mean Squared Deviation

In 1959, Box and Draper (6) criticized the previous approaches to deriving optimal designs for response surfaces on the grounds that they had only been concerned with the errors arising from sampling variation. They maintained that the fitted polynomial always fails, to some extent, to represent the true function and, therefore, there are two sources of discrepancy between the true function and the fitted equation to be considered. One source of discrepancy is due to the sampling variation and the other is because of the inadequacy of the fitted polynomial. The first one is called variance error and the second one is called bias error. Based on this logic, they derived new experimental designs that will be described next.

Let R be the immediate region of interest in the experimental region T. Also assume that a polynomial of degree d_1 is fitted to the

region R while the true function which provides an exact fit within the region T is of degree $d_2 > d_1$. Then the design should minimize:

$$J = \frac{N}{\sigma_E^2} \int_R E[\hat{Y}_z - G(z)]^2 \, dx \Big/ \int_R dx \tag{2.5}$$

where:

$G(z)$ = the true response at point z

$\hat{Y}_z$ = the estimated response at point z

N = the size of the experiment

σ_E^2 = the experimental error

$dx = dx_1, dx_2, \ldots, dx_k$

J gives the mean squared deviation from the true response, averaged over the region R and normalized with respect to the variance and the number of observations. It has two components: "variance error" and "bias error."

$$J = V + B$$

$$J = \frac{N\Omega}{2} \int_R V[\hat{Y}_z]dx + \frac{N\Omega}{2} \int_R [E\hat{Y}_z - G(z)]^2 dx \tag{2.6}$$

$$\Omega^{-1} = \int_R dx \tag{2.7}$$

where:

V = variance error

B = bias error.

For the situation where the true function is quadratic and a linear approximation was used, minimizing J resulted in an intuitively obvious result. If there is a strong belief about the adequacy of the linear model V alone should be minimized. On the other hand, if the sampling error is negligible and there is doubt about the linearity assumption, then B alone should be minimized. But one is very seldom confronted

with these extreme cases and of more value are cases in which variance and bias both occur. Investigation of these cases surprisingly revealed that the optimal design derived when bias and variance are minimized was very close to the one obtained when variance was totally ignored and bias alone was minimized.

To explain Box and Draper's (6) results, some terms need to be defined:

1. X_1 is a design matrix which includes terms of order d_1 and less.
2. c_{ij} is an element of the matrix $\underline{C}^{-1} = N(X_1'X_1)^{-1}$.
3. γ_i is the limit of the ith variance, i.e., $c_{11} \leq \gamma_1$.

When the surface is truly quadratic over the experimental region T and a linear polynomial is fitted to a smaller spherical region within T such that $\sum_{i=1}^{k} x_i^2 \leq 1$, it was concluded that:

(i) V + B is minimized for all β_{ij} and c_{ij}, when the third moments [ijk] of the design are chosen to be zero.
(ii) V alone is minimized, for T defined by $c_{ii} \leq \gamma_i$, when the design is chosen to be first order orthogonal with $c_{ii} = \gamma_i$, that is with the design of maximum possible size.
(iii) B alone is minimized when the design is chosen to be first order orthogonal with all third order moments zero and $c_{ij} = 1/(K+2)$.
(iv) V + B is minimized if values of β_{ij} averaged over all rotations are substituted, when the design has all third order moments zero and is first order orthogonal with the c_{ii} all equal (6, p. 638).

An optimal class of designs on the basis of these findings is fractional by replicated two-level factorial designs (in which no two factor interaction is confounded with the main effect) with added center points. These designs had already been applied to response surfaces by Box and Wilson (10). Box and Draper later discussed problems with cubic functions when the fitted polynomials are quadratic functions.

Designs for Cuboidal Experimental Regions

Draper and Lawrence (24) expanded Box and Draper's (6) methodology and examined situations with a cuboidal experimental region or when it can be made cuboidal by linear transformation of variables. For the all-biased case their designs are similar to Box and Draper's (6) rotatable designs. When both variance and bias are minimized they made the following recommendation:

Given

$$\gamma_u^2 = \sum_{i=1}^{k} x_{iu}^2 \qquad u = 1, 2, \ldots, N \tag{2.8}$$

then:

a. If a linear function is fitted to a quadratic surface, choose a design with large $\sum_{u=1}^{N} \gamma_u^4$.

b. If a quadratic function is fitted to a cubic surface choose a design with large $\sum_{u=1}^{N} \gamma_u^6$.

Additional Designs with Criterion of Mean Squared Deviation

In light of Box and Draper's results, Karson et al. (37), in 1969, suggested a new strategy for formulating optimum designs. Their method is designed to, first, minimize bias and then use any additional flexibility to minimize variance. To operationalize this idea, they developed an estimator such that for a given design:

1. Minimizes integrated square bias, B, due to terms of specified higher order omitted from the fitted polynomial.
2. Subject to (1) it achieves minimum integrated variance, V, for any fixed design.

Kupper and Meydrech (40), in 1973, made additional contributions to the formulation of efficient designs when integrated mean squared error is minimized. They advocated the use of $\underline{B}_1 = \underline{K}\underline{\beta}_1$, where K is a k x k diagonal matrix of appropriately chosen constants.[3] The "best" value of K, of course, depends on the unknown elements of the parameter vectors $\underline{\beta}_1$ and $\underline{\beta}_2$ ($\underline{\beta}_2$ represents the coefficients of the terms that have not been included in the model). But if based on the designer's knowledge some restriction can be imposed on one or more elements of $\underline{\beta}_1$, then it is possible to find a set of K's that result in J values smaller than K equal to an identity matrix for any choice of experimental design.

Although the approaches taken for designing efficient experiments have been different, the designs recommended for the most part have been the same. Complete factorial and fractional factorial designs are proposed for different reasons for estimating first order effects. To estimate second order effects, new experimental points are normally added to the result of factorial or fractional factorial designs. The design selected by the experimenter dictates the location and the number of additional points to be considered. The experimenter's choice of design itself depends on his knowledge of the situation. Any prior information about the response function enables him to economically find the optimum level of factors with more efficiency.

In the next chapter, Chapter III, the assignment of common, antithetic, and independent random numbers to the experimental points, for possible increases in efficiency, is discussed.

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[3] $\underline{B}_1$ and $\underline{\beta}_1$ are both k x 1 column vectors.

CHAPTER III

VARIANCE REDUCTION TECHNIQUES: COMMON AND ANTITHETIC RANDOM NUMBERS

Introduction

To implement a simulation experiment, after a model is built and validated, three critical phases remain to be considered. First, an appropriate computer language needs to be selected. Second, an experimental design that fits the situation should be formulated. Third, an efficient way of generating observations should be specified (17). Given the availability of many computer languages, the first phase will not create any difficulty for the designer. But the last two phases demand careful attention.

Simulation is a technique for performing sampling experiments on the abstract model of a real-world system. Therefore, all the experimental designs developed for physical experimentation are applicable to simulation experiments as well. The optimal design is undoubtedly the one that furnishes the maximum possible information with the minimum number of observations. The designs relevant to the purpose of this study were discussed in Chapter II and will not be repeated here.

Phase three deals with the efficiency of execution. Although it is possible to increase the precision in results by increasing the sample size, this is not usually a satisfactory or an economical solution.

Considerable progress has been made in developing techniques for increasing the efficiency of the desired estimators for a given sample size. These techniques, which were initially aimed at distribution sampling experiments, are called variance reduction techniques. The first complete survey of the literature in this field was conducted in 1964 by Hammersley and Handscomb (32).

Generally speaking, a technique is called variance-reducing if the reduction in variance is proportionately larger than the increase in the work involved. Thus, when comparing variance reduction techniques it is meaningless to look at the absolute reduction in variances without comparing the extra computer work involved. The most commonly known variance reduction techniques are:

1. Stratified Sampling,
2. Selective Sampling,
3. Control Variates,
4. Importance Sampling,
5. Antithetic Variates, and
6. Common Random Numbers.

Before examining the last two techniques in detail, it is necessary to clarify what is meant by increasing the precision of results or reducing variances. A variance reduction technique, when applied to an experimental design (as opposed to just one design point), may reduce the variances of some desired estimates but increase the variance of some other estimates as well. Therefore, care must be exercised in applying these techniques to avoid increase in the variances of the sensitive estimates. This issue will be clarified with respect to variance reduction techniques applied to response surface designs in Chapter IV.

This chapter focuses on the use of common and antithetic random numbers in simulation studies. In what follows, first, the rationale behind the use of these two techniques is explained. Second, the role of random numbers in running a simulation model is discussed. Third, the underlying statistical theory for very simple cases will be shown. Last, the possibility and the advantages of using the two techniques in the same simulation experiment will be examined.

Common and Antithetic Random Numbers Versus Other Variance Reducing Techniques

Many reasons can be cited for preferring common random numbers and antithetic variates techniques over the other variance reducing techniques. Some of the important reasons are as follows:

1. As mentioned earlier, the extra computer work involved for implementing each of the variance reduction techniques is a crucial factor in using them. But, unlike the first four techniques, antithetic variates and common random numbers require no or little extra computer programming time (38).

2. The purpose of many simulation analyses is to compare two or more systems. To have a fair comparison, it is natural to evaluate the performances of these systems under similar experimental conditions. In other words, the same random events should occur when each system is simulated. Using the same sequence of random numbers is one way of creating the same experimental circumstances.

3. Common random numbers and antithetic variates are capable of inducing positive and negative correlation between responses obtained

under different experimental conditions. The induced correlations can significantly increase the precision of simulation results. Schruben and Margolin (52) have shown situations in which improvement will occur regardless of the sign of correlations induced.

4. Simulations can be stopped and restarted without disturbing their stochastic properties permitting an early check on the sign of induced correlations.

The Role of Random Numbers

Simulations ordinarily have one or more stochastic variables with a known probability distribution. Therefore, a mechanism is needed for random selection of observations from the given probability distribution. Uniformly distributed random numbers have served this purpose for a long time. They can be either stored in the computer or be generated by the computer itself through the use of a sequential technique. Uniformly distributed random numbers (hereinafter called "random numbers") are a sequence of real numbers scaled to the interval [0,1] and meet two requirements:

1. They are statistically independent.
2. Each number in the sequence has an equal probability of taking on any value on the interval [0,1].

Since the random numbers generated by the computer are reproducible and predictable, they have sometimes been called pseudorandom numbers.

The three most common ways of generating random numbers are additive, multiplicative, and mixed congruential methods. These three techniques are based on recursive formulas which generate each random number from the knowledge of the previous one given an initial value,

called a seed, is provided. For example, the recursive formula for the mixed congruential method is:

$$r_{n+1} = (ar_n + c)(\text{modulo } m),$$

where a, c, and m are all positive integers such that a and c are both smaller than m (38). The relationship states that r_{n+1} is the remainder when $(ar_n + c)$ is divided by m. A complete discussion of these three and other random number generation techniques is given by a number of authors (39) and will not be covered here.

When a simulation consists of more than one stochastic component, separate streams of random numbers are normally used to derive each individual component. The logic behind this practice is to synchronize the output of different observations and increase the magnitude of the intended correlation between them (38). For the purpose of this study, the issues of how random numbers are generated and whether they contain one or more stream of random numbers are irrelevant and will not be discussed any further. However, it will be assumed that a common generator is used throughout the experiment to generate the random numbers needed.

Common Random Numbers

Two streams of random numbers will be identical if they have the same seed values. The use of common random numbers is recommended for maintaining homogeneous experimental conditions when the objective of simulation is to compare several alternatives. In order to compare two alternatives and make a statement about the relative superiority of one over the other, the differences among system responses, call it Γ,

should be calculated. Common random numbers can cause positive correlation between system responses which in turn leads to reduction in the variance of Γ. Let $\bar{y}_1$ denote the estimated response of system 1 and let $\bar{y}_2$ represent the estimated response of system 2, then the variance of can be expressed as:

$$\text{var}(\Gamma) = \text{var}(\bar{y}_1 - \bar{y}_2) = \text{var}(\bar{y}_1) + \text{var}(\bar{y}_2) - 2\ \text{cov}(\bar{y}_1, \bar{y}_2). \quad (3.1)$$

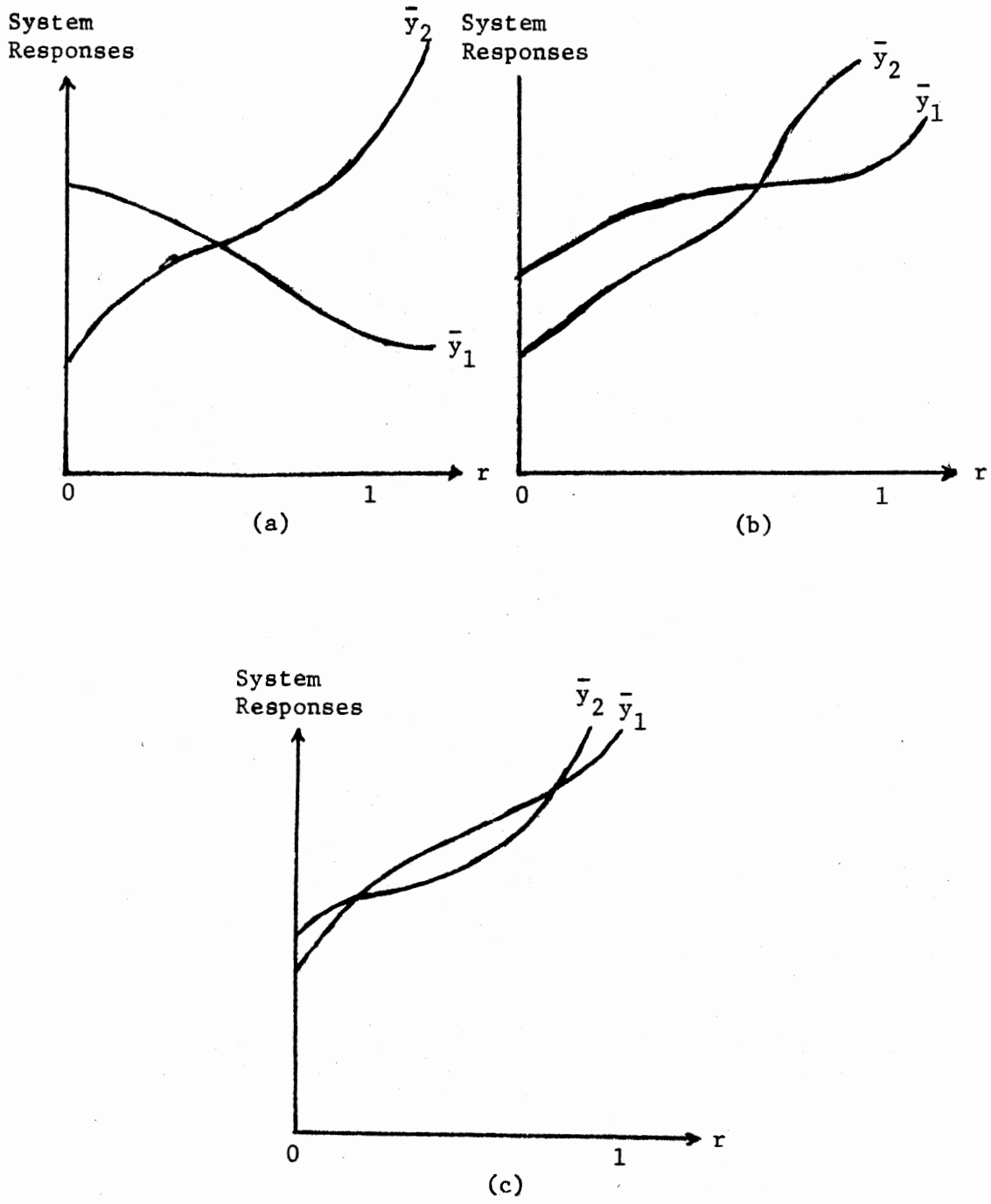
Thus, the variance of Γ will decrease whenever common random numbers make the covariance term positive. This will be the case only if both systems react similarly to the stochastic input variables. This point is graphically shown in Figure 7, adopted from Kleijnen (38).

Figure 7a illustrates a situation where assigning common random numbers results in negative instead of positive correlation. Application of random numbers to situations like Figure 7b leads to weak positive correlation. Figure 7c shows a situation where $\bar{y}_1$ and $\bar{y}_2$ will be positively correlated when using the same random numbers.

Although the relationship between the random numbers and the output in simulation is very complex, it is reasonable to assume that both systems react in the same direction, i.e., positive correlation is induced.

Antithetic Variates

The antithetic variates technique was devised by Hammersley and Morton (33) for creating negative correlations in Monte Carlo estimation of the value of an integral. Using this technique, one observation is generated from r, a random number, and the next one from (1 - r) for the same system. Let $\bar{y}_1$ represent the sample mean that is used for



Source: Kleijnen (38).

Figure 7. System Responses with the Same Random Numbers

estimating $\bar{G}$, the mean of the system responses. Also, let $\bar{y}_{11}$ and $\bar{y}_{12}$ denote the responses when r and (1 - r) are used respectively. Then,

$$\bar{y}_1 = 1/2(\bar{y}_{11} + \bar{y}_{12}) \tag{3.2}$$

$$\text{var}(\bar{y}_1) = 1/4[\text{var}(\bar{y}_{11}) + \text{var}(\bar{y}_{12}) + 2\ \text{cov}(\bar{y}_{11} + \bar{y}_{12})] \tag{3.3}$$

Therefore, if $\bar{y}_{11}$ and $\bar{y}_{12}$ are negatively correlated, the covariance term in (3.3) is negative, and the variance of $\bar{y}_1$ will consequently decrease.

To explain the logic behind the induction of negative correlations, the following three assumptions need to be made:

1. There is only one single value of an input variable affecting the output to be considered.
2. There exists an increasing monotonic relationship between the output and the input variable.
3. There is an increasing monotonic relationship between the input variable and r, the random number.

Now it is intuitively obvious that r and 1 - r generate high and low or low and high values of the input variable and consequently lead to negatively correlated responses under the foregoing assumptions.

In practice, however, the assumptions made are unrealistic and are almost always violated. The responses depend on a sequence of random numbers, there is more than one input variable involved, and the monotonic relationship is unjustified. When either one of these assumptions is relaxed it becomes very difficult, if not impossible, to show that the antithetic random numbers generate negative correlation. A complete discussion of common and antithetic random numbers techniques along with some empirical findings is given by Kleijnen (38).

Joint Application of Common and Antithetic Random Numbers

Few studies have been conducted to investigate the application of common and antithetic random numbers within the same simulation experiment. These studies fall into two categories: those which limit the use of antithetic random numbers to replicate observations within the same system and those which do not. In the first category, Kleijnen's (38) work is reviewed. Table II shows a situation where both common and antithetic random numbers are applied.

TABLE II

JOINT APPLICATION OF ANTITHETIC AND COMMON RANDOM NUMBERS

Run	System 1		System 2	
	Random Numbers	Response	Random Numbers	Response
1	$\underline{R}_1$*	$\bar{y}_{11}$	$\underline{R}_1$	$\bar{y}_{21}$
2	$\underline{1} - \underline{R}_1$	$\bar{y}_{12}$	$\underline{1} - \underline{R}_1$	$\bar{y}_{22}$
3	$\underline{R}_2$	$\bar{y}_{13}$	$\underline{R}_2$	$\bar{y}_{23}$
4	$\underline{1} - \underline{R}_2$	$\bar{y}_{14}$	$\underline{1} - \underline{R}_2$	$\bar{y}_{24}$
⋮	⋮	⋮	⋮	⋮

*Capital $\underline{R}$ represents a vector of random numbers and $\underline{1}$ is a vector of ones.

Source: Kleijnen (38, p. 210).

Denoting the difference between the two systems by $\bar{\Gamma}$, it follows:

$$\bar{\Gamma} = \bar{y}_1 - \bar{y}_2 \tag{3.4}$$

$$\text{var}(\bar{\Gamma}) = \text{var}\ \bar{y}_1 + \text{var}\ \bar{y}_2 - 2\ \text{cov}(\bar{y}_1, \bar{y}_2) \tag{3.5}$$

$$\text{var}(\bar{\Gamma}) = M^{-2} \sum_{i \neq g} \sum \text{cov}(\bar{y}_{1i}, \bar{y}_{1g}) + M^{-1}\sigma_1^2 +$$

$$N^{-2} \sum_{j \neq h} \sum \text{cov}(\bar{y}_{2j}, \bar{y}_{2h}) + N^{-1}\sigma_2^2 -$$

$$2M^{-1}N^{-1} \sum_{i=1} \sum_{j=1} \text{cov}(\bar{y}_{1i}, \bar{y}_{2j}) \tag{3.6}$$

where:

M = the number of runs for system 1.

N = the number of runs for system 2 which is not necessarily equal to M.

$$\sigma_1^2 = \text{var}(\bar{y}_{1i}) = \text{var}(\bar{y}_{1g}) \qquad i, g = 1, \ldots, M \tag{3.7}$$

$$\sigma_2^2 = \text{var}(\bar{y}_{2j}) = \text{var}(\bar{y}_{2h}) \qquad j, h = 1, \ldots, N \tag{3.8}$$

To reduce the variance of $\bar{d}$, the covariances in (3.6) should have the following signs:

$$\text{cov}(\bar{y}_{1i}, \bar{y}_{1g}) < 0 \qquad i \neq g \qquad k, g = 1, \ldots, M \tag{3.9}$$

$$\text{cov}(\bar{y}_{2j}, \bar{y}_{2h}) < 0 \qquad j \neq h \qquad j, h = 1, \ldots, N \tag{3.10}$$

$$\text{cov}(\bar{y}_{1i}, \bar{y}_{2j}) < 0 \qquad i = 1, \ldots M \quad j = 1, \ldots, N \tag{3.11}$$

Since the correlation between $\bar{y}_{1i}$ and $\bar{y}_{2i}$ is positive and the correlation between $\bar{y}_{2i}$ and $\bar{y}_{2,i+1}$ is negative, it follows that $\bar{y}_{1i}$ and $\bar{y}_{2,i+1}$ are negatively correlated. Similarly, $\bar{y}_{2i}$ and $\bar{y}_{1,i+1}$ are negatively correlated. These negative cross-correlations, corresponding to (3.11), are undesirable and will increase the variance. Thus,

Kleijnen's (38) analysis remains inconclusive. He then compared the efficiency of employing only common random numbers, only antithetic random numbers, and both antithetic and common random numbers within the same experiment. The empirical result did not favor any one of these techniques over others (38).

The motive behind the development of the second category stems from the difficulties of deriving mathematical proofs supporting generation of positive and negative correlations between simulation responses. The difficulty arises due to the nature of simulation. Simulations are mainly used when the analytical treatment of a situation is not possible. If all the relationships were mathematically well-defined, techniques other than simulation would be more efficient (55). That being the case, Fishman (27), in 1974, and very recently Schruben and Margolin (52) based their work on the following assumptions:

> Assumption 1: When two observations are made with the same randomly selected set of streams, a positive correlation of unknown magnitude is induced between the mean responses.
>
> Assumption 2: When two observations are made with the same randomly selected set of seeds, but with antithetic streams, a negative correlation of unknown magnitude is induced between the mean responses.
>
> Assumption 3: When two observations are made with different randomly selected streams, the mean responses have zero correlation (p. 508).

Although applying common and antithetic random numbers has in some cases decreased the sensitivity of the analysis, the empirical results in general support the above assumptions. These assumptions provide a simulation designer with three alternatives for assigning random numbers to each experimental point. First, a vector of random numbers

(VRN) used at another experimental point might be selected, causing positive correlation. Second, a VRN can be selected such that its elements are the same as another VRN subtracted from one, generating negative correlation. Finally, selecting a VRN not utilized at any other point will result in uncorrelated responses.

The objective of Fishman's (27) analysis was to detect the effects of using correlated random number streams in simulations with linear and quadratic response surfaces. The equations he examined were:

$$y_i = \beta_o + \beta_1 x_i + \varepsilon_i \tag{3.12}$$

$$y_i = \beta_o + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i \tag{3.13}$$

Two and three observations were used to estimate β coefficients in equations (3.12) and (3.13) respectively. Hence, correlations between the y's can be expressed as:

$$\text{cov}(Y) = \sigma_E^2 \begin{bmatrix} 1 & \phi \\ \phi & 1 \end{bmatrix} \tag{3.14}$$

where Y is the vector of y values and ϕ is the correlation between y_1 and y_2.

$$\text{cov}(Y) = \sigma_E^2 \begin{bmatrix} 1 & \phi_{12} & \phi_{13} \\ \phi_{12} & 1 & \phi_{23} \\ \phi_{13} & \phi_{23} & 1 \end{bmatrix} \tag{3.15}$$

where Y is again the vector of y values and ϕ_{ij} is the correlation between y_i and y_j.

Three criteria [(1) generalized variance, (2) prediction variance, (3) slope variance] were the basis for finding the optimal sign of the ϕ's. For the linear model it was shown that either positively or negatively correlated responses were superior over the independent

responses. For the quadratic case, 27 possible designs were considered. Six of these produced a smaller generalized variance and one resulted in smaller prediction variance. However, no plan guaranteed a smaller slope variance.

In contrast to the discouraging outcome of Fishman's (27) study, Schruben and Margolin (52) have obtained very promising results. The model they adopted was of the form:

$$\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon} \tag{3.16}$$

where $\underline{Y}$ is an N x 1 column vector, $\underline{\beta}$ is a k x 1 column vector, and $\underline{X}$ is an N x k matrix.

Their objective was to find the best design for efficient estimation of $\underline{\beta}$ in (3.16). The efficiency was measured by the determinant of the estimator dispersion matrix. In other words, the design with the smallest value for the determinant of the estimator dispersion matrix would be the most efficient design. Designs that minimize this determinant are called D optimal (8). After incorporating blocking into their analytical work, Schruben and Margolin (52) concluded:

> Assignment Rule: For the model in (3.16) with k+1 parameters, the N-point experimental design admits orthogonal blocking into two blocks of sizes N_1 and N_2, preferably chosen to be as nearly equal in size as possible; then for all N_1 design points in the first block, use a set of pseudorandom numbers $\underline{R}$, chosen randomly, and for all N_2 design points in the second block, use $\underline{1}-\underline{R}$ (p. 513).

The assignment rule will give ordinary least square estimators with smaller D value than will (1) the assignment of the same random number(s) to all the design points or (2) the assignment of different random numbers to the design points when the following inequality is met:

$$1 + (N - 1)\rho_+ - 2N^{-1}N_1N_2(\rho_+ + \rho_-)\ (1 - \rho_+)^k < 1 \tag{3.17}$$

> Theorem: Assume that the model in (3.16) consists of the mean plus a subset of $k(k < 2^{n-r})$ effects. Then, over the class of designs consisting of $N = 2^{n-r}(r \geq 0)$ design points (with replication allowed), together with all feasible induced correlation structures subject to $\rho_+ = \rho_- = \rho$,[1] a 2^{n-r} fractional factorial design with the Assignment Rule results in minimum generalized variance for either the OLS or WLS[2] estimators, i.e., the D criterion is minimized (p. 514).

The findings were proved by:

1. Assuming a unit variance for the responses.
2. Partitioning the $\underline{X}'\underline{X}$ matrix into two parts corresponding to the mean effect and all the remaining effects.
3. Making the appropriate substitution for the signs of the induced correlations.[3]
4. Calculating and comparing the determinants of the estimator dispersion matrix for the alternative assignment rules.[3]

The analytical conclusions were tested empirically by applying them to a hospital resource allocation problem. The empirical results, in general, confirmed the analytical findings except for the assumption that positive and negative correlations are of equal magnitude.

Since Schruben and Margolin's (52) assignment rule will be applied to response surface designs in the next chapter, a word of caution about the optimality of this assignment rule is in order. A necessary, but not sufficient, condition for superiority of the recommended rule over assignment of (1) common random numbers or (2) independent random

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[1] ρ is the correlation coefficient.

[2] OLS means ordinary least squares and WLS means weighted least squares.

[3] The results are shown and discussed in the next chapter.

numbers to each design point is that the systems responses behave similarly with a given set of random numbers. While most of the empirical results reported support such an assumption, it is not so difficult to find systems which violate this assumption.

Wright and Ramsey (56) recently presented some simulation problems for which the use of common random numbers augmented the variance. They showed, as the literature suggests, that the common random numbers technique is least effective when the policies compared are not small perturbations of each other. That being the case, extra care must be exercised in applying the common random numbers technique to response surface designs. Fortunately, however, simulation models can be stopped and restarted without disturbing the statistical properties of their results. Therefore, an early check on the sign and the magnitude of the assumed correlations will make it possible for a designer to test the validity of his assumptions.

In Chapter IV, first, a methodology will be developed to help simulation designers select an appropriate response surface design. Next, the application of Schruben and Margolin's (52) assignment rule to those designs will be examined. Last, an inventory simulation example will be evaluated.

CHAPTER IV

SELECTION OF A RESPONSE SURFACE DESIGN

Introduction

A problem that a simulation designer often faces is finding the relatively optimal values of the controllable conditions, i.e., the values that will optimize the simulated responses. For example, in an inventory simulation the objective could be to determine the ordering quantity and the reordering level that will result in minimum inventory cost. The first objective of this chapter is to develop a systematic procedure by which one can select a response surface design for simulation experiments. The selection will naturally be based on one's objective and his knowledge of the relationships involved in the problem. The second objective is to develop a methodology for incorporating a random numbers assignment rule, proposed by Schruben and Margolin, in response surface designs. The final objective is to provide an opportunity for demonstrating and testing the results by the use of an inventory simulation example. To begin the discussion, a few terms and concepts will be redefined.

Model

The equation that represents the assumed mathematical relationship between the simulated responses, G, and the controllable conditions, ξ's, can be written as:

$$G = f(\xi_1, \xi_2, \ldots, \xi_k) \tag{4.1}$$

To explore the unknown relationship (4.1), a polynomial equation is normally adopted. Denoting the observed simulated responses by y (which is different than the actual responses G), the polynomial equation can be expressed as:

$$y = \beta_0 + \beta_1\xi_1 + \beta_2\xi_2 + \ldots + \beta_k\xi_k + \beta_{11}\varepsilon_1^2 + \ldots + \beta_{kk}\varepsilon_k^2 + \beta_{12}\xi_1\xi_2 + \beta_{13}\xi_1\xi_3 + \beta_{k-1,k}\xi_{k-1}\xi_k + \beta_{111}\xi_1^3 + \ldots \tag{4.2}$$

Although the ultimate objective is to find the optimal values of the ξ's, an intermediate objective would be to estimate the β coefficients. Viewing the polynomial equation as a regression equation, β coefficients can be estimated through the least square procedure if an adequate number of observations (experimental points) are available. Each observation corresponds to a set of values for the controllable conditions with an observed simulated response for that combination.

Standardized Variables

Different simulation experiments have different controllable conditions. Therefore, to generalize the discussion, the controllable factors are assumed to be standardized as follows:

$$x_{iu} = \frac{(\xi_{iu} - \bar{\xi}_i)}{S_i} \tag{4.3}$$

where

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

It follows then that,

$$\sum_{u=1}^{N} x_{iu} = 0 \quad \text{and} \quad \sum_{u=1}^{N} x_{iu}^2 = N,$$

where N is the total number of observations.

The Search Technique

The search technique adopted for the methodology presented in this chapter is the steepest ascent technique. This technique was explained in Chapter II and will not be repeated here.

The Relative Scales of Variables

In the steepest ascent technique, the direction of search is determined by the magnitude and the signs of the first order coefficients, i.e., β_1, β_2, ..., β_k which are estimated through fitting a first order polynomial. The relative magnitude of these coefficients is heavily influenced by the units chosen for the variables. An example will clarify this point. In an inventory simulation, let the ordering quantity vary between 5,000 to 50,000 units. Also, let the experimental levels of this variable be -1, 0, and +1. The designer should then decide how many units of the ordering quantity will correspond to one experimental unit. If, for instance, 5,000 units of the ordering quantity represents one experimental unit, 5,000, 10,000, and 15,000 units will represent experimental levels of -1, 0, and +1 respectively. The decision is normally based on the designer's insight and the units selected for the other variables. It is wise and logical to choose the units such that the response varies symmetrically with respect to all

the factors. Failure to use the appropriate units will increase the amount of work required for finding the optimum conditions.

Experimental Region and Subregions

A set consisting of all the possible combinations of the values of the controllable conditions is called the experimental region. Due to the quantitative nature of these conditions, the set has an infinite number of points in it. Thus, an exhaustive search of the experimental region is not possible. When the steepest ascent technique is employed, the experimenter evaluates a small region (subregion) of the experimental region which leads to another subregion, etc.; this process continues until the region with the possible optimum is found. The designs that will be discussed in this chapter will explore spherical subregions with radii equal to one.

Features of the Designs

The designs to be presented in this chapter have been constructed to satisfy, to the extent possible, the following features:

1. The design should allow the approximating polynomial of degree d (tentatively assumed to be representationally adequate) to be estimated with satisfactory accuracy within the region of interest.
2. It should allow a check to be made on the representational accuracy of the assumed polynomial.
3. It should not contain an excessively large number of experimental points.
4. It should lend itself to "blocking".

5. It should form a nucleus from which a satisfactory design of order d+1 can be built in case the assumed degree of polynomial proves inadequate (9).

Experimenter's Priorities (Objectives)

Suppose a polynomial of degree d_1 is fitted to a small region (R) of an experimental region (T) that can truly be represented by a polynomial of degree $d_2 > d_1$. Also, assume that a least square regression with an N points design is used to fit the polynomial of degree d_1 to R. Denoting the true response for a point z by G(z), the estimated response by y(z), and the estimated experimental error by σ_E^2, the mean squared deviation, J, is given by:

$$J = \frac{N}{\sigma^2} \int_R E[y(z) - G(z)]^2 \, dx \Big/ \int_R dx \tag{4.4}$$

Expression (4.4) can be rewritten as:

$$J = V + B \tag{4.5}$$

$$J = \frac{N\Omega}{\sigma_E^2} \int_R V[y(z)]dx + \frac{N\Omega}{\sigma_E^2} \int_R [E[y(z)] - G(z)]^2 \, dx \tag{4.6}$$

where

$\Omega^{-1} = \int_R dx$,

V = variance error, and

B = bias error.

To select a response surface design, priorities need to be assigned to variance and bias portions of mean squared deviations. The priorities may take one of the following three forms:

1. Minimizing variance is more important than minimizing bias.

2. Minimizing bias is more important than minimizing variance.

3. Minimizing bias and variance are equally important.

The experimenter's knowledge of the problem dictates the alternative to be selected. This knowledge may be summarized as follows:

(i) The magnitude of the experimental errors.

(ii) The complexity of the response surface.

When the experimental errors are large, minimizing variance becomes more important. On the other hand, when the experimental errors are small and the response function is complex, minimizing bias becomes more important.

Assumption

In what follows it will be assumed that a linear or a quadratic equation adequately represents the true function. Therefore, the discussion will be limited to first and second order designs (models).

First Order Models

A plane is assumed to be adequate for representing the true function. The model to be fitted is:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_n x_n \qquad (4.7)$$

The β coefficients in (4.7) can be estimated through one of the paths indicated in the following tree diagram.

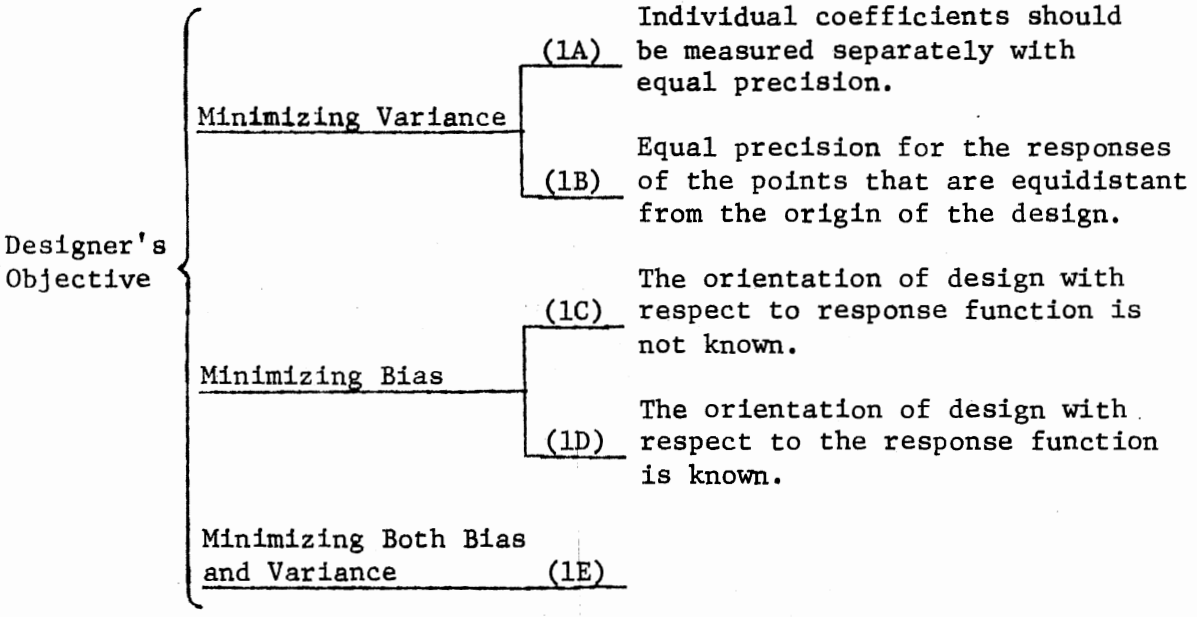

Figure 8. First Order Design Options

Case (1A)--Individual Coefficients Should Be Measured Separately with Equal Precision

Orthogonal designs will meet the above requirements. Two types of designs need to be distinguished at this point (10). Designs of type A provide unbiased estimated of linear coefficients, given that terms of higher order are insignificant. Designs of type B provide unbiased estimates of linear coefficients even though terms of second degree may exist.

For designs of type A, the number of observations, N, does not have to exceed the number of variables, M. For designs of type B, N must be larger than M to allow for disassociation of the linear coefficients from the second degree coefficients.

To estimate the β coefficients of a plane, the variables should take at least two different values. Therefore, complete and fractional factorial designs are used to construct designs of type A and B. If all the 2^k possible combinations are performed, the design will be a complete factorial; and when some of the combinations are not performed, the design will be an incomplete factorial. In the latter category, multifactor designs of Plackett and Burman (50) that furnish designs for 3, 7, 11, 15, ..., 4k-1, 99 factors in N = 4, 8, 12, 16, ..., 4k, 100 (excepting 92) are appropriate for designs of type A. The first column of these designs consists of entirely ones, and the remaining columns have equal numbers of +1 and -1. When N is a power of 2 these designs correspond to fractional factorial designs. For example, for k = 7 and N = 8, Plackett and Burman's design will be the same as 1/16 replication of the 2^7 factorial design. The design and its defining contrasts are shown in Table III.

For intermediate values of k the next higher value is used and the appropriate columns are omitted. For example, for k = 5, columns 6 and 7 of Table III will be deleted.

Duplicating Plackett and Burman's designs of appropriate size with reversed signs results in designs of type B. In other words, from a type A design with N-1 factors and N observations, one can obtain a type B design for N factors with 2N observations. For example, when all the entries of Table III are multiplied by a minus sign and are added to the original design, a type B design for eight factors will be obtained.

When fractional factorial designs are used in building designs of type A and B, the designer should not associate possible significant interaction effects with the linear effects. In other words, if there

is doubt about the interaction between two factors, the experiment should allow for isolating the suspicious interaction effect.

TABLE III

PLACKETT AND BURMAN'S DESIGN FOR SEVEN FACTORS, 1/16 REPLICATIONS OF 2^7 FACTORIAL DESIGN

Defining Contrasts: 127 = 135 = 146 = 236 = 245 = 347 = 567 = 1234 = 1256 = 1367 = 1457 = 2357 = 3467 = 3456 = 1234567 = -1

Factors	1	2	3	4	5	6	7
	+1	+1	+1	+1	-1	-1	-1
	+1	+1	-1	-1	+1	+1	-1
	+1	-1	+1	-1	-1	+1	+1
	+1	-1	-1	+1	+1	-1	+1
	-1	+1	+1	-1	+1	-1	+1
	-1	+1	-1	+1	-1	+1	+1
	-1	-1	+1	+1	+1	+1	-1
	-1	-1	-1	-1	-1	-1	-1

Case (1B)--Equal Precision for Responses of All the Points that are Equidistant from The Origin of the Design

Designs satisfying the above condition are called rotatable designs. A first order rotatable design should meet the following requirements:

1. All moments of order 1 should be zero. $\frac{\sum_{u=1}^{N} x_{iu}}{N} = 0$.

2. Mixed moments of order 2 must be zero. $\frac{\sum_{u=1}^{N} x_{iu} x_{ju}}{N} = 0$.

3. Pure quadratic moments should be equal to a constant. Given the scale convention, this constant is equal to 1. $\frac{\sum_{u=1}^{N} x_{iu}^2}{N} = 1$.

Orthogonal designs discussed for Case (1A) meet the above requirements. Therefore, first order orthogonal designs are first order rotatable designs as well. When the second order terms, contrary to the assumption, are significant, then the expected values of the β coefficients will be as follows (9):

$$E(\beta_0) = \beta_0 + \frac{\sum_{u=1}^{N} x_{iu}^2}{N} \sum_{m=1}^{k} \beta_{mm} \qquad m = 1, \ldots, k, \qquad (4.7)$$

$$E(\beta_m) = \beta_m + \frac{\sum_{u=1}^{N} x_{iu} x_{ju} x_{\ell u}}{N} \sum_{g=1}^{k} \sum_{h=1}^{k} \beta_{gh} \qquad g \text{ and } h = 1, \ldots, k \qquad (4.8)$$

Based on the scale convention, $\sum_{u=1}^{N} x_{iu} = 1$. Therefore, when the pure quadratic terms are present, the estimate of β_0 will certainly be biased. On the other hand, if the designed is formed such that the mixed third

order moments are zero, the estimates of the linear effects, β_m's, will be unbiased. Designs of this type may be obtained by duplicating any first order orthogonal design. Thus, designs of type B discussed in Case 1A will meet this requirement.

Case (1C)--Minimizing Bias When the Orientation of Design with Respect to the Response Function is Not Known

There will be interest in minimizing bias when a linear function is fitted but the true function is suspected to be quadratic. The proposed designs in this category are first order orthogonal designs with all the third order moments zero. The requirement that all third order moments should be zero is equivalent to choosing the factorial replicates so that no two factor interaction is confounded with a main effect. The legitimacy of this requirement was explained in case 1B. It is interesting to note that the minimiziation of bias separately requires the use of orthogonal designs which also minimize variance. Designs of type B satisfy the required condition.

A second requirement is that the variances of the β coefficients, assuming that the subregion under investigation is spherical with radius equal to one, must be equal to $\frac{1}{k+2}$ (6, p. 637). This, in turn, implies that the mean square distance (MSD) of the experimental points from the center of the design (or subregion) should be equal to $(\frac{k}{k+2})$.

$$MSD = \left(\sum_{m=1}^{k} x_m^2 \right)^{1/2} \quad \text{for all the N points.}$$

$$\left(\sum_{m=1}^{k} x_m^2\right)^{1/2} = \left(\frac{k}{k+2}\right)^{1/2} \quad \text{thus,} \tag{4.9}$$

$$x_m = \pm \left(\frac{1}{k+2}\right)^{1/2}$$

For example, when k = 4, the design to be adopted should be a type B design and the levels of the variables should be equal to the square roots of $\frac{1}{4+2}$, i.e., +.41 and -.41.

Case (1D)--Minimizing Bias When Orientation of Design with Respect to the Response Function is Known

In practice, examples of this case are hard to find. Nevertheless, when prior knowledge of the second degree equation is available, it might be possible to reduce bias by the orthogonal rotation of first order orthogonal designs. While orthogonal rotation of design will not affect the variances and covariances, it will change the magnitude and the arrangement of possible biases. Therefore, prior knowledge of the response function enables the designer to rotate the design until the arrangement that minimizes bias is obtained. A detailed discussion is given by Box (2).

Case (1E)--Minimizing Both Bias and Variance

The suggested designs again are first order orthogonal designs with third order moments zero and with the variances of the β coefficients all equal. With respect to the MSD of the experimental points from the center of the design, Box and Draper's analysis was led to an

intuitively obvious result: the MSD of the experimental points must be greater than $(\frac{k}{k+2})^{1/2}$ (the MSD for minimization of bias alone) and less than unity (the MSD for minimization of variance alone). Since it is unlikely for a designer to know, in advance, about the magnitude of the experimental errors as compared to the extent of bias, is it not possible to determine MSD precisely.

Recapitulation

First order orthogonal designs are the optimal designs in each of the above categories. The MSD of the experimental points help designers decide on the level of the variables. For example to minimize variance, designs with the largest possible MSD are recommended. In other words, the experimental points are located on the boundaries of the spherical subregion.

First order orthogonal designs, with a sufficient number of observations, will allow detection for departure from linearity so far as the interaction terms are concerned. However, to detect for the existence of pure quadratic terms in the true function, a number of experimental points should be added to the center of these designs i.e., where the x's are all equal to zero.

Second Order Designs

A designer may choose to fit a quadratic polynomial equation because of one of the following two reasons:

1. A linear equation has proved to be inadequate--the search process has probably been led to a stationary region. In this case, more observations will be added to the experimental

points of the last first order design to estimate quadratic and interaction coefficients.

2. The experimenter knows that the present conditions (the initial conditions) are close to the optimal conditions and progress may only be achieved through fitting a quadratic equation.

The equation to be fitted is:

$$Y = \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \ldots + \beta_{k-1,k} x_k x_{k-1} + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \ldots + \beta_{kk} x_k^2 \qquad (4.10)$$

To estimate the β coefficients in (4.10), the x's should take at least three different values. Consequently, the temptation is to employ 3^k factorial designs. However, there are two drawbacks in using these designs:

1. They require large sample sizes.
2. They estimate the quadratic coefficients with less precision than the interaction coefficients. Since the objective in the near stationary region is to approximate the true function by a polynomial, it is reasonable to expect that all the second order effects (interaction or quadratic coefficients) be measured with almost the same precision. The 3^k factorial designs estimate the quadratic coefficients with variances eight times larger than those of the interaction coefficients.

Since it is generally assumed that a quadratic equation will provide an adequate fit, attempts for building second order designs by and large have not been directed toward minimizing bias. Therefore, the criterion for evaluating first and second order designs are different. For example, while orthogonal designs are desirable for fitting linear

polynomials, they are not recommended for fitting a second degree equations. Second order response surface designs will basically fall into one of the following two categories:

1. Composite designs.
2. Rotatable designs.

An examination of these designs will explain the circumstances under which they should be applied. A tree diagram for second order designs is given in Figure 9.

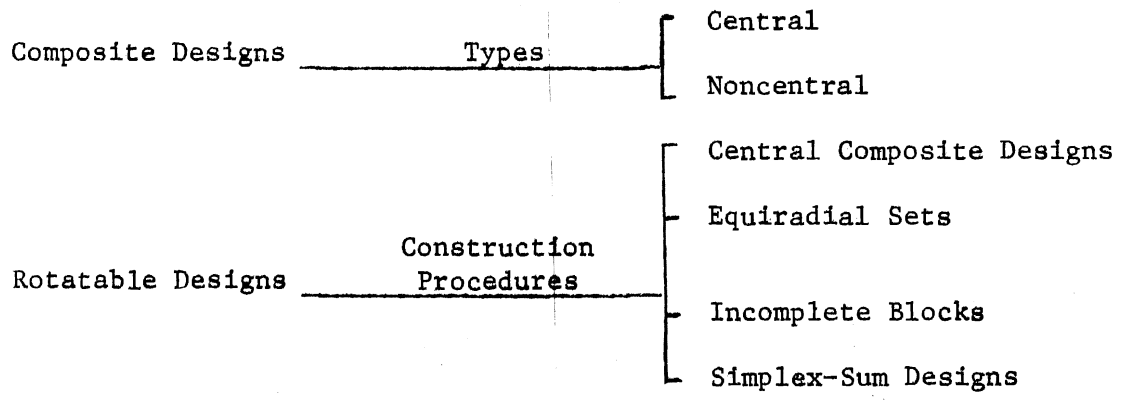

Figure 9. Second Order Designs

Composite Designs

Composite designs are obtained by adding experimental points to factorial or fractional factorial designs. Factorial or fractional factorial designs used for this purpose should be large enough to provide efficient and separate estimates of first order and mixed first order terms. A list of these designs, named type B' designs (10), is

given by Rao (51). When the first order design applied for the initial investigation of the present subregion is too small to provide separate estimates of mixed first order effects, new points should be added to form a B' design.

Central Composite Designs. Composite designs are either central or noncentral. Central composite designs are useful when the result of the first order design suggests that the surface is curved and the center of the design is close to the optimum. In this case, $2k + 1$ additional points are tested at

$(0, 0, \ldots, 0)$; $(-\alpha, 0, \ldots, 0)$; $(\alpha, 0, \ldots, 0)$; $(0, -\alpha, \ldots, 0)$;

$(0, \alpha, \ldots, 0)$; ... $(0, 0, \ldots, -\alpha)$; $(0, 0, \ldots, \alpha)$.

The value of α may be selected such that the design meets a desired property. For example, if a designer, for any reason, is interested in second order orthogonal designs, α should be set equal to $\{hN'/(4n^2)\}^{1/4}$ where:

$h = \{N^{1/2} - N'^{1/2}\}^2$,

N' = the number of observations in type B' design,

N = the total number of observations,

n = the number of times each extra observation is replicated; thus, $N - N' = n(2k + 1)$.

Or if it is desired to make the variances of the estimated second order coefficients (interaction as well as quadratic terms) equal, α can be calculated from equation (4.11).

$$2n(N' + n)\alpha^8 - 4nkN'\alpha^6 + N'\{nk(2k + 1) - 4(N' + 3n)\}\alpha^6 + 8(k - 1)N'^2\alpha^2 - 2(k - 1)(2k + 1)N'^2 = 0 . \quad (4.11)$$

After making the appropriate substitutions for n, k, and N' and also setting $\chi = \alpha^2$, equation (4.11) will have a real positive root for χ. Then α will be the square root of χ.

A value of α that makes the design rotatable will be given in the discussion of rotatable designs on page 67.

Noncentral Composite Designs. Noncentral composite designs are helpful when the initial investigation indicates that a factor combination other than the center is close to the optimum. Noncentral composite designs require k additional observations to be tested at points dictated by the combination close to the optimum. For example, in a problem with three factors, if the optimum is thought to be close to the point (-1, -1, 1), then the new combinations should be tested at

$$(-1-\alpha, -1, 1);\ (-1, -1-\alpha, 1);\ (-1, -1, 1+\alpha).$$

Rotatable Designs

A second order rotatable design should meet the following requirements:

1. All moments of order 1 should be zero. $\dfrac{\sum_{u=1}^{N} x_{iu}}{N} = 0$.

2. Mixed moments of order 2 must be zero. $\dfrac{\sum_{u=1}^{N} x_{iu}x_{ju}}{N} = 0,\ i \neq j.$

3. All moments of order 3 should be zero. $\dfrac{\sum_{u=1}^{N} x_{iu}^3}{N} = 0,$

$\dfrac{\sum_{u=1}^{N} x_{iu}x_{ju}}{N} = 0,$ $\dfrac{\sum_{u=1}^{N} x_{iu}x_{ju}x_{\ell u}}{N} = 0,\ i \neq j \neq \ell.$

4. Mixed moments of order 4 with at least one variable with an odd power must be zero. $\frac{\sum_{u=1}^{N} x_{iu}x_{ju}^3}{N} = 0$, $\frac{\sum_{u=1}^{N} x_{iu}x_{ju}^2x_{\ell u}}{N} = 0$, $\frac{\sum_{u=1}^{N} x_{iu}x_{ju}x_{\ell u}x_{mu}}{N} = 0$, $i \neq j \neq \ell \neq m$.

5. Pure quadratic moments should be equal to a constant. Given the scale convention this constant is equal to 1. $\frac{\Sigma x_i^2}{N} = 1$.

6. $\frac{\sum_{u=1}^{N} x_{iu}^4}{N}$ = constant = $3\lambda_4$.

7. $\frac{\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2}{N}$ = constant = (1/3) $\frac{\sum_{u=1}^{N} x_{iu}^4}{N}$.

8. $\lambda_4 > \frac{k}{k+2}$.

The first four conditions are tantamount to saying that all the moments of order 4 or less with at least one variable with an odd power must be zero. When the above conditions are met, the variance of the estimated response for a point, z, has been shown to be a function of p, the distance from z to the center, k, and the constant λ_4 (9). Therefore, from the class of rotatable designs, it is possible to choose one which produces a desired value for λ_4.

While large values of λ_4 increase the precision in the center of the design, it adversely affects bias for first order coefficients when third order terms are present in the model. A value of λ_4 recommended by Box and Hunter (9) makes the precision of responses at p = 0 equal to the precision of responses at p = 1. This value attaches equal

importance to the estimates of the responses within the region bounded by $p < 1$. Designs with this property are called uniform precision designs. Values of λ_4 resulting in uniform precision designs for various k are given in Table IV.

TABLE IV

VALUES OF λ_4 FOR SECOND ORDER DESIGNS WITH UNIFORM PRECISION

k	2	3	4	5	6	7	8
λ_4	0.7844	0.8385	0.8704	0.8918	0.9070	0.9184	0.9274

Source: Box and Hunter (9, p. 215).

When $\lambda_4 = 1$, the correlation coefficient between the quadratic terms becomes zero, making the design in a sense orthogonal. (The correlation coefficient between x_0 and x_i^2 for the obtained design is not zero, however.) A property of this design is that the variances of the pure quadratic coefficients are one half of those of the interaction coefficients.

A convenient method for altering the value of λ_4 is to increase the number of experimental points at the center. Although adding the points at the center may not generate an exact value for λ_4, the generated value will be close enough for most practical purposes. Addition of center points has also been used for satisfying the

inequality $\lambda_4 > \frac{k}{k+1}$. When λ_4 is equal to $\frac{k}{k+2}$, the X'X matrix is singular and, therefore, the β coefficients cannot be estimated. Increasing the number of points at the center will increase the value of λ_4 and, consequently, the inequality will be met.

The values of λ_4 are surely not limited to the values discussed before. The experimenter's judgment and his rationale could lead to other values for λ_4.

Construction of Rotatable Designs

A few alternatives are available for building designs that meet the second order rotatable designs requirements. While all the alternatives accomplish the same purpose, they are not normally equally attractive to a designer. The simplicity, the ease with which a method can be used for sequential experiments, and the method's efficiency are three logical criteria for selecting a procedure. The four procedures suggested in the literature are examined next.

1. Construction of Second Order Rotatable Designs via Central Composite Designs. In central composite designs when α is set equal to $(N')^{1/4}$, the design will become second order rotatable as well. N' is the number of observations in type B' design. Procedure 1 is easy to use and is quite adoptable for sequential experiments (9). The inventory example presented at the end of the chapter uses this procedure to construct a rotatable design.

2. Construction of Second Order Rotatable Designs by Using Equiradial Sets. This procedure was initially proposed by Box and Hunter (9) and was further developed by Draper (21) (22) (23),

Gardiner et al. (30), and Bose and Draper (1). Procedure 2 builds second order rotatable designs from a number of sets of points when the points in each set are equidistant from the origin. For example, a two-dimensional second order rotatable design may be constructed by combining some center points (one set) with a set consisting of five points equidistant from the origin. This arrangement is called pentagonal design. While one set in this example consists of the points at the center, this is not a needed requirement. This procedure is not based on the premise that second order designs are, by and large, applied when first order designs prove inadequate. Therefore, when applied to sequential experiments Procedure 2 is not convenient and as efficient as the first technique. References (9) and (21) furnish lists of second order rotatable designs built through this technique.

3. Construction of Rotatable Designs Through Balanced Incomplete Block Designs. Another procedure for building second order rotatable designs is to use balanced incomplete block designs. Using this procedure, the designs are formed by combining 2^k factorial designs with incomplete block designs in a particular way. Procedure 3 is best explained through an example. A balanced incomplete design for testing three factors in three blocks of size (S = 2) is given in Table V.

After replacing the asterisks in each row by the columns of 2^S factorial design (S = 2) and inserting a column of zeroes wherever there is no asterisk, and adding three center points (points 13, 14, and 15), a three level second order rotatable design is obtained as is shown in Table VI.

TABLE V

A BALANCED INCOMPLETE BLOCK DESIGN FOR THREE FACTORS IN THREE BLOCKS

Blocks	x_1	x_2	x_3
1	*	*	
2	*		*
3		*	*

TABLE VI

A SECOND ORDER ROTATABLE DESIGN FOR THREE FACTORS

Blocks	x_1	x_2	x_3
1	-1	-1	0
2	1	-1	0
3	-1	1	0
4	1	1	0
5	-1	0	-1
6	1	0	-1
7	-1	0	1
8	1	0	1
9	0	-1	-1
10	0	1	-1
11	0	-1	1
12	0	1	1
13	0	0	0
14	0	0	0
15	0	0	0

To obtain exact rotatability, the incomplete block designs recommended by Box and Behnken (4) require $q = 3\mu$, where q is the number of times each treatment is replicated and μ is the number of times each pair of treatments appear together in one block. Later, Das and Narasimham (18) developed a methodology for incomplete block designs with $q \neq 3\mu$. These authors provide a list of second order rotatable designs formed by utilizing incomplete block designs for three to sixteen factors.

In first order designs, the levels adopted for the factors are +1 and -1. However, for all the experimental points obtained through incomplete block designs, at least one factor has the value of zero. Consequently, this technique cannot form second order rotatable designs by adding experimental points to those of a first order design. Therefore, the technique is not efficient and suitable for sequential experiments.

4. Construction of Rotatable Designs by Using First Order Rotatable Designs (Simplex-Sum Designs). Because of the sequential nature of response surface experiments, this procedure seems to be more appealing than the last two procedures (5). Using procedure 4, a second order rotatable design is constructed by adding the rows of a first order design with minimum size ($n = k + 1$) i at a time, where $i = 1, 2, \ldots, k$ and multiplying the obtained rows by a set of constants, t_i, called radius multipliers. When the first order design, D, is of size n, the second order rotatable design, D', will have $2^n - 2$ points. Tables VII and VIII show designs D and D', respectively. D_i, in Table VIII, is an $\binom{n}{i}$ by k matrix whose rows are made up of all possible sums of the

rows of D taken i at a time. Since for $k \geq 5$ the number of design points required by this technique is large, Box and Behnken (5) recommend fractions of the derived designs which meet the necessary requirements. Fractional designs are found by setting some t_i's equal to zero. A list of simplex-sum designs for two to eight factors is given by Box and Behnken (5).

TABLE VII

FIRST ORDER DESIGN OF SIZE $n = k + 1$

$$D = \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_i \\ x_n \end{bmatrix}$$

TABLE VIII

SECOND ORDER ROTATABLE DESIGN

$$D' = \begin{bmatrix} t_1 D_1 \\ t_2 D_2 \\ \cdot \\ \cdot \\ \cdot \\ t_i D_i \\ t_k D_k \end{bmatrix}$$

Extensions

The designs classified in this chapter do not constitute an exhaustive list of response surface designs. First of all, since it was assumed that a quadratic equation will provide an adequate fit, third order designs were not discussed (7) (18) (30). Second, the designs that minimize bias and then use any additional flexibility to minimize variance were not mentioned (37) (40) (41). The reason behind the deletion is that a general class of designs of this type is not developed yet and each situation should be treated individually. Third, problems with cuboidal subregions were not discussed; this is a digression from the rest of the literature that is based on spherical subregions (24).

Random Number Assignment in Response Surface Designs

To eliminate the bias due to systematic disturbances, naturally, all the observations corresponding to any design should be performed in random order. However, some of the observations may be conducted under more homogeneous conditions than others. Specifically, response surface designs demand sets of experiments be conducted at different times. The procedure for taking advantage of these circumstances is called "blocking". All the observations taken at the same time or the observations with other similar conditions are placed in a block.

Response surface designs benefit from rich and well developed theories of blocking (9) (20) (47). Orthogonal blocking has been favored by the majority of the writers in the field. This technique

makes the estimated coefficients and the block effects orthogonal and reduces the residual sum of squares, which is highly desirable. However, when response surface designs are used in simulation experiments, the designer is able to manipulate the circumstances such that the experiments are conducted under similar conditions, therefore apparently eliminating the need for blocking.

But blocking within a different context may increase the efficiency of simulation results. The analytical work of Schruben and Margolin (52) recommended the use of two orthogonal blocks. The random numbers used in one block ($\underline{R}$) should be the antithesis ($\underline{1} - \underline{R}$) of the random numbers used in the other block. Applying this assignment rule to response surface designs will pose a problem. The difficulty will arise because of the sequentiality of response surface experiments, i.e., the uncertainty about the number of first order designs required before a second order design becomes necessary. The Proposed Methodology (hereinafter written by capital M) developed next will overcome this problem and will conduct all the experiments in two orthogonal blocks regardless of the number of first order designs needed before a second order design is used. In the discussion that will follow, methodology refers to the strategies developed for assigning random numbers to response surface designs; and assignment rule refers to part of the strategy that assigns random numbers to the points of the individual designs.

The proposed Methodology functions as follows: Sets of experiments that are used for estimating first order effects are conducted in two orthogonal blocks. All the observations in one block use $\underline{R}$ and those in the second block use $\underline{1} - \underline{R}$. When the search leads to the near stationary region, i.e., estimating second order effects becomes

desirable, the additional observations will be divided into two parts. Half of the additional observations will be added to those in one block (responses will be generated by $\underline{R}$) and the other half will be added to those in the second block (responses will be generated by $\underline{1} - \underline{R}$) while the orthogonality of the two blocks is maintained.

The simulation responses obtained through this Methodology are more efficient than those generated by applying common or different random numbers throughout the experiments. This result directly follows from the work of Schruben and Margolin as is indicated next. Assume that for response surface experiments, in general, n - 1 first order designs are employed before the search effort dictates the desirability of using a second order design. Also assume that the extra observations are added to those of the nth first order design to form a second order design. This concept is graphically shown in Figure 10.

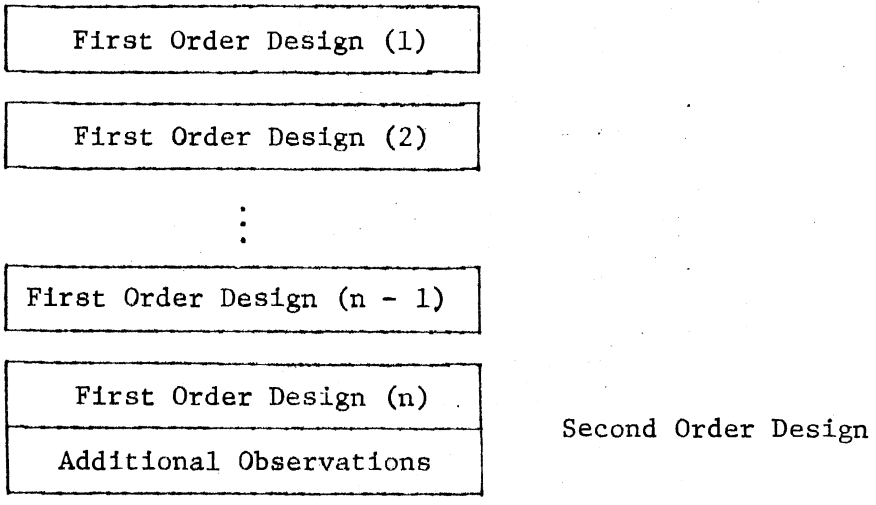

Figure 10. Graphical Illustration of the Search Method for Response Surfaces

Since in the first order design 1 through n the observations will be divided into two orthogonal blocks and Schruben and Margolin's assignment rule will be applied, it then follows that the responses obtained, for all the n cases, will be more efficient than those obtained from using common or different random numbers. Also because Schruben and Margolin's assignment rule will be applied to the second order design formed by adding the extra observations to the nth first order design, the estimates obtained in this last stage are also more efficient than those provided by the alternative assignment rules.

Yet another methodology for assigning random numbers to response surface experiments was proposed by Schruben and Margolin (52, p. 514). Their methodology applies $\underline{R}$ to all the observations of the first order design and $\underline{1} - \underline{R}$ to all the observations that are added for forming a second order design. This methodology is consistent with orthogonal blocking of response surface experiments when they are used in physical experiments. It is reasonable to have all the observations of the first order design which probably are conducted at the same time in one block, and the additional observations in the second block. The Methodology proposed here improves Schruben and Margolin's methodology for response surface experiments in three respects.

First, Schruben and Margolin's methodology applies only to the last stage of response surface experiments while the one suggested here applies to every stage. Second, although both approaches apply the original Schruben and Margolin's assignment rule to the second order design and are equally attractive, the method developed in this paper provides more efficient estimates for the nth first order design. The justification for this claim is the superiority of using $\underline{R}$ and $\underline{1} - \underline{R}$

(when the conditions are met) to the use of $\underline{R}$ for all the experimental points. Third, to apply Schruben and Margolin's methodology, the value of α should be calculated such that the additional observations will form a block orthogonal to the one formed by the observations of the first order design. But for the proposed Methodology, the value of α is immaterial in building the two orthogonal blocks and could be calculated to meet an auxiliary condition.

To operationalize the proposed Methodology, first order designs and second order designs described before should be divided into two orthogonal blocks. Fortunately, these designs can conveniently form two orthogonal blocks.

Complete and fractional factorial designs used for estimating first order coefficients can easily form two orthogonal blocks. For example, for $k = 3$, the 2^3 factorial design may be split into two orthogonal blocks, each with four observations by using the three factors interaction as the defining contrast. When complete or fractional factorial designs are performed in blocks, the estimates of some of the coefficients will be confounded with block constrasts. In other words, the reduction in the size of blocks is obtained by the loss of accuracy on certain high order interaction coefficients. The estimates of the interaction coefficients which are used for assigning the observations to blocks will be mixed with the estimates of the block differences. For example, if the three factors interaction is used to assign the observations of a 2^3 factorial to two blocks (an observation is assigned to the first block when the multiplication of the values of the three factors is equal to one and to the second block when the multiplication is equal to minus one), then the estimate obtained for

the three factors interaction will represent the blocks differences as well. The discussion of which interaction coefficient(s) should be confounded is beyond the scope of this paper and will not be presented here. Confounding is discussed in detail in the books written on the subject of experimental design (19) (44).

Plackett and Burman's (50) designs can be split into two orthogonal blocks leading to the estimates of the main effects for 4k-2 factors in 4k observations. These designs normally provide estimates of 4k-1 factors in 4k observations. The estimation of a main factor is sacrificed for splitting the designs into two parts. No effort is needed for forming two orthogonal blocks in case of type B designs because they are made up of two orthogonal blocks. (Duplicating designs of type A with reverse signs results in formation of type B designs.)

Designs of type B' will form two orthogonal blocks as shown in Table IX.

TABLE IX

DESIGNS OF TYPE B' FORMED IN TWO ORTHOGONAL BLOCKS

Factorial Design	Number of Factors	Defining Contrast
2^3	2, 3	AB=I, ABC=I
2^4	4	ABCD=I
2^5	5, 6, 7	*
2^6	8, 9, 10	*
2^7	11	*

*The sufficient condition for dividing these designs into two blocks is that all combinations of every five factors involving the first three occur equally, i.e., the first three factors interaction is used for comparing the groups (51).

Designs of type B' are the most appropriate designs for the Methodology being discussed here. An examination of the necessary conditions for performing the second order designs into two orthogonal blocks will elaborate on this point (9). A second order design with N points assigned to w = 2 blocks with n_1 and n_2 points in each block may be expressed as

$$Y_u = \sum_{w=1}^{2} \beta_{ow} Z_{wu} + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \sum_{j=1}^{k} \beta_{ij} x_{iu} x_{ju} , \qquad (4.12)$$

where β_{ow} is the expected value of the response in the wth block corresponding to the conditions at the origin of the design, and Z_{wu} is a block variable taking the value unity for the observations in the wth block and zero otherwise.

Equation (4.12) can be rewritten as

$$Y_u = \beta_o + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \sum_{j=1}^{k} \beta_{ij} x_{iu} x_{ju} + \sum_{w=1}^{2} \delta_w (Z_{wu} - \bar{Z}_w) \qquad (4.13)$$

where

$$\beta_o = \sum_{w=1}^{2} \frac{n_w}{N} \beta_{ow} , \quad \delta_w = \beta_{ow} - \beta_o , \text{ and } \bar{Z}_w = \frac{n_w}{N} .$$

Block variables, $Z_{wu} - \bar{Z}_w$, will be orthogonal to the variables $x_1, x_2, \ldots, x_k, x_1^2, x_2^2, \ldots, x_k^2, x_1, x_2, \ldots, x_{k-1}x_k$ when

$$\sum_{u=1}^{N} x_{iu} x_{ju} (Z_{wu} - \bar{Z}_w) = 0 \qquad (i, j = 0, 1, \ldots, k) \qquad (4.14)$$

(4.14) is equivalent to

$$\sum_{u=1}^{N} x_{iu} x_{ju} Z_{wu} = \bar{Z}_w \sum_{u=1}^{N} x_{iu} x_{ju} . \qquad (4.15)$$

In a second order rotatable or composite designs for $i \neq j$, $\sum_{u=1}^{N} x_{iu}x_{ju} = 0$. Thus, it becomes necessary for orthogonal blocking that

$$\sum_{u=1}^{n_1} x_{iu}x_{ju} = 0, \quad i \neq j. \tag{4.16}$$

$$\sum_{u=1}^{n_2} x_{iu}x_{ju} = 0, \quad i \neq j. \tag{4.17}$$

Condition I: All the sums of products between x's within each block should be zero.

Substituting $i = j$ in equation (4.15) leads to another requirement

$$i = j \rightarrow \frac{\sum_{u=1}^{n_1} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_1}{N} \text{ and } \frac{\sum_{u=n_1+1}^{n_2} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_2}{N} . \tag{4.18}$$

Condition II: The contribution of each block to the sum of squares for each variable should be proportional to the number of observations in that block.

The points to be added to a first order design in order to form a second order rotatable or composite design are:

$(\alpha, 0, 0, \ldots, 0)$; $(-\alpha, 0, 0, \ldots, 0)$; $\ldots$; $(0, 0, 0, \ldots, \alpha)$; $(0, 0, 0, \ldots, -\alpha)$

It is clear that these experimental points will always satisfy the first condition regardless of the block to which they are assigned. Therefore, to satisfy the first condition for the second order design as a whole, the columns associated with the x's in the first order design must be mutually orthogonal. Fortunately, first order designs of type B' which are used for forming second order designs meet this requirement.

Designs of type B' that are made up of two orthogonal blocks meet the second condition as well. So, care must be taken to assure the satisfaction of the second condition when designs are supplemented by additional observations. To do so, the points with positive and negative α for each factor should not be assigned to the same block. A systematic procedure would be to assign all the points with positive α to one block and the points with negative α to the second block. Since the sum of squares for each variable is the same for both blocks, an equal number of observations in each block satisfies the second condition. If central points are needed, equal numbers of them should be added to each block.

Discussion

A technical discussion of the proposed Methodology can be based on the dispersion matrices of the $\underline{\beta}$ coefficients for different assignment rules as derived by Schruben and Margolin (52). After partitioning the $\underline{X}$ matrix as $(\underline{1}, \underline{X}^*)$ and assuming a unit variance for the dispersion matrix, the dispersion matrices for Schruben and Margolin's assignment rule, the common streams of random numbers, and independent streams of random numbers are given by (4.19), (4.20), and (4.21) respectively.[1]

$$\beta_{OLS} = \left[\begin{array}{c|c} \rho_+ - (2N_1N_2/N^2)(\rho_+ - \rho_-) + N^{-1}(1 - \rho_+) & 0 \\ \hline 0 & (X^{*\prime}X^*)^{-1} \cdot (1 - \rho_+) \end{array}\right] \qquad (4.19)$$

[1] ρ_+ and ρ_- denote positive and negative correlations, and N_1 and N_2 represent the number of observations in the first and second block.

$$\beta_{OLS} = \left[\begin{array}{c|c} \rho_+ + N^{-1}(1 - \rho_+) & 0 \\ \hline 0 & (X^*'X^*)^{-1}(1 - \rho_+) \end{array}\right] \tag{4.20}$$

$$\beta_{OLS} = \left[\begin{array}{c|c} N^{-1} & 0 \\ \hline 0 & (X^*'X^*)^{-1} \end{array}\right] \tag{4.21}$$

Schruben and Margolin's assignment rule and the common streams of random numbers are equally efficient in estimating all the main and interaction effects (β_1, β_2, ..., β_j, β_{12}, ...), and they are both more efficient in estimating those effects than the assignment rule using independent streams of random numbers. However, the common streams of random numbers provides the least efficient estimate of the mean effect (β_0). The issue of whether Schruben and Margolin's assignment rule is more efficient than the independent streams of random numbers in estimating the mean effect and the extent of its efficiency over the common streams of random numbers is decided by the magnitude of ($\rho_+ - \rho_-$) (see equations 4.19, 4.20, and 4.21). Clearly the larger the magnitude of the negative correlations induced, the more efficient Schruben and Margolin's assignment will be. While not discussed by Schruben and Margolin, it is interesting to note that even if the antithetic random numbers produce zero correlations or positive correlations less than ρ_+ (the positive correlation induced between the points in the first block by $\underline{R}$), Schruben and Margolin's rule will still be more efficient than the common streams of random numbers for estimating the mean effect.

The objective of a designer in early stages of response surface methodology is to estimate the main effects as accurately as possible to determine the steepest ascent or descent path. Thus the proposed Methodology that uses Schruben and Margolin's assignment rule and the

common streams of random number methodology are both more efficient than the independent streams of random numbers methodology. Also, because it provides a better estimate of the mean than the common streams methodology, the proposed Methodology appears to be the optimal choice.

When the search process has been led to the near-stationary region, the efficiency of the interaction effects then becomes as important as the efficiency of the main effects. An argument against the proposed Methodology would be that it confounds the estimate of one or more interaction effects in dividing the observations into two orthogonal blocks. However, in a problem with more than two factors, it is not hard to find a high-order interaction effect that is expected to be insignificant and can be used for dividing the observations into two blocks.

Although it is possible for the proposed Methodology to produce a more efficient estimate of the mean than the independent streams methodology, a conservative approach would be to use independent streams of random numbers when an efficient estimate of the mean is desired. Two other issues related to the proposed Methodology are discussed next.

The construction of second order designs alone appears to assume that designs of type B' are used for fitting first order polynomials. This practice could be criticized because the number of observations required for designs of type B' is larger than the number of observations of type A or B. In fact, one may argue that the increase in efficiency obtained through conducting the experiments into two orthogonal blocks might be offset by the increase in the number of observations. These arguments are refuted on the ground that the proposed Methodology assumes the utilization of B' designs only when the search effort has been led

to the near stationary region and it will surely be supplemented by additional observations for estimating second order coefficients. Therefore, if the prevailing conditions are far from the optimum (for example, around the initial conditions), designs of type A and B could be used.

Also, the procedure adopted for building rotatable designs in two orthogonal blocks is one of the four possible procedures discussed earlier in this chapter. Consequently, questions could be raised about the merits of the remaining three procedures. A brief examination of these procedures will provide support for the selected procedure. Second order rotatable designs built through incomplete block designs or equiradial sets are not efficient and suitable for sequential experiments for the following reason: While some of the experimental points required for the two methods are those presumably performed in the previous phase of the analysis, none of the two will form a second order rotatable design in conjunction with all the experiments used in the previous phase. Thus, some of the observations performed for estimating the first order effects will not contribute to the estimation of the second order effects.

The third procedure, simplex-sum designs, constructs second order designs from first order designs with $k + 1$ observations. Methodologically, this approach seems to be appropriate for sequential experiments. However, it is very unlikely for a designer to recognize the need for fitting a second order polynomial with only $k + 1$ observations. (A first order orthogonal design with $k + 1$ observations furnishes neither an estimate of any interaction effect nor an estimate of the experimental error.) When the number of observations utilized for estimating the

first order coefficients is larger than k + 1, then some of them will not be used for estimating the second order coefficients. Therefore, based on the criteria of efficiency and adoptability for sequential experiments, the central composite design procedure is likely to be favored over other techniques available for building second order rotatable designs.

Empirical Evaluation of Results

The contribution of the first part of this chapter, which was developing a new method for presenting response surface designs, remains to be evaluated. The classification presented in this chapter will hopefully stimulate the interest in applying response surface designs to simulation through collecting the designs under one cover and presenting them in a logical sequence.

The contribution to be made by the second part of this chapter is, however, more difficult to gauge. In other words, it is not possible to say that conducting the experiments in two orthogonal blocks will bring about the maximum possible efficiency in simulation results. All that really can be said is that the proposed Methodology is superior to (1) the assignment of the same random number(s) to all the design points, and (2) the assignment of different random numbers to all the design points only when the following two conditions are met:[2]

1. The use of common random numbers and antithetic random numbers will generate positive and negative correlations between responses, respectively.
2. $\{1 + (N - 1)\rho_{+} - 2N^{-1}N_1N_2\ (\rho_{+} + \rho_{-})\}(1 - \rho_{+})^{k} < 1$ (4.22)

---

[2]The second condition is necessary only for the superiority of the Methodology to the assignment of different random numbers.

While Schruben and Margolin provide empirical support for the optimality of their random number assignment rule, Wright and Ramsay (56) recently presented simulation problems for which the use of common random numbers increased the variance. As a result of their findings, Wright and Ramsay reiterated the argument that the common random numbers technique fails to induce the desired correlations if the policies compared are not small perturbations of each other. This argument implies caution in assuming the generation of positive correlations for response surface experiments. For example, in a simulation with two variables, depending upon the units of the variables the design point (-1, -1) might be too far apart from the design point (+1, +1).

Simulations are normally developed when a problem cannot be solved analytically. In other words, the response function, $G = f(x)$, cannot be written in a deterministic mathematical form. Additionally, the form of the response function and the way random numbers, which generate some of the variables, affect the responses differ in different simulations. Therefore, the nature of simulation seems to defy a general analytical investigation of random number assignment rules. The analytical and empirical investigations of the assignment of random numbers only recommend possible ways for increasing the efficiency of certain simulations. It is the responsibility of a simulation designer to be familiar with the alternative assignment rules and, based on his knowledge of the problem or a few pilot runs, assign the random numbers appropriately.

To supplement and complete the discussions in this chapter, and to also evaluate the application of the proposed Methodology, and example of an inventory simulation case is presented next.

The Characteristics of the Inventory Simulation

The inventory simulation used for empirical investigation is developed by Professor Billy M. Thornton of the Oklahoma State University. The input parameters of this simulation are as follows:

a. Inventory Situation Characteristics

1--The initial inventory level (50,000 units)

2--Maximum inventory size (100,000 units)

3--Cost of carrying inventory per unit ($.35)

4--Ordering cost ($2,000 per order)

5--Shortage cost ($5 per unit)

6--Temporary storage cost ($7 per unit)

7--Number of warm-up periods (15)

8--Number of periods in the simulation (104)

The numbers inside the parentheses were used in an example.

b. Demand Distributions

1--The number of different demand segments--all are assumed to be normally distributed (1)

2--The number of periods in each segment (104)

3--Means and standard deviations for the demand segments (12,500 units, 500 units)

4--A random number seed for demand generator

The number inside the parentheses were used in an example.

c. Delivery Time Distributions

1--The number of different delivery time periods--all are assumed to be normally distributed (1)

2--The number of periods in each segment (104)

3--Means and standard deviations for the delivery time segments (3.5 and 1)

4--A random number seed for the delivery time generator

d. Policy Variables (Controllable Conditions)

1--The number of policy segments (1)

2--The number of periods in each policy segment (104)

3--Ordering quantity and reordering level for each policy segment

e. Process Generators

Random numbers are generated through a subprogram which is a part of the simulation program. The following subroutine calls the subprogram to generate normal random variates using the Central Limit Theorem (48, p. 95).

```
SUBROUTINE NORMAL (EX, STDX, X)
SUM = 0.0
DO 5 I = 1, 12
R = RND(R)
5 SUM = SUM + R
X = STDX * (SUM - 6.0) + EX
RETURN
```

Two other methods for generating normal random variates are the Direct Approach and the Fast Procedure (48, p. 95). The Direct Approach furnishes two normal random variates by using two random variates as is shown below.

$$\text{Normal random variate 1} = (-2 \log_e r_1)^{1/2} \cos 2\pi r_2 \qquad (4.23)$$

$$\text{Normal random variate 2} = (-2 \log_e r_1)^{1/2} \sin 2\pi r_2 \qquad (4.24)$$

The Fast Procedure calculates normal random variates from the mixture of three densities given below.

$$f(x) = .09578\ g_1(x) + .0395\ g_2(x) + 0.0027\ g_3(x).$$

In validating the simulation model, the normal random variates produced by the Central Limit Theorem were compared to those produced by the other two techniques. This comparison did not suggest any one of these techniques to be superior to others.

An Illustrative Example

Given the numbers inside the parentheses, the objective of the example was to find the ordering quantity and the reordering level that minimize the average inventory cost for a year. The steepest descent technique was used to search for the optimum point. Based on the demand distribution (mean = 12,500 units per week, standard deviation = 500) and the delivery time distribution (mean = 3.5 weeks, standard deviation = 1 week) the search effort was subjectively determined to start from the point at which the ordering quantity is 45,000 units and the reordering level is 40,000 units. Additionally, this point was considered to be far from the optimum conditions, therefore a design that provides estimates of the main effects and the interaction effects would be appropriate. Moreover, since it was not essential to discover the nature of the relationships involved, the experimenter's priority was to choose a design that would minimize variance (Figure 8, page 54). Denoting the ordering quantity by x_1 and the reordering level by x_2, a 2^2 factorial design, as shown in Table X, was used to fit a first order polynomial to the subregion around the selected point. (A 2^2 factorial design will satisfy both conditions 1A and 1B in Figure 8.)

TABLE X

FACTOR LEVELS FOR THE FIRST EXPERIMENT

Factor	-1	+1
x_1 the ordering quantity	44,000	46,000
x_2 the reordering level	39,000	41,000

Note: "1,000 units" was subjectively set equal to one experimental unit for both variables.

Simulation runs were made for the four experimental points and the center point with the following three alternative random numbers assignment rules.

1. Independent streams of random numbers.
2. Common random numbers.
3. Schruben and Margolin's assignment rule.

The obtained responses are shown in Tables XI, XII, and XIII respectively.

The responses shown in Table XI, XII, and XIII were obtained by dividing the total inventory costs by 104 (the periods in the simulation). The 104 period costs were punched on computer cards and were used by a FORTRAN Program to calculate the induced correlations between the trials. The correlation coefficients for the five trials when the independent streams of random numbers were used are shown in Table XIV.

TABLE XI

THE FIRST EXPERIMENT WITH INDEPENDENT STREAMS OF RANDOM NUMBERS

Trial	Factor Level		Response
	x_1	x_2	y
1	-1	-1	$25,461
2	-1	+1	24,544
3	+1	-1	24,440
4	+1	+1	24,774
5	0	0	25,100

TABLE XII

THE FIRST EXPERIMENT WITH COMMON STREAMS OF RANDOM NUMBERS

Trial	Factor Level		Response
	x_1	x_2	y
1	-1	-1	$25,314
2	-1	+1	24,610
3	+1	-1	23,503
4	+1	+1	23,503
5	0	0	24,600

TABLE XIII

THE FIRST EXPERIMENT WITH SCHRUBEN AND MARGOLIN'S ASSIGNMENT RULE

Trial	Factor Level		Response
	x_1	x_2	y
1	-1	-1	$25,314
2	-1	+1	24,895
3	+1	-1	25,081
4	+1	+1	23,503
5	0	0	24,600

TABLE XIV

CORRELATION COEFFICIENTS FOR INDEPENDENT RANDOM NUMBERS CASE

Trial* \ Trial*	1	2	3	4	5
1	1	-.25	.27	.01	-.27
2	---	1	-.02	-.04	.15
3	---	---	1	-.03	-.19
4	---	---	---	1	.01
5	---	---	---	---	1

*The trial numbers correspond to the previous tables.

Although some of the coefficients in Table XIV are close to zero, the independent streams of random numbers did not generate absolutely independent responses. The obtained correlations may be attributed to one or both of the following two factors.

1. The nature of the adopted simulation.
2. The policies (the experimental points) are too far apart.

The next set of trials will be closer to each other and will provide an opportunity for examining the validity of the second factor. To evaluate the efficiency of this assignment rule as compared to the other two, the standard errors of the β coefficients need to be compared. The evaluation will be presented after the correlation coefficients for the other two random numbers assignment rules are discussed.

The correlation matrix for the observations of the common random numbers rule are given in Table XV.

TABLE XV

CORRELATION COEFFICIENTS FOR COMMON RANDOM NUMBERS ASSIGNMENT RULE

Trial \ Trial	1	2	3	4	5
1	1	.66	.39	.39	.45
2	---	1	.18	.18	.21
3	---	---	1	1.00	.99
4	---	---	---	1	.99
5	---	---	---	---	1

The correlation coefficients presented in Table XV support the hypothesis that the common random numbers assignment rule induces positive correlations between the simulation responses. However, more than half of the coefficients show only weak correlations. Two possible explanations behind obtaining such correlation coefficients are the ones described in the case of independent streams of random numbers. A more plausible explanation appears to be the dependence of the magnitude of the induced correlations on the specific pairs of the design points.

The correlation coefficients between the responses for the use of Schruben and Margolin's assignment rule is given in Table XVI.

TABLE XVI

CORRELATION COEFFICIENTS BETWEEN RESPONSES FOR SCHRUBEN AND MARGOLIN'S ASSIGNMENT RULE

Trial \ Trial		$\underline{R}$ 1	$1 - \underline{R}$ 2	$\underline{1} - \underline{R}$ 3	$\underline{R}$ 4	$\underline{R}$ 5
$\underline{R}$	1	1	-.31	-.10	.39	.45
$1 - \underline{R}$	2	---	1	.07	-.09	-.13
$\underline{1} - \underline{R}$	3	---	---	1	-.24	-.25
$\underline{R}$	4	---	---	---	1	.99
$\underline{R}$	5	---	---	---	---	1

The four trials corresponding to the 2^2 factorial experiment are divided into two orthogonal blocks. But adding one observation to the center of design for estimating the standard errors and including it in the first block violates that orthogonality condition. However, slight deviation from the orthogonality is not expected to affect the efficiency of the assignment rule. The sign of the induced correlations between the trials that use the same streams of random numbers was expected to be positive; and the sign of the generated correlations between the trials that use $\underline{R}$ and $\underline{1} - \underline{R}$ was expected to be negative. Although the signs of all the correlation coefficients in Table XVI are as anticipated, their magnitudes are not. The same factors that caused the weak correlations in case of the common streams of random numbers are possibly at work here, too.

The standard errors of the β coefficients obtained by each of the alternative assignment rules is given in Table XVII.

TABLE XVII

STANDARD ERRORS OF THE β COEFFICIENTS FOR THE THREE ALTERNATIVES

Alternatives	Standard Error			
	β_0	β_1	β_2	β_{12}
1. Independent Streams	109	114	148	133
2. Common Streams	261.9	184	67.7	67.7
3. Schruben and Margolin	44.9	33.7	42.8	55.56

The common streams of random numbers as expected has the largest variance for β_0. The use of the common streams of random numbers did, however, reduce the variances for β_2 and β_{12}. The reason that the variance for β_1 was not reduced is the magnitude of some of the correlation coefficients in Table XV. Schruben and Margolin's assignment rule, which is part of the proposed Methodology, has the most efficient estimates. This assignment rule reduces the variance of β_{12} with a lesser degree than it reduces the variances of β_1 and β_2. A reasonable explanation is that the estimate of the interaction effect, β_{12}, is confounded with the estimate of the blocks contrast. Theoretically, the variances of β_1, β_2, and β_{12} for common streams of random numbers and Schruben and Margolin's assignment rule must be equal. That would be the case only if first all the positive and negative correlations have equal magnitudes; second, if the experimental errors for the two regression equations are equal.

The next step in the search process is to examine the magnitude and the signs of the estimated coefficients. This examination will, first, show the nature of the present subregion; and, second, the steepest descent path in case the subregion under investigation is not the near stationary subregion. The estimate of the β coefficients according to Schruben and Margolin's assignment (the most efficient one) are shown in Table XVIII.

TABLE XVIII

THE ESTIMATES OF THE β COEFFICIENTS

$\hat{\beta}_1$	= -406.25
$\hat{\beta}_2$	= -499.25
$\hat{\beta}_{12}$	= -289.75

Since the estimates of the main effects, β_1 and β_2, are relatively larger than the estimate of the interaction effect, it was realized that reduction in the average inventory cost moving down on the steepest descent path might be possible. The calculation of the steepest descent path and the trials performed on the path are shown in Table XIX.

After performing 12 trials, the point associated with trial 11 was selected to be the center of the next first order design. The observations of the second 2^2 factorial design are shown in Table XX.

In light of the magnitude of main effects obtained previously, the units adopted in the second set of experiments for x_1 and x_2 are 407 and 500 units respectively. While the relative magnitude of the units was dictated by the slopes, the absolute magnitude of the units was determined subjectively.

Simulation runs were made for the four experimental points and the center point with the three random numbers assignment rules. The results are shown in Tables XXI, XXII, and XXIII.

The correlation coefficients between the responses when independent streams of random numbers were employed are given in Table XXIV.

TABLE XIX

CALCULATION OF STEEPEST DESCENT PATH AND SUBSEQUENT TRIALS ON THE PATH

Variables	Ordering Quantity x_1	Reordering Level x_2	
Base level	45,000 units	40,000 units	
Unit	1,000 units	1,000 units	
Estimated slope x(-)*	406.25	499.25	
Unit x slope	406250	499250	
Change in level per 1,000 units for x_1	814	1,000**	
Subsequent points on the path:			
Point			Responses
1	45,814	41,000	23,725
2	46,628	42,000	22,845
3	47,442	43,000	21,992
4	48,256	44,000	21,173
5	49,070	45,000	20,397
6	49,884	46,000	19,307
7	50,698	47,000	19,079
8	51,512	48,000	18,289
9	52,326	49,000	18,260
10	53,140	50,000	18,027
11	53,954	51,000	17,964
12	54,768	52,000	18,295

*Because the objective is cost minimization, the negative sign is required.

**1,000 units was determined subjectively.

TABLE XX

FACTOR LEVELS FOR THE SECOND 2^2 FACTORIAL DESIGN

Factors	-1	+1
Ordering Quantity x_1	53,547	54,361
Reordering Level x_2	50,500	51,500

TABLE XXI

THE SECOND 2^2 FACTORIAL DESIGN WITH INDEPENDENT STREAMS

Trial	Factor Level		Response
	x_1	x_2	y
1	-1	-1	17,766
2	-1	+1	19,894
3	+1	-1	18,230
4	+1	+1	19,498
5	0	0	18,494

TABLE XXII

THE SECOND 2^2 FACTORIAL DESIGN WITH COMMON STREAMS OF RANDOM NUMBERS

Trial	Factor Level x_1	Factor Level x_2	Response y
1	-1	-1	18,507
2	-1	+1	17,831
3	+1	-1	18,448
4	+1	+1	18,631
5	0	0	17,964*

*The seed value that was used for trial five in the previous table was repeated for all the trials in Table XXII.

TABLE XXIII

THE SECOND 2^2 FACTORIAL DESIGN WITH SCHRUBEN AND MARGOLIN'S ASSIGNMENT RULE

Trial	Factor Level x_1	Factor Level x_2	Response y
1	-1	-1	18,507
2	-1	+1	18,740
3	+1	-1	18,011
4	+1	+1	18,631
5	0	0	17,964

TABLE XXIV

CORRELATION COEFFICIENTS FOR INDEPENDENT STREAMS OF RANDOM NUMBER CASE

Trial \ Trial	1	2	3	4	5
1	1	-.15	.08	-.03	.02
2	---	1	-.20	.31	-.14
3	---	---	1	-.14	.42
4	---	---	---	1	-.16
5	---	---	---	---	1

The correlation coefficients in Table XXIV do not show absolute independency between the responses, but show weak positive or negative correlations. The experimental points under consideration here are closer to each other than the ones considered before. Since the correlation coefficients in Table XXIV are not an improvement over those in Table XIV, it may be concluded that the distance between the experimental points is not affecting the magnitude of the correlations between the responses. The factor then to blame would be the nature of the adopted simulation. Had, for example, the standard deviations of the demand and the delivery time been larger, the entries of Table XXIV might have shown weaker positive and negative correlations.

The correlation coefficients between the responses when they were generated by the same stream of random numbers is given in Table XXV.

TABLE XXV

CORRELATION COEFFICIENT BETWEEN RESPONSES FOR THE COMMON RANDOM NUMBERS ASSIGNMENT RULE

Trial \ Trial	1	2	3	4	5
1	1	.87	.22	.23	.86
2	---	1	.14	.15	.95
3	---	---	1	.99	.23
4	---	---	---	1	.25
5	---	---	---	---	1

The use of common streams of random numbers generated positive correlations between the responses; however, in terms of the magnitude of the induced correlations, the correlation coefficients are not better than those presented in Table XXV. Therefore, in this simulation, the distance between the experimental points does not seem to be the reason behind the weak correlations. For the adopted simulation, the magnitude of the positive correlations induced is ostensibly dependent upon the specific pairs of the design points. (Schruben and Margolin assumed that the induced correlations are independent of the design points.)

The last correlation coefficients between responses was obtained when Schruben and Margolin's assignment rule was applied. These coefficients are shown in Table XXVI.

TABLE XXVI

THE CORRELATION COEFFICIENT BETWEEN RESPONSES FOR SCHRUBEN AND MARGOLIN'S ASSIGNMENT RULE

Trial \ Trial	1	2	3	4	5
$\underline{R}$ 1	1	.05	.08	.23	.86
$\underline{1} - \underline{R}$ 2	---	1	.18	.00	.08
$\underline{1} - \underline{R}$ 3	---	---	1	.00	.10
$\underline{R}$ 4	---	---	---	1	.25
$\underline{R}$ 5	---	---	---	---	1

The entries that were expected to be negative in Table XXVI show either zero or weak positive correlations. Also, except for ρ_{15}, the anticipated positive correlations show only weak correlations. The possible explanations for the performance of the common streams of random numbers are the ones discussed before. The failure of the antithetic random numbers to generate negative correlations may be attributed to the nature of this simulation, the variability of demand and the delivery time in particular. The more variations in the demand and the delivery time, the more fluctuations will be caused between the inventory costs by low and high, and high and low random numbers. It is interesting to note that for the adopted simulation, moving the experimental points closer to each other adversely affects the performance of the antithetic random numbers.

The standard error of the β's for the three alternative random numbers assignment rules are shown in Table XXVII.

TABLE XXVII

THE STANDARD ERROR OF THE β'S FOR THE ALTERNATIVE RANDOM NUMBERS ASSIGNMENT RULE

Alternatives	Standard Error			
	β_0	β_1	β_2	β_{12}
1. Independent Streams	141.4	139	190	144.25
2. Common Streams	268	217	46.17	46.17
3. Schruben and Margolin	192	144.2	146	172

As in the case of the initial first order design, the common streams or random numbers increased the variance of β_0 and reduced the variances of β_2 and β_{12}. The increase in the variance of β_1 can be traced back to the weak correlation coefficients presented in Table XXV. The inefficiency associated with Schruben and Margolin's assignment rule is because of the large experimental error of its corresponding regression analysis. The mean square error of the regression analysis for observations of Table XXIII was about twice larger than the mean square error of the regression equation using independent streams of random numbers responses and the regression equation using common streams of

random numbers responses. Had the mean square errors for the three regression equations been equal, Schruben and Margolin's assignment rule would have been more efficient than the other two assignment rules.

The variability in mean square errors of the different regression equations is caused by the volatile nature of the adopted simulation. Certainly, one would increase the consistency of the responses by running the individual simulations for longer periods of time. For simulations with a volatile nature, the experimental errors are large and consequently making the application of the response surface methodology inappropriate. The success of the response surface methodology very much depends on the magnitude of the experimental errors. However, this problem could be overcome by, first, selecting the experimental points closer to one another. Second, by increasing the number of periods for which each experimental point is run.

Since the proposed Methodology was used in the initial stage of the analysis, the search process continued with the estimates obtained through it. Table XXVIII shows the estimates of the β coefficients.

TABLE XXVIII

THE ESTIMATES OF THE β COEFFICIENTS

$\hat{\beta}_1 = 348.75$
$\hat{\beta}_2 = -286.75$
$\hat{\beta}_{12} = -403.25$

Since the estimate of the interaction effect is large as compared to the estimates of the main effects, a second degree polynomial needs to be fitted. An examination of the responses in Table XXIII led to the adoption of a second order composite rotatable design. The value of α for this design based on the formula given in page 67 is equal to $(4)^{1/4}$. This value of α will make it possible to compare Schruben and Margolin's methodology with the proposed Methodology. So the additional experimental points are:

	x_1	x_2
1	1.414	0
2	-1.414	0
3	0	1.414
4	0	-1.414
5	0	0

To conform to the orthogonality requirement, the experimental points 1 and 3 were simulated using $\underline{R}$ and the rest were simulated using $\underline{1} - \underline{R}$. Table XXIX shows the results. (Also, 1 and 3 were simulated using $\underline{1} - \underline{R}$ and the rest were simulated using $\underline{R}$.)

TABLE XXIX

THE ADDITIONAL EXPERIMENTAL POINTS AND THEIR RESPONSES

Trial	Factor Level		Response
	x_1	x_2	y
1	1.414	0	$18,524
2	-1.414	0	18,895
3	0	1.414	17,964
4	0	-1.414	19,966
5	0	0	19,545

The correlation coefficients between the ten observations of the second order rotatable designs when they were all generated by the common streams of random numbers are shown in Table XXX.

TABLE XXX

CORRELATION COEFFICIENTS BETWEEN RESPONSES OF THE SECOND ORDER ROTATABLE DESIGN FOR COMMON STREAMS OF RANDOM NUMBERS

Trial \ Trial		1	2	3	4	5	6	7	8	9	10
	1	1	.87	.22	.23	.86	.99	.22	.29	.86	.86
	2	--	1	.14	.15	.95	.86	.14	.20	.95	.95
	3	--	--	1	.99	.23	.18	.94	.90	.23	.23
	4	--	--	--	1	.25	.20	.93	.91	.25	.25
	5	--	--	--	--	1	.82	.24	.30	1	1
$(-\alpha, 0)$	6	--	--	--	--	--	1	.19	.25	.82	.82
$(\alpha, 0)$	7	--	--	--	--	--	--	1	.83	.24	.24
$(0, -\alpha)$	8	--	--	--	--	--	--	--	1	.30	.30
$(0, \alpha)$	9	--	--	--	--	--	--	--	--	1	1
(0, 0)	10	--	--	--	--	--	--	--	--	--	1

Table XXX provides further support for the claim that the magnitude of the induced correlations, in this simultion, depends on the pairs of the design points. The common streams of random numbers generate strong positive correlations between the responses only when the policies (the design points) compared are similar or are close in nature. While the distances between the design points may, in some cases, indicate the degree of similarity between the policies, it will not do so in general.

The correlation coefficients between the design points of Table XXX when Schruben and Margolin's methodology was applied are presented in Table XXXI.

TABLE XXXI

CORRELATION COEFFICIENTS BETWEEN THE RESPONSES OF THE SECOND ORDER ROTATABLE DESIGN FOR SCHRUBEN AND MARGOLIN'S METHODOLOGY

Trial \ Trial	1	2	3	4	5	6	7	8	9	10
R	1	1	.87	.22	.23	.86	.05	.07	.09	.02	.09
R	2	--	1	.14	.15	.95	.05	.09	.10	.02	.10
R	3	--	--	1	.99	.23	-.01	-.01	-.02	-.05	.00
R	4	--	--	--	1	.25	.00	.00	.01	.04	.01
R	5	--	--	--	--	1	.08	.10	.12	.02	.12
1 - R	6	--	--	--	--	--	1	.15	.18	.60	.20
1 - R	7	--	--	--	--	--	--	1	.90	.30	.89
1 - R	8	--	--	--	--	--	--	--	1	.38	.96
1 - R	9	--	--	--	--	--	--	--	--	1	.40
1 - R	10	--	--	--	--	--	--	--	--	--	1

All entries which are located at the intersection of the first five rows and the last five columns were expected to be negative and the remaining coefficients were expected to be positive. Because of the factors explained before most of the coefficients in Table XXXI do not show strong positive or negative correlations. The correlation coefficients between the experimental points when the proposed Methodology was used are given in Table XXXII.

TABLE XXXII

CORRELATION COEFFICIENTS BETWEEN THE RESPONSES OF THE SECOND ORDER ROTATABLE DESIGN FOR THE PROPOSED METHODOLOGY

Trial	Trial	1	2	3	4	5	6	7	8	9	10
R	1	1	.05	.08	.23	.86	.05	.22	.09	.86	.09
1 - R	2	--	1	.18	.00	.08	1	.01	.20	.08	.22
1 - R	3	--	--	1	.00	.10	.16	-.01	.92	.10	.90
R	4	--	--	--	1	.25	.00	.93	-.01	.25	.01
R	5	--	--	--	--	1	.08	.24	.12	1	.12
1 - R	6	--	--	--	--	--	1	.02	.18	.08	.20
R	7	--	--	--	--	--	--	1	-.03	.24	.00
1 - R	8	--	--	--	--	--	--	--	1	.12	.96
R	9	--	--	--	--	--	--	--	--	1	.12
1 - R	10	--	--	--	--	--	--	--	--	--	1

As in the previous table, the antithetic random numbers generated zero or weak correlations between the responses. An examination of the standard errors of the β coefficients for the common random numbers methodology, Schruben and Margolin's methodology, and the proposed Methodology is given next. Table XXXIII shows the standard errors for the β coefficients.

For the second order composite rotatable design, the proposed Methodology has produced the most efficient results. However, as before, part of the efficiency is caused by the mean square errors of the regression equations. The standard error of β_0 for the common streams of random numbers is larger than the standard error of β_0 for the other two alternatives. This result is consistent with the analytical discussion presented before. The standard errors of all the other

coefficients would have been the same if 1) all the positive correlations and also all the negative correlations would have been equal and 2) if the mean square errors for the three regression equations would have been equal. The last stage in the search process is evaluation of the near stationary region which is presented below.

TABLE XXXIII

THE STANDARD ERROR OF THE β COEFFICIENTS FOR ALTERNATIVE RANDOM NUMBERS METHODOLOGIES

Alternatives	Standard Error					
	β_0	β_1	β_2	β_{12}	β_{11}	β_{22}
1. Common Random Numbers	4,560	3,118	1,389	404	1,172	1,587
2. Schruben and Margolin's Methodology	2,812	2,017	1,064	358	949	1,123
3. The Proposed Methodology	521	390	311	248	98	351

Analysis of the Fitted Surface

Based on the estimates obtained by the proposed Methodology, the mathematical relationship between the inventory cost and the ordering quantity and the reordering level is:

$$y = 18{,}754 + 108\, x_1 - 497\, x_2 - 403\, x_1 x_2 + 11\, x_1^2 + 139\, x_2^2 \qquad (4.25)$$

To find the stationary point in the near stationary region, partial derivatives with respect to x_1 and x_2 for equation (4.25) were calculated.

After setting the results equal to zero, a system of two equations and two unknowns was solved. The values of x_1 and x_2 obtained for the stationary point are:

$$x_1 = .20$$
$$x_2 = 1.25$$

These values correspond to 54,463 units for the ordering quantity and 51,100 units for the reordering level. The inventory cost of this policy is $18,389. The response for the stationary point is not better than all the other responses obtained before. However, since the inventory simulation under consideration is probabilistic and the trials are not replicated, this is a likely occurrence.

A closer examination of the stationary point was made possible by the method of canonical analysis. By transferring the origin of the second order design to the stationary point and measruing the variables along the new axes, denoted by X_1 and X_2, the following canonical equation was obtained.

$$y = 18,389 - 136.5\ X_1^2 + 286.5\ X_2^2 \qquad (4.26)$$

If the coefficients for X_1^2 and X_2^2 were both positive, the stationary point would have been a true minimum. Since one coefficient is positive and the other is negative the stationary point is a saddle point. The fitted contours are hyperbolas elongated in the direction of the X_1 axis. Therefore, no conclusion can be drawn about the presence of a global minimum.

Analysis

Although the empirical investigation was limited to the application of response surface methodology to an inventory simulation case, the results do have direct implications for other forms of simulation. The potential of response surface methodology stems from the efficiency by which it discovers an unknown relationship or finds the optimum point regardless of the nature of a problem. Since the objective(s) of many simulation problems coincide with the rationale behind the use of response surface methodology, as was the case in the inventory problem, it is natural for most other simulation problems to benefit from it, too.

The inventory simulation example indicated that the response surface methodology is a strong and an efficient technique for simulation. The average inventory cost which was more than 24,000 for the initial experiments was substantially reduced to less than 18,000. Only about 20 experiments were needed to discover the relationship between the simulation responses and the controllable conditions.

The examination of the example reported here and other examples not reported in detail provided valuable insight about the application of response surface methodology in simulation. Some of the pitfalls in applying response surface methodology to simulation and the way to minimize their impact are as follows.

General speaking, the performance of response surface methodology strongly depends on the magnitude of the experimental error. The response surface methodology is successful when the experimental error is small. The stochastic nature of simulation causes volatility in responses that can lead to large experimental errors. This problem

is aggrevated when the experimental points under investigation are too far apart.

Therefore, successful application of response surface methodology to simulation requires, first, the units selected for the variables to be small so that the experimental points are not too far apart. Secondly, each experimental point should be run for adequate intervals or periods of time to allow for erosion of erratic variations. Another strategy would be replication of observations at each experimental point. Replication of observations is in contrast to the spirit of this research, that is accomplishing the objective of a simulation study with the least possible number of observations. Additionally, very little discussion exists in the literature about the assignment of random numbers to the experiomental points of a design when the trials are replicated.

To increase the efficiency of results in a simulation that uses response surface designs, it was shown that it is wise to take advantage of efficient random numbers assignment rules that are available. The common random numbers technique consistently performed better than the independent streams of random numbers. For the regressions with comparable experimental errors, the Methodology proposed in this paper was more efficient than Schruben and Margolin's methodology, the common random numbers methodology, and the independent random numbers methodology when the expected positive correlations between the responses were induced.

Due to the nature of simulation, no recommendation regarding random numbers assignment rule can be made from the empirical findings of a simulation. The findings of this study do not support the argument that

the common random numbers technique performs better when the policies compared are small perturbations of each other. The findings, however, suggest that the magnitude of the induced positive correlations depends on the specific pairs of the design points. With respect to the antithetic random numbers, the magnitude of the induced negative correlations was larger when the experimental points were further apart. In other words, moving the experimental points closer to each other adversely affected the magnitude of the negative correlations. The magnitude of the induced negative correlations could have increased, to a limited extent, by the increase in the variability of demand. While no specific random numbers assignment rule can be recommended, the following two approaches will help one decide on the assignment rule.

First, a few pilot runs in the beginning will enable the designer to discover the signs and magnitudes of the induced correlations. Second, simulations can be stopped and restarted without disturbing their statistical properties. Therefore, an early check on the signs and magnitudes of induced correlations will allow the designer to test the validity of his assumptions. If the expected negative (or zero) and positive correlations between the responses are realized, the proposed Methodology will be more efficient than the common random numbers rule. If only positive correlations are generated, the common random numbers might be more efficient than the proposed Methodology.

The reclassification of response surface designs supplemented by the discussion of random numbers assignment rules will, hopefully, stimulate future application of response surface methodology in simulation. A summary of the conclusions, and the recommendations for future research will be given in Chapter V.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

This study was designed to develop a methodology for assigning random numbers to the experimental points of response surface designs used in simulation. The proposed Methodology was based on the analytical findings of Schruben and Margolin (52). Additionally, the study was intended to create a presentation scheme for response surface designs to facilitate their applications to simulation.

In pursuing the objectives of the paper, first, the literature of response surface methodology was reviewed and presented in Chapter II. Second, the developments in the area of random numbers assignment were examined. Third, two tree diagrams were drawn to help designers find their appropriate designs. Fourth, a methodology was presented for incorporating Schruben and Margolin's random number assignment rule in response surface designs used in simulation. Last, the analytical discussions were applied to an inventory simulation case. A summary of the findings is given below.

Response surface methodology is rich and advanced in theory. A number of first order, second order, and third order designs have been developed for fitting polynomials to different problems. Experimenters in chemical laboratories have well taken advantage of response surface methodology in their experiments. The limited application of response surface methodology to simulation may, in the researcher's opinion, be

attributed to 1) the availability of inefficient but simple enumerative approaches and 2) the lack of an exhaustive and a cohesive presentation of the subject. Although many books have devoted a chapter to this subject, the discussions have been basically fragmented and categorical (16) (19) (45). In 1971, a complete discussion of the subject was given by Myers (47). The objective of Myer's book was to create a continued awareness of response surface methodology techniques among potential users. The book is not oriented toward simultion, and unless one reads it in entirety, he will not be in a position to decide which design to use. The tree diagrams and their associated discussion in Chapter IV facilitates the selection process, and through references, provides an opportunity for further evaluation of the selected design.

The tree diagram representing first order designs (see Figure 8) has five branches. Each branch corresponds to a possible objective of the designer influenced by his knowledge of the problem. Two of the branches are associated with minimizing variance. Variance can be minimized for either the individual coefficients of the response as a whole. Two other branches are related to minimizing bias. Whether the orientation of design with respect to response function is known or not will affect the method used for minimizing bias. Minimization of both bias and variance is shown on the last branch.

Orthogonal designs are used for all the above cases. However, the size of designs will not be the same for all the categories. To estimate the first order coefficients, variables should be varied at least at two levels. Thus, complete and fractional factorial designs are the most appropriate first order orthogonal designs.

The second order design tree (Figure 9) has two branches representing second order composite and second order rotatable designs. For estimating the coefficients of a second order polynomial, variables should take at least three different values. A class of designs more efficient than 3^k factorial designs is called composite designs (10). These designs are obtained by adding experimental points to a first order design which is large enough to estimate the main effects as well as the first order interaction effects. Composite designs are either central or noncentral. Central composite designs are appropriate when the optimum point is suspected to be around the origin of the design. On the other hand, noncentral composite designs are desirable when the optimum point is suspected to be close to a combination other than the origin. Composite designs are easy to apply and are suitable for sequential experiments. They provide a designer with the opportunity to form second order orthogonal designs, second order designs with equal precision for quadratic and interaction effects, and second order rotatable designs.

Second order rotatable designs are useful when the objective is to have equal precision for all the responses that are equidistant from the origin. There are four possible procedures for constructing second order ratatable designs and depending upon the circumstances, one might be preferred over others. The procedures are:

1. Equiradial sets procedure.
2. Composite designs procedure.
3. Imcomplete block designs procedure.
4. Simplex-sum designs procedure.

The most attractive procedure seems to be composite designs method.

Since second order designs are normally built by adding points to first order designs, composite designs and central composite rotatable designs are widely applied in practice. The other methods developed for forming second order rotatable designs do not use all the observations employed for estimating first order effects and, therefore, are not as efficient.

One characteristic of sequential experiments is that sets of experiments are conducted at different times leading to a possible source of variation among observations. Consequently, blocking techniques have been developed to take into account time variation and other heterogeneous experimental conditions. In simulation, however, one is generally able to control the experimental conditions and, therefore, eliminate the need for blocking. But blocking, through random numbers, has been considered as a means for increasing the efficiency of simulation. Most empirical findings to date indicate that simulation responses generated by the same random numbers are positively correlated. Similarly, responses generated by a random number and its antithesis are negatively correlated. Having taken these findings for granted, Schruben and Margolin (52) investigated alternative assignment of random numbers and concluded the following: If N experimental points admit orthogonal blocking into two blocks, preferably chosen to be equal, then assigning a set of random numbers to the observations in one block and its antithetic set to the second block results in a smaller D-value than the assignment of common random numbers to all the design points or different random numbers to all the design points. D-value refers to the determinant of the estimator dispersion matrix.

When response surface designs are planned and performed at one time, the application of the aforementioned assignment rule will not pose any problem. But, because response surface methodology is performed in steps, appropriate measures need to be taken to assure compliance with the rule. Specifically, addition of experimental points to first order designs conducted in two orthogonal blocks should keep the blocks orthogonal.

Factorial and fractional factorial designs recommended for fitting first order polynomials can be divided into two orthogonal blocks by identifying a defining contrast(s). Theories of confounding help one decide which contrasts should be selected for blocking purposes.

When the objective is to form second order designs in two orthogonal blocks by adding points to a first order design, the first order design should be large enough to provide estimates of the main effects plus those of paired interaction effects. First order designs meeting this condition are labeled as designs of type B' and a list of them was given in Chapter IV. Additionally, it was shown how designs of type B' and its associated second order designs can be performed in two orthogonal blocks.

It is important to emphasize that not all the first order designs used at different stages for estimating first order effects have to be designs of type B'. Except for the last first order design that will be augmented by additional observations to estimate second order coefficients, the rest could be designs with fewer number of observations. The designer's knowledge about the problem is the key determinant of the number of experimental points. For instance, if the designer knows that the initial experiments are far from the optimum,

he may decide to use a design with the minimum number of observations just to estimate the main effects.

The Methodology presented in this paper and the common streams of random numbers are equally efficient in estimating all the main and interaction effects; and they are both more efficient than the independent streams of random numbers in estimating those effects. However, the common streams of random numbers provides the least efficient estimate of the mean effect. The question of whether the proposed Methodology is more efficient than the independent streams of random numbers in estimating the mean effect and the extent of its efficiency over the common streams of random numbers is answered by the magnitude of the positive and negative correlations. It was shown that, the larger the magnitude of the negative correlations induced, the more efficient the proposed Methodology will be. However, even if the antithetic random numbers produce zero or positive correlations less than the positive correlation induced between the points in the first block, the proposed Methodology will still be more efficient than the common streams methodology for estimating the mean.

The objective of a designer in early stages of response surface methodology is to estimate the main effects as accurately as possible to determine the steepest ascent or descent path. Thus the proposed Methodology that uses Schruben and Margolin's assignment rule and the common streams of random numbers are both more efficient than independent streams of random numbers. Also, because of providing a better estimate of the mean as compared to the common streams of random numbers, the proposed Methodology appears to be the best choice.

When the search process has been led to the near-stationary region, the efficiency of the interaction effects then becomes as important as the efficiency of the main effects. An argument against the recommended Methodology would be that it confounds the estimate of one or more interaction effects in dividing the observations into two orthogonal blocks. However, in a problem with more than two factors, it is not hard to find a high-order interaction effect that is expected to be insignificant and can be used for dividing the observations into two blocks.

The result of the empirical work strongly supported the idea of using response surface methodology in simulation. Response surface methodology required a limited number of trials to either find the optimum (local) or to discover the functional relationship between the controllable conditions and the simulation responses.

The examination of the example reported in Chapter IV and other examples not reported in detail provided valuable insight about the application of response surface methodology in simulation. Some of the pitfalls in applying response surface methodology to simulation and the way to minimize their impact are as follows.

Generally speaking, the performance of the response surface methodology strongly depends on the magnitude of the experimental error. The response surface methodology is successful when the experimental error is small. The stochastic nature of simulation causes volatility in responses that can lead to large experimental errors. This problem is aggrevated when the experimental points under investigation are too far apart.

Therefore, successful application of response surface methodology to simultion requires, first, the units selected for the variables to be

small so that the experimental points are not too far apart. Second each experimental point should be run for adequate intervals or periods of time to allow for erosion of erratic variations. Another strategy would be replication of observations at each experimental point. Replication of observations is in contrast to the spirit of this research, that is, accomplishing the objective of a simulation study with the least possible number of observations. Additionally, very little discussion exists in the literature about the assignment of random numbers to the experimental points of a design when the trials are replicated.

With respect to random numbers assignment rules, the findings of this study do not support the argument that the common random numbers technique performs better when the policies compared are small perturbations of each other. The findings, however, suggest that the magnitude of the induced positive correlations depends on the specific pairs of the design points. With respect to the antithetic random numbers, the magnitude of the induced negative correlations was larger when the experimental points were further apart. In other words, moving the experimental points closer to each other adversely affected the magnitude of the negative correlations. The magnitude of the induced negative correlations could have been increased, to a limited extent, by the increase in the variability of demand.

Due to the nature of simulation no specific recommendation can be made about the assignment of random numbers to response surface designs used in simulation. However, the empirical findings lend support to the belief that the deliberate manipulation of random numbers in most cases will enhance the efficiency of the simulation results. A few

pilot runs and an early check on the signs and magnitudes of the induced correlations will signal the appropriateness of an assignment rule.

In summary, this study developed an efficient methodology for assigning random numbers to the experimental points of response surface designs used in simulation. Moreover, it developed a different format for presentation and categorization of response surface designs to encourage and facilitate their future application mainly in simulation. A simulation designer with some knowledge of a problem and an objective will, hopefully, be able to appreciate this presentation and use it for selecting an appropriate design.

Recommendations

Response surface methodology is the union between the fields of nonlinear programming and experimental designs. While steepest ascent method is an improvement over using the "one variable at a time" technique, its superiority over other nonlinear optimization tools is questionable. There is a need for a study to examine the feasibility of applying more efficient nonlinear optimization tools to response surfaces.

Response surface methodology has, so far, been limited to unconstrained optimization problems. However, there are circumstances in which the optimum conditions should be found given that a number of constraints are present. Thus, a new direction of research would be examination of experimental designs as they apply to constrained optimization problems.

Another avenue of future research lies in application of multivariate analysis, canonical correlation analysis in particular, to problems with multiple responses.

When response surface methodology is used in simulation, the magnitude of the experimental error may make it desirable to replicate the observations at each design point. The analytical and empirical investigation of random number assignment rules for designs with replicated observations accouter an opportunity for future research.

Generation of response surface designs of higher order or with new features is also a challenge to be confronted in the future. But with the theory far ahead of the practice, and given the adequacy of second order polynomials in most cases, the gain to be obtained by pressing for new designs does not appear to be of a great value.

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