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MINIMUM BIAS DESIGNS FOR RESPONSE SURFACES

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SUMMARY

This thesis presents the topic of minimum bias designs in response surfaces with a view toward organizing the material and illustrating it in a comprehensive manner stressing interrelationships among various modern design criteria. In particular, it examines the assumptions which have been made concerning minimum bias designs and certain aspects of the results obtained.

The research also develops other traditional criteria and stresses the importance of rotatability to modern design criteria. Application of two traditional criteria, orthogonality and uniform precision, to certain minimum bias rotatable designs was demonstrated by the writer to have no meaning, since they are mutually exclusive relationships.

The major thrust of this research was directed at deriving a method to apply minimum bias estimation to the problem of estimating the slope of a response surface. This was accomplished for the case of a single factor. Simple design applications were also demonstrated. These results closely parallel previous work with minimum bias estimation and demonstrate the superiority of minimum bias estimation to least squares estimation for designs which seek to minimize integrated mean square error.

CHAPTER I

INTRODUCTION

Since its inception in the late 1940's and early 1950's by George E. P. Box and K. B. Wilson, response surface methodology has come into widespread prominence because of the simple yet effective manner in which these techniques may be used to experimentally determine optimum conditions for some process or phenomenon. Initial applications were in the field of chemistry and chemical engineering, although in recent years response surface methodology has been applied in tool life wear determination, food stuff production, education, econometrics, and traffic control.

Implicit in the concept of response surface methodology is the assumption that there exists a smooth functional relationship between the characteristic of interest, called the response, and the independent variables which influence this response. It is further assumed that such a function can be adequately represented by a low-order polynomial within the area of potential interest.

Suppose the experimenter is interested in exploring the functional relationship

$$\eta = f(\xi_1, \xi_2, \xi_3 \xi \ldots, \xi_k) + \varepsilon \qquad (1.1)$$

where η is the response, the ξ_i's are the independent factors which influence the response, ε is the random experimental error, and the function

$\mathcal{f}$ is usually of an unknown form. In the experimental design literature, the function $\mathcal{f}$ is usually called a response surface. The experimenter decides that the actual relationship can be approximated by a graduating polynomial such as

$$y(\xi) = g(\underline{\xi},\underline{\beta}) = g(\xi_1,\xi_2,\ldots,\xi_p,\beta_1,\beta_2,\ldots,\beta_p) + \epsilon, p \leqq k \tag{1.2}$$

over some specified region of interest, where $\underline{\beta}$ is a vector of unknown parameters.

Typically, the experimenter will fit an estimated response surface by estimating the unknown parameters in Equation (1.2). This will require that at least k observations on the response at various levels of the independent variables be taken and some procedure used to compute estimates of $\underline{\beta}$, say $\hat{\underline{\beta}}$. This fitted model may now be written as

$$\hat{y}(\underline{\xi}) = \hat{y} = g(\underline{\xi},\hat{\underline{\beta}}) \tag{1.3}$$

In estimating the parameters, it is usually possible to control the levels of the independent variables ξ_i. Thus the experimenter is faced with the problem of choosing these levels, or a problem of experimental design. Experimental designs for estimating the unknown parameters in a model such as Equation (1.2) are often called response surface designs.

The fitting of the graduating polynomial can be treated as a particular case of multiple linear regression. The N sample levels of the ξ_{iu} and the associated response y_u can be represented as

$$\underset{\sim}{\xi} = \begin{bmatrix} \xi_{11} & \xi_{21} & \cdot & \cdot & \cdot & \cdot & \cdot & \xi_{p1} \\ \xi_{12} & \xi_{22} & \cdot & \cdot & \cdot & \cdot & \cdot & \xi_{p2} \\ \xi_{13} & \xi_{23} & \cdot & \cdot & \cdot & \cdot & \cdot & \xi_{p3} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \xi_{1N} & \xi_{2N} & \cdot & \cdot & \cdot & \cdot & \cdot & \xi_{pN} \end{bmatrix}, \quad \underset{\sim}{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \cdot \\ \cdot \\ y_N \end{bmatrix} \tag{1.4}$$

As was indicated above, the actual plan of experimental levels in the ξ's is called the experimental design.

In much of the work which follows, it is convenient to adopt the scaling convention that the design levels are coded such that

$$\sum_{u=1}^{N} x_{iu}^2 = N, \tag{1.5}$$

and $\qquad (i = 1,2,3,\ldots,p)$

$$\sum_{u=1}^{N} x_{iu} = 0.$$

If the actual value of the u^{th} level of the variable i is denoted by ξ_{iu}, then the corresponding coded value is

$$x_{iu} = \frac{\xi_{iu} - \bar{\xi}_i}{S_i}, \tag{1.6}$$

where

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

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

The least squares estimators of the β_i, say $\hat{\beta}_i$, are chosen so as to minimize the sum of the squares of the deviations

$$L = \sum_{i=1}^{N} \epsilon_i^2 = \underline{\epsilon}'\underline{\epsilon} \tag{1.7}$$

It is well known that

$$\underline{Y} = \underline{X\beta} + \underline{\epsilon} , \tag{1.8}$$

or

$$\underline{Y} - \underline{X\beta} = \underline{\epsilon} . \tag{1.9}$$

Substituting into (1.7) and expanding one obtains

$$L = \underline{Y}'\underline{Y} - 2\underline{\beta}'\underline{X}'\underline{Y} + \underline{\beta}'\underline{X}'\underline{X}\ \underline{\beta} , \tag{1.10}$$

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

$$\frac{\partial L}{\partial \underline{\beta}} = -2\underline{X}'\underline{Y} + 2(\underline{X}'\underline{X})\ \underline{\beta} . \tag{1.11}$$

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

$$\hat{\underline{\beta}} = (\underline{X}'\underline{X})^{-1}\ \underline{X}'\underline{Y} \tag{1.12}$$

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

It is now possible to estimate each of the model parameters and obtain a fitted equation of the response surface. Also, one may test various hypotheses about the parameters in the model (1.8). This is discussed extensively in Graybill (13).

There are two different objectives which influence the choice of a response surface design; that of estimating the model parameters and that of estimating the response surface itself. Of course, the appropriate strategy for investigation is heavily dependent upon the experimenter's own knowledge of the important variables; on the one hand he may know the entire functional form of the true surface, while at the other extreme he may not know which variables are pertinent to the investigation. This situation will lead the experimenter into screening experiments to gain some insight into these important factors.

Concurrent with the development of response surface designs, Box (2) sought to develop requirements for the evaluation of these experimental designs. An experimental design should be such that it

1. allows the graduating polynomial to estimate the response surface throughout the region of interest,
2. insures that $\hat{y}$ is as close as possible to η,
3. gives good detectability of "lack of fit,"
4. allows transformations to be fitted,
5. allows experiments to be performed in blocks,
6. allows designs of increasing order to be built up sequentially,
7. provides an internal estimate for error,
8. is insensitive to wild observations,
9. requires a minimum number of observations,
10. provides patterning of data allowing for visual appreciation,
11. insures simplicity of calculation, and
12. behaves well when errors occur in the settings of the control-

lable factors (ξ's).

Requirements two and three provide the primary impetus for modern criteria in experimental design. While satisfying these requirements, modern experimental design criteria deal with the second objective of response surface design, that of estimating the response surface itself. In particular, if one considers the squared differences between the true model and the fitted surface, then this error measurement can be divided into two components; a bias component due to model inadequacy, and a variance component due to sampling error. Box and Draper were instrumental in developing designs which attempt to minimize this squared error. The topic of modern design criteria is a major area of study in the recent response surface literature and will form the basis for this investigation.

Nature of This Investigation

The objective of this investigation involves the analysis of modern criteria for response surface design. These concepts have been largely developed by Box, Draper, and other writers, and are alternatives to the "classical" criteria of rotatability, uniform precision, and minimum variance.

The first objective is to discuss, analyze, and develop modern design criteria with a view toward organizing this material and presenting it in a comprehensive manner stressing the interrelationships between these criteria. The second objective will be to apply the concept of minimum bias estimation due to Karson *et al*. (17) to the problem of estimating the slope of a response surface. The final objective will be to integrate modern design criteria with other traditional criteria such as rotatability, uniform precision, etc. in order to more fully explain and differentiate important characteristics for their application.

CHAPTER II

LITERATURE SURVEY

A survey of the pertinent literature, along with some of the simpler concepts of minimum bias designs will be presented in this chapter. However, because of their importance, a detailed presentation of fundamental concepts will be developed in the following chapters along with descriptions, extensions, and applications to specific response surface designs.

The Work of Box and Wilson

The concept of response surface methodology can be traced to Yates (19) in 1935. Further work in its development can be attributed to Hotelling (15) in 1941 and Friedman and Savage (12) in 1947. The original paper by Box and Wilson (6) in 1951 introduced little in the way of statistical or analytical techniques but rather introduced a simple but ingenious technique aimed at problem solving, coupled with some well known mathematical and statistical techniques. The real merit of the original work was in the field of experimental design.

As was indicated previously, Box and Wilson used the method of least squares to estimate the coefficients of the fitted polynomial, but quickly realized the inadequacy of the factorial design when estimating quadratic and higher order coefficients. As an alternative to this design, Box and Wilson proposed the Central Composite Design (CCD) to overcome two major obstacles which were inherent in the older 3^p factorial designs; that is, significantly reducing the number of trials when compared with the factorial design, and secondly obtaining an important increase in the precision when estimating the coefficients of the quadratic and higher order terms of the approximating polynomial.

The central composite design is in reality a 2^p factorial or suitable fraction thereof, augmented by additional points to allow estimates of the coefficients of the higher order polynomial. For the case of three variables the design matrix is given by

$$D = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ -\alpha & 0 & 0 \\ +\alpha & 0 & 0 \\ 0 & -\alpha & 0 \\ 0 & +\alpha & 0 \\ 0 & 0 & -\alpha \\ 0 & 0 & +\alpha \end{bmatrix} \end{array} \qquad (2.1)$$

where (-1, +1) represent the coded levels of the independent variables, $(-\alpha, +\alpha)$ represent axial points of a cube and (0,0,0) represents center points of the design. Figure 1 gives a geometric illustration of the three variable CCD. In general, the p variable CCD consists of a factorial portion (usually a 2^p or a suitable fraction thereof), an axial portion with 2p observations, and n_o center points.

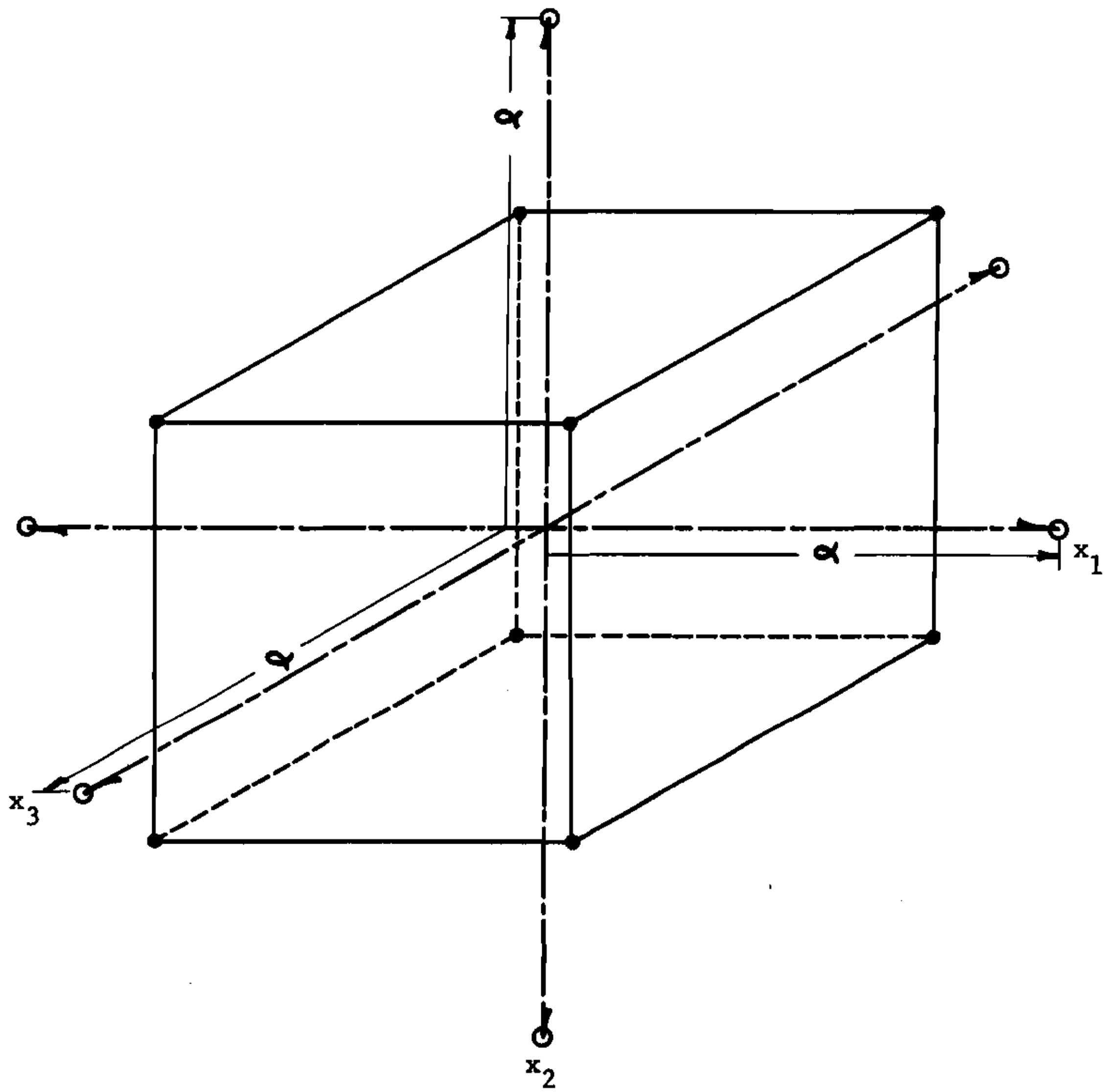

Figure 1. Three Variable Central Composite Design

In order to locate the region of the optimum, when remote from the initial starting conditions, Box and Wilson used a 2^p factorial design (or a suitable fraction thereof) to fit a first order polynomial and moved along the direction of greatest slope. When it appeared that near optimal conditions had been reached, the authors used the Central Composite Design to fit a second order polynomial and located the stationary point by calculus methods. If the stationary point indicated a maximum or minimum, the optimum conditions were thought to have been determined. This approach gave the experimenter added insight into the experimental process and also some appreciation for the type of response surface involved. Box and Wilson further demonstrated that the method converged rapidly on the optimum and would lead the experimenter to an efficient empirical exploration of the system.

In the early years of the development of response surface designs, it was always assumed that the problem of choosing a "best" design would be interpreted as choosing a design whereby the coefficients (β) of the controllable factors, could be estimated with minimum variance. For a first order model, this criterion necessitated the choice of a diagonal $(\underline{X}'\underline{X})$ matrix, or an orthogonal experimental design. For higher-order polynomials, it may not always be clear how the design must be chosen.

Box and Hunter's Criteria

A second criterion for a "best" design was proposed by Box and Hunter (5), whereby overall response is based upon the joint consideration of the accuracy of the response coefficients. This paper was the first to place attention on estimating the response surface itself as such, rather than on simply estimating the parameters of the model. This design criterion is called a "rotatable" design. The concept of rotatability requires that all points equidistant from the center of the experimental design have a common variance. That is, for any k-dimensional design, the variance of the estimated response is a function of distance only. The variance contours are simply spheres centered at the origin.

A secondary benefit, but of great importance is the significant reduction in the treatment combinations which will provide precise estimates of the polynomial coefficients. Coupled with the natural benefit of rotatability, which allows the experimenter to overcome the problem of orientation of the response surface with respect to some predetermined axis in the design of the experiment, this new design criterion provided a great breakthrough over previous designs.

To this point, the problem of "bias," or the lack of fit of the graduating polynomial to the true surface has not been mentioned, and in fact, it has been assumed that the experimenter had complete knowledge of the surface to be approximated. Of course, this is really not the case at all. If in fact the terms of higher order are not negligible, Box and Hunter (5) sought to choose a design which gives some protection against bias from higher order terms, while still giving a high degree of precision near the center of the design. This criterion, called uniform precision, causes the variance at the center of the design to be equal to the variance at some arbitrary distance, usually $\rho = 1$, where

$$\rho^2 = \sum_{i=1}^{\rho} x_i^2 \qquad (2.2)$$

The value of ρ depends upon the scaling convention.

It would seem appropriate at this point to digress momentarily to develop some of the concepts of rotatability and uniform precision and their associated underlying definitions because of their fundamental importance to response surface design. The moment matrix of a design is given by $N^{-1}\underline{X}'\underline{X}$ where N is the total number of runs specified by the design. For a first order design the moment matrix is

$$N^{-1}\underline{X}'\underline{X} = \begin{array}{c} \\ \left[\begin{array}{ccccc} & x_1 & x_2 & \cdots & x_k \\ [1] & [1] & [2] & & [k] \\ & [11] & [12] & & [1k] \\ & & [22] & & [2k] \\ & & & & \cdot \\ & & & & [kk] \end{array}\right] \end{array} \qquad (2.3)$$

where

$$[i] = 1/N \sum_{u=1}^{N} x_{iu}$$

$$[ij] = 1/N \sum_{u=1}^{N} x_{iu}x_{ju} \quad .$$

The quantities [i] and [ij] are called first and second order design moments, respectively. Hence one sees that the moment matrix is just a matrix containing the design moments. The elements of $N^{-1}\underline{X}'\underline{X}$ in (2.3) can be easily verified by obtaining the sums of squares and products in the appropriate $\underline{X}'\underline{X}$ matrix. For a second order model one may verify that

$$N^{-1}\underline{X}'\underline{X} = \begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\ \end{array}$$
$$\begin{bmatrix} [1] & [1] & [2] & [11] & [22] & [12] \\ & [11] & [12] & [111] & [122] & [112] \\ & & [22] & [112] & [222] & [122] \\ & & & [1111] & [1122] & [1112] \\ & & & & [2222] & [1222] \\ & & & & & [1122] \end{bmatrix} \qquad (2.4)$$

where, as before

$$[1122] = 1/N \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$$

$$[1111] = 1/N \sum_{u=1}^{N} x_{iu}^4 \quad .$$

The inverse $N(\underline{X}'\underline{X})^{-1}$ is called the precision matrix and contains elements which are related to the variances and covariances of the model coefficients.

Box and Hunter further demonstrated that a necessary and sufficient condition for a d^{th} order design to be rotatable is that the moments of order up to 2d be of the form:

$$\left[1^{\delta_1} 2^{\delta_2}, \ldots, p^{\delta_p}\right] = N^{-1} \sum_{u=1}^{N} x_{1u}^{\delta_1} x_{2u}^{\delta_2}, \ldots, x_{pu}^{\delta_p} = \frac{\lambda_\delta \prod_{i=1}^{p} (\delta_i)\,!}{2^{\delta/2} \prod_{i=1}^{p} (\frac{1}{2}\delta_i)!} \qquad (2.5a)$$

for all δ_i (δ_i is an index) even and

$$\left[1^{\delta_1} 2^{\delta_2}, \ldots, p^{\delta_p}\right] = N^{-1} \sum_{u=1}^{N} x_{1u}^{\delta_1} x_{2u}^{\delta_2}, \ldots, x_{pu}^{\delta_p} = 0 \qquad (2.5b)$$

if any δ_i odd where $\delta = \sum_{i=1}^{p} \delta_i$. Here λ_δ represents the design moment. For first order designs, it can be shown that an orthogonal design is also rotatable. However, this is not the case for a second order design. It is easily seen that [11] and [22], from (2.5) have the value λ_2, and [1111] and [2222] have the value $3\lambda_4$. Further [1122] has the value λ_4. The moment matrix for a second order rotatable design is given by

$$N^{-1}(X'X) = \begin{array}{c} \begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & \lambda_2 & \lambda_2 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_2 & 0 & 0 & 0 \\ \lambda_2 & 0 & 0 & 3\lambda_4 & \lambda_4 & 0 \\ \lambda_2 & 0 & 0 & \lambda_4 & 3\lambda_4 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_4 \end{bmatrix} \end{array} . \qquad (2.6)$$

It is important to note that the fourth moments [iiii] have the value $3\lambda_4$, and the fourth moments [iijj] have the value λ_4. From (2.6) it can be seen that there is a certain amount of flexibility in choosing a value for λ_4. The parameter λ_4 = [iijj] can be conveniently altered without loss of rotatability. In certain designs this may be accomplished by adding center points to the basic design configuration. Box and Hunter sought to give some protection against higher order bias while still giving a high degree of precision near the center of the design. This new criterion fixed the value for λ_4 and gave a "uniform precision" rotatable design. Box and Hunter further demonstrated that λ_4 could be chosen so as to give an orthogonal second order design.

Minimization of Mean Square Error

In examining the criteria of rotatability and uniform precision, Box and Draper (3) considered a more careful appraisal of the effectiveness of the design, and in particular, requirements two and three of Box's ideal design. They developed a new criterion--minimization of the mean square error over the region of interest.

If $\hat{y}$ (ξ) denotes the response estimated by the approximating polynomial, we desire to choose the design matrix D so that the expected squared difference $E\{\hat{y}(\xi) - \eta(\xi)\}^2$ will be minimized over the region of interest R. It is convenient as before to transform the independent variables to a new set of variables $x_1, x_2, \ldots x_p$ in such a way that the center of interest becomes the origin of the x's and are scaled relative to one another. Thus the measure of effectiveness becomes

$$E\{\hat{y}\ (x) - \eta(x)\}^2 \tag{2.7}$$

where $\hat{y}$ (x) and $\eta(x)$ represent the approximating polynomial and the true surface, respectively. This difference, when averaged over the region R, is

$$\Omega\int_R E\{\hat{y}\ (x) - \eta(x)\}^2\ dx \tag{2.8}$$

where

$$\Omega^{-1} = \int_R dx \quad .$$

Since it is important to be able to compare designs which do not contain equal numbers of points, our overall measure of effectiveness becomes

$$J = \frac{N\Omega}{\sigma^2} \int_R E\{\hat{y}\ (x) - \eta(x)\}^2\ dx \quad . \tag{2.9}$$

Thus J is simply the expected value of the squared difference between the true surface and the fitted model over the region R and normalized with respect to the number of observation and the variance. Now

$$\{\hat{y}\ (x) - \eta(x)\} = \{\hat{y}\ (x) - E[\hat{y}\ (x)]\} + \{E[\hat{y}\ (x)] - \eta(x)\}, \tag{2.10}$$

and substituting (2.10) into (2.9) one obtains

$$J = \frac{N\Omega}{\sigma^2} \int_R E\{\hat{y}\ (x) - E[\hat{y}\ (x)] + E[\hat{y}\ (x)] - \eta(x)\}^2\ dx \tag{2.11}$$

which can be rewritten as

$$J = \frac{N\Omega}{\sigma^2}\left[\int_R E\{\hat{y}(x) - E[\hat{y}(x)]\}^2\, dx + \int_R \{E[\hat{y}(x)] - \eta(x)\}^2\, dx \right] . \quad (2.12)$$

The first integral is simply the variance of y(x) and the second integral is the bias. Thus

$$J = V + B, \quad (2.13)$$

with the corresponding obvious notation.

Box and Draper were thus able to show that the criterion of integrated mean square error was simply composed of two components--bias and variance. They ultimately obtained the somewhat surprising conclusion that the optimal design for a situation in which both bias and variance occurred would be nearly the same as if the variance component were ignored and the experiment were designed to minimize the bias alone.

Integrated Mean Square Error and Rotatability

Further work into the criterion of minimum integrated mean square error evaluated the assumptions which were made by Box and Draper in their original article. In a second article (4) they established a more generalized model for integrated mean square error, over some new general region, say O, as

$$J = \int_O w(x)\, E(\hat{y}(x) - \eta(x))^2\, dx \quad (2.14)$$

where

$$\int_{o} w(x)\ dx = 1$$

and

$$w(x) = \begin{cases} \Omega \text{ in R the region of interest} \\ 0 \text{ elsewhere} \end{cases}$$

The quantity $w(x)$ is a weight function which gives more weight to error at one point than at another point, and one sees that Equation (2.8) is a special case of (2.14).

In this second article Box and Draper also examine the choice of region of interest--a spherical region or a cuboidal region. Box and Draper chose to deal with the spherical region of interest, first because it was probably the most frequently encountered and second because it lent itself to the important property of rotatability. Box and Draper were able to show that designs which minimize bias were rotatable designs which depend on the order of the true function and the order of the graduating polynomial.

Box and Draper further concluded that as the experimenter expects less and less effect from the bias of the approximating polynomial, more and more center points should be added and the spread of the experimental points along their respective axes should be made as large as possible from the origin, and they should include points <u>outside</u> the region of interest.

Cuboidal Regions

Draper and Lawrence (8) continued the research into the assumptions made by Box and Draper regarding the region of interest. They chose to explore the concept of a cuboidal region of interest. Draper and Lawrence were able to construct designs utilizing this particular region of interest, but these designs did not enjoy any of the other useful properties such as rotatability. Further work by Draper and Lawrence (9) included the choice of a "wrong" region on the part of the experimenter. For example, if one chose a spherical design and the region was in fact cuboidal or vice versa. It was found that each design (with one rare exception) worked best over its own particular region of interest.

Weighted Regions of Interest

A second assumption explored by Draper and Lawrence (10) was the use of a uniform weight function throughout the region of interest. In this article Draper and Lawrence point out and prove general conditions for minimization of bias. An unpublished theorem by Mallows (as referenced by Draper and Lawrence (17)) shows that bias can be minimized by choosing the moments of the design such that they will equal the moments of the weight function. This is equal to the sum of the order of the fitted polynomial plus the order of the surface against which bias is to be guarded.

Draper and Lawrence assumed that interest varied according to the distribution of a symmetric multivariate weighting function over the particular region of interest. This concept has an inherent appeal to the experimenter because now the total interest was not focused about the center of the design, but some weight was given to clusters which might appear at the periphery. The authors developed rotatable designs which give additional flexibility to the spherical weight function designs.

Other Recent Work

Recently there have appeared several other articles which deal with related aspects of modern response surface designs. Herzberg (14) examined the behavior of the variance function of the difference between two estimated responses. She developed rotatable designs with this criterion in mind, but did not consider the problem of bias. She assumed a total knowledge of the order of the surface on the part of the experimenter. Herzberg's research concluded that the variance function is a function of the distance of the two points from the origin (the design center) and the angle subtending the two points at the origin. When the variance function is considered alone, for second-order rotatable designs, the second and fourth design moments should be made as large as possible.

A more recent article by Davies (7) uses the criterion of Box and Draper to investigate the relationship between the response and the exclusion of certain independent variables, both in the design portion of the experiment and in the analysis portion of the experiment. Davies gives further guidelines regarding the exclusion of these design factors and discusses certain criteria for the exclusion of these variables. These criteria are highly dependent upon an intimate knowledge of the process on the part of the experimenter and upon previous experimentation.

Minimum Bias Estimation by Design

The last three articles, which form the primary basis for the thrust of this research, also concern minimum bias designs. The original article by Karson, Manson, and Hader (17) provides a new dimension to the principle of minimization of integrated mean square error. Rather than using the concept of least squares estimation to minimize bias, the authors proceed to minimize bias by design. The authors demonstrate that the case of least squares estimation is a special case of minimization of bias by design. Once bias has been minimized, the authors then minimize variance subject to the criterion of minimum bias and develop designs using both criteria. The real advantage for minimum bias estimation by design is that it gives values of integrated mean square error which are approximately equal for a wide range of design parameters and other factors.

Karson (16) in a later article examines the original criterion and introduces a protection criterion for designs in which higher order terms have been omitted. The criterion introduced gives a constant estimator for the difference between the true surface and the graduating polynomial consistant with minimum bias estimation.

Estimation of the Slope of a Response Surface

In a recent paper by Atkinson (1), an application of Box and Draper's criterion with a view toward estimating the slope of a response surface is given. The author assumes that the emphasis is upon the differences in response rather than upon the estimation of the highest response as is most often the case. Atkinson concludes by showing that designing experiments to estimate the slope of a response surface in any direction is equivalent to designing the experiment to obtain precise estimates of the slopes, strictly along the axes of the independent variables.

Atkinson contrasts his designs for estimating slope with rotatable designs. His designs depend upon the region of interest, but are not necessarily centered upon the region. On the other hand, the rotatable design must be centered upon the region of interest and must be scaled according to that region.

CHAPTER III

MINIMUM BIAS DESIGNS

As was demonstrated in the preceding chapter, minimizing integrated mean square error provided an additional area of investigation in the evaluation of response surface designs. The overriding importance of bias in comparison with variance is borne out by the work of Box and Draper who demonstrated that only when the variance contribution is at least six times the bias is there any significant difference in J, in comparison with the all-bias design. Most previous response surface designs considered only the criterion of variance.

In order to more fully develop an appreciation for an analysis of modern criteria in response surface designs, the development of the concepts behind minimum bias designs shall be considered in more detail. It has already been demonstrated that the integrated mean square error, J, is composed of a bias component, B, and a variance component, V. A useful demonstration at this point might be the development of rotatability, orthogonality, and uniform precision with this type of design. It would seem appropriate to assume that the experimenter is attempting to fit a quadratic response surface, but that the true function can be best described by a cubic polynomial.

A brief introduction to the topic of bias is important to understanding further concepts in this area. One can assume that the model to be fitted is of order d_1 and of the form

$$\hat{y} = \underline{x}_1'\underline{\beta}_1 + \epsilon \tag{3.1}$$

where

$$\underline{x}_1' = [1, x_1, \ldots, x_k, x_1^2, \ldots, x_k^2, x_1x_2, \ldots, x_{k-1}x_k] \tag{3.1a}$$

$$\hat{\underline{\beta}}_1 = [b_0, b_1, \ldots, b_k, b_{11}, \ldots, b_{kk}, b_{12}, \ldots, b_{k-1}b_k] \tag{3.1b}$$

but in actuality the true form is of order d_2 and is represented by

$$y = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2 + \epsilon \tag{3.2}$$

where $\underline{x}_1'$ and $\underline{\beta}_1$ are as in (3.1) and

$$\underline{x}_2' = [x_1^3, x_1x_2^2, \ldots, x_1x_k^2, x_2^3, x_2x_1^2, \ldots, x_2x_k^2, \ldots, x_k^3, x_kx_1^2, \tag{3.2a}$$
$$\ldots, x_kx_{k-1}^2, \ldots, x_1x_2x_3, x_1x_2x_4, \ldots, x_{k-2}x_{k-1}x_k]$$

$$\underline{\beta}_2 = [\beta_{111}, \beta_{122}, \ldots, \beta_{1kk}, \beta_{222}, \beta_{211}, \ldots, \beta_{2kk}, \ldots, \beta_{kkk}, \tag{3.2b}$$
$$\beta_{k11}, \ldots, \beta_{kk-1k-1}, \ldots, \beta_{123}, \beta_{124}, \ldots, \beta_{k-2k-1k}]$$

Now the matrix $\underline{X}_1$ is of the form

$$\underline{X}_1 = \begin{bmatrix} 1, x_{11}, x_{21}, \ldots, x_{k1}, x_{11}^2, \ldots, x_{k1}^2, x_{11}x_{21}, \ldots, x_{k-1,1}x_{k,1} \\ 1, x_{12}, x_{22}, \ldots, x_{k2}, x_{12}^2, \ldots, x_{k2}^2, x_{12}x_{22}, \ldots, x_{k-1,2}x_{k,2} \\ \cdots \\ 1, x_{1N}, x_{2N}, \ldots, x_{kN}, x_{1N}^2, \ldots, x_{kN}^2, x_{1N}x_{2N}, \ldots, x_{k-1,N}x_{k,N} \end{bmatrix}. \tag{3.3}$$

The matrix $\underline{X}_2$ is given by

$$\underline{X}_2 = \left[\begin{matrix} x_{11}^3, x_{11}x_{21}^2, \ldots, x_{11}x_{k1}^2, x_{21}^3, x_{21}x_{11}^2, \ldots, x_{21}x_{k1}^2, \ldots, x_{k1}^3, \\ x_{12}^3, x_{12}x_{22}^2, \ldots, x_{12}x_{k2}^2, x_{22}^3, x_{22}x_{12}^2, \ldots, x_{22}x_{k2}^2, \ldots, x_{k2}^3, \\ \cdots \\ x_{1N}^3, x_{1N}x_{2N}^2, \ldots, x_{1N}x_{kN}^2, x_{2N}^3, x_{2N}x_{1N}^2, \ldots, x_{2N}x_{kN}^2, \ldots, x_{kN}^3, \end{matrix}\right. \tag{3.4}$$

$$\left.\begin{matrix} x_{k1}x_{11}^2, \ldots, x_{k1}x_{k-1,1}^2, \ldots, x_{11}x_{21}x_{31}, \ldots, x_{k-2,1}x_{k-1,1}x_{k,1} \\ x_{k2}x_{12}^2, \ldots, x_{k2}x_{k-1,2}^2, \ldots, x_{12}x_{22}x_{32}, \ldots, x_{k-2,2}x_{k-1,2}x_{k,2} \\ \cdots \\ x_{kN}x_{k2}^2, \ldots, x_{kN}x_{k-1,N}^2, \ldots, x_{1N}x_{2N}x_{3N}, \ldots, x_{k-2,N}x_{k-1,N}x_{k,N} \end{matrix}\right]$$

The problem is to estimate $\underline{\beta}_1$. By the method of least squares, one obtains from (1.12)

$$\hat{\underline{\beta}}_1 = (\underline{X}_1'\underline{X}_1)^{-1}\underline{X}_1'\underline{Y} . \tag{3.5}$$

Taking expectation

$$E(\hat{\underline{\beta}}_1) = E[(\underline{X}'\underline{X})^{-1}\underline{X}_1\underline{Y}] \tag{3.6}$$

$$= (\underline{X}_1'\underline{X}_1)^{-1}\underline{X}_1\underline{E}(\underline{Y}) \ . \tag{3.7}$$

From (3.2), the true value of $E(\underline{Y})$, upon substituting into (3.5) is

$$E(\hat{\underline{\beta}}_1) = (\underline{X}_1'\underline{X}_1)^{-1}(\underline{X}_1'\underline{X}_1)\ \underline{\beta}_1 + (\underline{X}_1'\underline{X}_1)^{-1}(\underline{X}_1'\underline{X}_2)\ \underline{\beta}_2 \tag{3.8}$$

$$= \underline{\beta}_1 + (\underline{X}_1'\underline{X}_1)^{-1}(\underline{X}_1'\underline{X}_2)\ \underline{\beta}_2 \tag{3.9}$$

$$= \underline{\beta}_1 + \underline{A\beta}_2 \tag{3.10}$$

where $\underline{A} = (\underline{X}_1'\underline{X}_1)^{-1}(\underline{X}_1'\underline{X}_2)$ is called the "alias" matrix. Equation (3.10) indicates the extent of biasing in the coefficients $\hat{\underline{\beta}}_1$ from higher order terms.

It can be seen that the variance function for the fitted model can be written as

$$\text{Var}\ (\hat{y}) = \text{Var}\ (\underline{x}_1\hat{\underline{\beta}}_1) \tag{3.11}$$

$$= \underline{x}_1'\ (\text{Var}\ \hat{\underline{\beta}}_1)\underline{x}_1 \tag{3.12}$$

$$= \sigma^2\ \underline{x}_1'\ (\underline{X}_1'\underline{X}_1)^{-1}\underline{x}_1 \tag{3.13}$$

or

$$\text{Var}\ (\hat{y}/\sigma^2) = \underline{x}_1'\ (\underline{X}_1'\underline{X}_1)^{-1}\underline{x}_1 \tag{3.14}$$

The integrated variance from (2.12) can now be written as

$$V = N\,\Omega \int_R \underline{x}_1'(\underline{X}_1'\underline{X}_1)^{-1}\underline{x}_1 \, d\underline{x} \tag{3.15}$$

Also, the bias at a point $(x_1,x_2,\ldots,x_k)$ can be written using the results of (3.10) as

$$E[\underline{x}_1'\underline{\beta}_1 - (\underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2)] = \underline{x}_1'(\underline{\beta}_1 + \underline{A\beta}_2) - \underline{x}_1'\underline{\beta}_1 - \underline{x}_2'\underline{\beta}_2 \tag{3.16}$$

$$= x_1'A\beta_2 - x_2'\beta_2 , \tag{3.17}$$

and the bias portion of J, from (2.12), becomes

$$B = \frac{N\,\Omega}{\sigma^2} \int_R (\underline{x}_1\underline{A\beta}_2 - \underline{x}_2'\underline{\beta}_2)^2 \, d\underline{x} \tag{3.18}$$

$$= \frac{N\,\Omega}{\sigma^2} \int_R \underline{\beta}_2' \, (\underline{A}'\underline{x}_1 - \underline{x}_2)(\underline{x}_1\underline{A} - \underline{x}_2) \, \underline{\beta}_2 \, d\underline{x} \tag{3.19}$$

Equation (3.19) can be rearranged as

$$\Omega^{-1}B = \frac{N}{\sigma^2}\Big[\underline{\beta}_2' \, \underline{A}' \left(\int_R \underline{x}_1\underline{x}_1' \, d\underline{x}\right) \underline{A\beta}_2 - 2\underline{\beta}_2 \left(\int_R \underline{x}_2\underline{x}_1' \, d\underline{x}\right) \underline{A\beta}_2 \tag{3.20}$$

$$+ \underline{\beta}_2' \left(\int_R \underline{x}_2\underline{x}_2' \, d\underline{x}\right) \underline{\beta}_2\Big]$$

It can be seen that the derived expressions for V and B are quite general and are valid for any d_1 and any $d_2 > d_1$. If the region R is assumed to be a unit hypersphere, i.e., the region defined by

$$\sum_{i=1}^{p} x_i^2 \leqq 1 \ , \tag{3.21}$$

the variables can be scaled to conform to this region and then integrals of the form

$$\int_R x_1^{\delta_1} x_2^{\delta_2}, \ldots, x_p^{\delta_p} \, d\underline{x} \tag{3.22}$$

must be evaluated in (3.20). For the region as defined above, the integral (3.22) can be shown to be

$$\int_R x_1^{\delta_1} x_2^{\delta_2}, \ldots, x_p^{\delta_p} \, d\underline{x} = \begin{cases} 0 \text{ if any } \delta_i \text{ odd;} \\ \dfrac{\Gamma\left(\frac{\delta_1+1}{2}\right) \Gamma\left(\frac{\delta_2+1}{2}\right), \ldots, \Gamma\left(\frac{\delta_p+1}{2}\right)}{\Gamma\left[\sum_{i=1}^{p} \frac{(\delta_i+1)}{2} + 1\right]}, \\ \text{for all } \delta_i \text{ even.} \end{cases} \tag{3.23}$$

writing (3.15) as

$$\Omega^{-1}V = \sum_{i=1}^{p} \sum_{j=1}^{N} c^{ij} \int_R \underline{x}_i \underline{x}_j' \, d\underline{x} \ , \tag{3.24}$$

where c^{ij} is the ij^{th} element of the precision matrix $N(\underline{X}_1'\underline{X}_1)^{-1}$ and the term x_o is assumed to be unity, then for $i \neq j$ from (3.21)

$$\int_R x_i x_j' \, d\underline{x} = 0 \ ,$$

for $i = j = 0$

$$\int_R x_i x_j' \, d\underline{x} = p \ ,$$

and for i = j = (1,2,..., p)

$$\int_R x_i x_j \, d\underline{x} = \frac{\Gamma(3/2)\ \Gamma(1/2),\ldots,\ \Gamma(1/2)}{\Gamma\ (\frac{2+p}{2} + 1)}$$

$$= \frac{1/2(\Pi)^{p/2}}{\frac{p+2}{2}\ \Gamma(\frac{p+2}{2})},$$

There are exactly p-1 functions of the form $\Gamma(1/2)$ in the numerator. From (3.21), in a similar manner, it is easily seen that

$$\Omega^{-1} = \int_R d\underline{x} = \frac{\{\Gamma(1/2)\}^p}{\Gamma(\frac{p}{2} + 1)} = \frac{(\Pi)^{p/2}}{\Gamma\ (\frac{p+2}{2})} \qquad (3.26)$$

At this time, consider the case of the second order central composite design. From (3.25) and (3.26) the second moment is simply

$$[ii] = \Omega \int_R x_i^2 \, d\underline{x} = \frac{1}{(p+2)} \ , \qquad (3.27)$$

the fourth pure design moment is

$$[iiii] = \Omega \int_R x_i^4 \, d\underline{x} = \frac{\Omega\ (\Pi)^{p/2}\ (3/4)}{\Gamma\ (\frac{p+6}{2})} \qquad (3.28a)$$

$$= \frac{3}{(p+2)(p+4)} \ ,$$

and the fourth moment of the region

$$[iijj] = \Omega \int_R x_i^2 x_j^2 \, d\underline{x} = \frac{\Omega \ (\Pi)^{p/2} \ (1/4)}{\Gamma(\frac{p+6}{2})} = \frac{1}{(p+2)(p+4)} \ , \qquad (3.28b)$$

which agrees with the principle that, for a rotatable design, the fourth mixed moment is one-third the fourth pure design moment. Thus the moments required for this design have been shown, but as yet J, the quantity of interest, has not been minimized.

At this point, it is appropriate to return to (3.15) and (3.18) and develop the concept of minimum integrated mean square error. Define the matrices of the design moments

$$\underline{M}_{11} = N^{-1}(\underline{X}_1'\underline{X}_1) \ , \qquad (3.29a)$$

$$\underline{M}_{12} = N^{-1}(\underline{X}_1'\underline{X}_2) \ , \qquad (3.29b)$$

and

$$\underline{M}_{22} = N^{-1}(\underline{X}_2'\underline{X}_2) \ , \qquad (3.29c)$$

which follow from the definition of moment matrices in (2.4). Further, define matrices of the region R as

$$\underline{\mu}_{11} = \int_R \underline{x}_1\underline{x}_1' \, d\underline{x} \qquad (3.30a)$$

$$\underline{\mu}_{12} = \int_R \underline{x}_1\underline{x}_2' \, d\underline{x} \qquad (3.30b)$$

$$\underline{\mu}_{22} = \int_R \underline{x}_2\underline{x}_2' \, d\underline{x} \qquad (3.30c)$$

These integrals can further be defined as moment matrices of a uniform probability distribution over the region of interest R.

Substituting (3.15) and (3.20) into the original expression for J and using the above definitions, one obtains

$$J = \mathrm{Tr}\,[\mu_{11}\, \underline{M}_{11}^{-1}] + \underline{\beta}_2' \,[\mu_{22} - \mu_{12}' \,\mu_{11}^{-1}\, \mu_{12}) + (\underline{M}_{11}^{-1} - \underline{M}_{12} - \mu_{11}^{-1}\mu_{12})' \tag{3.31}$$

$$\mu_{11}\, (\underline{M}_{11}^{-1}\, \underline{M}_{12} - \mu_{11}^{-1}\, \mu_{12})]\, \underline{\beta}_2$$

The variance is represented by the first term and bias by the second term. In choosing the design matrix D in such a manner that J is minimized, one sees that the variance portion of (3.31) does not depend on $\underline{\beta}_2$ at all, but depends only on D while the bias portion depends on both D and $\underline{\beta}_2$. Thus minimization of J depends on the assigned value of $\underline{\beta}_2$.

It can be shown that the minimum integrated mean square bias error which can be achieved is

$$\underline{\beta}_2' \,(\mu_{22} - \mu_{12}' \,\mu_{11}^{-1}\, \mu_{12})\, \underline{\beta}_2 \tag{3.32}$$

This quantity has an intuitive appeal to the experimenter, since this means that

$$(\underline{M}_{11}^{-1}\, \underline{M}_{12} - \mu_{11}^{-1}\, \mu_{12})' \,\mu_{11}\, (\underline{M}_{11}^{-1}\, \underline{M}_{12} - \mu_{11}^{-1}\, \mu_{12}) = 0 \tag{3.33}$$

and that

$$\underline{M}_{11}^{-1}\, \underline{M}_{12} = \mu_{11}^{-1}\, \mu_{12}\ , \tag{3.34}$$

or

$$\underline{M}_{11} = \mu_{11} \qquad \text{Design moments through order } 2d_1 \ (d_1 = 2) \tag{3.35}$$

$$\underline{M}_{12} = \mu_{12} \qquad \text{Design moments through order 5, for } d_1 = 2 \text{ and } d_2 = 3 \tag{3.36}$$

This is simply a statement that the moments of the design should be equal to the moments of the region up to and including order $(d_1 + d_2)$. For a second order design protecting against cubic bias, this implies that the design moments through order five must be equal to the corresponding moments of the region R, along with the requirements of (3.27), (3.28a), and (3.28b), the necessary moments for a rotatable design.

As was pointed out previously, designs from this class which minimize J where both bias and variance are contributors have design parameters which are very close to those which minimize J if bias were considered alone. By restricting oneself to rotatable designs with fifth moments equal to zero, designs which minimize J can be developed. Box and Draper (4) present curves which give values of λ_2 and λ for those designs which minimize J, where V/B ranges from 0 to ∞. λ is defined as λ_4/λ_2^2. In these curves, zero represents the all-variance design (true surface and fitted model are the same) and infinity the all-bias design (no experimental error) for values of p running from one to five, where p represents number of factors.

An Example Design

In this section, a rotatable central composite design is given which systematically protects against both bias and variance. Table 1 presents, for the case p = 2, the number of center points, n_o, together with the corresponding values of the design parameters, x, α, corresponding to the design moments, λ_2 and λ. Here again, α represents the distance of the axial points from the center of the central composite design and x the side length (see Fig. 1).

Table 1. Parameter Values for a CCD When p = 2*

n_o	$\lambda_2^{1/2}$	λ	x	α
0	0.628	1.500	0.628	0.888
1	0.578	1.688	0.613	0.867
2	0.505	1.875	0.565	0.799
3	0.583	2.063	0.684	0.967
4	0.627	2.250	0.768	1.086
5	0.663	2.438	0.846	1.196
6	0.696	2.625	0.921	1.303
7	0.727	2.813	0.996	1.408
8	0.757	3.000	1.070	1.514
9	0.785	3.188	1.145	1.619
10	0.813	3.375	1.220	1.725
11	0.840	3.563	1.295	1.832
12	0.867	3.750	1.371	1.939

*After Box and Draper, reference 4.

From Table 1, it can be seen that, as one expects less effect from bias, more center points are added to the design, and points are placed further from the origin, even outside the region of interest. On the other hand, if bias is thought to be large and variance is thought to be small, the region of interest is contracted and only a small number of center points is used to provide an estimate of σ^2.

The experimenter should use a design with large values of λ_2 if bias is considered to be relatively unimportant; on the other hand, if uncertainty arises regarding the adequacy of the second order model, smaller values of λ and λ_2 should be selected.

Minimization of Integrated Mean Square Error, Orthogonality, and Uniform Precision

It would seem appropriate as a logical extension to the criterion of minimization of rotatable integrated mean square error designs (MMSE) to develop the dual criteria of MMSE and orthogonality or MMSE and uniform precision, as an alternative to MMSE alone. The attempt to incorporate these ideas will be for the Central Composite Design (CCD) with $p = 2$. The basic requirements for orthogonality must still hold, in other words, the fourth pure design moment must be equal to unity. The value of the design moments, although basically set by choice of the design points, can be altered by the addition of center points to the central composite design, the design moments are directly related to x, the length of the side of the cube (see Fig. 1), and the number of center points added.* At the same time, to maintain rotatability, the axial points must be related to the side length of the cube as follows

$$\alpha = 2^{1/2p} x \tag{3.37}$$

*Once again α represents the distance from the center of the CCD to the axial points.

The design moments are

$$\lambda_2 = (2^p + 2^{1/2(p+2)})\ x^2/N \tag{3.38}$$

$$\lambda = 3\lambda_4/\lambda_2^2 = 3N/(2 + 2^{1/2p})^2\ , \tag{3.39}$$

where

$$N = 2^p + 2p + n_o \tag{3.40}$$

It would seem that one could easily determine a value for n_o for which $\lambda_4 = 1$; however, the value of λ_4 reaches a minimum between $n_o = 17$ and $n_o = 18$, at which point $\lambda_4 \approx 1.55$. At this point, the value of the second moment is equal to unity. Thus it can be seen that the concept of minimum bias designs with orthogonality and minimum bias designs with uniform precision have no meaning. The same argument holds for designs of $p = 3, 4, 5$.

It is important to note the following points about what has been developed above. As more and more center points are added, the moments are altered and become smaller and begin to take the form of an all-variance design. Secondly, the number of center points required for orthogonality or uniform precision becomes completely out of proportion to the rest of the design. Lastly, as one attempts to gain orthogonality for the design, design points are placed outside the region of interest, which may be a poor experimental strategy.

CHAPTER IV

MINIMUM BIAS ESTIMATION OF THE SLOPE OF A RESPONSE SURFACE

Application of the criterion of minimization of bias by design alone due to Karson _et al_. (16) will be presented in the following paragraphs. This criterion will be applied to the problem of estimating the slope of a response surface. Previous development in the field has tended to emphasize the absolute response rather than differences in response. If differences are important, this implies that estimation of the local slope may also be of interest. Thus one sees the importance of the topic.

Minimization of Bias

The concept of minimum bias estimation will be developed and then applied to estimating the slope of a response surface. Once again, assume that the true form of the response surface can be represented as a function

$$\eta = \mathcal{f}(\xi_1, \xi_2, \ldots, \xi_k) + \epsilon \qquad (4.1)$$

which has been transformed into variables $x_1, x_2, \ldots, x_p$ such that the variables become the origin of the x's and are scaled relative to each other (see Equation 1.6). This polynomial is of degree d_2 and of the form

$$\eta(x) = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2 \tag{4.2}$$

but for some reason the experimenter has chosen to deal with an approximating polynomial of the form

$$\hat{y}(x) = \underline{x}_1'\underline{b}_1 \tag{4.3}$$

This polynomial is of degree d_1 ($d_2 > d_1$). As was demonstrated in Chapter III, to minimize bias alone, the experimenter had to satisfy the necessary and sufficient condition

$$(\underline{X}_1'\underline{X}_1)^{-1}\underline{X}_1'\underline{X}_2 = \underline{\mu}_{11}^{-1}\,\underline{\mu}_{12} \tag{4.4}$$

where $\underline{X}_1$ is as defined earlier, and $\underline{X}_2$ is the matrix of values taken by the variables $\underline{x}_2'$ (the omitted portion of the model), and

$$\underline{\mu}_{11} = \int_R \underline{x}_1\underline{x}_1'\,d\underline{x} \tag{4.5}$$

$$\underline{\mu}_{12} = \int_R \underline{x}_1\underline{x}_2'\,d\underline{x}$$

As an alternative to the traditional method of least squares estimation, Karson et al. (16) proposed the concept of minimum bias estimation. The polynomial which best approximates the true surface is given by (4.2) and the fitted model by (4.3). It is desired to minimize the bias component of (2.12), that is

$$B = \frac{N\,\Omega}{\sigma^2} \int_R \{E\,[\hat{y}(x)] - \eta(x)\}^2\, dx \tag{4.6}$$

where the quantity $E\,[\hat{y}(x)]$ is a polynomial of degree d_1, say

$$E\,[\hat{y}(x)] = \underline{x}_1'\underline{\alpha}_1 \tag{4.7}$$

Substituting into (4.6) one obtains

$$B = \frac{N\,\Omega}{\sigma^2} \int_R [\underline{x}_1'\ (\underline{\alpha}_1 - \underline{\beta}_1) - \underline{x}_2'\underline{\beta}_2]^2\, dx \tag{4.8}$$

$$= \frac{N\,\Omega}{\sigma^2} \int_R [\underline{\alpha}_1 - \underline{\beta}_1)'\ \underline{x}_1\underline{x}_1'\ (\underline{\alpha}_1 - \underline{\beta}_1) - 2(\underline{\alpha}_1 - \underline{\beta}_1)'\ \underline{x}_1\underline{x}_2'\ \underline{\beta}_2 \tag{4.9}$$

$$+ \underline{\beta}_2'\ \underline{x}_2\underline{x}_2'\ \underline{\beta}_2\ d\underline{x}]$$

$$= \frac{N\,\Omega}{\sigma^2} \int_R (\underline{\alpha}_1 - \underline{\beta}_1)'\ \underline{x}_1\underline{x}_1\ (\underline{\alpha}_1 - \underline{\beta}_1)\ d\underline{x} - \frac{2N\,\Omega}{\sigma^2} \int_R (\underline{\alpha}_1 - \underline{\beta}_1)' \tag{4.10}$$

$$\underline{x}_1\underline{x}_2'\ \underline{\beta}_2\ d\underline{x} + \frac{N\,\Omega}{\sigma^2} \int_R \underline{\beta}_2'\ \underline{x}_2\underline{x}_2'\ \underline{\beta}_2\ d\underline{x}\ .$$

Define the quantity

$$\underline{\mu}_{22} = \int_R \underline{x}_2\underline{x}_2'\ d\underline{x}\ . \tag{4.11}$$

Using this definition along with the definitions of (4.5), one obtains

$$B = \frac{N}{\sigma^2} [(\underline{\alpha}_1 - \underline{\beta}_1)' \, \underline{\mu}_{11} \, (\underline{\alpha}_1 - \underline{\beta}_1) - 2(\underline{\alpha}_1 - \underline{\beta}_1)' \, \underline{\mu}_{12} \, \underline{\beta}_2 \tag{4.12}$$

$$+ \underline{\beta}_2' \, \underline{\mu}_{22} \, \underline{\beta}_2] \; .$$

Differentiating this expression with respect to the vector $\underline{\alpha}_1$ and equating to zero yields

$$\frac{\partial B}{\partial \underline{\alpha}_1} = 2 \, \underline{\mu}_{11} \, (\underline{\alpha}_1 - \underline{\beta}_1) - 2 \, \underline{\mu}_{12} \, \underline{\beta}_2 = 0 \tag{4.13}$$

and solving for $\underline{\alpha}_1$

$$\underline{\alpha}_1 = \underline{\beta}_1 + \underline{\mu}_{11}^{-1} \, \underline{\mu}_{12} \, \underline{\beta}_2 \tag{4.14}$$

or

$$\underline{\alpha}_1 = \underline{A\beta} \; ,$$

where

$$\underline{A} = (\underline{I} \; : \; \underline{\mu}_{11}^{-1} \, \underline{\mu}_{12}) \; , \tag{4.15}$$

and

$$\underline{\beta}' = (\underline{\beta}_1' \; : \; \underline{\beta}_2') \; .$$

Here A is the identity matrix augmented by the product of two matrices which contain the moments of the region R. Thus the necessary and sufficient condition for minimum bias estimation is that

$$E \, [\hat{y}(x)] = \underline{x}_1' \underline{A\beta} \tag{4.16}$$

or

$$E \, (\underline{b}_1) = \underline{A\beta} \; . \tag{4.17}$$

One may write $\underline{b}_1$ as a linear transformation of the observations, say

$$\underline{b}_1 = \underline{T}'\underline{Y} . \tag{4.18}$$

Since E $(\underline{Y}) = \underline{X\beta}$ and E $(\underline{b}_1) = \underline{A\beta}$; therefore, $\underline{T}'$ must satisfy the relationship

$$\underline{T}'\underline{X} = \underline{A} \tag{4.19}$$

where

$$\underline{X} = (\underline{X}_1 : \underline{X}_2) .$$

One can readily see that the necessary and sufficient conditions of equation (4.4) are satisfied as a special case by least squares estimation if

$$T' = (\underline{X}_1'\underline{X}_1)^{-1} \underline{X}_1 . \tag{4.20}$$

Thus the minimum bias, from (4.12), is simply

$$\text{Min } \{B\} = \frac{N}{\sigma^2} \underline{\beta}_2' \{\underline{\mu}_{22} - \underline{\mu}_{12}' \underline{\mu}_{11}^{-1} \underline{\mu}_{12}\} \underline{\beta}_2 . \tag{4.21}$$

Estimating the Slope of a Response Surface

This principle may be applied to the problem of estimating the slope of a response surface, which was solved by Atkinson (1) using the traditional method of least squares. At this time it must be pointed out that the development of this topic will be directed at the special case of a single variable; however, later discussion will demonstrate its application to the multivariable case.

The true surface can be represented by a polynomial of degree d_3

$$\eta(x) = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2 + \underline{x}_3'\underline{\beta}_3 \tag{4.22}$$

For this problem, the vectors $\underline{x}_3'$ and $\underline{x}_2'$ are vectors which contain only the elements of degree d_3 for vector $\underline{x}_3'$ and $\underline{d}_3 - 1$ for vector $\underline{x}_2'$. All other elements are contained in vector $\underline{x}_1'$. The fitted model is represented by a polynomial of degree $d_3 - 1$ (which can be easily extended to $d_3 - k$)

$$\hat{y}(x) = \underline{x}_1'\underline{b}_1 + \underline{x}_2'\underline{b}_2 \tag{4.23}$$

The slope of the true surface is simply the derivative

$$\frac{d[\eta(x)]}{dx} = d_2\underline{x}_1' \, \underline{\beta}_I + d_3\underline{x}_2' \, \underline{\beta}_{II} \, , \tag{4.24}$$

where d_2 represents all constants arising from the differentiation of the polynomial, d_3 is the coefficient of the highest order term, $\underline{\beta}_I = (\beta_1, \beta_{11}, \beta_{111}, \ldots, \beta_{d_3-1})$, and $\underline{\beta}_{II} = (\beta_{d_3})$. The slope of the fitted model is

$$\frac{d[\hat{y}(x)]}{dx} = d_2\underline{x}_1' \, \underline{\gamma}_1 \tag{4.25}$$

where d_2 is as defined previously and $\underline{\gamma}_1 = (b_1, b_{11}, b_{111}, \ldots, b_{d_3-1})$. Now the expected value of this polynomial is a polynomial of degree

$d_3 - 2$, say

$$E\left\{\frac{d[\hat{y}(x)]}{dx}\right\} = d_2\underline{x}_1'\ \underline{\alpha}_1 \tag{4.26}$$

From Equation (4.6) it can be seen readily that the bias of the slopes is

$$B = \frac{N\ \Omega}{\sigma^2}\int_R \left\{E\left(\frac{d[\hat{y}(x)]}{dx}\right) - \frac{d[\eta(x)]}{dx}\right\}^2 dx\ . \tag{4.27}$$

Substitution of (4.24) and (4.26) into (4.27) yields

$$B = \frac{N\ \Omega}{\sigma^2}\int_R \{\underline{x}_1'\ (d_2\underline{\alpha}_1 - d_2\underline{\beta}_I) - d_3\underline{x}_2'\ \underline{\beta}_{II}\}^2\ dx\ . \tag{4.28}$$

Expanding

$$B = \frac{N\Omega}{\sigma^2}\int_R [(d_2\underline{\alpha}_1 - d_2\underline{\beta}_I)'\ (\underline{x}_1\underline{x}_1')\ (d_2\underline{\alpha}_1 - d_2\underline{\beta}_I) - 2(d_2\underline{\alpha}_1 \tag{4.29}$$

$$- d_2\underline{\beta}_I)'\ (\underline{x}_1\underline{x}_2')\ (d_3\underline{\beta}_{II}) + (d_3\underline{\beta}_{II})'\ (\underline{x}_2\underline{x}_2')\ (d_3\underline{\beta}_{II})]\ dx\ .$$

Substitution from Equation (4.5) and (4.11) for their appropriate integrals yields

$$B = \frac{N}{\sigma^2}\ (d_2\underline{\alpha}_1 - d_2\underline{\beta}_I)'\ \underline{\mu}_{11}\ (d_2\underline{\alpha}_1 - d_2\underline{\beta}_I) - 2(d_2\underline{\alpha}_1 - d_2\underline{\beta}_I)' \tag{4.30}$$

$$\underline{\mu}_{12}\ (d_3\underline{\beta}_{II}) + (d_3\underline{\beta}_{II})'\ \underline{\mu}_{22}\ (d_3\underline{\beta}_{II})\ .$$

Differentiating (4.30) with respect to $\underline{\alpha}_1$ and equating to zero yields

$$\frac{dB}{d\underline{\alpha}_1} = 0 = 2\,\underline{\mu}_{11}\, d_2\, (d_2\underline{\alpha}_1 - d_2\underline{\beta}_I) - 2\underline{\mu}_{12}\, d_2\, d_3\underline{\beta}_{II}\ , \qquad (4.31)$$

or

$$\underline{\alpha}_1 = \underline{\beta}_I + \frac{d_3}{d_2}\,\underline{\mu}_{11}^{-1}\,\underline{\mu}_{12}\,\underline{\beta}_{II}\ . \qquad (4.32)$$

By taking the second derivative of B with respect to $\underline{\alpha}_1$, one can see that B is minimized since μ_{11} is positive definite.

Or

$$\underline{\alpha}_1 = \underline{A\beta}\ , \qquad (4.33)$$

where

$$\underline{A} = \left(\underline{I}\ :\ \frac{d_3}{d_2}\,\underline{\mu}_{11}^{-1}\,\underline{\mu}_{12}\right)\ , \qquad (4.34)$$

and

$$\underline{\beta}' = (\underline{\beta}_I'\ :\ \underline{\beta}_{II})\ . \qquad (4.35)$$

One quickly notes the similarity of these results to Karson's conditions for minimum bias estimation of a response surface. In fact, these results differ by a constant multiplier and the loss of the original intercept term, which is now the term corresponding to the linear coefficient.

Similarly, extension of these results to the case of multiple factor designs means simply that differentiation of Equation (4.20) will yield a matrix of coefficients. The direction in which the slope is to be estimated must also be considered. Examples of the single factor design will be discussed in Chapter V.

CHAPTER V

DESIGNS FOR USE IN PRACTICE

Presentation of a single factor design for use in practice is made. This design is representative of the various criteria that have been discussed in previous chapters. At the same time, an attempt will be made to integrate these criteria with each other and to gain further insight into the application of these designs.

Box and Draper's Criterion (3)

Once again assume the true conditions are represented by

$$\eta(x) = \beta_o + \beta_1 x + \beta_{11} x^2 , \tag{5.1}$$

and the fitted model is

$$\hat{y}(x) = b_o + b_1 x . \tag{5.2}$$

The design matrix is

$$\underline{D} = \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_N \end{bmatrix} . \tag{5.3}$$

The region of interest R is the segment of the real line from -1 to 1. If one assumes that the design is symmetric about the midpoint of the interval R, then $\sum_{u=1}^{N} x_u = 0$. From Equation (2.12) the integral J can be written as

$$J = \frac{N\,\Omega}{\sigma^2}\left\{\int_{-1}^{1} [\mathrm{Var}\ b_o + x^2\ \mathrm{Var}\ b_1]\,dx + \int_{-1}^{1} [E\ (\hat{y}(x)) - \beta_o - \beta_1 x - \beta_{11}x^2]^2\ dx\right\} \tag{5.4}$$

$$\Omega = \int_{-1}^{1} dx = 2 \tag{5.5}$$

The variance portion of J can be evaluated immediately as $\mathrm{Var}\ b_o = \sigma^2/N$ and $\mathrm{Var}\ (b_1) = \sigma^2/(N[11])$ where [11] is evaluated as in Equation (2.3). Therefore, the integrated variance is

$$V = 1/2 \int_{-1}^{1} (1 + x^2/[11])\ dx \tag{5.6}$$

$$= 1 + 1/3\ [11]\ . \tag{5.7}$$

In order to evaluate the bias portion of J, one must recall the expression for the alias matrix from Equation (3.10). The matrices $\underline{X}_1$ and $\underline{X}_2$ are given by

$$\underline{X}_1 = \begin{bmatrix} 1 \, , & x_1 \\ 1 \, , & x_2 \\ \cdots & \cdots \\ 1 \, , & x_N \end{bmatrix} , \quad \text{and} \quad \underline{X}_2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \cdots \\ x_N^2 \end{bmatrix} . \tag{5.8}$$

The alias matrix $\underline{A} = (\underline{X}_1'\underline{X}_1)^{-1}\underline{X}_1'\underline{X}_2$ is

$$\underline{A} = \begin{bmatrix} 1/N & 0 \\ 0 & 1/(N[11]) \end{bmatrix} \begin{bmatrix} N[11] \\ N[111] \end{bmatrix} , \tag{5.9}$$

or

$$\underline{A} = \begin{bmatrix} [11] \\ [111]/[11] \end{bmatrix} . \tag{5.10}$$

Therefore

$$E(b_o) = \beta_o + [11] \, \beta_{11} \tag{5.11}$$

and

$$E(b_1) = \beta_1 + \{[111]/[11]\} \, \beta_{11} \, . \tag{5.12}$$

Now using Equations (5.2), (5.11), and (5.12)

$$E \, [\hat{y}(x)] = \beta_o + \beta_1 x + \beta_{11} \, \{[11] + [111]x/[11]\} \, . \tag{5.13}$$

From Equation (5.4) the bias portion of J can now be written as

$$B = \frac{N \, \beta_{11}^2}{2\sigma^2} \int_{-1}^{1} \{[11] + [111]x/[11] - x^2\}^2 \, dx \tag{5.14}$$

$$= \frac{N\,\beta_{11}^2}{\sigma^2} \{[11]^2 - 2/3\,[11] + 1/5 + [111]^2/(3[11]^2)\} \tag{5.15}$$

Once again it can be seen that B is minimized with respect to the third moment by making this moment equal to zero. Thus

$$J = 1 + 1/(3[11]) + \frac{N\,\beta_{11}^2}{\sigma^2} \{([11] - 1/3)^2 + 4/45\} \tag{5.16}$$

Therefore, one sees that, if the experimenter suspects substantial bias in $\hat{y}(x)$, B should be minimized, whereas, if the bias is expected to be negligible, the second moment should be made as large as possible. Bias can be minimized by making $[11] = 1/3$.

A Three Point Design

Suppose it is desired to allocate N trials, where N is divisible be three, at three levels, $x = 0$ and $x = \pm\, a$. From the discussion above, we know that if bias is suspected one should make the second moment equal to one-third. Therefore,

$$\frac{1}{N}\left[\sum_{i=1}^{N/3} a^2 + \sum_{i=1}^{N/3} 0 + \sum_{i=1}^{N/3} (-a)^2\right] = 1/3\ , \tag{5.17}$$

$$2/3\ a^2 = 1/3\ , \tag{5.18}$$

$$a^2 = 1/2\ ,$$

or

$$a = 0.707\ .$$

Therefore space the observations at $x = \pm\ 0.707$.

Minimum Bias Estimation and the Three Point Design

In applying this criterion, it will be assumed that the true surface can be represented as

$$\eta(x) = \beta_0 + \beta_1 x + \beta_{11} x^2 \tag{5.19}$$

and the fitted model as

$$\hat{y}(x) = b_0 + b_1 x\ . \tag{5.20}$$

The familiar $\underline{X}$, $\underline{Y}$, and $(\underline{X}'\underline{X})^{-1}$ matrices are

$$\underline{X} = (\underline{X}_1 : \underline{X}_2) = \begin{bmatrix} 1 & -a & : & a^2 \\ 1 & 0 & : & 0 \\ 1 & a & : & a^2 \end{bmatrix}, \qquad \underline{Y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}, \tag{5.21}$$

and

$$(\underline{X}'\underline{X})^{-1} = \begin{bmatrix} 1 & 0 & -a^2 \\ 0 & 1/2\ a^2 & 0 \\ -a^{-2} & & (3/2)a^{-4} \end{bmatrix}. \tag{5.22}$$

From Equations (5.4) and (3.25), each of the following quantities can be evaluated

$$\Omega^{-1} = 2 \ , \ \underline{\mu}_{11} = \begin{bmatrix} 1 & 0 \\ 0 & 1/3 \end{bmatrix}, \ \underline{\mu}_{12} = \begin{bmatrix} 1/3 \\ 0 \end{bmatrix}, \ \underline{\mu}_{22} = [1/5] \ . \tag{5.23}$$

Therefore

$$\underline{A} = \underline{I} : \underline{\mu}_{11}^{-1} \underline{\mu}_{22} = \begin{bmatrix} 1 & 0 & : & 1/3 \\ 0 & 1 & : & 0 \end{bmatrix}, \tag{5.24}$$

and from Equation (4.18)

$$\underline{b}_1 = \underline{T}'\underline{Y} = \underline{A}(\underline{X}'\underline{X})^{-1}\underline{X}'\underline{Y} \tag{5.25}$$

$$= \frac{1}{6a^2} \begin{bmatrix} 1 & 2(3a^2-1) & 1 \\ -3a & 0 & 3a \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \tag{5.26}$$

From Equation (5.25)

$$E(\underline{b}_1) = \underline{A\beta} = \begin{bmatrix} \beta_0 & + 0 & + & 1/3\beta_{11} \\ 0 & + \beta_1 & + & 0 \end{bmatrix} \tag{5.27}$$

or

$$E[\hat{y}(x)] = \beta_0 + 1/3 \ \beta_{11} + \beta_1 x \tag{5.28}$$

From Equation (4.21)

$$\text{Min } B = \frac{N}{\sigma^2} \underline{\beta}_{11}' \ (\underline{\mu}_{22} - \underline{\mu}_{12}' \underline{\mu}_{11}^{-1} \underline{\mu}_{12}) \ \underline{\beta}_{11} \tag{5.29}$$

$$= \frac{3}{\sigma^2} \frac{4}{45} \beta_{11}^2$$

which is independent of a. Solving for the variance function,

$$\text{Var } \hat{y}(x) = \text{Var } (\underline{x}_1'\underline{b}_1) = \sigma^2 \underline{x}_1'\underline{T}'\underline{T}\underline{x}_1 \tag{5.30}$$

$$= \sigma^2 \underline{x}_1'\underline{A}(\underline{X}'\underline{X})^{-1}\underline{A}'\underline{x}_1 \tag{5.31}$$

Therefore

$$V = \frac{N\,\Omega}{\sigma^2}\int_{-1}^{1} \text{Var } \hat{y}(x)\, dx = 3 - \frac{3}{2a^2} + \frac{1}{2a^4}\,, \tag{5.32}$$

and

$$J = 3 - \frac{3}{2a^2} + \frac{1}{2a^4} + \frac{12}{45\sigma^2}\,\beta_{11}^2 \tag{5.33}$$

Using the method of least squares for the same three point design, it can be seen that the bias is

$$B^* = \frac{3\beta_{11}^2}{\sigma^2}\left\{\frac{4a^4}{9} - \frac{4a^2}{9} + \frac{1}{5}\right\}. \tag{5.34}$$

The variance function is

$$V^* = 1 + \frac{1}{2a^2} \tag{5.35}$$

Thus

$$J^* = 1 + \frac{1}{2a^2} + \frac{3\beta_{11}^2}{\sigma^2}\left\{\frac{4a^4}{9} - \frac{4a^2}{9} + \frac{1}{5}\right\}. \tag{5.36}$$

In the following two figures, a graphical presentation will be made using minimum bias estimation and least squares estimation, utilizing the three point design. Now from the results of (5.16), it was seen that the

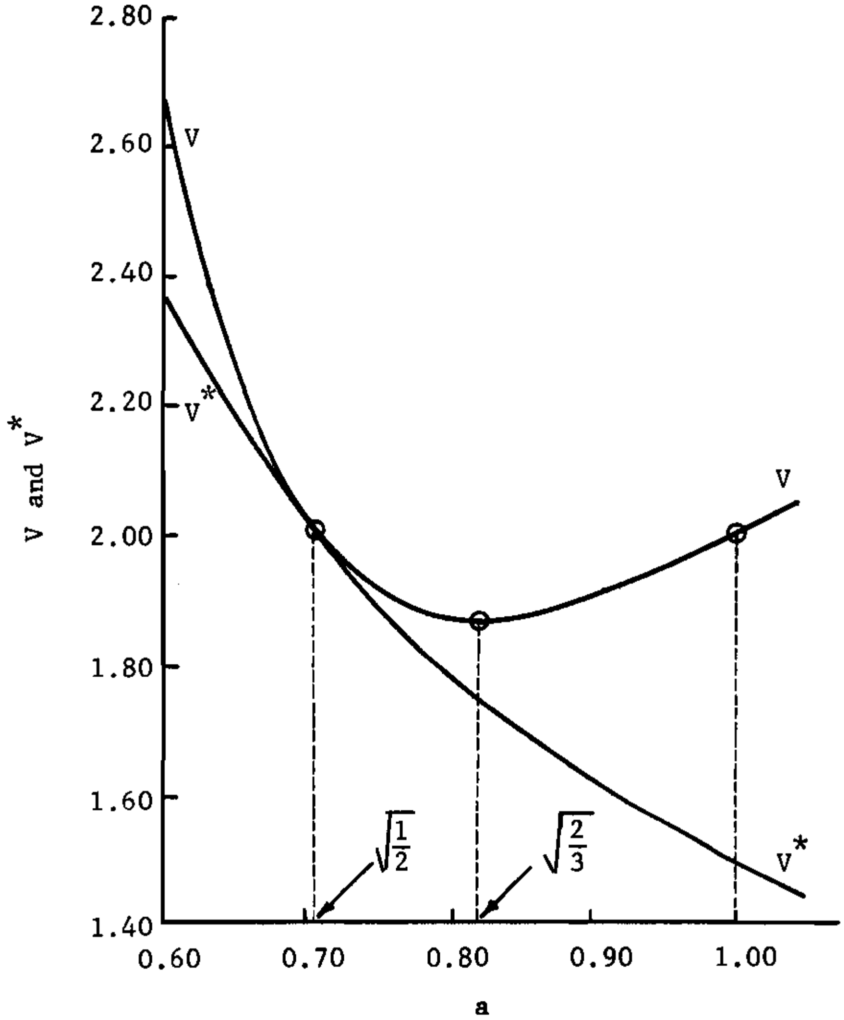

Figure 2. V and V^* versus a (after Karson <u>et</u> <u>al</u>. reference 17)

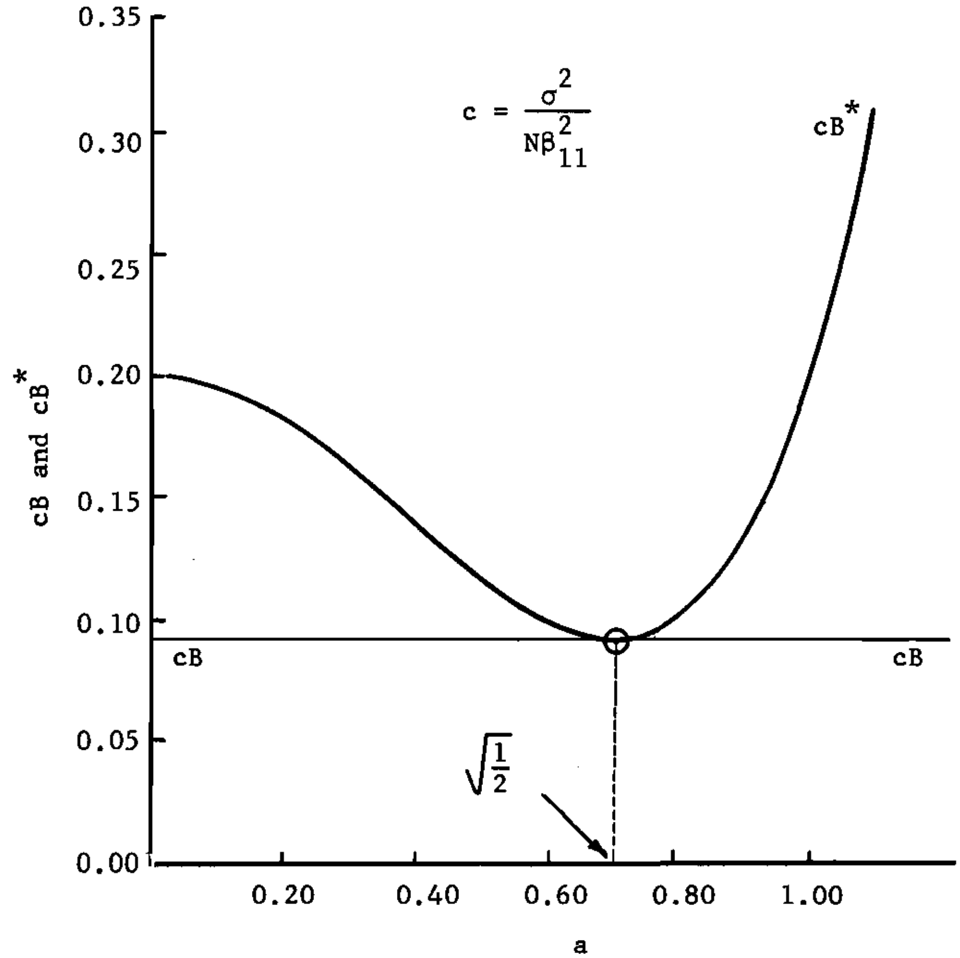

Figure 3. B and B* versus a (after Karson *et al.* reference 17)

minimum bias was achieved, using the method of least squares, at $a = 0.707$; however, looking at Figure 3, it is seen that a has no effect on bias when using minimum bias estimation and is, in fact, independent of bias. At the same time, examining Figure 2, it can be seen that, in the vicinity of $a = \sqrt{2/3}$, minimum bias can still be obtained while achieving a smaller J. This means that minimum bias estimation gives values of integrated mean square error which are approximately equal for a wide range of the design parameter, a.

Minimized Bias of the Slope Using Minimum Bias Estimation (MBE)

Application of (MBE) to the problem of estimating slope can be demonstrated for the single factor three point design. The true model is

$$\eta(x) = \beta_0 + \beta_1 x + \beta_{11} x^2 + \beta_{111} x^3 , \qquad (5.36)$$

and the fitted model is represented by a second order surface

$$\hat{y}(x) = b_0 + b_1 x + b_{11} x^2 . \qquad (5.37)$$

The derivatives of the true surface and the fitted model are

$$\frac{d[\eta(x)]}{dx} = \beta_1 + 2\beta_{11} x + 3\beta_{111} x^2 , \qquad (5.38)$$

and

$$\frac{d[\hat{y}(x)]}{dx} = b_1 + 2b_{11} x .$$

The $\underline{X}$, $\underline{Y}$, and $(\underline{X}'\underline{X})^{-1}$ matrices are as follows:

$$\underline{X} = (\underline{X}_1 : \underline{X}_2) = \begin{bmatrix} 1 & -a & : & a^2 \\ 1 & 0 & : & 0 \\ 1 & a & : & a^2 \end{bmatrix}, \quad \underline{Y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \tag{5.39}$$

$$(\underline{X}'\underline{X})^{-1} = \begin{bmatrix} 1 & 0 & -a^{-2} \\ 0 & 1/2a^{-2} & 0 \\ -a^{-2} & 0 & (3/2)a^{-4} \end{bmatrix}$$

The area and region moments from (5.24) are given by

$$\Omega^{-1} = 2 \, , \; \underline{\mu}_{11} = \begin{bmatrix} 1 & 0 \\ 0 & 1/3 \end{bmatrix}, \; \underline{\mu}_{12} = \begin{bmatrix} 1/3 \\ 0 \end{bmatrix}, \; \underline{\mu}_{22} = [1/5] \tag{5.40}$$

From Equation (4.29), the $\underline{A}$ matrix is

$$\underline{A} = \left[\underline{I}_2 : \frac{d_3}{d_2} \underline{\mu}_{11}^{-1} \underline{\mu}_{12}\right] = \begin{bmatrix} 1 & 0 & : & 1/2 \\ 0 & 1 & : & 0 \end{bmatrix} \tag{5.41}$$

Substituting Equation (4.29) into (4.27) one obtains

$$\text{Min } B = \frac{N}{\sigma^2} \{d_3 \ (\underline{\mu}_{11}^{-1} \underline{\mu}_{12})' \ \underline{\beta}_{II}' \ \underline{\mu}_{11} \ d_3 \ (\underline{\mu}_{11}^{-1} \underline{\mu}_{12}) \ \underline{\beta}_{II} \tag{5.42}$$

$$- 2d_3 \ (\underline{\mu}_{11}^{-1} \underline{\mu}_{12})' \ \underline{\beta}_{II}' \ \underline{\mu}_{12} \ d_3 \ \underline{\beta}_{II} + d_3 \ \underline{\beta}_{II}' \ \underline{\mu}_{22} \ d_3 \ \underline{\beta}_{II}\}$$

Substituting for the appropriate values yields

$$\text{Min } B = \frac{3}{\sigma^2} = \left\{9\beta_{111}^2 \ [1/3 \quad 0] \begin{bmatrix} 1 & 0 \\ 0 & 1/3 \end{bmatrix} \begin{bmatrix} 1/3 \\ 0 \end{bmatrix} - 18\beta_{111}^2 \right. \tag{5.43}$$

$$\left. [1/3 \quad 0] \begin{bmatrix} 1/3 \\ 0 \end{bmatrix} + 9\beta_{111}^2 \ [1/5] \right\} = \frac{3}{\sigma^2} \frac{4}{5} \beta_{111}^2 \ ,$$

which again is independent of a. The variance can be obtained as

$$\text{Var} \left\{\frac{d[\hat{y}(x)]}{dx}\right\} = \sigma^2 d_2' \underline{x}_1' \ \underline{T}'\underline{T}\underline{x}_1 d_2 \tag{5.44}$$

$$= \sigma^2 d_2' \underline{x}_1' \ \underline{A}(\underline{X}'\underline{X})^{-1} \ \underline{A}'\underline{x}_1 d_2$$

$$V = \frac{N \ \Omega}{\sigma^2} \int_{-1}^{1} \text{Var} \left\{\frac{d[\hat{y}(x)]}{dx}\right\} dx = 3 - \frac{1}{a^2} + \frac{9}{8a^4} \tag{5.45}$$

Atkinson's Criterion to Estimate Slope (1)

This problem will demonstrate the method of least squares to the problem of estimating slope. Once again the true surface will be represented by the polynomial of Equation (5.36) and the fitted model by the polynomial of Equation (5.37). The slopes of these surfaces are represented by Equations (5.38). Again it can be seen that $E(\hat{b}_1)$ is

$$E(\hat{b}_1^*) = \beta_1 + (\underline{X}_1'\underline{X}_1)^{-1}\ \underline{X}_1'\underline{X}_2\beta_2\ . \tag{5.46}$$

Rewriting in matrix notation gives

$$E\left\{\frac{d[\hat{y}(x)]}{dx}\right\} = d_2\underline{x}_1'\underline{b}_1^* \tag{5.47}$$

The minimized bias can be written as

$$B^* = \frac{N\,\Omega}{\sigma^2}\int_R \left\{E\ \frac{d[\hat{y}(x)]}{dx} - \frac{d[\eta(x)]}{\partial dx}\right\}^2 dx\ . \tag{5.48}$$

The $(\underline{X}'\underline{X}\ )^{-1}$ and $(\underline{X}_1'\underline{X}_2)$ matrices are given by

$$(\underline{X}_1'\underline{X}_1)^{-1} = \begin{bmatrix} 1/N & 0 \\ 0 & 1/N[11] \end{bmatrix}, \qquad (\underline{X}_1'\underline{X}_2) = \begin{bmatrix} N[11] \\ N[111] \end{bmatrix} \tag{5.49}$$

where $[11] = \frac{1}{N}\sum_{i=1}^{N} x_1^2 = \frac{2}{3}a^2$ for $N = 3$.

Now

$$E\left\{\frac{d[\hat{y}(x)]}{dx}\right\} = E\ (b_1 + d_2 b_{11}x) \tag{5.50}$$

$$= \beta_1 + 2[11]\beta_{111} + d_2 x\left\{\beta_{11} + 2\,\frac{[111]}{[11]}\,\beta_{111}\right\},$$

and substituting into (5.48) yields

$$B^* = \frac{N\,\Omega}{\sigma^2}\int_{-1}^{1} \beta_1 + 2[11]\beta_{111} + 2x\beta_{11} + 4x\,\frac{[111]}{[11]}\,\beta_{111} - \beta_1 \tag{5.51}$$

$$- 2\beta_{11}x - 3\beta_{111}x^2\Big\}^2\,dx\ .$$

Subtracting and expanding yields

$$B^* = \frac{N}{\sigma^2}\,\beta_{111}^2 \int_{-1}^{1} \Big[4[11]^2 + 16x[111] + 16\,\frac{[111]^2}{[11]^2}\,x^2 \tag{5.52}$$

$$- 12x^2[11] - 24x^3\,\frac{[111]}{[11]} + 9x^4\Big]\,dx\ .$$

Integrating (5.52), substituting for [11], and setting the third moment to zero yields

$$B^* = \frac{N}{\sigma^2}\,\beta_{111}^2\left\{\frac{16}{9}\,a^4 - \frac{8}{3}\,a^2 + \frac{9}{5}\right\} = \frac{3}{\sigma^2}\,\beta_{111}^2\left[\left(\frac{4}{3}\,a^2 - 1\right)^2 + \frac{4}{5}\right] \tag{5.53}$$

From Equations (5.4) and (5.7), the variance can be obtained as

$$V^* = \frac{3}{\sigma^2}\int_{-1}^{1} \mathrm{Var}\left\{\frac{d[\hat{y}(x)]}{dx}\right\}dx = 1 + \frac{4}{3[11]} = 1 + \frac{2}{a^2} \tag{5.54}$$

A graphical presentation of the two designs demonstrates that, in a similar manner to Karson's original article, the least squares estimation of the slope of a response surface is a special case of minimizing bias by direct estimation.

In Figure 4, V and V^* are plotted against a. At the same time, it can be seen that $V^* \leqq V$ except at the point $a = \sqrt{3/4}$, the minimum value achieved by least squares estimation where $V = V^*$. In a similar manner, a plot of B versus B^* as a function of a indicates that, for minimum bias estimation, minimum bias is achieved for any value $a \neq 0$. At the same time, B^* reaches a minimum at $a = \sqrt{3/4}$, the value achieved by least squares estimation. Thus combining the knowledge of both graphs it can be seen that

$$J = V + B = J^* \ (a = \sqrt{3/4}) \tag{5.55}$$

on the interval $\sqrt{3/4} \leqq a \leqq 1$. At the same time, it must be pointed out that minimum V is not achieved until $a = \sqrt{6}$ which is outside the region of interest, i.e., $x_i \leqq 1$. Consequently, the only limitation on the design is the inherent design limitation defined by the region of interest.

The last situation that will be considered is the estimation of the slope where the true surface is quadratic and the fitted model is linear; that is,

$$\eta(x) = \beta_0 + \beta_1 x + \beta_{11} x^2 \tag{5.56}$$

$$\hat{y}(x) = b_0 + b_1 x \ .$$

The slopes of the fitted model and the true surface are

$$\frac{d[\eta(x)]}{dx} = \beta_1 + 2\beta_{11} x \tag{5.57}$$

(Continued)

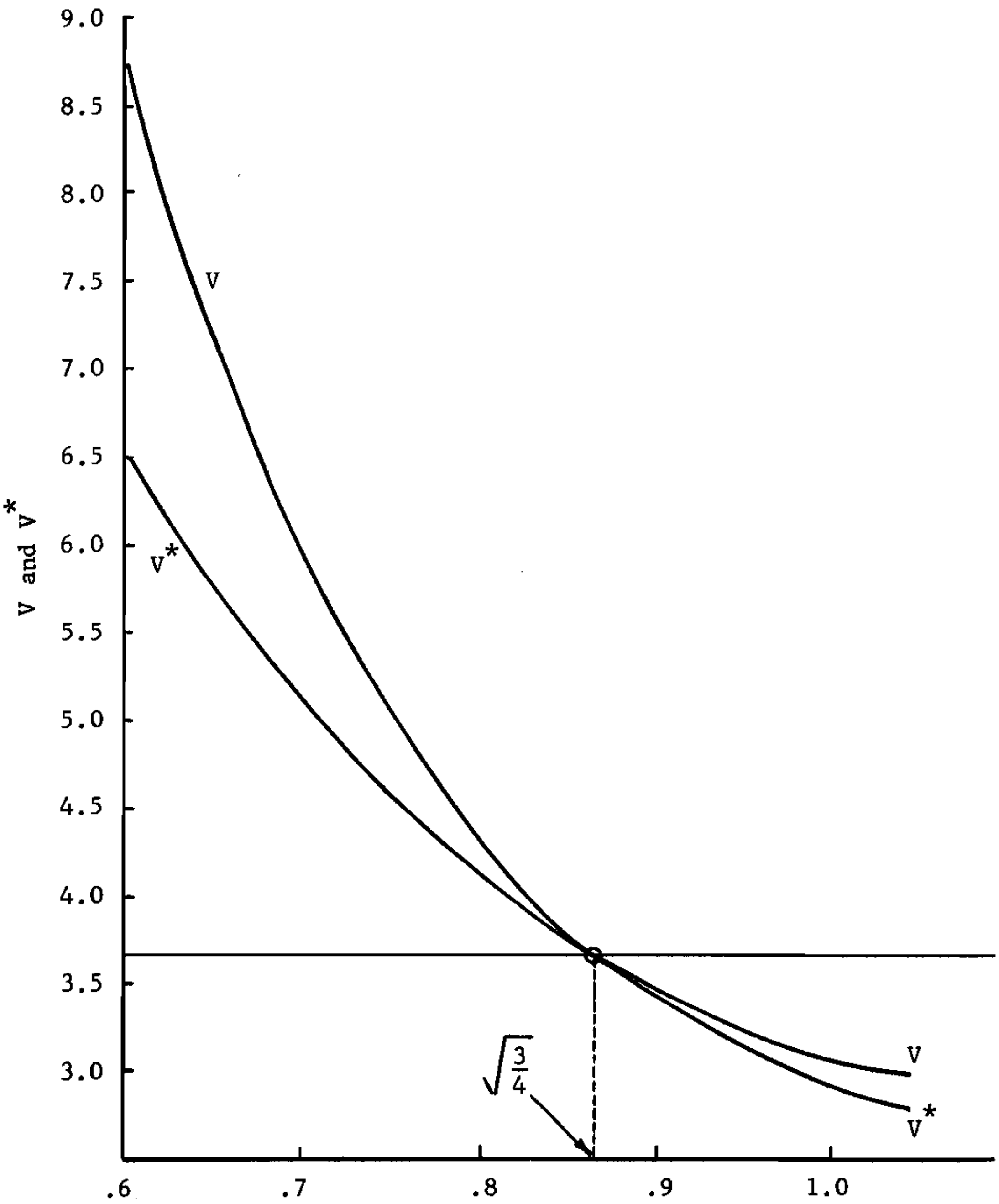

Figure 4. V and V^* versus a

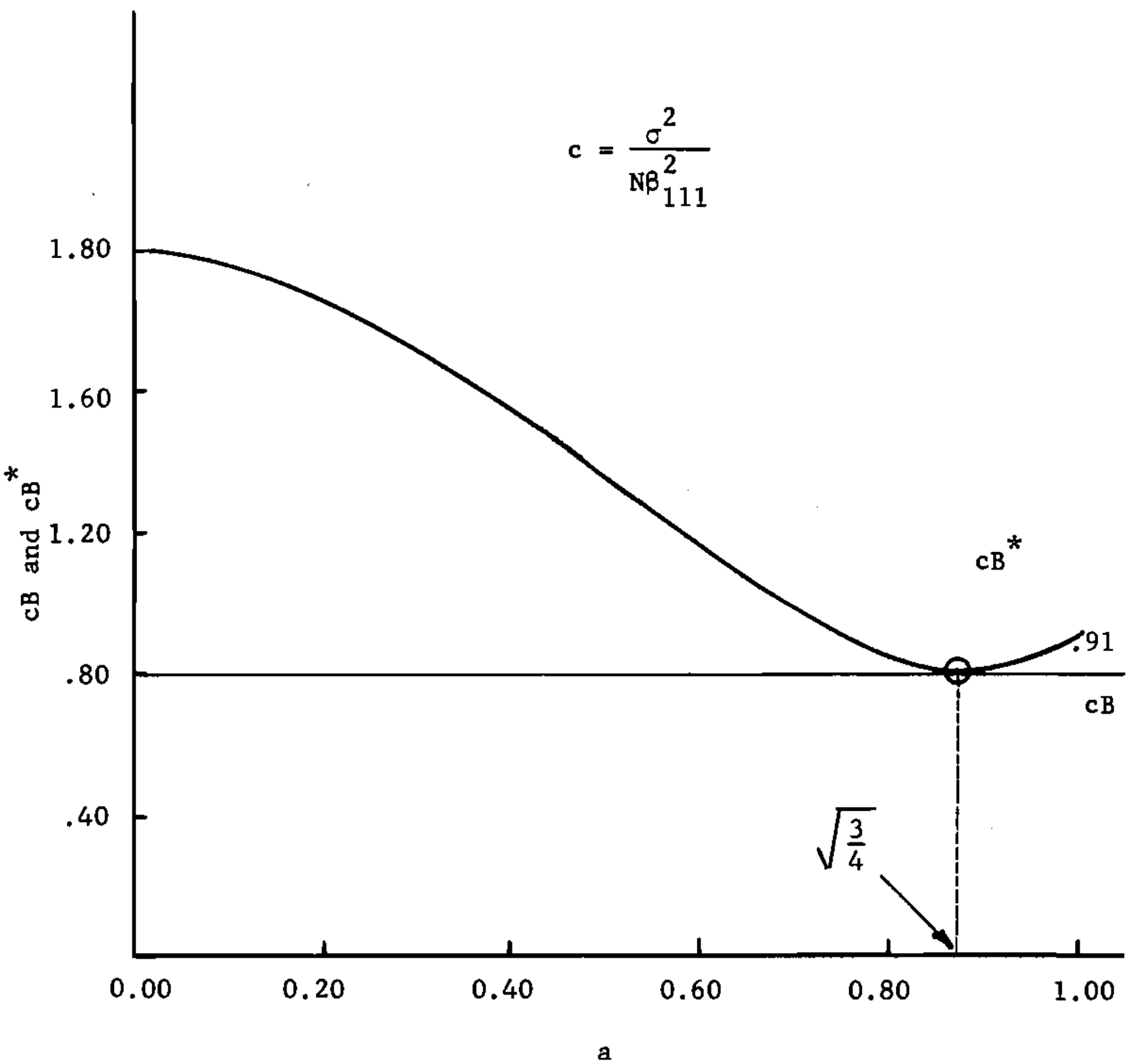

Figure 5. B and B* versus a

$$\frac{d[\hat{y}(x)]}{dx} = b_1$$

The $\underline{X}_1$ and $\underline{X}_2$ matrices are given by

$$\underline{X}_1 = \begin{bmatrix} 1\ , & x_1 \\ 1\ , & x_2 \\ . & . \\ 1\ , & x_N \end{bmatrix}, \quad \text{and} \quad \underline{X}_2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ . \\ x_N^2 \end{bmatrix}. \tag{5.58}$$

Using least squares estimation, the alias matrix obtained is

$$\underline{A} = (\underline{X}_1'\underline{X}_1)^{-1}\ \underline{X}_1'\underline{X}_2 \tag{5.59}$$

Thus

$$E(b_1) = \beta_1 + ([111]/[11])\ \beta_{11}\ . \tag{5.60}$$

From Equation (5.4), the bias portion of J can be written as

$$B = \frac{N\ \Omega}{\sigma^2} \int_{-1}^{1} \{\beta_1 + ([111]/[11])\ \beta_{11} - \beta_1 - 2\beta_{11}x\}^2\ dx\ . \tag{5.61}$$

$$= \frac{N\ \Omega}{\sigma^2} \int_{-1}^{1} \{([111]/[11])\ \beta_{11} - 2\beta_{11}x\}^2\ dx\ . \tag{5.62}$$

Examining the equation above, one sees that, if the design is centered at the point where the slope is estimated, the bias term is zero, since the third moment is zero. This was pointed out by Atkinson (1) and he developed designs which are not centered at the point of slope estimation.

Using MBE with the same true surface and fitted response, the slopes are as shown in (5.57). The expected value of b_1 is some polynomial of degree zero, say α_1. The problem is to minimize B with respect to α_1. From (5.4) the bias portion of J can be written as

$$B = \frac{N\,\Omega}{\sigma^2}\int_{-1}^{1} \{\alpha_1 - (\beta_1 + 2\beta_{11}x)\}^2\, dx\ . \tag{5.63}$$

Rewriting this equation

$$= \frac{N\,\Omega}{\sigma^2}\int_{-1}^{1}\ \alpha_1 - \beta_1) - 2\beta_{11}x\}^2\, dx\ . \tag{5.64}$$

Expanding yields

$$B = \frac{N\,\Omega}{\sigma^2}\int_{-1}^{1} \left[(\alpha_1 - \beta_1)^2 - 4(\alpha_1 - \beta_1)x\ \beta_{11} + 4\beta_{11}x_{11}^2\right] dx\ . \tag{5.65}$$

Looking at Equation (5.65), it can be seen that the term $4(\alpha_1 - \beta_1)\ x\beta_{11}$ is zero since from (3.23) this integral is zero if any δ_i odd. Differentiating (5.65) with respect to α_1 gives

$$\frac{d\ B}{d\ \alpha_1} = 2(\alpha_1 - \beta_1) = 0 \qquad \text{or} \qquad \alpha_1 = \beta_1\ . \tag{5.66}$$

This simply means that the least squares estimator is equivalent to the MBE.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

Summary of Results

This thesis discusses an approach to minimum bias designs for response surface methodology. Three important areas of minimum bias designs were considered: 1) organization of the topic of minimum bias designs and presenting it in a comprehensive manner; 2) integration of modern and classical design criteria to more fully explain and differentiate characteristics of importance; 3) application of minimum bias estimation to the problem of estimating the slope of a response surface.

A detailed development and explanation of the assumptions of Box and Draper was presented to demonstrate the importance of each assumption to each type of minimum bias designs. At the same time, development of rotatability was considered in detail because of its fundamental importance to basic assumptions for minimum bias designs as well as its basic importance in the development of additional criteria in minimum bias designs.

Minimum bias designs were also examined with the purpose of developing additional design criteria to include orthogonality and uniform precision. However, these were shown to be mutually exclusive concepts. The development and examination of minimum bias estimation was considered in great detail. An extension of minimum bias estimation to estimate the slope of a response surface was developed and applied to a three point design. Within this context it must be pointed out that designs for estimating the slope of a response surface seem somewhat limited since the method degenerates into a least squares estimation procedure in linear models, which is probably the most frequently encountered case on the part of the experimenter.

Conclusions

The conclusions derived from this study are the following:

1. A literature survey revealed the importance of the assumptions surrounding each criterion of modern response surface design. This study clearly demonstrates the importance of rotatability to modern design criteria and its application to new areas of response surface design.

2. Rotatable minimum bias designs with uniform precision or orthogonality are mutually exclusive categories. Although moments were achieved which are somewhat near these criteria, the corresponding cost in terms of additional experiments and the spread of the design, outside the region of interest, are in most cases undesirable.

3. The superiority of minimum bias estimation to the traditional method of least squares estimation was mathematically and pictorially demonstrated for a single variable, with regard to integrated mean square error as a design criterion for response surface designs. This technique allows the experimenter to select a considerable range for the design parameter over which the integrated mean square error is approximately equal. This allows the experimenter further design flexibility to satisfy other design criteria.

Recommendations for Further Study

Although the concept of estimation of slope was developed in detail, there appear to be many areas of potential research which remain open, both related to modern design criteria as well as other topics of basic interest in response surface methodology. The following is a brief outline of recommendations for further research in the area.

1. Develop a protection criterion for minimum bias estimation of slope. Based upon the protection criteria developed by Karson (16) for estimation of response surfaces as well as the developments of this study, this would seem to be a feasible topic for further development.

2. Does minimum bias design lend itself to the development of other design criteria, such as the protection criterion developed by Karson? Potentially this topic is the area of greatest importance; however, the topic would be the most difficult to develop.

3. Apply Karson's minimum bias estimation to spherical weight functions and develop design criteria for this type of response surface design.

4. A relatively unknown article by Nelder (18) concerning inverse polynomials and their application to response surface methodology provides a wide area for new further research in response surfaces. Can rotatability for this type of design be demonstrated? How does this design affect minimum bias design and "lack of fit"?

5. Develop further types of approximating polynomials to be utilized for response surface design. If this is feasible, what characteristics of item 3 above can be applied to these designs?

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