OPTIMALITY CRITERIA APPLIED TO
CERTAIN RESPONSE SURFACE DESIGNS

by

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(ABSTRACT)

The estimation of a particular matrix of coefficients of a second-order polynomial model was shown to be important in Response Surface Methodology (RSM). This led naturally to designing RSM experiments for best estimation of these coefficients as a primary goal. A design criterion, D_s-optimality, was applied to several classes of RSM designs to find optimal choices of design parameters. Further, previous results on D-optimal RSM designs were extended. The designs resulting from the use of the two criteria were compared.

Two other design criteria were also studied. These were IV, the prediction variance of $\hat{y}$ integrated over a region R, and IV*, sum of the variances of $\partial\hat{y}/\partial\underline{\alpha}$ again integrated over R. Three different choices of the region R were used. The object of the study was not only to identify optimal choices of design parameters, but also to compare the resulting designs with those obtained using the determinantal criteria.

An extension of a method for constructing D-optimal designs was used to construct D_s-optimal central composite designs. This involved viewing the design points as having continuous weights. D_s-best

central composite designs were constructed either analytically or numerically for a fixed axial point distance. The results of previous work by other authors were extended for D-optimality by varying the axial point distance. Other design classes studied were Box-Behnken, equiradial, and some small composite designs.

The novel study of IV and the extended IV, called IV*, was done for each of the four design classes mentioned previously. The results of the study were presented graphically, or tabularly. The best designs according to IV and IV* were compared with the D_s-best designs.

Composite designs performed well in all criteria, with the central composite designs performing best. The Box-Behnken and equiradial seemed to suffer from a lack of flexibility. The D_s-best designs agreed well with the designs suggested by the IV* criteria.

DEDICATION

To my family for making me want it, and to Barbara for making it possible.

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TABLE OF CONTENTS

TABLE OF CONTENTS (cont.)

TABLE OF CONTENTS (cont.)

LIST OF TABLES

LIST OF FIGURES

LIST OF FIGURES (cont.)

LIST OF FIGURES (cont.)

CONVENTION

Throughout this thesis, the plots will have the following legend

number of center points	symbol
0	————————
1	- - - - - - - -
2	— — — — —
3	—— —— —— ——
4	- — - — - —

CHAPTER I

INTRODUCTION

In many exploratory and research situations a researcher may want to model some important response as a function of several controllable variables or factors. After modeling the response, the researcher may want to find conditions on the controllable variables which optimize the response, along with other related objectives.

Generally, it is assumed that the response, say y, is a function, whose form is unknown, of the k controllable and quantitative factors, $w_1, w_2, \ldots, w_k$. Written succinctly, this is

$$y = f(w_1, w_2, \ldots, w_k) \quad . \tag{1.1}$$

Since the form of $f(\cdot)$ is unknown, it is generally approximated in a region of k-space by a low order polynomial in the k controllable factors. This is done by expanding $f(\cdot)$ in a Taylor series about some point w_0. A first order expansion can be written as

$$f(\underline{w}) \simeq \gamma_0 + \sum_{i=1}^{k} \gamma_i w_i \quad , \tag{1.2}$$

while a second order expansion can be written as

$$f(\underline{w}) \simeq \gamma_0 + \sum_{i=1}^{k} \gamma_i w_i + \sum_{i \leq j}^{k} \gamma_{ij} w_i w_j \quad . \tag{1.3}$$

The point w_0 is assumed to be $(0,0,\ldots,0)'$, here. The coefficients are $\gamma_0 = f(w_0)$, $\gamma_i = \left.\frac{\partial f(\underline{w})}{\partial w_i}\right|_{\underline{w}=\underline{w}_0}$, and $\gamma_{ij} = \frac{\partial^2 f(\underline{w})}{\partial w_i \partial w_j}$. This type of approximation is the basis of much of regression analysis.

The experimenter may be interested, as mentioned above, in several things. First, he may be interested in estimation of the surface determined by the response. He may also wish to locate the position of the optimum response and estimate the response at this point. The methods of doing this estimation and optimization are contained in a collection of methods called Response Surface Methodology (the acronym RSM will be used hereafter).

The following thesis will consist of four parts. The first part will describe the methods of RSM and will include a discussion of RSM experimental designs used when the approximating model is second order. This discussion will include properties designs may possess as well as criteria for constructing designs. The second part gives the results of a statistical experiment which justify the use of a design criterion suggested by Kiefer (1961) to construct RSM designs. This part will also present conditions for choosing an optimal RSM design in a well known, much used class of RSM designs. The third part will apply the design criteria suggested by Kiefer to another group of RSM designs, not so widely used. The final portion of the thesis will consider a very different design criterion. This criterion will be applied to the same classes of RSM designs to allow comparisons between the criteria to be made. Conclusions will be drawn regarding the criteria and suggestions will be included for construction of designs for better determination of the response surface.

CHAPTER II

LITERATURE REVIEW

2.1 Response Surface Methodology

The techniques of RSM were first discussed by Box and Wilson (1951) and will be repeated for clarity and emphasis. The text by Myers (1976) provides a unified, thorough, and concise discussion of the topics presented here. The interested reader is referred there.

2.2 Basic Assumptions in RSM

It is generally assumed in RSM that the response, y, can be approximated by a polynomial in a set of factors $\underline{w} = (w_1, w_2, \ldots, w_k)'$. This polynomial is usually assumed to be first or second order in the factors $\underline{w}$. This thesis will be concerned only with second order models and the discussion will be restricted to these models in the succeeding.

Suppose that N observations are made on the response y at N settings of the controllable variables (not necessarily all distinct settings). Assume also that the observed response is, in fact, the true response plus a random disturbance. Symbolically,

$$Y(\text{observed}) = y(\text{true}) + \text{error} . \tag{2.2.1}$$

Let ε_u, $u = 1, 2, \ldots, N$ denote this additive random variable. The vector of random disturbances $\underline{\varepsilon} = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_N)'$ is assumed to have a mean vector of $\underline{0} = (0,0,\ldots,0)'$ and $\mathrm{Var}(\underline{\varepsilon}) = \sigma^2 I$. It is also often assumed the $\underline{\varepsilon}$ has a multivariate normal probability distribution. The second order model may now be written as

$$Y_u = \gamma_0 + \sum_{i=1}^{k} \gamma_i w_{iu} + \sum_{i\le j}^{k} \gamma_{ij} w_{iu} w_{ju} + \varepsilon_u , \qquad (2.2.2)$$

$$u = 1, 2, \ldots, N .$$

This can be written concisely as,

$$\underline{y} = W\underline{\gamma} + \underline{\varepsilon} , \qquad (2.2.3)$$

where $\underline{y} = (Y_1,\ldots,Y_N)'$, $\underline{\varepsilon} = (\varepsilon_1,\ldots,\varepsilon_N)'$, $\underline{\gamma} = (\gamma_0,\gamma_1,\gamma_2,\ldots,\gamma_k,$ $\gamma_{11},\ldots,\gamma_{kk},\gamma_{12},\ldots,\gamma_{k-1k})$, and

$$W = \begin{bmatrix} 1 & w_{11} & \cdots & w_{k1} & w_{11}^2 & \cdots & w_{k1}^2 & w_{11}w_{21} & \cdots & w_{k-11}w_{k1} \\ 1 & w_{12} & \cdots & w_{k2} & w_{12}^2 & \cdots & w_{k2}^2 & w_{12}w_{22} & \cdots & w_{k-12}w_{k2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 1 & w_{1N} & \cdots & w_{kN} & w_{1N}^2 & \cdots & w_{kN}^2 & w_{1N}w_{2N} & \cdots & w_{k-1N}w_{kN} \end{bmatrix} .$$

The matrix W will be called the W-model matrix.

The goal of the experimenter is to estimate the surface. This estimation is done by the method of least squares. This gives an estimate of $\underline{y}$ denoted by $\hat{\underline{y}}$ (see, for example, Draper and Smith (1981)),

$$\hat{\underline{y}} = W(W'W)^{-1}W'\underline{y} . \qquad (2.2.4)$$

The vector $\underline{\gamma}$ can also be estimated in this way, and the least squares estimator of γ is $\hat{\gamma} = (W'W)^{-1}W'\underline{y}$.

Under the limited assumptions of $E(\underline{\varepsilon}) = \underline{0}$, $\mathrm{Var}(\underline{\varepsilon}) = \sigma^2 I$, the estimator $\hat{\underline{\gamma}}$ is BLUE (see Graybill (1976)). Including the assumption of normality, the estimator is UMVU (again, see Graybill (1976)).

It is typical in RSM to redefine the k controllable variables as centered and scaled variables in the following way:

$$x_{iu} = \frac{w_{iu}-a_i}{b_i}\ , \quad i=1,\ldots,k;\ u=1,\ldots,N\ . \tag{2.2.5}$$

The variables, x_i, will be called *design variables* hereafter. The γ_0, γ_i, γ_{ij}, $i=1,\ldots,k$; $i \le j = 1,\ldots,k$, are redefined also. The model (2.2.2) becomes

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i\le j}^{k} \beta_{ij} x_{iu} x_{ju} + \varepsilon_u\ ,$$

$$u = 1,\ldots,N\ . \tag{2.2.6}$$

This model has a corresponding X-model matrix, which will hereafter be called the model matrix dropping the X-prefix. Another matrix which will be useful later is the moment matrix of the design given by

$$\frac{X'X}{N} =$$

$$\begin{bmatrix}
1 & [1] & [2] & \cdots & [k] & [11] & \cdots & [kk] & [12] & [13] & \cdots & [k\text{-}1k] \\
 & [11] & [12] & \cdots & [1k] & [111] & \cdots & [1kk] & [112] & [113] & \cdots & [1k\text{-}1k] \\
 & & \ddots & & & & & & & & & \\
 & & & & [kk] & [1kk] & \cdots & [kkk] & [12k] & [13k] & \cdots & [k\text{-}1kk] \\
 & & & & & [1111] & \cdots & [11kk] & [1112] & [1113] & \cdots & [11k\text{-}1k] \\
 & & & & & & \ddots & & & & & \\
 & & \text{symmetric} & & & & & [kkkk] & [12kk] & [13kk] & \cdots & [k\text{-}1kkk] \\
 & & & & & & & & [1122] & [1123] & \cdots & [12k\text{-}1k] \\
 & & & & & & & & & [1133] & \cdots & [13k\text{-}1k] \\
 & & & & & & & & & & \ddots & \\
 & & & & & & & & & & & [k\text{-}1k\text{-}1kk]
\end{bmatrix}$$

where $[i] = \frac{1}{N}\sum_{u=1}^{N} x_{iu}$, $[ij] = \frac{1}{N}\sum_{u=1}^{N} x_{iu}x_{ju}$, $[ijk] = \frac{1}{N}\sum_{u=1}^{N} x_{iu}x_{ju}x_{ku}$,
and $[ijk\ell] = \frac{1}{N}\sum_{u=1}^{N} x_{iu}x_{ju}x_{ku}x_{\ell u}$.

Equation (2.2.6) can be expressed more concisely as,

$$y_u = \beta_0 + \underline{x}_u'\underline{\beta}^L + \underline{x}_u'\beta^q\underline{x}_u + \varepsilon_u, \quad u = 1,\ldots,N, \tag{2.2.7}$$

where $\underline{x}_u = (x_{1u}, x_{2u}, \ldots, x_{ku})$, $\underline{\beta}^L = (\beta_1,\ldots,\beta_k)'$ and β^q is a $k \times k$ symmetric matrix of the form

$$\beta^q = \frac{1}{2}\begin{bmatrix} 2\beta_{11} & \beta_{12} & \cdots & \beta_{1k} \\ \beta_{12} & 2\beta_{22} & \cdots & \beta_{2k} \\ \vdots & \vdots & & \vdots \\ \beta_{1k} & \beta_{2k} & \cdots & 2\beta_{kk} \end{bmatrix} .$$

The matrix β^q will be very important later in this thesis.

2.3 Optimization

Consider equation (1.3). This relationship can be expressed in terms of the design variables as

$$y(\underline{x}) = \beta_0 + \underline{x}'\underline{\beta}^L + \underline{x}'\beta^q\underline{x} \quad . \tag{2.3.1}$$

The results which follow pertaining to (2,3.1) can be found in a different form in Myers (1976). They are repeated here for emphasis and later reference.

The location of the stationary point, $\underline{x}_0$, of the quadratic surface defined by (2.3.1) is found by differentiation of that expression with respect to $\underline{x}$ and setting the result equal to a k-vector of zeroes. This gives

$$\underline{x}_0 = -(\tfrac{1}{2}) \cdot (\beta^q)^{-1}\underline{\beta} \quad . \tag{2.3.2}$$

Also,

$$y(\underline{x}_0) = \beta_0 - \frac{1}{4}\,\underline{\beta}'(\beta^q)^{-1}\underline{\beta} \; . \tag{2.3.3}$$

Whether this stationary point is a maximum, a minimum, or neither is determined by β^q. β^q is a $k \times k$ symmetric matrix so (see Graybill (1976))

$$\beta^q = V'\Lambda V \ , \quad V'V = VV' = I \ .$$

Let $\underline{z} = \underline{x} - \underline{x}_0$. Then

$$y(\underline{x}) = \beta_0 + (\underline{x}_0 + \underline{z})'\underline{\beta} + (\underline{x}_0 + \underline{z})'\beta^q(\underline{x}_0 + \underline{z}) \ .$$

Substituting $\underline{x}_0 = -(\frac{1}{2})(\beta^q)^{-1}\underline{\beta}$ and collecting terms,

$$y(\underline{x}) = y(\underline{x}_0) + \underline{z}'\beta^q\underline{z} \ .$$

Hence,

$$y(\underline{x}) = y(\underline{x}_0) + \underline{z}'V'\Lambda V\underline{z}$$

so,

$$y(\underline{x}) = y(\underline{x}_0) + \underline{w}'\Lambda\underline{w}$$

or,

$$y(\underline{x}) = y(\underline{x}_0) + \sum_{i=1}^{k} w_i^2\lambda_i \ . \qquad (2.3.4)$$

Therefore if

(i) $\lambda_i < 0$ for all i, the point $\underline{x}_0$ will be a point of maximum response.

(ii) $\lambda_i > 0$ for all i, the point $\underline{x}_0$ will be a point of minimum response.

(iii) λ_i are mixed in sign or zero, the point $\underline{x}_0$ will be neither a maximum or a minimum and will be called a *saddle point*.

To this point, the parameters β_0, $\underline{\beta}^L$, β^q have been assumed known. This will generally not be the case. It is standard procedure in RSM to act as if the fitted surface is the true approximating surface, and hence, substitute the estimated parameter values into equations (2.3.1), (2.3.2), (2.3.3), and (2.3.4) giving

$$\hat{y}(\underline{x}) = b_0 + \underline{x}'\underline{b} + \underline{x}'B\underline{x}$$

$$\hat{\underline{x}}_0 = -(\tfrac{1}{2})B^{-1}\underline{b}$$

$$\hat{y}(x_0) = b_0 - (\tfrac{1}{4})\underline{b}'B^{-1}\underline{b}$$

$$\hat{\lambda}_i = \ell_i, \quad \ell_i \text{ is the } i^{th} \text{ largest eigenvalue of } B,\ i=1,\ldots,k\,. \tag{2.3.5}$$

2.4 Constrained Optimization

Often not all of the estimated eigenvalues are appropriately signed. For instance, a maximum is desired, but a single eigenvalue of B is positive. The stationary point is a saddle point. Hoerl (1959) exposited a method for doing the optimization in a constrained region. Draper (1963) made the exposition precise. The suggested method locates the optimum point when the region of interest is constrained to be the surface of a k-dimensional hypersphere. Briefly,

$$\text{one optimizes } \hat{y} \text{ subject to } \underline{x}'\underline{x} = R^2 \ . \qquad (2.4.1)$$

Whether maximization or minimization is required, the first step in the optimization is to establish the function $\phi(\underline{x})$ using a Lagrange multiplier, where

$$\phi(\underline{x}) = \hat{y} - \mu(\underline{x}'\underline{x} - R^2) \ ,$$

where μ is the Lagrangian multiplier. Differentiating, the following equation results

$$(B - \mu I)\underline{x}_0 = -\frac{1}{2}\underline{b} \ . \qquad (2.4.2)$$

A particular choice of μ defines a choice of the radius R of the hypersphere. Also, by choosing μ, the experimenter determines whether the resulting $\underline{x}_0$ will be a constrained maximum or minimum. The conditions on μ necessary for a maximum or a minimum will be stated here without derivation.. The interested reader may see Myers (1976) and Draper (1963).

(i) If a constrained maximum is desired, choose $\mu > \ell_i$ $(i=1,\ldots,k)$.

(ii) If a constrained minimum is desired, choose $\mu < \ell_i$ $(i=1,\ldots,k)$. (2.4.3)

This method of contrained optimization is commonly called *ridge analysis*.

2.5 Confidence Region for x_0

Box and Hunter (1954) presented a method of constructing a $(1-\alpha)\times 100\%$ confidence region for x_0, the location of the stationary point of a quadratic surface. The method will be described here for later reference.

As mentioned above, the estimated location of the stationary point is obtained by solving the equation

$$b + 2B\underline{x} = \dot{0} \ . \tag{2.5.1}$$

Let $\underline{\delta} = \underline{b} + 2B\underline{x}$, and $V = \mathrm{Var}(\underline{\delta})$. Then $\frac{\underline{\delta}'V^{-1}\underline{\delta}}{ks^2}$ has a central $F(k,\phi)$ distribution, where s^2 is an estimate of the variance of the error with ϕ degrees of freedom. A $(1-\alpha)\times 100\%$ confidence interval for the location of the stationary point is then

$$\{\underline{x}\colon \underline{\delta}'V^{-1}\underline{\delta} \le ks^2F(k,\phi,\alpha)\} \ . \tag{2.5.2}$$

Box and Hunter discuss at length the nature of the resulting confidence regions. One of the most interesting comments they make is that the shape of the resulting region is dependent on B. In particular, the shape of the surface is dependent on the conditioning of B. They also mention that the choice of the design will have an effect on the confidence regions defined by (2.5.2).

2.6 Design of Experiments

The design of experiments in RSM consists of telling the experimenter what settings should be made on the controllable factors. It will be assumed throughout that no blocking is needed. Also, only designs for second-order models will be considered.

In the remainder of this section four important and useful design classes will be presented. Criteria and design properties useful for choosing amongst the designs in a class will also be presented. Where such exist in the literature, conditions on the design parameters will be presented to make a design fit a particular criterion or have a certain property.

2.7 Central Composite Designs

This class of designs was first introduced by Box and Wilson (1951) in their pioneering paper. These designs are easy to construct and hence are widely used. The design consists of three portions. One portion simply consists of center points, i.e. n_0 (k-vectors) points of the form $(0,0,\ldots,0)$. Another portion of the design is the axial portion. It is made up of k pairs of points. The i^{th} pair is $(0,0,\ldots,0,\alpha,0,\ldots,0)$ and $(0,0,\ldots,0,-\alpha,0,\ldots,0)$ where α, $-\alpha$ occur in the i^{th} position in the k-vector. It is called the axial portion since all points lie on the k axes, α units from the origin. There are 2k points in this portion. The final part of the central composite design is a full or fraction of a 2^k factorial. The fraction is usually chosen so that no main effects or two factor interactions are aliased with a main effect or two factor interaction. The fractionation is done for $k \geq 5$, when the cost of taking observations is large.

An example of a central composite design for $k = 3$ is given below. The reader can easily see the three portions described above.

$$D = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \\ \alpha & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & \alpha \\ 0 & 0 & -\alpha \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \end{bmatrix}, \quad N = 8 + 6 + n_0 \,. \qquad (2.7.1)$$

2.8 Small Composite Designs

Small composite designs for estimating second order models were suggested first by Hartley (1959) and later Westlake (1965). A recent work by Draper (1984) also deals with such designs.

This class of design takes advantage of the fact that not all of the coefficients in the second order model require the use of factorial points in their estimation. Hartley (1965) noticed that it is only necessary that two-factor interactions be unaliased with each other. Using this idea, he constructed saturated or nearly-saturated designs for various k.

Westlake (1965) used irregular fractions of 2^n factorials to construct the factorial portion of a central composite design. Draper (1984) used portions of Plackett-Burman (1946) designs to make up the factorial section of his designs.

These designs will be used subsequently for comparison with the other design classes. The comparisons will be done for each of the design criteria being studied.

2.9 Box-Behnken Designs

Box and Behnken (1960) presented a method for constructing second order designs using balanced incomplete block designs. The motivation was to locate designs with a smaller number of points than the corresponding central composite design. For small k ($k = 3,4,5$), the designs are of a simple form. An example for $k = 3$ is as follows:

$$D = \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ -1 & -1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ -1 & 0 & -1 \\ 0 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & -1 & -1 \\ \underline{0} & \underline{0} & \underline{0} \end{bmatrix} \tag{2.9.1}$$

As can easily be seen, the design consists of three 2^2 factorials in all possible choices of pairs of the factors. A vector of zeroes is included. For $k = 4$, 5 this simple form is retained. For $k \geq 6$, the construction is more complicated. The reader is referred to the original paper for more detail. These designs will be used as yet another class to compare and contrast with the central composite design.

2.10 Equiradial Designs

This class of designs was suggested by Box and Hunter (1957) for the case when $k = 2$. The design consists of two parts. One portion is a set of n_1 points equally spaced around a circle of radius ρ. The other part is a set of n_0 center points, (0,0). The design can be written in general as

$$D = \begin{bmatrix} \rho\cos(\theta) & \rho\sin(\theta) \\ \rho\cos(\theta+\frac{2\pi}{n_1}) & \rho\sin(\theta+\frac{2\pi}{n_1}) \\ \rho\cos(\theta+\frac{4\pi}{n_1}) & \rho\sin(\theta+\frac{4\pi}{n_1}) \\ \vdots & \vdots \\ \rho\cos(\theta+\frac{2\pi(n_1-1)}{n_1}) & \rho\sin(\theta+\frac{2\pi(n_1-1)}{n_1}) \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix}, \quad (2.10.1)$$

where θ is the angle the first point makes with the real axis. The experimenter is allowed the freedom to choose ρ, n_0, n_1.

2.11 Design Criteria and Properties

As mentioned above, much of the research on second order designs has focused on the construction of designs with a chosen property or which are best with respect to some criterion. This section will be dedicated to several criteria and properties prevalent in the literature, indicating, where possible, what conditions on the design parameters will give a design that has the property or is best.

2.12 Rotatability

A design is *rotatable* if the variance of the estimated response at a particular point is a function only of the distance of that point from the center of the design (see Box and Hunter (1957)).

That is, if $x'x = R^2$, then $\mathrm{Var}(\hat{y}(\underline{x})) = g(R^2) \cdot \sigma^2$. This means that predicted values at points on the same k-dimensional hypersphere will have equal variances. Rotatability is a design property that can be obtained by the appropriate choice of the design parameters. Box and Hunter (1957) showed that a general condition sufficient to insure rotatability is that [iiii] = 3[iijj] for all i, j = 1, ..., k, and that all design moments of order 1 or 3 be 0.

Using the condition for rotatability, Box and Hunter showed (see also Myers (1976)) that the central composite design is rotatable with $\alpha = (F)^{1/4}$, where F is the number of factorial points in the design. It is easy to see that the Box-Behnken designs for k = 4, 6 are rotatable also, as is the equiradial design.

2.13 Integrated Variance

A rotatable design has equal variances on hyperspheres. This is a special class of designs. Box and Draper (1959) suggested a variance criterion for comparing designs found by averaging the variance of the predicted responses over a region.

<u>Definition:</u>

The integrated variance over the region R of a design D with model matrix X is defined by

$$\mathrm{I.V.}(D) = \frac{KN}{\sigma^2} \int_R \mathrm{Var}(\hat{y}(\underline{x}))\, d\underline{x}$$

$$= KN \int_R \underline{x}'(X'X)^{-1}\underline{x}\, d\underline{x} \qquad (2.13.1)$$

where $K^{-1} = \int_R dx$, N is the number of points in the design. A design will be best with respect to integrated variance in a class of designs if it has the smallest integrated variance.

Draper (1982) studied the effect that the number of center points in a rotatable central composite design had on the design's integrated variance. Recommendations were made there for the number of center points to be used for various values of k. No similar study has been done to find the best choice of α for a given range of α. This type of study will be a part of this thesis.

Integrated variance has been ignored in the cases of small composite, Box-Behnken and equiradial designs. The criterion will be studied here in those cases, also.

2.14 D-optimality

The criterion of D-optimality was first studied extensively by Kiefer (1961) and Kiefer and Wolfowitz (1959, 1960). The criterion is easily seen in a quite general form and then specialized to the specific case of RSM designs. Kiefer and his co-workers used the mathematical abstraction that a design could be generalized to be a probability measure on the set of possible choices of design levels for the factors. The notion of a moment matrix introduced above is generalized in the sense that $[ijk\ell] = \sum_{u=1}^{N} x_{iu}x_{ju}x_{ku}x_{\ell u}$ is replaced by $m_{ijk\ell} = \int x_i x_j x_k x_\ell \, d\xi$, where ξ is the probability measure defining the design. A design is called D-optimal if it maximizes the determinant of M, the moment matrix. For an extensive and fairly recent bibliography see St. John and Draper (1975).

Box and Draper (1971) applied the notion of D-optimality as a criterion for choosing amongst RSM designs. In this paper, they used a method due to Kiefer (1961) to find optimal central composite designs. This method is useful and will be extended below, so a complete description is necessary here.

Box and Draper classified the points of a central composite design into three types: center points, factorial points, and axial points. Each set of points was given a weight, w_0, w_1, and w_2, respectively, with the conditions that $1 \geq w_i \geq 0$, $i = 0, 1, 2$, and $\sum_{i=0}^{2} w_i = 1$. The determinant of the moment matrix can then be written in terms of these weights. In fact, for $\alpha = 1$ (see Box and Draper (1971, 1973))

$$\det(M) = (w_1 + \frac{w_2}{k})^k (w_1)^{\binom{k}{2}} (\frac{w_2}{k})^{k-1} \{(kw_1 + \frac{w_2}{k}) - k(w_1 - \frac{w_2}{k})^2\} \quad , \tag{2.14.1}$$

for a k-variable central composite design. Using this expression and results given in Kiefer (1961, page 315), Box and Draper (1971, 1973) give optimal choices of weights for the central composite design with various k. The weights can be considered as the relative importance of the points to the criterion.

Recently, a group of papers (Chatterjee and Mandel (1981), Mandel (1982)) have considered the use of an extended D-optimality criterion in constructing designs which are best when locating the position of optimum response is of interest. These papers use the notion of a design as a probability measure and give weight to each point in the chosen design. In the construction of the designs, Chatterjee and Mandel, and Mandel assume that the location of the optimum point has a prior distribution whose first and second moments are known. The Chatterjee and Mandel (1981) paper makes further assumptions about the coefficients in the matrix β^q. The notion of the vague prior is certainly open to criticism from a practical point of view. However, it is interesting to note that the designs which result must be rotatable. It turns out that a rotatable central composite design is D-optimal in the sense of Chatterjee and Mandel for $k = 2$. It is also interesting to note that both papers used the idea of designs as probability measures and gave weights to points.

The D-optimality criterion of Kiefer has been given several interpretations (see St. John and Draper (1975)). The most compelling is the minimum volume confidence region interpretation. That is, a D-optimal design will yield the smallest volume $(1-\alpha) \times 100\%$ confidence ellipsoid for the parameters of the model.

It should be noted that the designs suggested in the paper by Box and Draper are not universally D-optimal (except in the case of $k = 2$). Instead, they are D-best in the class of central composite designs. The criterion is used then as a method for choosing between the designs in a class, not for finding the overall best design. It will be used in this sense below when the equiradial and Box-Behnken designs are studied with respect to this criterion.

2.15 D_s-optimality

In some cases, the whole parameter set is not of interest, but only a subset of the parameters. A determinant criterion has been suggested in the literature for this case. It was first suggested by Kiefer (1961) and his results were extended by Karlin and Studden (1965). This criterion will be used extensively in what follows so a thorough definition and explanation is necessary.

Let $\mathcal{D}$ be a class of designs with members D. Let X_D be the model matrix corresponding to D. Let M(D) be the moment matrix defined by D. Let $\underline{\beta}$ be a (p×1) vector representing the coefficients in the model. Partition $\underline{\beta} = (\underline{\beta}_{p-s}, \underline{\beta}_s)$, and assume $\underline{\beta}_s$(s×1) are the parameters of interest. Partition M to conform to $\underline{\beta}$, that is

$$M = \begin{array}{cc} \left[\begin{array}{cc} M_{11} & M_{12} \\ & \\ M'_{12} & M_{22} \end{array}\right] & \begin{array}{c} p-s \\ \\ p \end{array} \\ \begin{array}{cc} p-s & \quad p \end{array} & \end{array} \tag{2.15.1}$$

Definition:

A design D* will be D_s-optimal in the class $\mathcal{D}$

$$\text{if } \max_{D\in\mathcal{D}}\{\det(M_{22}(D) - M'_{12}(D)M_{11}^{-1}(D)M_{12}(D))\}$$

$$= \det(M_{22}(D^*) - M'_{12}(D^*)M_{11}^{-1}(D^*)M_{12}(D^*)) \ .$$

This can be viewed as making the determinant of the variance-covariance matrix corresponding to the $\underline{\beta}_s$ estimator in least squares as small as possible. More precisely,

Proposition:

The volume of the $(1-\alpha) \times 100\%$ confidence set for $\underline{\beta}_s$ is proportional to $\det(M^{22}) = \det(M_{22} - M_{12}' M_{11}^{-1} M_{12})^{-1}$.

Proof:

The $(1-\alpha) \times 100\%$ confidence region for $\underline{\beta}_s$ is $\{\underline{\beta}_s\colon (\underline{\beta}_s - \hat{\underline{\beta}}_s)'(M^{22})^{-1}(\underline{\beta}_s - \hat{\underline{\beta}}_s) \le s^2\}$ and $\int_{\{x:\ \underline{x}'M\underline{x} < 1\}} d\underline{x} = |M|^{-1/2} \int_{\{y'y \le 1\}} d\underline{y}$, where $\underline{y} = M^{1/2}\underline{x}$.

This explanation of the criterion is given in Hill and Hunter (1974), without proof. The proof is provided for clarity.

The D_s-criterion has not been studied in the literature of RSM extensively. As mentioned, Hill and Hunter (1974) have presented a short treatment. They do not deal with choosing between standard RSM designs using this criterion. This will be a major portion of the following chapter.

CHAPTER III

DETERMINANT CRITERIA

As mentioned above, the criteria for constructing optimal experimental designs in a regression setting have been studied for many years. A much studied criterion is D-optimality, that is, one chooses the design whose moment matrix has the largest determinant in a class of designs (see Section 2.14).

Another, less studied, criterion is called D_s-optimality. A D_s-optimal design is one which maximizes the determinant of the inverse of a particular submatrix of M^{-1}. Designs chosen using the D_s-criterion are best in the estimation of a selected subset of the parameter vector, $\underline{\beta}$, whereas designs selected using the D-criterion are best in the estimation of the whole vector $\underline{\beta}$. In the following chapter, the D_s- and D-criteria will be used as selection criteria to choose between competing response surface designs. No claim will be made as to the universal optimality of the chosen designs. This chapter will focus on the designs described in Chapter II and will present new results for each class of designs and each criterion. The results of Box and Draper (1969, 1971) and Lucas (1974) on the D-criterion in composite designs will be extended. The D_s-criterion will be studied and results obtained using the tools presented in the papers by Box and Draper. These results will be the major portion of the chapter as this criterion has not been studied in the response surface setting.

3.1 The D_s-criterion in RSM

As mentioned, designs chosen according to the D_s-criterion will be best in the estimation of a subset of the parameter vector, $\underline{\beta}$. This is a natural criterion in RSM for a variety of reasons.

The goal of RSM is the estimation of the response surface, and once the estimation is done, the location of optimal response is estimated. As was shown above, the matrix β^q plays a large role in both of these objectives. In particular, the matrix β^q completely determines the nature of the response surface (whether the surface has a maximum, a minimum, or a saddle point) through its eigenvalues, λ_1, λ_2, ..., λ_k. The matrix β^q also enters into the equations for the location of the optimum response and the value of the optimum response. Hence, it seems that the matrix β^q should be well-estimated. That is, if the elements of β^q, $\underline{\beta}_s = (\beta_{11},\beta_{22},\ldots,\beta_{kk},\beta_{12},\ldots,\beta_{k-1k})'$ are estimated well, then the nature of the surface will be well determined, and the location and value of the optimal response will be estimated well.

It is also interesting to note that the matrix β^q plays a large role in the constrained optimization procedure of ridge analysis as discussed in Chapter II. Recall from that chapter that the location of the point of constrained optimum is the solution of the equation

$$(\beta^q-\mu I)\underline{x}_0 = -\frac{1}{2}\underline{\beta}^L \quad .$$

The parameter μ is a Lagrangian multiplier, and the choice of μ determines the nature of the solution $\underline{x}_0$. Recall from Chapter II that if

(i) $\mu > \lambda_i$, $\forall_i$ then the point $\underline{x}_0$ is a point of constrained maximum.

(ii) $\mu < \lambda_i$, $\forall_i$ then the point $\underline{x}_0$ is a point of constrained minimum.

The choice of μ also determines the value R, the radius of the hypersphere on whose surface the optimization is done. So, if the λ_i, $i = 1, 2, \ldots, k$ are estimated well, the choices of μ will be expanded and so the choices of surfaces on which to do the constrained optimization.

From the above, it seems clear that the D_s-criterion is a reasonable design criterion for the construction of response surface designs. The study of this criterion will produce designs which will be useful in RSM.

3.2 A Statistical Experiment

A statistical experiment was done to illustrate the capability of the D_s-criterion to determine RSM designs which will perform well according to certain desirable measures. The performance of the designs will be assessed by examining the standard deviation of the mean of the eigenvalue estimates and by considering the mean width of confidence intervals for the eigenvalues. The method used in the construction of the confidence intervals is of interest in itself, and will be discussed. First, however, a description of the experiment will be given.

The experiment used two underlying models. Each was a second degree polynomial in two variables. One model had a single eigenvalue that was small in magnitude. Hence the resulting surface was attenuated in the direction of the corresponding eigenvector. This surface will henceforth be called badly-determined. The other model was a very steep, bowl-shaped, surface with large, in magnitude, eigenvalues. This surface will henceforth be called well-determined. The two surfaces are displayed in Figure 3.1 and Figure 3.2.

For each surface, observations were generated by evaluating the polynomial at selected points. In this manner, observations were generated for each of the two surfaces for six different RSM designs. Each design was a two-factor central composite design. Three different values of α and two different numbers of center points, n_0, were used to generate the six designs. The values of α used were $\alpha = 1.0$, 1.414, and 2.5, while $n_0 = 1, 4$.

These three choices of α represent three different philosophies for choosing the axial distance. When $\alpha = 1.0$, a 3^2 factorial design results when at least one center point is included. Choosing $\alpha = 1.414$ results in a central composite design with the property of rotatability. Finally, the choice of $\alpha = 2.5$ is meant to represent the philosophy of choosing the axial points at a distance as far away from the origin as practicable.

The choices of n_0 were made for more practical reasons. Without a center point, the rotatable design has a singular moment matrix (see Myers (1976)). The choice of four center points was made to

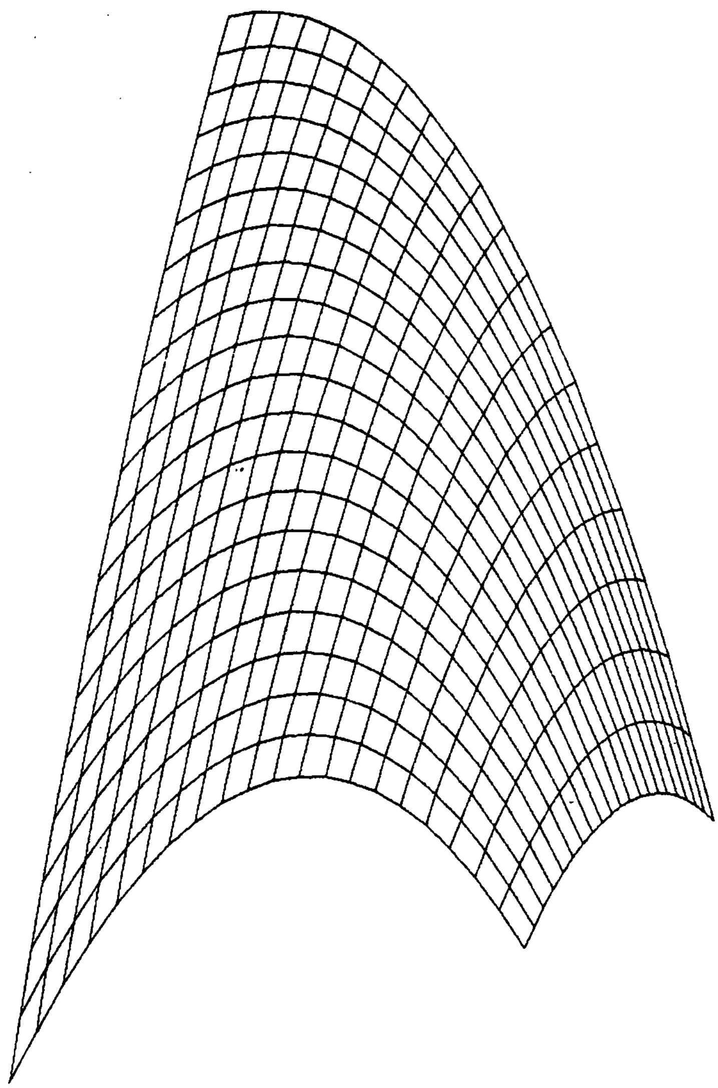

Figure 3.1

Badly Determined, Beta = (10,1,1,-3,-1,3)

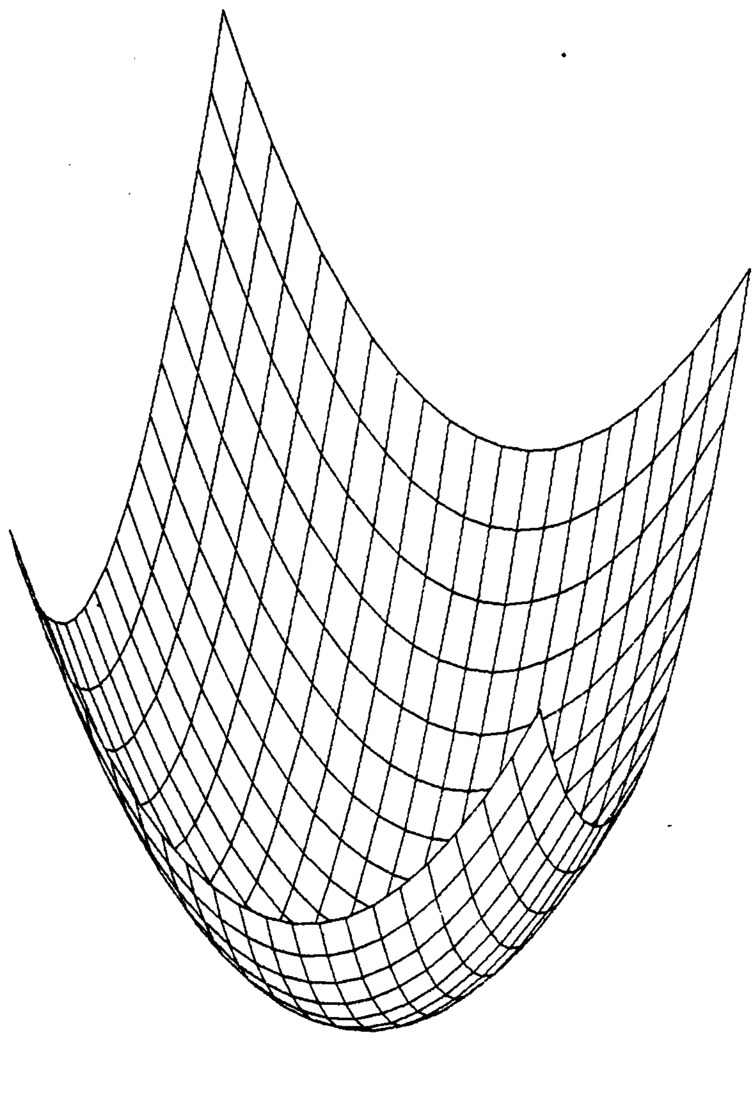

Figure 3.2

Well Determined, Beta = (10,1,1,15,15,1) contrast low number of center points with high number of center points, $n_0 = 4$ representing the high number.

Twelve data sets result from the method described. For each set, a pseudo-random standard normal variate was added to each observation in a set. The variates were generated by the function RANNOR in the Statistical Analysis System (SAS).

3.3 Construction of Confidence Intervals for the λ_i

The evaluation of the designs chosen for the experiment was done partly by constructing confidence intervals for λ_2, the largest eigenvalue of β^q. Work on methods of constructing approximate $(1-\alpha) \times 100\%$ confidence intervals for $Y(\underline{x}_0)$ and λ_i, $i = 1, 2, \ldots, k$ has been done by Carter, Myers and Campbell (1984). A method for constructing intervals for $Y(\underline{x}_0)$ was presented by Khuri and Conlin (1981) but the method is conditional and seems to have other philosophical problems.

The method of Carter, Myers and Campbell was used in a program written by this author and will be explained here. The program is given in Appendix I. The method makes use of a general notion for constructing approximate confidence intervals for a function of a set of parameters (see Rao (1973)).

3.4 Method of Construction of Confidence Intervals on λ_2

In general, assume $\underline{\theta}$ is a $(k \times 1)$ vector of unknown parameters. Further assume $g(\underline{\theta})$ is a function of the parameters for which a confidence interval is required. The form of $g(\underline{\theta})$ is known, and

$g\colon R^k \to R^1$. Let $S(\underline{x})$ be a $(1-\alpha)\times 100\%$ confidence set for θ based on the random vector, $\underline{x}$. Define $G(\underline{x}) = \{t\colon t=g(\underline{s}),\ \underline{s}\in S(\underline{x})\}$. Then $P(g(\underline{\theta})\in G(\underline{x})) \geq P(\underline{\theta}\in S(\underline{x}))$, with equality if g is one-to-one. The set $G(\underline{x})$ is a confidence set for $g(\underline{\theta})$ with confidence coefficient at least $(1-\alpha)$. Practically, the minimum and maximum value in $G(\underline{x})$ define a confidence interval with confidence coefficient at least $(1-\alpha)$.

The theory requires that the function $g(\cdot)$ be evaluated at each point $\underline{s}\in S(\underline{x})$. Realistically, this is not possible since $S(\underline{x})$ contains, in general, an uncountably infinite number of points. Instead, the values of $g(\cdot)$ could be generated at a selected set of points in $S(\underline{x})$ and the approximate confidence interval generated from these points. A computer program was written using these ideas and PROC MATRIX in SAS to construct $(1-\alpha)\times 100\%$ confidence interval for λ_1, λ_2 and $Y(\underline{x}_0)$. A sketch of the idea of the program will be included here and the actual computer program is in Appendix I, as mentioned above.

Step one is to generate a $(1-\alpha)\times 100\%$ confidence region for $\underline{\beta}$. Since the usual linear model

$$Y = X\underline{\beta} + \underline{\varepsilon}\ , \tag{3.4.1}$$

with $\underline{\varepsilon}$ having a multivariate normal distribution with mean $\underline{0}$ and variance $\sigma^2 I_k$ is assumed, a $(1-\alpha)\times 100\%$ confidence ellipsoid for $\underline{\beta}$ is given by

$$\{\underline{\beta}\colon\ (\underline{\beta}-\underline{\hat{\beta}})'(X'X)(\underline{\beta}-\underline{\hat{\beta}}) \leq s^2\cdot p\cdot F(p,\phi,\alpha)\}\ , \tag{3.4.2}$$

where $\underline{\hat{\beta}} = (X'X)^{-1}X'\underline{y}$, s^2 is the usual estimate of σ^2 with ϕ degrees of freedom and $F(p,\phi,\alpha)$ is the point such that α probability is to the right in the $F(p,\phi,\alpha)$ distribution (see Graybill (1976)). From this p-variate ellipsoid, a set of concentric ellipsoids are generated with the outermost being the confidence region itself. The function of interest is then evaluated at a set of points on the surface of the ellipsoids and the resulting values collected. These values are then sorted to find the maximum and minimum values. These two values determine the approximate $(1-\alpha) \times 100\%$ confidence interval.

3.5 Results of the Experiment

First, the criterion was calculated for each of the designs used in the experiment. Table 3.1 provides this information. As can easily be seen, the $\det(M^{22})^{-1}$ is increasing as α increases when n_0 is fixed. This suggests that the designs with $\alpha = 2.5$ should be best in terms of the estimation of the quadratic and cross-product coefficients, for a fixed n_0.

Comparisons will not be made between designs with a different number of center points. The estimate of the variance σ^2 will have different degrees of freedom as n_0 changes, resulting in smaller confidence regions for $Y(\underline{x}_0)$, λ_1, and λ_2 independent of the criterion of interest.

Only the largest eigenvalue will be considered since the eigenvalues will have the same variances for $k = 2$. Hence, the confidence

Table 3.1

$\mathrm{Det}(M^{22})^{-1}$ for Various Alpha and n_0

n_0 \ alpha	1	1.414	2.5
1	2.195×10^{-2}	7.797×10^{-2}	1.098×10^{1}
4	1.852×10^{-2}	9.868×10^{-2}	7.369×10^{0}

interval widths will be the same for both eigenvalues, as will all other design discriminating statistics.

A measure of the performance of the designs is the average width of the confidence intervals for the largest eigenvalue. The D_s-criterion predicts that the mean width should decrease as α increases. The results for the experiment are presented in Table 3.2.

The results of Table 3.2 are very clear. As α increases, the confidence interval width decreases. For each number of center points and each model, the design with $\alpha = 2.5$ has mean width approximately one-half that of the design with $\alpha = 1$. It is also interesting to note that, for a fixed n_0, the repetitions with the well-conditioned surface gave smaller widths than those for the badly-conditioned surface. This emphasizes the point made in Box and Hunter (1954) that the conditioning of the response surface will affect the confidence regions for x_0, the stationary point.

The standard errors of the mean widths are included in Table 3.2, in parentheses. Again, the pattern is clear; as α increases, the standard errors decrease. Also, the model underlying the repetition affects the standard errors. The pattern for the mean widths holds for the standard errors, also.

Another measure of the performance of the designs in the experiment is the number of times a confidence interval on the eigenvalue closest to zero actually covered zero. If a confidence interval on an eigenvalue covers zero, the nature of the surface cannot be determined.

Consider the following: Let $\beta^q = V\Lambda V'$, where $V'V = VV' = I_k$ and Λ is a diagonal matrix with the eigenvalues of β^q on the diagonal. So,

Table 3.2

Mean Width and Standard Deviation of Width
for 250 Repetitions of Experiment;
Confidence Interval on λ_2*

badly conditioned	well conditioned	Design
2.90 1.20 (7.59×10^{-2})	2.58 0.97 (6.13×10^{-2})	$\alpha = 1$ $n_0 = 1$
2.57 1.04 (6.58×10^{-2})	2.32 0.88 (5.57×10^{-2})	$\alpha = 1.414$ $n_0 = 1$
1.37 0.56 (3.54×10^{-2})	1.19 0.46 (2.91×10^{-2})	$\alpha = 2.5$ $n_0 = 1$
1.96 0.54 (3.42×10^{-2})	1.78 0.47 (2.97×10^{-2})	$\alpha = 1$ $n_0 = 4$
1.65 0.46 (2.91×10^{-2})	1.48 0.40 (2.53×10^{-2})	$\alpha = 1.414$ $n_0 = 4$
1.01 0.29 (1.83×10^{-2})	0.88 0.24 (1.52×10^{-2})	$\alpha = 2.5$ $n_0 = 4$

*Top number is the sample mean width of the 250 repetitions, and the bottom number is sample standard deviation. The number in parentheses is the standard error of the mean.

$$\underline{x}_0 = -\frac{1}{2}V\Lambda^{-1}V'\underline{\beta}^L \quad , \tag{3.5.1}$$

and

$$Y(\underline{x}_0) = \beta_0 - \frac{1}{4}\,\underline{\beta}^{L1}V\Lambda^{-1}V'\underline{\beta}^L \quad . \tag{3.5.2}$$

Let $\underline{\delta} = \dfrac{V'\underline{\beta}^L}{2}$. Then

$$\underline{x}_0 = -\frac{1}{2}V\Lambda^{-1}\underline{\delta} \tag{3.5.3}$$

and

$$Y(\underline{x}_0) = \beta_0 - \underline{\delta}'\Lambda^{-1}\underline{\delta} \tag{3.5.4}$$

or

$$Y(\underline{x}_0) = \beta_0 - \sum_{i=1}^{k} \delta_i^2/\lambda \ . \tag{3.5.5}$$

From the formulations (3.5.3) and (3.5.5) it is clear that a confidence interval covering zero will imply that $\underline{x}_0$ could have at least one component that has infinite magnitude. Also, $Y(\underline{x}_0)$ will possibly be infinite in magnitude.

Table 3.3 is a tabulation of the results on the number of times a confidence interval covered zero in the experiment. The results are reported only for the badly conditioned surface, since this is the only time in the experiment that intervals covered zero.

Table 3.3

Percentage of Intervals Covering
Zero for Badly Conditioned Surface

$\alpha = 1$ $n_0 = 1$	47.6
$\alpha = 1.414$ $n_0 = 1$	38.2
$\alpha = 2.5$ $n_0 = 1$	1.2
$\alpha = 1$ $n_0 = 4$	14.4
$\alpha = 1.414$ $n_0 = 4$	5.6
$\alpha = 2.5$ $n_0 = 4$	0

The results in Table 3.3 are again very clear. As alpha increases for fixed n_0, the percentage of times that the confidence intervals cover zero decreases. This conclusion agrees with those reached after examining Table 3.2.

Finally, consider the observed standard deviations of the largest eigenvalue. That is, for each of the twelve different experiments, the sample standard deviation was calculated based on 249 degrees of freedom. Table 3.4 contains a summary of the results.

Again the general pattern of best designs being those with large α holds. There is, however, one anomaly. This occurs in the entry for the well conditioned surface, $\alpha = 1.414$ and $n_0 = 1$. This design is very nearly singular, and this anomaly can probably be explained by that.

The overall conclusion from the experiment must be that the D_s-criterion is appropriate for predicting the ability of response surface designs to estimate λ_i, $i = 1, \ldots, k$ well. This ability to estimate the eigenvalues well will help in the estimation of $Y(\underline{x}_0)$ and $\underline{x}_0$, as evidenced by (3.5.3) and (3.5.5), respectively. The D_s-criterion will be studied extensively throughout the remainder of this chapter, for various classes of response surface designs, not just those used in this experiment.

Table 3.4

Observed Standard Deviations of ℓ_2
for 250 Repetitions of Experiment

badly conditioned	well conditioned	Design
0.69	0.59	$\alpha = 1$ $n_0 = 1$
0.62	0.61	$\alpha = 1.414$ $n_0 = 1$
0.21	0.28	$\alpha = 2.5$ $n_0 = 1$
0.55	0.46	$\alpha = 1$ $n_0 = 4$
0.39	0.38	$\alpha = 1.414$ $n_0 = 4$
0.20	0.27	$\alpha = 2.5$ $n_0 = 4$

3.6 D_s- and D-Criteria in Central Composite Designs

The central composite design was first suggested by Box and Wilson (1951), and was discussed in Chapter II of this thesis. This class of response surface designs is widely used in practice and has been widely studied in the literature. An example of a central composite design was given in Section 2.7. The experimenter must choose values for two design parameters, α, the axial distance, and n_0, the number of center points. The value of α is typically chosen so that the resulting design has some desirable property (e.g. rotatability), or so that the design achieves some design criterion. This portion of this thesis will discuss choices of α and n_0 that result in central composite designs that are best according to one of two design criteria, D_s- and D-optimality.

In general, assume that the factorial points in the design are replicated s times, the axial points are replicated t times and there are n_0 center points. Assume $s \geq 1$, $t \geq 1$, and $n_0 \geq 0$. Usually, s and t will have value 1. Using this, the moment matrix of a k-factor central composite design may be written as

$$M = \begin{bmatrix} 1 & \underline{0}' & a\underline{1}_k' & \underline{0}' \\ \underline{0} & aI_k & \phi & \phi \\ a\underline{1}_k & \phi & bI_k + c\underline{1}_k'\underline{1}_k & \phi \\ \underline{0} & \phi & \phi & cI_\ell \end{bmatrix}, \qquad (3.6.1)$$

where $a = \frac{Fs + 2t\alpha^2}{N}$, $b = \frac{2t\alpha^2}{N}$, $c = \frac{Fs}{N}$, F is the number of distinct points in the factorial portion, $\ell = \binom{k}{2}$, and 1_k is a $(k \times 1)$ vector of ones. Using (3.6.1), det(M) may be written as

$$\mathrm{Det}(M) = a^k c^\ell b^{k-1} D , \tag{3.6.2}$$

where $D = N(ksF + 2t\alpha^4) - k(Fs + 2t\alpha^2)^2$. This result is obtained by using a well-known result from matrix theory (see Graybill (1976)). Using the form (2.1.2) and the same matrix theory result,

$$\mathrm{Det}(M^{22})^{-1} = c^\ell \cdot b^{k-1} \cdot D . \tag{3.6.3}$$

The results of the statistical experiment described in Section 3.5 suggest that choosing α as large as practicable will yield a central composite design which is best according to the D_s-criterion for a fixed number of points. This conclusion is supported by plots of $\log(\det(M^{22}))$ versus α when each point other than center points is unreplicated. The plots, Figure 3.3 through Figure 3.9, suggest that $\log(\det(M^{22}))$ decreases as α increases, hence, $\log(\det(M^{22})^{-1})$ is increasing with increasing α. This conjecture is confirmed by the following theorem.

Theorem 3.1:

If the factorial points are replicated s times, the axial t times, and the center points n_0 times in a central composite design, then $\det(M^{22})$ is decreasing in α when

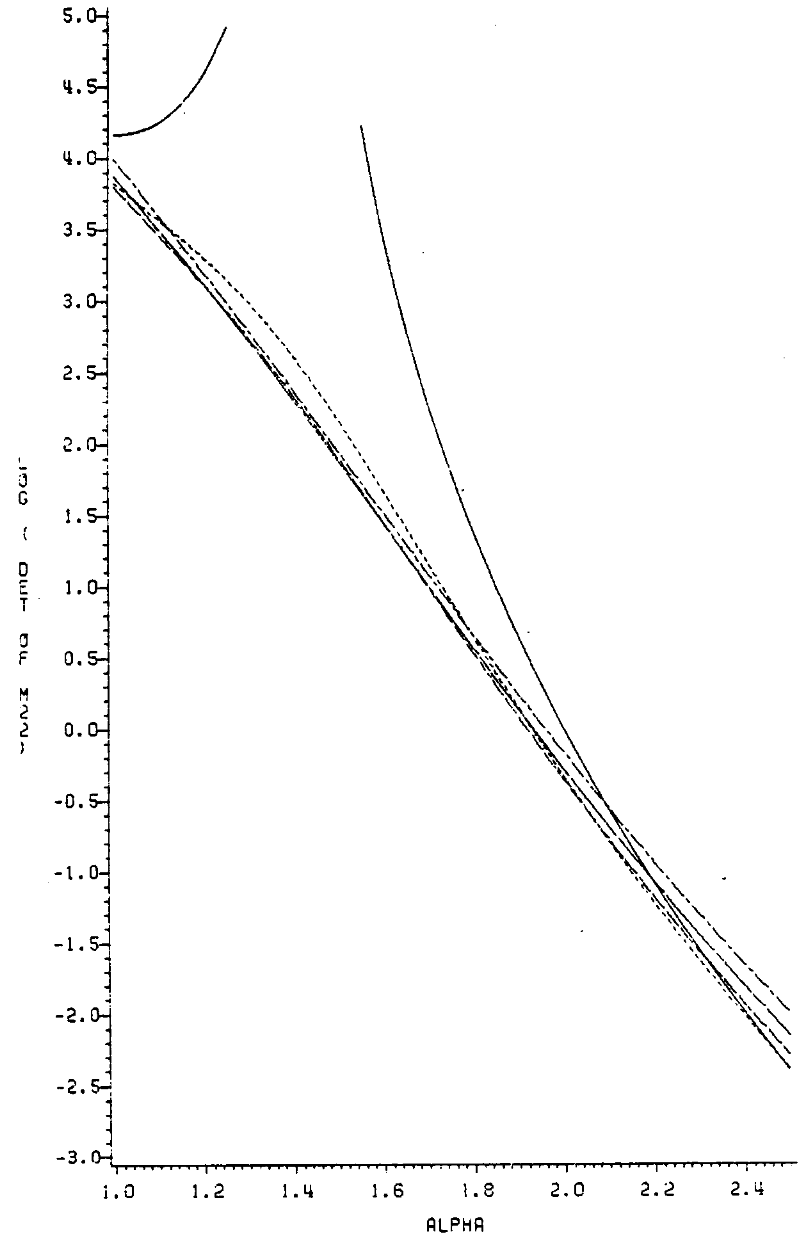

Figure 3.3

$\log(\mathrm{Det}(M^{22}))$, ccd, $k = 2$

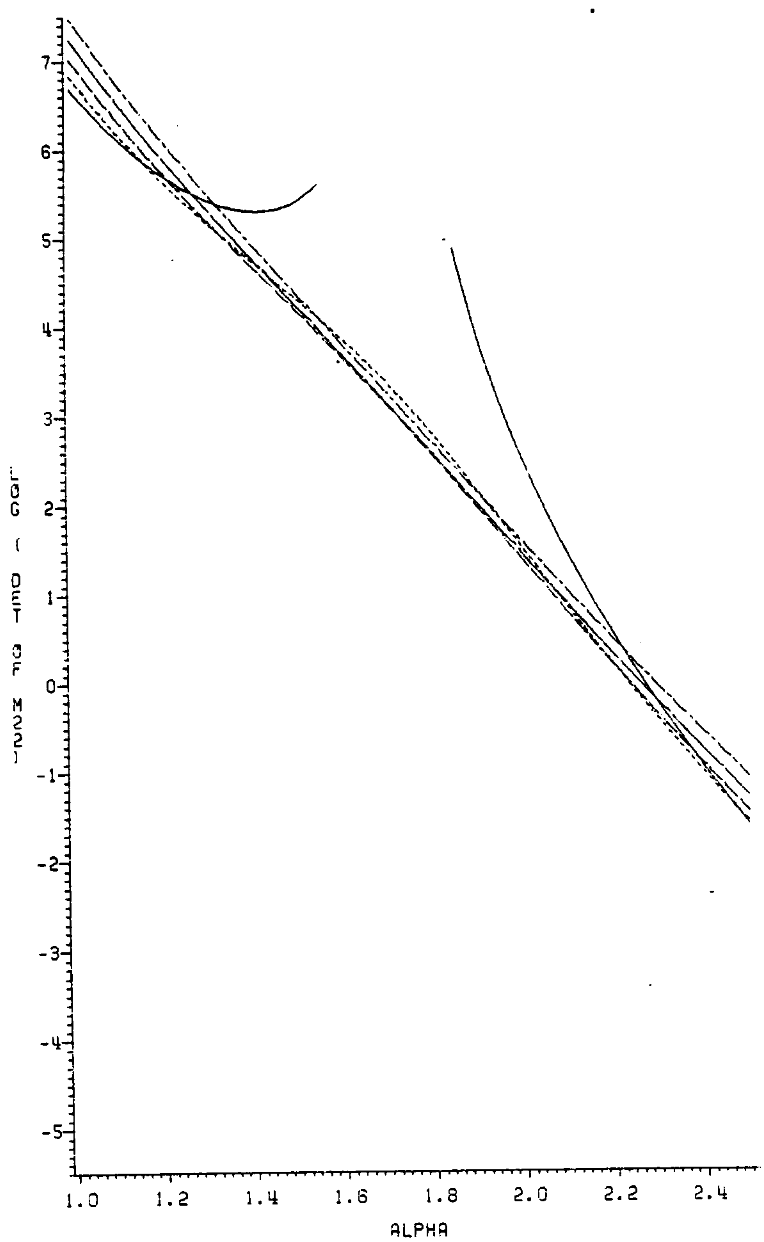

Figure 3.4

$\log(\mathrm{Det}(M^{22}))$, ccd, $k = 3$

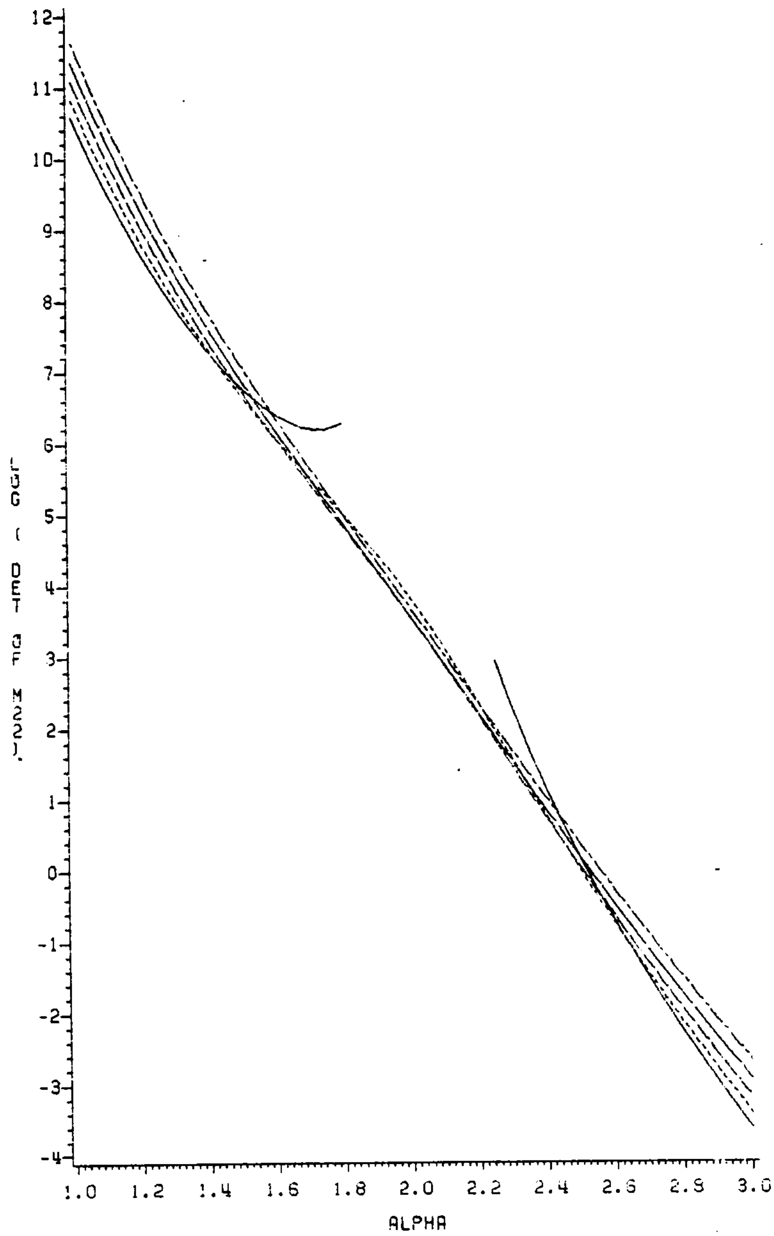

Figure 3.5

$\log(\mathrm{Det}(M^{22}))$, ccd, $k = 4$

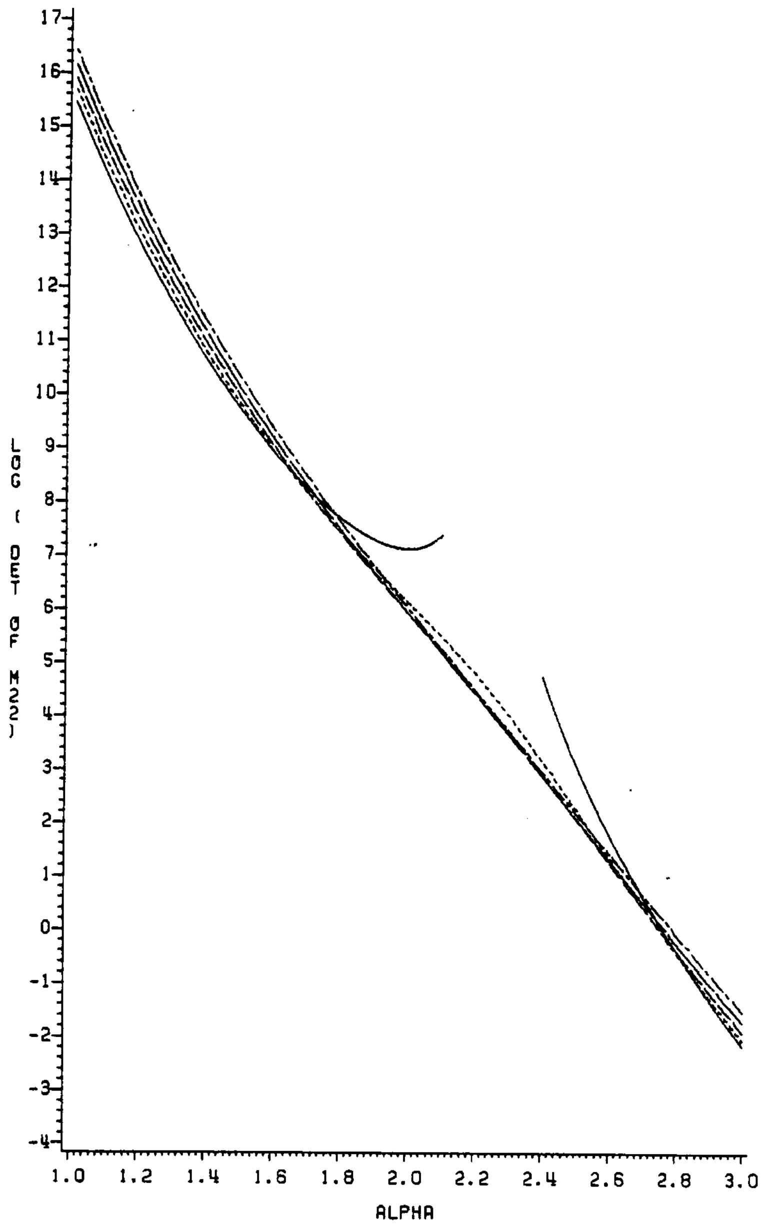

Figure 3.6

log(Det(M^{22})), ccd, k = 5

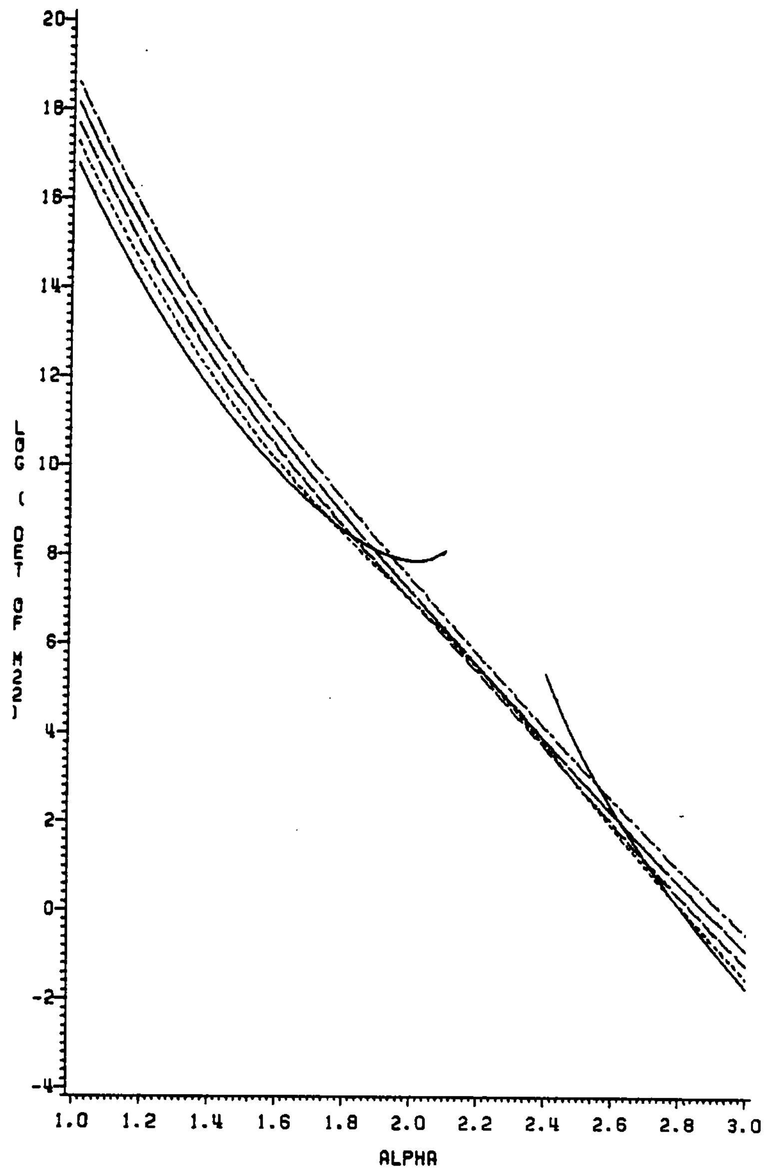

Figure 3.7

$\log(\mathrm{Det}(M^{22}))$, ccd, $k = 5$ ($\frac{1}{2}$ fraction)

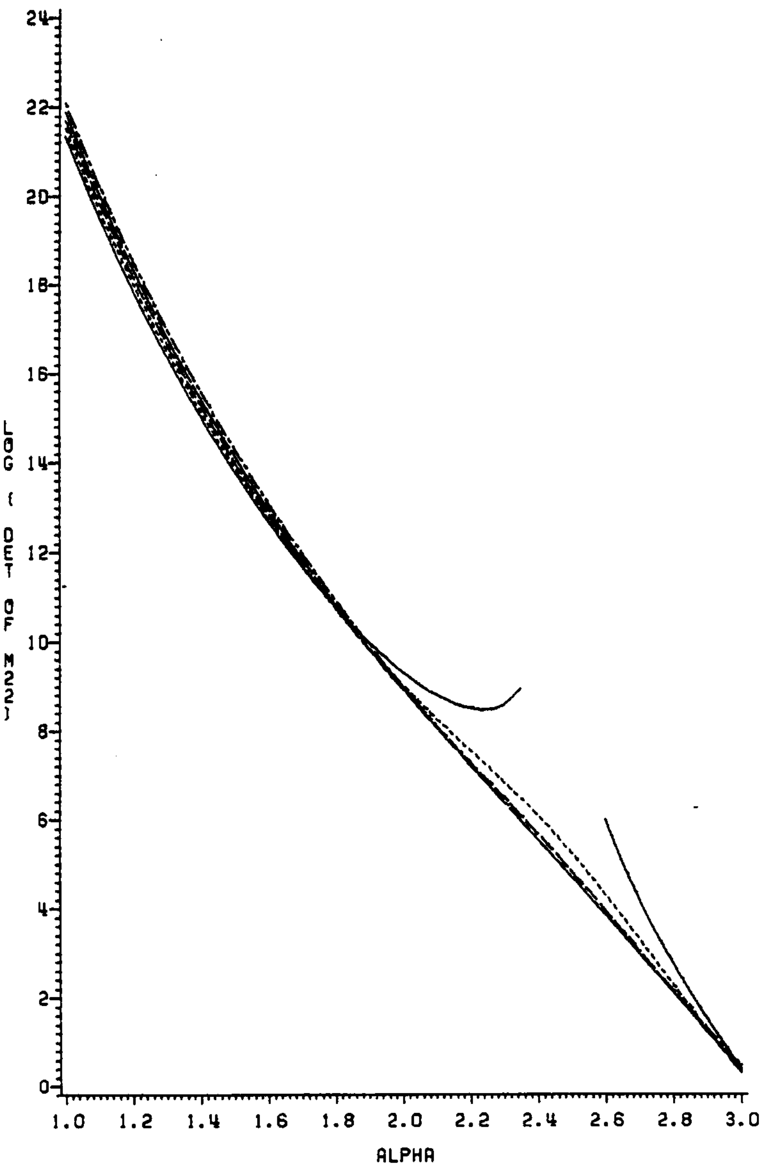

Figure 3.8

$\log(\mathrm{Det}(M^{22}))$, ccd, $k = 6$

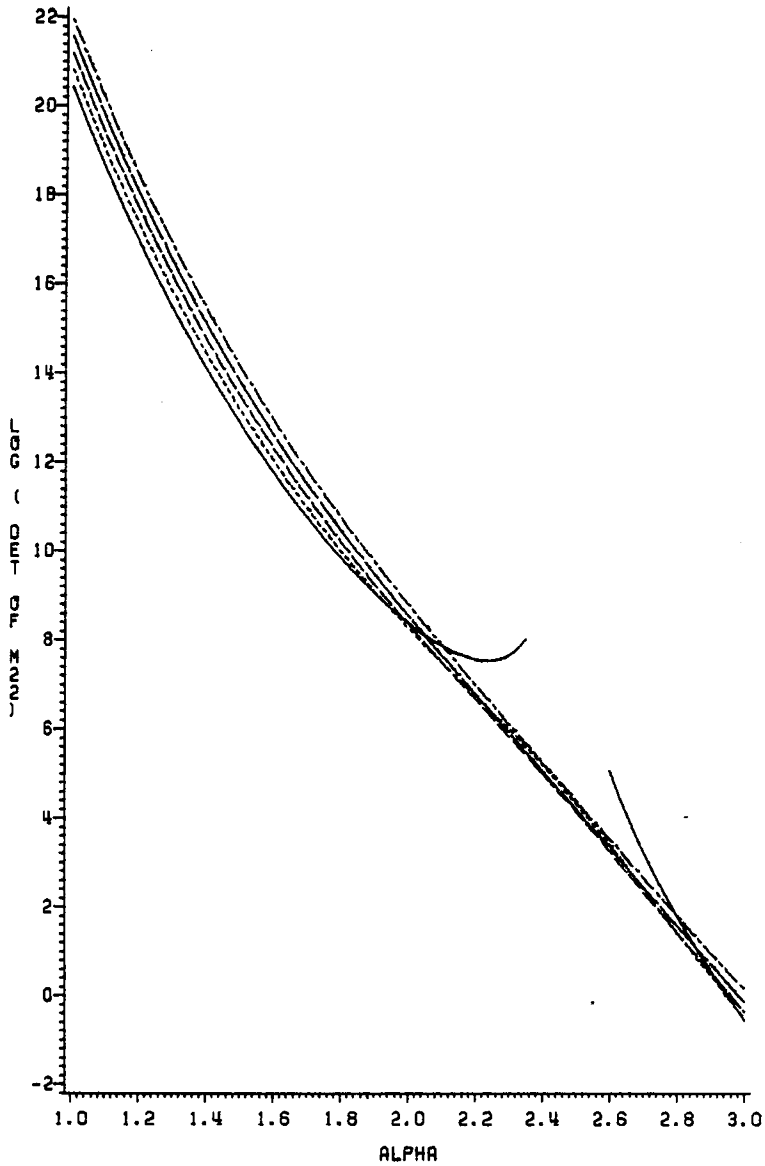

Figure 3.9

log(Det(M^{22})), ccd, k = 6 ($\frac{1}{2}$ fraction)

$$2(k-1)n_0N - tFs > 0 .$$

In particular, if $s = t = 1$, and $n_0 \geq 1$, then $\det(M^{22})$ is decreasing in α.

<u>Proof</u>:

Let $\phi(\alpha) = \log(\det(M^{22}))$. Then

$$\phi(\alpha) = C - 4(k-1)\log(\alpha) - \log(D) , \tag{3.6.4}$$

where C is a constant with respect to α.

$$\frac{\partial\phi(\alpha)}{\partial\alpha} = \frac{-4(k-1)}{\alpha} - \frac{\frac{\partial D}{\partial\alpha}}{D} \tag{3.6.5}$$

The method of proof will be to show (3.6.5) is negative when the conditions of the hypothesis hold. After simplication, (3.6.5) becomes

$$\frac{\partial\phi(\alpha)}{\partial\alpha} = \frac{8tk(2kt-N)\alpha^4 + 8kFst(2k-1)\alpha^2 - 4(k-1)kFs(N-Fs)}{\alpha D} . \tag{3.6.6}$$

The denominator of (3.6.6) is positive, so we may concentrate on showing that the numerator is negative.

Let $y = \alpha^2$. The numerator of (3.6.6) is

$$f(y) = 8tk(2kt-N)y^2 + 8kFst(2k-1)y - 4(k-1)kFs(N-Fs) . \tag{3.6.7}$$

Equation (3.6.7) is of the form $f(y) = Ay^2 + By + C$ which is a downturned parabola with a stationary point at $y_0 = -\frac{B}{2A}$. Now,

$$f(-\frac{B}{2A}) = \frac{4AC - B^2}{4A} . \qquad (3.6.8)$$

Replacing A, B, and C by their equivalents we obtain the value of $f(-\frac{B}{2A})$. Let $T = N - Fs$, and $W = N - 2kt$. Then,

$$f(-\frac{B}{2A}) = \frac{128k\ (k-1)tFsTW - 64k\ t\ F\ s\ (2k-1)}{32tk(2kt-N)} . \qquad (3.6.9)$$

The denominator of (3.6.9) is always negative. We may now concentrate on showing the numerator of (3.6.9) is positive. This numerator is given by

$$64k^2Fst\{2(k-1)TW - tFs(2k-1)^2\} . \qquad (3.6.10)$$

The quantity in the brackets of (3.6.10) is

$$\{2(k-1)(2kt+n_0)(sF+n_0) - tFs(2k-1)^2\} , \qquad (3.6.11)$$

which may be written as

$$\{tFs[4(k-1)k - (2k-1)^2] + 2(k-1)n_0N\} . \qquad (3.6.12)$$

Simplifying, (3.6.12) becomes

$$\{2(k-1)n_0N - tFs\} . \qquad (3.6.13)$$

Hence, if (3.6.13) is positive the numerator of (3.6.9) is positive and the theorem is proved.

The conjecture is thus proved correct. For most choices of t and s the condition in the hypothesis of the theorem will hold. When this is the case, the experimenter should choose α as large as possible.

This result agrees with intuition. That is, as α increases, the quadratic coefficients will be better estimated, and to do the estimation best α should be as large as possible.

The plots in Figure 3.3 through Figure 3.9 suggest some other general conclusions.

(i) When α is chosen near $\sqrt{k}$, the number of center points required by the D_s-criterion is larger than for other values of α. More will be written on this point in the next section.

(ii) If α is chosen different from $\sqrt{k}$, the number of center points required becomes smaller. Practically, this suggests that an experimenter does not need a large number of center points when α is chosen to be as large as practicable as this generally would result in an α larger than $\sqrt{k}$.

3.7 D_s- and D-Best Replicated Central Composite Designs

In the foregoing, a discussion of the number of center points needed to yield a D_s-best central composite design was given. In this discussion, generated from the plots of $\log(\det(M^{22}))$ versus α, the factorial and axial points were assumed to be unreplicated. As shown by many real-world situations, one has the capability of replicating all design points. In this case, an approach due to Box and Draper (1969), adapted from a technique of Kiefer (1961) for constructing D-best composite designs, will be extended. This approach will also be used to construct D_s-best central composite designs. The approach uses the mathematical abstraction of considering a design as a discrete probability measure. This idea was mentioned in Section 2.14, and will be discussed more fully here.

We allow the set of factorial points to be assigned weight w_1, the axial points are assigned weight w_2, and the center point is assigned weight w_0. Since the design is a probability measure, $0 \leq w_i \leq 1$, $i = 0, 1, 2$ and $w_0 + w_1 + w_2 = 1$. Each point in the factorial set of points has weight w_1/F. Similarly, each axial point has weight $w_2/2k$, and each center point has weight w_0/n_0. This formulation is just a special case of a more general theory due in large part to Kiefer (1961) and Kiefer and Wolfowitz (1959, 1960).

Box and Draper (1971, 1973) gave optimal weights for the central composite designs with the artifical choice of $\alpha = 1$ when the D-optimality criterion is used. They maximized det(M) subject to the necessary restrictions. In the following, α will be unrestricted. Det(M) may be written as a function of the weights and α. That is,

$$\det(M) = (w_1 + \frac{w_2}{k}\alpha^2)^k \cdot w_1^{\ell} \cdot (\frac{w_2}{k}\alpha^4)^{k-1}(\frac{w_2}{k}\alpha^4 + w_1 k - k(w_1 + \frac{w_2}{k}\alpha^2)^2). \tag{3.7.1}$$

Also,

$$\det(M^{22})^{-1} = w_1^{\ell} \cdot (\frac{w_2}{k}\alpha^4)^{k-1}(\frac{w_2}{k}\alpha^4 + kw_1 - k(w_1 + \frac{w_2}{k}\alpha^2)^2). \tag{3.7.2}$$

A central composite design here will consist of weights (w_0, w_1, w_2). A design will be D-best if the weights are the solution to the optimization problem,

$$\max \det(M) \text{ subject to } \sum_{i=0}^{2} w_i = 1, \quad 0 \le w_i \le 1 \quad i = 0, 1, 2 . \qquad (3.7.3)$$

Likewise, a design will be D_s-best if the weights are the solution to the optimization problem,

$$\max \det(M^{22})^{-1} \text{ subject to } \sum_{i=0}^{2} w_i = 1, \quad 0 \le w_i \le 1 \quad i = 0, 1, 2 . \qquad (3.7.4)$$

In (3.7.3) and (3.7.4) the parameter α must be chosen before the optimization problem is solved. This α corresponds to the parameter α that the experimenter chooses when constructing a central composite design. Choosing α is equivalent to choosing the ratio of the axial distance to the factorial point's distance from the origin. This choice is restricted only by the experimenter's choice of a model. One possible choice of α is $\alpha = \sqrt{k}$. With this choice, the axial distance and factorial distance are identical. This results in a rotatable or near rotatable design. The following theorems give weights for designs with $\alpha = \sqrt{k}$.

Theorem 3.2:

If $\alpha = \sqrt{k}$ in a k-factor central composite design, then the D-optimal weights are

$$w_1 = \frac{(\ell+2k)}{(\ell+k-1)(\ell+2k+1)}\ ,\ w_2 = \frac{(k-1)(\ell+2k)}{(\ell+k-1)(\ell+2k+1)}\ ,\ w_0 = 1 - w_1 - w_2\ . \tag{3.7.5}$$

Proof:

$\text{Det}(M) = k^k(w_1+w_2)^{k+1} w_1^{\ell}\, w_2^{k-1}(1-w_1-w_2)$ when $\alpha = \sqrt{k}$. Let

$$\phi(w_1,w_2) = \log(\det(M))\ . \tag{3.7.6}$$

Then the solution to $(\frac{\partial\phi}{\partial w_1}, \frac{\partial\phi}{\partial w_2}) = (0,0)$ will give the optimal weights.

$$\begin{pmatrix} \frac{\partial\phi}{\partial w_1} \\ \\ \frac{\partial\phi}{\partial w_2} \end{pmatrix} = \begin{pmatrix} \frac{k+1}{w_1+w_2} + \frac{\ell}{w_1} - \frac{1}{1-w_1-w_2} \\ \\ \frac{k+1}{w_1+w_2} + \frac{k-1}{w_2} - \frac{1}{1-w_1-w_2} \end{pmatrix} \tag{3.7.7}$$

Setting the vector in (3.7.7) equal to $\binom{0}{0}$ we obtain

$$\begin{pmatrix} \frac{\ell}{w_1} \\ \\ \frac{k-1}{w_2} \end{pmatrix} = \begin{pmatrix} \frac{1}{1-w_1-w_2} - \frac{k+1}{w_1+w_2} \\ \\ \frac{1}{1-w_1-w_2} - \frac{k+1}{w_1+w_2} \end{pmatrix}\ ,$$

so $\frac{\ell}{w_1} = \frac{k-1}{w_2}$. Hence, $w_1 = \frac{\ell}{k-1} w_2$. Substituting back into (3.7.7), we obtain

$$(\ell+2k)((k-1)-w_2(\ell+k-1)) = w_2(\ell+k-1) \ .$$

Hence, $w_2 = \dfrac{(\ell+2k)(k-1)}{(\ell+k-1)(\ell+2k+1)}$.

Theorem 3.3:

If $\alpha = \sqrt{k}$ in a k-factor central composite design, then the D_s-optimal weights are

$$w_1 = \frac{(\ell+k)\ell}{(\ell+k+1)(\ell+k-1)} \ , \ w_2 = \frac{(k-1)(\ell+k)}{(\ell+k+1)(\ell+k-1)} \ , \ w_0 = 1 - w_1 - w_2 \ . \tag{3.7.8}$$

Proof:

$\mathrm{Det}(M^{22})^{-1} = k^k w_1^{\ell} w_2^{k-1}(w_1+w_2)(1-w_2-w_1)$ when $\alpha = \sqrt{k}$. Now proceed as in Theorem 3.2.

Comparing the results of the two theorems, conclusions about the relative importance of the sets of points can be made.

(i) For both criteria, the ratio of the weight assigned to the factorial points to the weight assigned to the axial points is k/2. This suggests that the relative importance of the two sets of points to each of the criteria is the same when $\alpha = \sqrt{k}$. The fact that the criteria do not discriminate between the two sets of points for this case is intuitive. When $\alpha = \sqrt{k}$, the factorial and axial points lie on a single sphere of radius $\sqrt{k}$. They appear as a single set of points to each criterion. The results of the theorems reflect this.

(ii) For the D-criterion, the ratio w_1/w_0 is $\ell(\ell+2k)/(\ell+k-1)$.

(iii) For the D_s-criterion, the ratio w_1/w_0 is $\ell(\ell+k)/(\ell+k-1)$.

(iv) From (ii) and (iii), one can see that center points are more important to the D_s-criterion than to the D-criterion. Also, center points are always required by both criteria when $\alpha = \sqrt{k}$. This is reasonable, as $\alpha = \sqrt{k}$ results in a design with a singular or near singular moment matrix if no center points are included.

Choosing $\alpha = \sqrt{k}$ is not the only possible choice of α. As shown in Theorem 3.1, under certain conditions on the number of replications, large values of α are best. Other choices of α should then be investigated. Using the idea of a design as a probability measure, the criteria can be optimized as a function of w_0, w_1, w_2. To do this optimization, an algorithm due to Nelder-Mead (1965) can be used. The optimization problems involve solving (3.7.3) and (3.7.4) with α fixed. Table 3.5 through Table 3.9 provide the optimal weights, for k = 2, 3, 4, 5, 6, for the D-criterion. Table 3.10 through Table 3.14 provide weights for the D_s-criterion.

Consider first the D-criterion, Tables 3.5 - 3.9. The conclusions which may be drawn from these are:

(i) The weight placed on the center point increases to a maximum at $\sqrt{k}$, then decreases. If α is substantially different from $\sqrt{k}$, the weight on the center point is 0.

(ii) The weights given by the Nelder-Mead routine agree with the Box-Draper (1971) solution for $\alpha = 1$. Also, when

Table 3.5

Optimal Weights for D-Criterion

k=2

α	w_1	w_2	w_0
1.00	0.583	0.321	0.096
1.05	0.573	0.314	0.112
1.10	0.561	0.312	0.126
1.15	0.547	0.315	0.138
1.20	0.529	0.323	0.147
1.25	0.509	0.336	0.155
1.30	0.484	0.355	0.161
1.35	0.455	0.380	0.165
1.40	0.425	0.408	0.167
1.45	0.396	0.438	0.166
1.50	0.371	0.465	0.164
1.55	0.351	0.489	0.160
1.60	0.336	0.509	0.155
1.65	0.326	0.525	0.150
1.70	0.319	0.538	0.143
1.75	0.315	0.549	0.136
1.80	0.313	0.558	0.129
1.85	0.313	0.566	0.121
1.90	0.314	0.573	0.113
1.95	0.317	0.578	0.105
2.00	0.321	0.583	0.096
2.05	0.325	0.587	0.087
2.10	0.331	0.591	0.078
2.15	0.337	0.594	0.069
2.20	0.344	0.597	0.059
2.25	0.351	0.600	0.049
2.30	0.359	0.602	0.039
2.35	0.367	0.604	0.028
2.40	0.376	0.606	0.018
2.45	0.385	0.608	0.007
2.50	0.390	0.610	0.000

Table 3.6

Optimal weights for D-Criterion

k=3

α	w_1	w_2	w_0
1.00	0.655	0.345	0.000
1.05	0.651	0.349	0.000
1.10	0.646	0.354	0.000
1.15	0.640	0.360	0.000
1.20	0.636	0.348	0.017
1.25	0.631	0.337	0.032
1.30	0.625	0.329	0.046
1.35	0.618	0.324	0.058
1.40	0.611	0.321	0.069
1.45	0.603	0.320	0.077
1.50	0.593	0.322	0.085
1.55	0.583	0.326	0.090
1.60	0.572	0.333	0.095
1.65	0.560	0.342	0.098
1.70	0.548	0.352	0.100
1.75	0.536	0.365	0.100
1.80	0.523	0.378	0.099
1.85	0.512	0.392	0.096
1.90	0.503	0.405	0.092
1.95	0.495	0.418	0.087
2.00	0.488	0.430	0.081
2.05	0.484	0.442	0.075
2.10	0.481	0.452	0.067
2.15	0.480	0.461	0.059
2.20	0.480	0.469	0.050
2.25	0.482	0.477	0.041
2.30	0.485	0.484	0.031
2.35	0.489	0.490	0.021
2.40	0.494	0.495	0.011
2.45	0.500	0.500	0.000
2.50	0.496	0.504	0.000

Table 3.7

Optimal weights for D-Criterion

k=4

α	w_1	w_2	w_0
1.00	0.708	0.292	0.000
1.05	0.706	0.294	0.000
1.10	0.703	0.297	0.000
1.15	0.700	0.300	0.000
1.20	0.697	0.303	0.000
1.25	0.694	0.306	0.000
1.30	0.691	0.309	0.000
1.35	0.688	0.312	0.000
1.40	0.684	0.316	0.000
1.45	0.681	0.316	0.004
1.50	0.677	0.308	0.015
1.55	0.673	0.301	0.025
1.60	0.669	0.297	0.034
1.65	0.665	0.294	0.042
1.70	0.660	0.292	0.048
1.75	0.654	0.292	0.054
1.80	0.648	0.293	0.059
1.85	0.642	0.296	0.062
1.90	0.636	0.300	0.065
1.95	0.629	0.305	0.066
2.00	0.622	0.311	0.067
2.05	0.615	0.319	0.066
2.10	0.609	0.327	0.065
2.15	0.602	0.336	0.062
2.20	0.597	0.345	0.058
2.25	0.592	0.354	0.054
2.30	0.588	0.363	0.049
2.35	0.585	0.372	0.042
2.40	0.584	0.381	0.035
2.45	0.583	0.389	0.028
2.50	0.584	0.397	0.019
2.55	0.586	0.404	0.011
2.60	0.588	0.409	0.003
2.65	0.630	0.370	0.000
2.70	0.630	0.370	0.000
2.75	0.630	0.370	0.000
2.80	0.630	0.370	0.000
2.85	0.630	0.370	0.000
2.90	0.630	0.370	0.000
2.95	0.630	0.370	0.000
3.00	0.630	0.370	0.000

Table 3.8

Optimal weights for D-Criterion

k=5

α	w_1	w_2	w_0
1.00	0.747	0.253	0.000
1.05	0.745	0.255	0.000
1.10	0.744	0.256	0.000
1.15	0.742	0.258	0.000
1.20	0.740	0.260	0.000
1.25	0.738	0.262	0.000
1.30	0.736	0.264	0.000
1.35	0.734	0.266	0.000
1.40	0.732	0.268	0.000
1.45	0.730	0.270	0.000
1.50	0.728	0.272	0.000
1.55	0.725	0.275	0.000
1.60	0.723	0.277	0.000
1.65	0.720	0.280	0.000
1.70	0.718	0.278	0.004
1.75	0.715	0.273	0.012
1.80	0.713	0.269	0.019
1.85	0.710	0.265	0.025
1.90	0.707	0.263	0.031
1.95	0.703	0.262	0.035
2.00	0.700	0.261	0.039
2.05	0.696	0.262	0.042
2.10	0.692	0.263	0.045
2.15	0.688	0.266	0.046
2.20	0.683	0.269	0.047
2.25	0.679	0.273	0.048
2.30	0.675	0.278	0.047
2.35	0.671	0.284	0.046
2.40	0.666	0.290	0.043
2.45	0.663	0.297	0.040
2.50	0.660	0.304	0.037
2.55	0.657	0.311	0.032
2.60	0.655	0.318	0.027
2.65	0.654	0.326	0.021
2.70	0.653	0.333	0.014
2.75	0.653	0.340	0.007
2.80	0.654	0.346	0.000
2.85	0.651	0.349	0.000
2.90	0.630	0.370	0.000
2.95	0.630	0.370	0.000
3.00	0.630	0.370	0.000

Table 3.9

Optimal weights for D-Criterion

k=6

α	w_1	w_2	w_0
1.00	0.776	0.224	0.000
1.05	0.758	0.242	0.000
1.10	0.774	0.226	0.000
1.15	0.773	0.227	0.000
1.20	0.771	0.229	0.000
1.25	0.770	0.230	0.000
1.30	0.769	0.231	0.000
1.35	0.768	0.232	0.000
1.40	0.766	0.234	0.000
1.45	0.765	0.235	0.000
1.50	0.763	0.237	0.000
1.55	0.762	0.238	0.000
1.60	0.760	0.240	0.000
1.65	0.759	0.241	0.000
1.70	0.757	0.243	0.000
1.75	0.755	0.245	0.000
1.80	0.754	0.246	0.000
1.85	0.752	0.248	0.000
1.90	0.750	0.250	0.000
1.95	0.748	0.245	0.007
2.00	0.746	0.242	0.012
2.05	0.744	0.239	0.017
2.10	0.742	0.237	0.022
2.15	0.740	0.235	0.025
2.20	0.737	0.234	0.028
2.25	0.735	0.234	0.031
2.30	0.732	0.235	0.033
2.35	0.729	0.236	0.035
2.40	0.726	0.238	0.035
2.45	0.723	0.241	0.036
2.50	0.720	0.244	0.035
2.55	0.717	0.248	0.034
2.60	0.715	0.253	0.033
2.65	0.712	0.258	0.031
2.70	0.709	0.263	0.028
2.75	0.707	0.268	0.024
2.80	0.705	0.274	0.020
2.85	0.704	0.280	0.015
2.90	0.703	0.287	0.010
2.95	0.703	0.293	0.004
3.00	0.702	0.298	0.000

Table 3.10

Optimal Weights for D_s-Criterion

k=2

α	w_1	w_2	w_0
1.00	0.472	0.352	0.176
1.05	0.465	0.342	0.194
1.10	0.456	0.336	0.209
1.15	0.445	0.333	0.221
1.20	0.434	0.335	0.231
1.25	0.421	0.340	0.239
1.30	0.407	0.348	0.245
1.35	0.393	0.359	0.248
1.40	0.379	0.371	0.250
1.45	0.366	0.385	0.249
1.50	0.355	0.398	0.248
1.55	0.346	0.410	0.244
1.60	0.340	0.421	0.239
1.65	0.336	0.431	0.233
1.70	0.334	0.439	0.227
1.75	0.333	0.447	0.220
1.80	0.335	0.453	0.212
1.85	0.337	0.459	0.203
1.90	0.341	0.464	0.194
1.95	0.346	0.469	0.185
2.00	0.352	0.472	0.176
2.05	0.358	0.476	0.166
2.10	0.365	0.479	0.156
2.15	0.373	0.482	0.145
2.20	0.382	0.484	0.134
2.25	0.391	0.486	0.123
2.30	0.400	0.488	0.111
2.35	0.410	0.490	0.100
2.40	0.421	0.492	0.087
2.45	0.432	0.493	0.075
2.50	0.443	0.495	0.063

Table 3.11

Optimal Weights for D_s-Criterion

k=3

α	w_1	w_2	w_0
1.00	0.571	0.429	0.000
1.05	0.571	0.429	0.000
1.10	0.570	0.420	0.009
1.15	0.568	0.400	0.033
1.20	0.564	0.382	0.053
1.25	0.561	0.368	0.071
1.30	0.557	0.357	0.086
1.35	0.553	0.348	0.099
1.40	0.548	0.341	0.110
1.45	0.543	0.337	0.120
1.50	0.539	0.334	0.127
1.55	0.533	0.333	0.133
1.60	0.528	0.334	0.138
1.65	0.523	0.336	0.141
1.70	0.517	0.340	0.143
1.75	0.513	0.345	0.143
1.80	0.508	0.350	0.142
1.85	0.505	0.356	0.139
1.90	0.502	0.362	0.136
1.95	0.501	0.369	0.131
2.00	0.500	0.375	0.125
2.05	0.500	0.381	0.118
2.10	0.502	0.387	0.111
2.15	0.505	0.393	0.102
2.20	0.509	0.398	0.094
2.25	0.513	0.403	0.084
2.30	0.519	0.407	0.074
2.35	0.526	0.411	0.063
2.40	0.533	0.415	0.052
2.45	0.541	0.419	0.041
2.50	0.549	0.422	0.029

Table 3.12

Optimal Weights for D_s-Criterion

k=4

α	w_1	w_2	w_0
1.00	0.630	0.370	0.000
1.05	0.630	0.370	0.000
1.10	0.630	0.370	0.000
1.15	0.630	0.370	0.000
1.20	0.630	0.370	0.000
1.25	0.630	0.370	0.000
1.30	0.636	0.364	0.000
1.35	0.636	0.364	0.000
1.40	0.635	0.355	0.009
1.45	0.633	0.343	0.024
1.50	0.631	0.332	0.036
1.55	0.629	0.324	0.047
1.60	0.627	0.316	0.057
1.65	0.624	0.311	0.065
1.70	0.622	0.306	0.072
1.75	0.619	0.303	0.078
1.80	0.616	0.301	0.083
1.85	0.614	0.300	0.086
1.90	0.611	0.300	0.089
1.95	0.608	0.301	0.090
2.00	0.606	0.303	0.091
2.05	0.604	0.306	0.090
2.10	0.602	0.309	0.089
2.15	0.601	0.313	0.086
2.20	0.600	0.317	0.083
2.25	0.600	0.321	0.079
2.30	0.601	0.326	0.074
2.35	0.602	0.331	0.068
2.40	0.604	0.335	0.061
2.45	0.607	0.340	0.053
2.50	0.610	0.345	0.045
2.55	0.615	0.349	0.036
2.60	0.620	0.353	0.027
2.65	0.625	0.358	0.017
2.70	0.632	0.361	0.007
2.75	0.630	0.370	0.000
2.80	0.630	0.370	0.000
2.85	0.630	0.370	0.000
2.90	0.630	0.370	0.000
2.95	0.630	0.370	0.000
3.00	0.630	0.370	0.000

Table 3.13

Optimal Weights for D_s-Criterion

k=5

α	w_1	w_2	w_0
1.00	0.687	0.313	0.000
1.05	0.687	0.313	0.000
1.10	0.687	0.313	0.000
1.15	0.687	0.313	0.000
1.20	0.687	0.313	0.000
1.25	0.687	0.313	0.000
1.30	0.687	0.313	0.000
1.35	0.688	0.312	0.000
1.40	0.688	0.312	0.000
1.45	0.688	0.312	0.000
1.50	0.687	0.313	0.000
1.55	0.688	0.312	0.000
1.60	0.687	0.313	0.000
1.65	0.687	0.307	0.006
1.70	0.685	0.298	0.016
1.75	0.684	0.291	0.025
1.80	0.683	0.285	0.032
1.85	0.681	0.280	0.039
1.90	0.680	0.275	0.045
1.95	0.678	0.272	0.050
2.00	0.677	0.269	0.054
2.05	0.675	0.268	0.057
2.10	0.673	0.267	0.060
2.15	0.672	0.267	0.061
2.20	0.671	0.267	0.062
2.25	0.669	0.268	0.062
2.30	0.668	0.270	0.062
2.35	0.667	0.272	0.061
2.40	0.667	0.275	0.058
2.45	0.667	0.278	0.056
2.50	0.667	0.281	0.052
2.55	0.668	0.285	0.048
2.60	0.669	0.289	0.043
2.65	0.670	0.293	0.037
2.70	0.673	0.297	0.030
2.75	0.676	0.301	0.023
2.80	0.679	0.305	0.016
2.85	0.683	0.309	0.008
2.90	0.687	0.313	0.000
2.95	0.688	0.312	0.000
3.00	0.687	0.313	0.000

Table 3.14

Optimal Weights for D_s-Criterion

k=6

α	w_1	w_2	w_0
1.00	0.727	0.273	0.000
1.05	0.727	0.273	0.000
1.10	0.727	0.273	0.000
1.15	0.727	0.273	0.000
1.20	0.727	0.273	0.000
1.25	0.727	0.273	0.000
1.30	0.727	0.273	0.000
1.35	0.727	0.273	0.000
1.40	0.728	0.272	0.000
1.45	0.728	0.272	0.000
1.50	0.728	0.272	0.000
1.55	0.727	0.273	0.000
1.60	0.727	0.273	0.000
1.65	0.727	0.273	0.000
1.70	0.727	0.273	0.000
1.75	0.727	0.273	0.000
1.80	0.727	0.273	0.000
1.85	0.727	0.272	0.000
1.90	0.726	0.265	0.008
1.95	0.725	0.260	0.015
2.00	0.724	0.255	0.021
2.05	0.723	0.250	0.026
2.10	0.723	0.247	0.031
2.15	0.721	0.244	0.035
2.20	0.720	0.241	0.038
2.25	0.719	0.240	0.041
2.30	0.718	0.239	0.043
2.35	0.718	0.238	0.044
2.40	0.717	0.238	0.045
2.45	0.716	0.239	0.045
2.50	0.715	0.240	0.045
2.55	0.715	0.241	0.044
2.60	0.714	0.243	0.043
2.65	0.714	0.245	0.041
2.70	0.714	0.248	0.038
2.75	0.715	0.251	0.035
2.80	0.716	0.254	0.031
2.85	0.717	0.257	0.026
2.90	0.719	0.261	0.021
2.95	0.721	0.264	0.015
3.00	0.723	0.268	0.009

$\alpha = \sqrt{k}$, the weights predicted by Theorem 3.2 are also given by the numerical routine.

(iii) For most values of k, the weight placed on the axial points increases with increasing α.

Next, consider the D_s-criterion, that is Tables 3.10 - 3.14. The conclusions drawn are:

(i) The weight placed on the center point is a maximum at $\alpha = \sqrt{k}$.

(ii) For $\alpha = \sqrt{k}$, the results of Theorem 3.3 and the Nelder-Mead routine are identical.

(iii) For all k, the weight on the axial points, w_2, decreases, then increases, as does w_1. The two weights, however, reach their minima at different values of α.

Finally, a comparison of the tables for fixed k reveals some further conclusions.

(i) Most importantly, the weight placed on the center points by the D_s-criterion is at least as large, and usually much larger, than that placed by the D-criterion. This can be explained by noting that the D_s-criterion has estimation of quadratic coefficients as a primary concern. Center points help in this estimation.

(ii) The ratio w_1/w_2, weight on the factorial portion to weight on the axial portion, depends on α. This ratio is higher for the D-criterion than for the corresponding ratio for the D_s-criterion when α less than $\sqrt{k}$. For $\alpha > \sqrt{k}$, the reverse is true.

3.8 Using the Weights

The weights given in Table 3.5 through 3.14 can be used in practical situations to give composite designs with replicated points. Two examples are now given to illustrate the use of these weights in real world applications.

Example 1:

A researcher has decided that the time required, t, to drive a spike into a block of wood using constant force is a function of the diameter of the spike and the water content of the wood. The experimenter has decided that t can be modeled adequately by a second order polynomial in the two factors. Let w_1 = diameter of the spike, and w_2 = water content of the wood. The region in which the model is thought to function properly is

$$\begin{aligned} 1 \text{ cm} \leq w_1 \leq 5 \text{ cm} \\ 0.1 \text{ g/cm}^3 \leq w_2 \leq 1.0 \text{ g/cm}^3 \quad . \end{aligned} \tag{3.8.1}$$

After questioning, the experimenter revealed that the region in which the model would function correctly is not a rectangle. That is, if w_1, w_2 are both set to their extreme values, the model will not function correctly. This suggests that the restrictions given by

(3.8.1) determine the axial distance and the design should be constructed accordingly.

Define

$$x_1 = \frac{w_1 - 3}{1.414}$$

$$x_2 = \frac{w_2 - 0.55}{.3182} \tag{3.8.2}$$

Equation (3.8.2) gives the design variables for this problem. The design levels are (±1.414, 0, ±1), with corresponding natural levels of (1, 1.59, 3, 4.41, 5) and (0.10, 0.232, 0.55, 0.868, 1.00). Using the results from Theorem 3.2 and Theorem 3.3, a D_s- and D-best central composite design may be constructed for this problem. The designs are

Natural Variable	Design Variable	Number of Replications for D_s-criterion	Number of Replications for D-criterion
(4.41,0.868)	(1,1)	3	5
(4.41,0.232)	(1,-1)	3	5
(1.59,0.868)	(-1,1)	3	5
(1.59,0.232)	(-1,-1)	3	5
(1,0.55)	(-1.414,0)	3	5
(5,0.55)	(1.414,0)	3	5
(3,0.10)	(0,-1.414)	3	5
(3,1.00)	(0,1.414)	3	5
(3,0.55)	(0,0)	8	8
	Total points	32	48

Example 2:

The patient load of a community hospital is being simulated by use of a simulation model involving two variables. The variables are

$$w_1 = \frac{\text{population in community}}{\text{number of MDs}}$$

$$w_2 = \text{average length of stay} \quad . \tag{3.8.3}$$

The goal of the study is to minimize the number of unused beds. The cost of generating a single observation at a particular setting of w_1 and w_2 is small, hence, the points may be replicated a large number of times.

From previous experience the researcher has decided that the quadratic model will function well when

$$1{,}000 \le w_1 \le 5{,}000$$

$$4 \le w_2 \le 12 \quad . \tag{3.8.4}$$

The experimenter wants to restrict the study to a smaller region, namely

$$2{,}000 \le w_1 \le 4{,}000$$

$$6 \le w_2 \le 10 \quad . \tag{3.8.5}$$

Let

$$x_1 = \frac{w_1 - 3{,}000}{1000}$$

$$x_2 = \frac{w_2 - 8}{2} \quad . \tag{3.8.6}$$

Then the approximate design for both criteria are given below.

Natural Variables.	Design Variables	Number of Replications for D_s-criterion	Number of Replications for D-criterion
(4000,10)	(1,1)	9	8
(4000,6)	(1,-1)	9	8
(2000,10)	(-1,1)	9	8
(2000,6)	(-1,-1)	9	8
(5000,6)	(2,0)	12	15
(1000,8)	(-2,0)	12	15
(3000,12)	(0,2)	12	15
(3000,4)	(0,-2)	12	15
(3000,8)	(0,0)	18	10
		102	102

CHAPTER IV

OTHER DESIGNS

This chapter will focus on three classes of RSM designs discussed in Chapter II. They are the equiradial, Box-Behnken and small composite designs. Conditions for choosing the D- and D_s-best k-factor design will be given for the equiradial and certain Box-Behnken designs. The small composite designs will be studied using tables and figures.

4.1 Equiradial Design

The equiradial design was introduced in Chapter II. The design matrix was given there and consisted of $n_0 + n_1 = N$ points with n_1 points of the form

$$[\rho \cos(\theta + \frac{(u-1)2\pi}{n_1}),\ \rho \sin(\theta + \frac{(u-1)2\pi}{n_1})] , \quad u = 1, 2, \ldots, n_1 , \tag{4.1.1}$$

where θ is the angle the first point makes with the real axis and ρ is the distance of the points from the center of the design. The remaining n_0 points are of the form [0,0]. The final design consists of n_1 points equally spaced on a circle of radius ρ, around n_0 center points.

The moment matrix for this general design is given in Myers (1976) as

$$M = \begin{bmatrix} 1 & 0 & 0 & a & a & 0 \\ 0 & a & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 \\ a & 0 & 0 & b & c & 0 \\ a & 0 & 0 & c & b & 0 \\ 0 & 0 & 0 & 0 & 0 & c \end{bmatrix}, \qquad (4.1.2)$$

where $a = \frac{\rho^2 n_1}{2N}$, $b = \frac{3\rho^4 n_1}{8N}$, and $c = \frac{\rho^4 n_1}{8N}$.

To calculate the det(M) and $\mathrm{Det}(M^{22})^{-1}$ write M as

$$M = \begin{bmatrix} A & C \\ C' & B \end{bmatrix}. \qquad (4.1.3)$$

Then,

$$\mathrm{Det}(M) = \det(A) \cdot \det(B - C'(A)^{-1}C), \qquad (4.1.4)$$

and

$$\mathrm{Det}(M^{22})^{-1} = \det(B - C'(A)^{-1}C). \qquad (4.1.5)$$

Calculating (4.1.4) it is easy to see that $\det(A) = a^2$ and $\det(B - C'A^{-1}C) = c \cdot ((b^2 - c^2) - 2a^2(b - c))$. Substituting the equivalent of a, b and c we obtain

$$\det(M) = \frac{\rho^{16} n_1^5 n_0}{256N^6} \qquad (4.1.6)$$

and

$$\det(M^{22})^{-1} = \frac{\rho^{12} n_1^3 n_0}{64N^4} . \tag{4.1.7}$$

These results are obtained by using the fact that the matrix M is a partition matrix and then using the results given in Graybill (1976) on such matrices.

It is obvious from the expressions for det(M), and $\det(M^{22})^{-1}$ that, in both cases, the functions are increasing in ρ. This implies that both criteria will be best if ρ is chosen as large as possible. The experimenter should act accordingly.

The following theorems give the requirements on the ratio of circle points to center points for both criteria.

Theorem 4.1:

An equiradial design with ρ fixed will be D-best in the class of equiradial designs if the ratio of points on the circle to points in the center is 5:1.

Proof:

Let $\frac{n_1}{N} = w_1$, and so $w_0 = 1 - w_1 = \frac{n_0}{N}$. Let $\phi(w_1) = \det(M) = \frac{\rho^{16}}{256} w_1^5(1-w_1)$.

$$\frac{\partial\phi(w_1)}{\partial w_1} = \left(\frac{\rho^{16}}{256}\right)(5w_1^4 - 6w_1^5) = 0 ,$$

so $w_1 = \frac{5}{6}$.

Fox example, the design with radius ρ and twelve total points, will be D-best if ten points are placed on the circle and two points are placed in the center. A very similar result holds for the D_s-criterion.

Theorem 4.2:

An equiradial design with ρ fixed will be D_s-best in the class of equiradial designs if the ratio of points on the circle to center points is 3:1.

Proof:

Let $w_1 = \frac{n_1}{N}$, again. Hence,

$$\det(M^{22})^{-1} = \frac{\rho^{12}}{64} w_1^3(1-w_1) .$$

Using the same technique as in Theorem 4.1, the maximum is found to occur at $w_1 = 3/4$.

The results of the last two theorems agree with the results of Theorem 3.2 and Theorem 3.3 for the central composite design when $k = 2$, and $\frac{n_1}{N}$ in the equiradial design is equated with $w_1 + w_2$ in the ccd. This agreement should occur, since for $n_1 = 8$ circle points and $n_0 \geq 1$ center points, the equiradial design is just a rotation of a central composite design. The equiradial design allows fewer or more points to be placed on the circle than the ccd, so in this sense it is more general. Hence, the results of Theorem 4.1 and Theorem 4.2 are necessary.

Comparing the results of the two theorems, 4.1 and 4.2, the D-criterion places less weight on the center points than the D_s-criterion. This is again caused by the different objectives of the two criteria as discussed in Chapter III. Again, the D_s-criterion requires center points to aid in the estimation of quadratic coefficients.

4.2 Box-Behnken Designs

Box and Behnken (1960) introduced a set of incomplete 3^k factorial designs for use in response surface problems. The construction of these designs is not of interest here and is discussed in the original paper. The interested reader is referred to that paper for details. Keeping with the pattern set in the preceding, only designs for k = 3, 4, 5, and 6 will be discussed. The results can sometimes be generalized to other k, and the k for which this is possible will be noted.

Following Hussey (1983), the moment matrix of a Box-Behnken design for k = 3, 4, 5 can be written as

$$M = \begin{bmatrix} 1 & \underline{0}' & A\underline{1}_k' & \underline{0}' \\ \underline{0} & AI_k & \phi & \phi \\ A\underline{1}_k & \phi & (A-B)I_k + BJ_k & \phi \\ \underline{0} & \phi & \phi & BI_\ell \end{bmatrix}, \qquad (4.2.1)$$

where $A = \frac{a}{N}$, $B = \frac{b}{N}$, J_k is a (k k) matrix of ones, $\underline{1}_k$ is a (k×1) vector of ones, $\ell = \binom{k}{2}$ and I_k is the (k×k) identity. The parameter a is the number of non-zero entries in a column of the model matrix representing a linear term, while b is the number of non-zero entries in a column representing an interaction term. The value of a is constant for all i = 1, 2, ..., k, and b is constant for all i < j = 1, 2, ...,k.

Using the matrix M, the determinants of interest can be found by applying results on partition matrices. Let the matrix M of (4.2.1) be written as

$$M = \begin{bmatrix} 1 & 0 & A\underline{1}_k' & 0 \\ 0 & AI_k & \phi & \phi \\ A\underline{1}_k & \phi & B^* & \phi \\ 0 & \phi & \phi & BI_\ell \end{bmatrix} . \tag{4.2.2}$$

Then, det(M) can be written as

$$\det(M) = A^k \cdot B^\ell \cdot \det(B^* - A^2 J_k) . \tag{4.2.3}$$

Equation (4.2.3) may now be written as

$$\det(M) = c_1 \cdot \frac{N(a+(k-1)b) - ka^2}{N^p} \tag{4.2.4}$$

and

$$\det(M^{22})^{-1} = c_2 \cdot \frac{N(a+(k-1)b) - ka^2}{N^m} \quad , \qquad (4.2.5)$$

where $c_1 = a^k \cdot b^{\ell} \cdot (a-b)^{k-1}$, $c_2 = b^{\ell} \cdot (a-b)^{k-1}$, $p = \frac{(k+1)(k+2)}{2}$, and $m = p - k - 1$.

For $k = 3, 4, 5$, the numerator term, given by $N(a+(k-1)b) - ka^2 = n_0(a+(k-1)b)$, where n_0 is the number of center points. Thus, the determinants become

$$\det(M) = c_1' \cdot \frac{n_0}{N^p} \qquad (4.2.6)$$

and

$$\det((M^{22})^{-1}) = c_2' \cdot \frac{n_0}{N^m} \quad . \qquad (4.2.7)$$

Using this form, the following theorem results.

<u>Theorem 4.3</u>:

If $k = 3, 4, 5$ and a Box-Behnken design is used with

$$\text{(i)} \quad n_0 = \frac{n_1}{p-1} \quad , \qquad (4.2.8)$$

$$\text{(ii)} \quad n_0 = \frac{n_1}{m-1} \quad , \qquad (4.2.9)$$

where n_1 is the number of non-center points, $n_1 + n_0 = N$, then the resulting design will be, respectively,

(i) D-best in the class of k-factor Box-Behnken ,

(ii) D_s-best in the class of k-factor Box-Behnken .

Proof:

Both determinants are of the form

$$\phi(n_0) = c(a,b) \cdot \frac{n_0}{(n_0 + n_1)^s} \quad . \tag{4.2.10}$$

$$\frac{\partial \phi}{\partial n_0} = c(a,b) \cdot \frac{n_1 - (s-1)n_0}{(n_0 + n_1)^{s+1}} \quad . \tag{4.2.11}$$

Setting (4.2.11) equal to zero, one obtains

$$\tilde{n}_0 = \frac{n_1}{s-1} \tag{4.2.12}$$

as the location of the stationary point of this function. Also,

$$\frac{\partial^2 \phi}{\partial n_0^2} = \frac{s((s-1)n_0 - 2n_1)}{(n_0 + n_1)^{s+1}} \quad . \tag{4.2.13}$$

Evaluating (4.2.13) at $\tilde{n}_0 = \frac{n_1}{s-1}$, one obtains

$$\left. \frac{\partial^2 \phi}{\partial n_0^2} \right|_{n_0 = \frac{n_1}{s-1}} = \frac{s(n_1 - 2n_1)}{(n_0 + n_1)^{s+2}} < 0 \ . \tag{4.2.14}$$

Hence, (4.2.10) has a maximum at $n_0 = \frac{n_1}{s-1}$.

In fact, this theorem will hold for any Box-Behnken design constructed using a BIBD with $\lambda = 1$ (see Box and Behnken (1960), Hinkelmann and Kempthorne (1982)). In particular, for the designs presented in the original paper by Box and Behnken for k = 7 and 11, the results of the theorem will hold. The values of n_0 required by the theorem, as well as the practical, approximate choice of n_0 for each k are illustrated in Table 4.1.

For $k = 6$, the design given in the 1960 paper is constructed using a partially balanced incomplete block design (PBIBD) (see, again, Hinkelmann and Kempthorne (1982)) with two associate classes. The general form of the determinant exhibited above will no longer hold. Because of this, a general theorem like Theorem 4.3 will not be possible. To study this design, a table of the two criteria was constructed, and is presented in Table 4.2. From this table, the number of center points to be D_s-best is 2 while the number to be D-best is also 2.

From Table 4.1 and Table 4.2 the following conclusion may be drawn. Different values of k require different numbers of center points for both criteria. Generally, the D_s-criterion requires more center points than the D-criterion. Again, this conclusion has been reached with the other design classes (see Section 3.7 and 4.1).

Table 4.1

Required Center Points for D_s- and D-best Box-Behnken Designs

k	p	m	n_1	$\tilde{n}_0$ for D_s	$\tilde{n}_0$ for D	n_0 for D_s	n_0 for D
3	10	6	12	2.4	$1.\overline{3}$	2	1
4	15	10	24	$2.\overline{6}$	1.714	3	2
5	21	15	40	2.851	2	3	2
7	36	28	56	2.074	1.6	2	2
11	78	66	176	2.708	2.286	3	2

Table 4.2

Determinant Criteria for $k = 6$

Box-Behnken Design

number of center points	Det(M)	$\det(M^{22})^{-1}$
1	2.599×10^{-18}	1.936×10^{-16}
2	2.952×10^{-18}	2.483×10^{-16}
3	2.544×10^{-18}	2.409×10^{-16}
4	1.969×10^{-18}	2.095×10^{-16}
5	1.444×10^{-18}	1.723×10^{-16}
6	1.027×10^{-18}	1.370×10^{-16}
7	7.166×10^{-19}	1.068×10^{-16}
8	4.945×10^{-19}	8.208×10^{-17}
9	3.389×10^{-19}	6.256×10^{-17}
10	2.314×10^{-19}	4.741×10^{-17}

4.3 Small Composite Designs

Small composite designs were introduced in Section 2.8 of this thesis. Examples of the designs suggested by Hartley (1959) and Westlake (1965) are given in Appendix II. Both of these types of designs use extensive aliasing of main effects to achieve their goal of a minimal number of points. The information lost on the main effects in the factorial portion is partially made up by the fact that the axial portion of the design helps in the estimation of main effects. This aliasing causes non-zero covariance between certain main effects and interactions. This covariance structure will result in non-zero elements in the upper right-hand submatrix of X'X. This very complicated structure of X'X for Westlake's designs will prohibit general formulations of the type given in Section 3.6. The analysis of this design class will therefore be carried out by the inspection of figures showing the various design criteria.

Draper (1985) has recently suggested a method of constructing small composite designs using portions of Plackett-Burman (1946) designs. The designs constructed by Draper have an extensive covariance structure, also. This will again prohibit a general form for each of the determinant criteria. Again, Draper's designs will be studied by examining plots of the criteria against the choice of α.

Small composite designs are used when the cost of obtaining a data point is very large. This fact also rules out the formulation of Section 3.6. If points are expensive, replication of points seems unreasonable. Center points may be an exception to this rule. However, a large number of center points will probably not be realistic. It also seems reasonable to expect that both determinant criteria will require center points for certain values of α, namely those near $\alpha = \sqrt{k}$.

Hartley's designs for k = 4 and 6 use a relatively simple system of confounding. Because of this, the determinant criteria can be written down in a general form. The next section will provide that form and show that the determinant criteria are increasing as functions of α. Following that section, a discussion of the plots of the criteria for the more intricate designs of Draper and Westlake will be given.

4.4 Hartley's Small Composite Designs

As mentioned previously, Hartley noticed that the factorial portion of a composite design may have a main effects aliased with a two-factor interaction as long as no main effect is aliased with other main effects and the two-factor interactions are not aliased with other two-factor interactions. Hartley realized that information on the main effects is obtained from the axial portion of the design. For k = 4 and 6, Hartley gave the defining equations to construct the fractions. These defining relations are

$$k=4,\ x_1 = x_2x_3 \tag{4.4.1}$$

$$k=6,\ x_1 = x_2x_3,\ x_4 = x_5x_6,\ x_1x_2x_3 = x_4x_5x_6\ . \tag{4.4.2}$$

Using this aliasing structure, the (X'X) matrix of Hartley's designs can be written as

$$X'X = \begin{bmatrix} \underline{N} & \underline{0}' & (F+2\alpha^2)1_k' & \underline{0}' \\ \underline{0} & (F+2\alpha^2)I_k & \phi & A' \\ (F+2\alpha^2)1_k & \phi & 2\alpha^4 I_k + FJ_k & \phi \\ \underline{0} & A & \phi & FI_\ell \end{bmatrix}, \qquad (4.4.3)$$

where A is a $k \times \ell$ matrix with elements

$$(a_{ij}) = \begin{cases} F & \text{if } j^{th} \text{ main effect is aliased with } i^{th} \text{ interaction} \\ 0 & \text{otherwise} \end{cases} . \qquad (4.4.4)$$

From (4.4.3) and results found in Graybill (1976),

$$\det(X'X) = N(F+2\alpha^2)^k \cdot \det\left\{ \begin{bmatrix} 2\alpha^4 I_k + FJ_k & \phi \\ \phi & FI_\ell \end{bmatrix} - \begin{bmatrix} (F+2\alpha^2)1_k & \phi \\ \underline{0} & A \end{bmatrix} \begin{bmatrix} 1/N & \underline{0}' \\ \underline{0} & \frac{1}{F+2\alpha^2} I_k \end{bmatrix} \begin{bmatrix} (F+2\alpha^2)1_k' & \underline{0}' \\ \phi & A' \end{bmatrix} \right\}, \qquad (4.4.5)$$

and $\det(M) = N^{-p} \cdot \det(X'X)$, $p = \frac{(k+1)(k+2)}{2}$. The form in the curly brackets of (4.4.5) is merely $N^{(p-k-1)} \det(M^{22})^{-1}$. From (4.4.5), the two determinant criteria may be calculated.

$$N^{(p-k-1)} \cdot \det(M^{22})^{-1} =$$

$$\det\left\{\begin{bmatrix} 2\alpha^4 I_k + (F - \frac{(F+2\alpha^2)^2}{N}) J_k & \phi \\ \phi & FI_\ell - (\frac{1}{F+2\alpha^2}) AA' \end{bmatrix}\right\}, \quad (4.4.6)$$

and

$$N^p \cdot \det(M) = (F+2\alpha^2)^k \cdot (N^{p-k-1} \cdot \det(M^{22})^{-1}) . \quad (4.4.7)$$

Now (4.4.6) can be calculated easily as

$$\det(M^{22})^{-1} =$$

$$N^{-(p-k-1)} (F - \frac{F^2}{F+2\alpha^2})^m \cdot F^{\ell-m} \cdot (2\alpha^4)^{k-1} (2\alpha^4 + kF - \frac{k(F+2\alpha^2)^2}{N}) , \quad (4.4.8)$$

where, $m \leq k$ is the number of aliased main effects. From (4.4.8) it is mere manipulation to show,

$$\det(M^{22})^{-1} =$$

$$N^{-(p-k-1)} (\frac{2\alpha^2}{F+2\alpha^2})^m \cdot F^\ell \cdot (2\alpha^4)^{k-1} \quad (2\alpha^4 + kF - \frac{k(F+2\alpha^2)^2}{N}) . \quad (4.4.9)$$

Using (4.4.9),

det(M) =

$$N^{-(p-1)}(F+2\alpha^2)^k \cdot (\frac{2\alpha^2}{F+2\alpha^2})^m \cdot F^{\ell} \cdot (2\alpha^4)^{k-1} \cdot (2\alpha^4 + kF - \frac{k(F+2\alpha^2)^2}{N}) \quad . \tag{4.4.10}$$

Both (4.4.9) and (4.4.10) are the determinant criteria obtained for the usual central composite design multiplied by $(\frac{2\alpha^2}{F+2\alpha^2})^m$. Hence, it is easy to see that the following theorem must be true.

Theorem 4.4:

Det(M) and $\det(M^{22})^{-1}$ are increasing functions of α for Hartley's small composite designs given in Appendix II when $n_0 \geq 1$.

Proof:

Let $\phi(\alpha)$ be the determinant criterion (Det(M) or $\mathrm{Det}(M^{22})^{-1}$) from the central composite designs of Chapter III. Then for Hartley's designs the corresponding criterion is

$$\tilde{\phi}(\alpha) = (\frac{2\alpha^2}{F+2\alpha^2})^m \cdot \phi(\alpha) \quad . \tag{4.4.11}$$

$$\frac{\partial\tilde{\phi}(\alpha)}{\partial\alpha} = (\frac{2\alpha^2}{F+2\alpha^2})^m \cdot \frac{\partial\phi(\alpha)}{\partial\alpha} + m(\frac{2\alpha^2}{F+2\alpha^2})^{m-1} \cdot \frac{4F\alpha}{(F+2\alpha^2)^2}\,\phi(\alpha) \quad . \tag{4.4.12}$$

The quantity (4.4.12) must be positive, since $\frac{\partial\phi(\alpha)}{\partial\alpha}$ is positive from Theorem 3.1 for D_s-optimality or from Lucas (1974) for D-optimality, and $\phi(\alpha)$ is positive, since (X'X) is positive definite. Hence, $\tilde{\phi}(\alpha)$ is increasing in α.

The plots given in Figure 4.1 and Figure 4.2 are $\log(\mathrm{Det}(M^{22}))$ against α for Hartley's designs of k = 4 and 6. From these plots, the results of Theorem 4.4 can be easily seen. That is, $\det(M^{22})^{-1}$ is increasing in α since $\det(M^{22})$ is decreasing in α. Hence, large α is optimal. A further point, previously noticed in the other design classes, is also seen most clearly for k = 4. As α approaches $\sqrt{k}$, the moment matrix becomes closer to singularity.

Figures 4.3 and 4.4 present plots of $\log(\mathrm{Det}(M^{-1}))$ against α for k = 4 and 6, respectively. Again, the result of Theorem 4.4 is evidenced. Also, it is interesting to note that the D-criterion requires fewer center points than the D_s-criterion, especially when $\alpha = \sqrt{k}$. Notice, when k = 4, the D_s-criterion requires two center points while the D-criterion requires only one.

4.5 Westlake's and Draper's Small Composite Designs

Westlake (1965) and Draper (1985) have suggested designs to be used when observations are expensive. This thesis has restricted study to designs for $k \leq 6$. Both authors have suggested designs for the case of k = 5. These designs will be studied in the following. Examples of these designs are given in Appendix II.

The aliasing used in the construction of both types of designs is very extensive. The resulting form of the X'X matrix will not allow a general analysis as was done with Hartley's designs. These designs, for k = 5, will be studied by plots of the criterion of

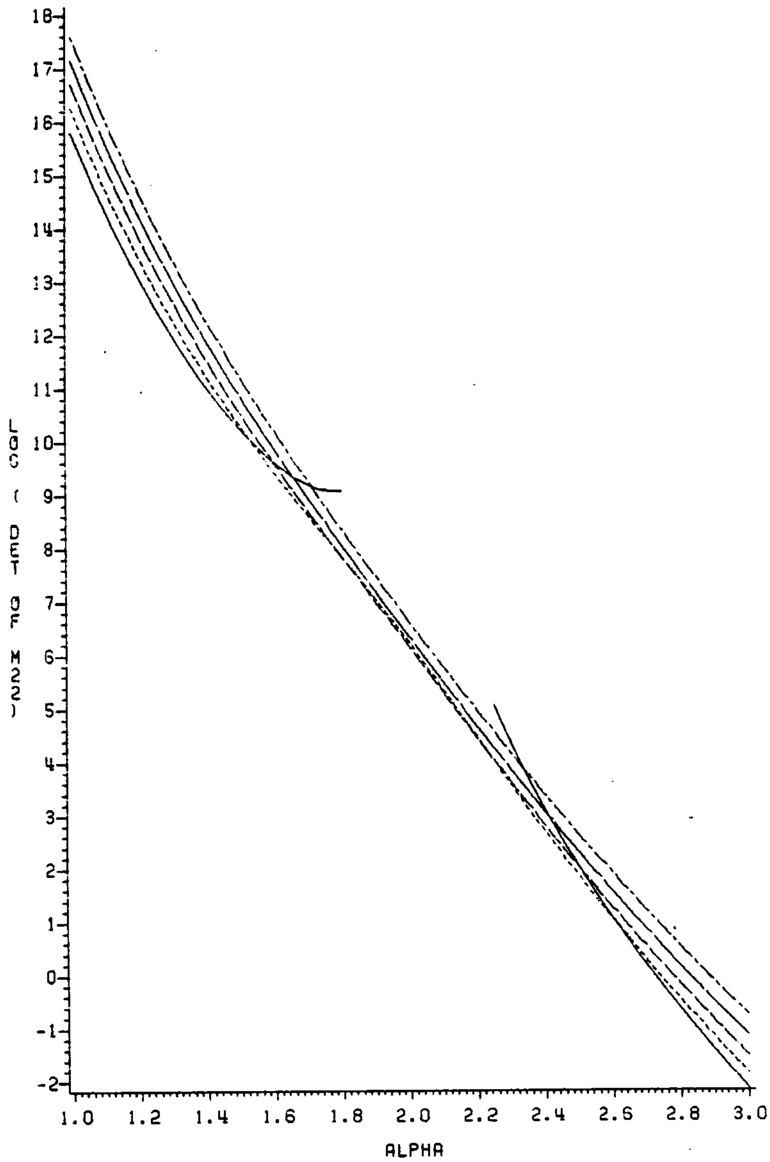

Figure 4.1

log(Det(M^{22})), Hartley $k = 4$

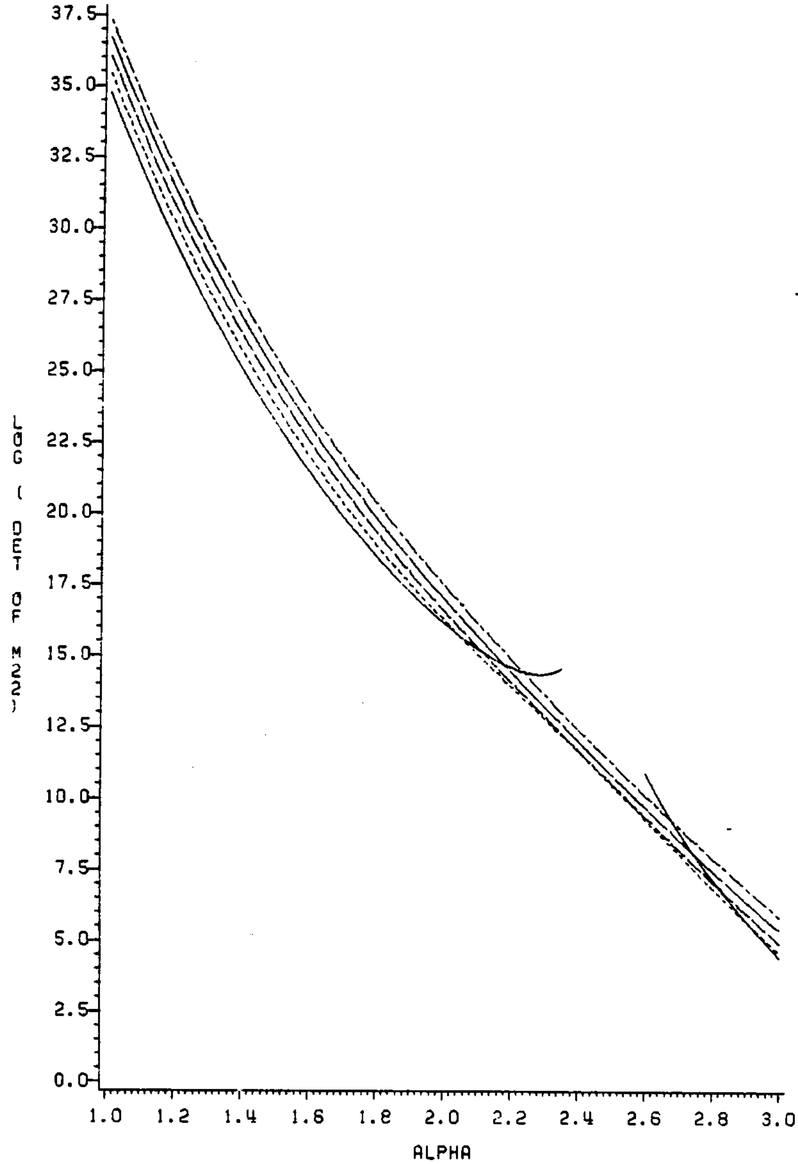

Figure 4.2

log(Det(M^{22})), Hartley k = 6

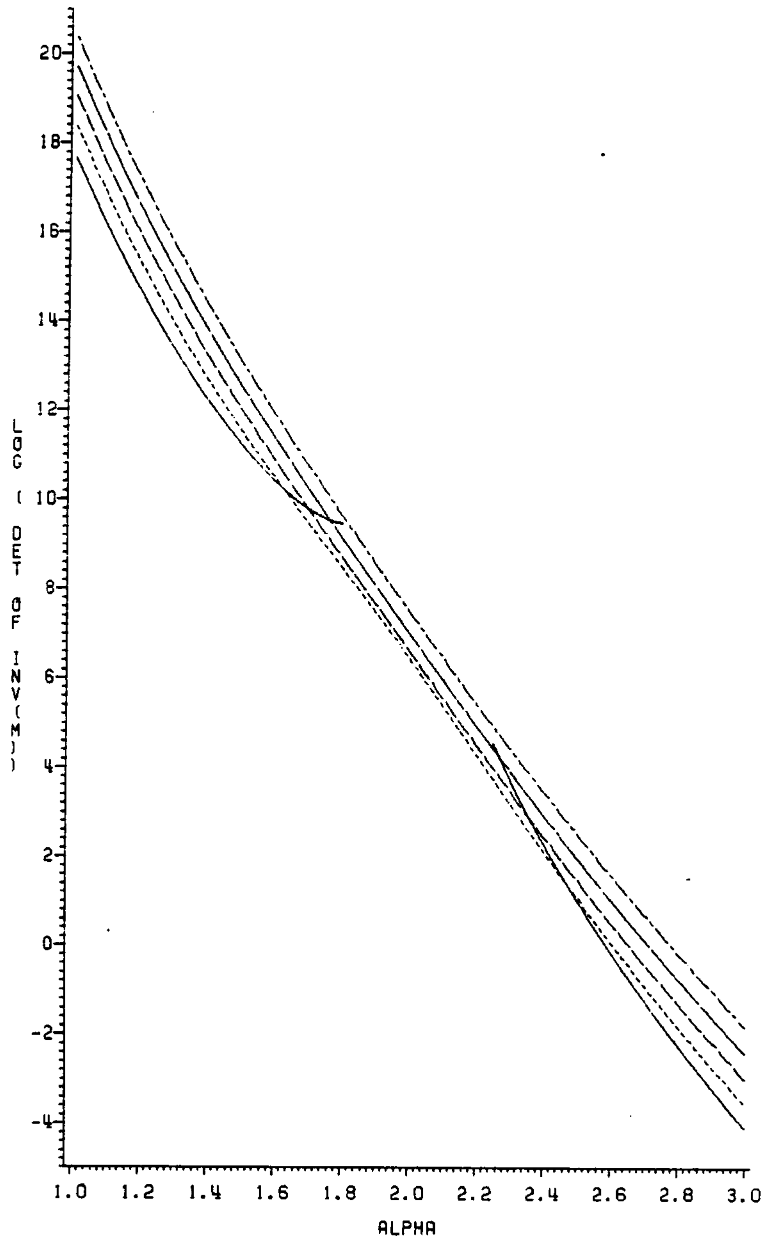

Figure 4.3

log(Det(M^{-1})), Hartley k = 4

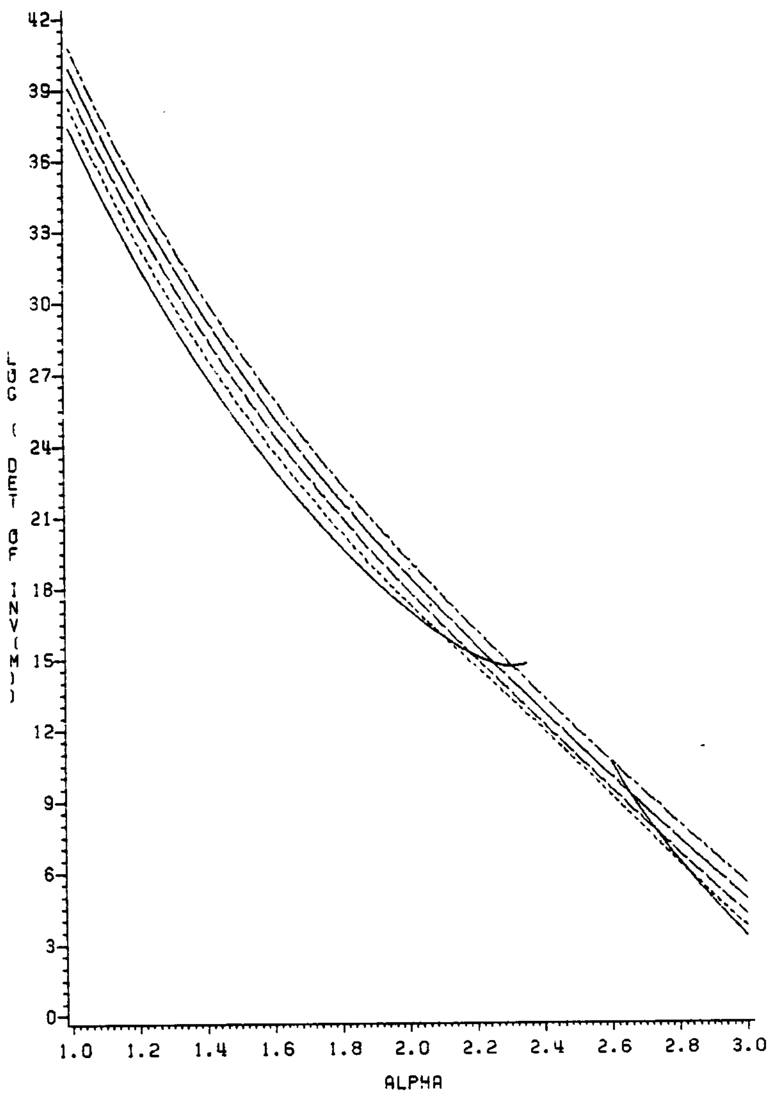

Figure 4.4

$\log(\mathrm{Det}(M^{-1}))$, Hartley $k = 6$

interest against α. The discussion below will first consider the D_s-criterion, then the D-criterion.

Figures 4.5 through 4.8 are plots of $\log(\mathrm{Det}(M^{22}))$ against α for each of the designs under study. From these plots, some conclusions are possible.

(i) Again, as α increases, $\det(M^{22})$ decreases, hence $\det(M^{22})^{-1}$ increases. Therefore, α as large as possible is the best choice.

(ii) Small numbers of center points are best. For α near $\sqrt{k}$, a single center point is best. For very large or very small α, zero center points are best.

(iii) The ordering of designs according to the D_s-criterion is

1. Westlake's #1
2. Westlake's #3
3. Westlake's #2
4. Draper's .

This ordering can probably be attributed to the amount of aliasing. It seems that designs with more aliasing will not estimate the coefficients as well.

Figures 4.9 through 4.12 are plots of $\log(\mathrm{Det}(M^{-1}))$ against α for each of the four k = 5 designs. Some general conclusions may be drawn from these plots.

(i) Again, as α increases, $\det(M^{-1})$ decreases, so $\mathrm{Det}(M)$ increases. Hence, large α is again optimal with respect to D-optimality.

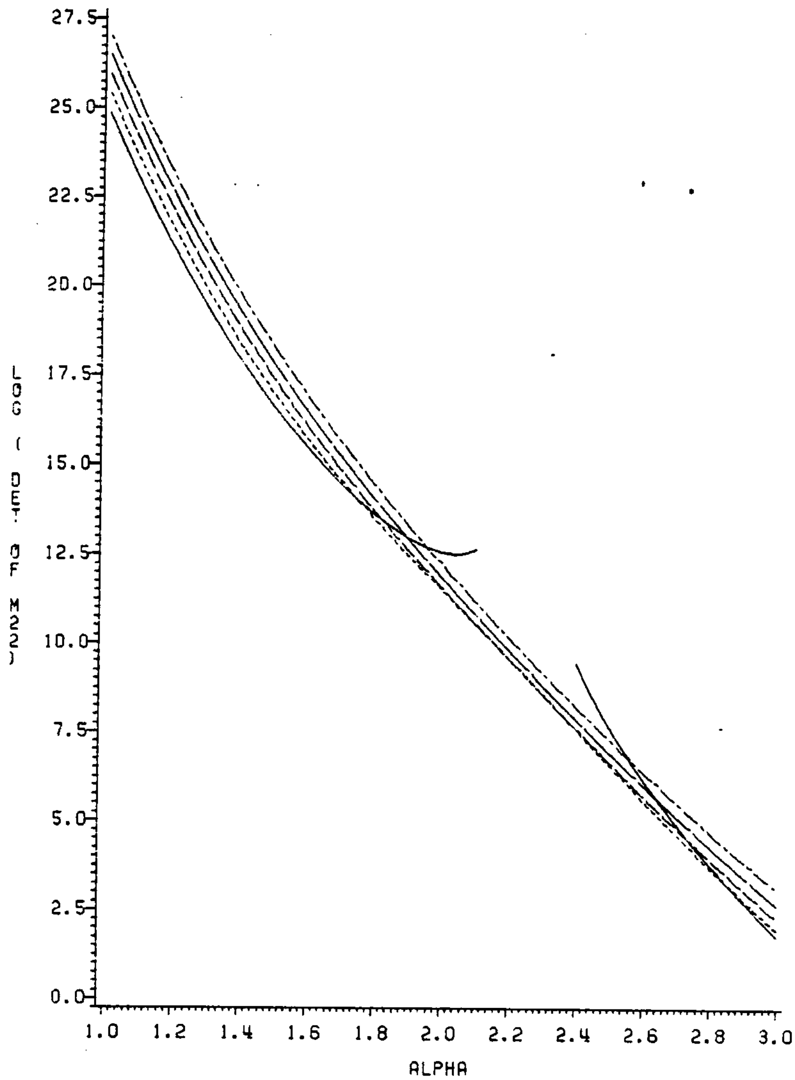

Figure 4.5

$\log(\mathrm{Det}(M^{22}))$ Westlake #1 $k = 5$

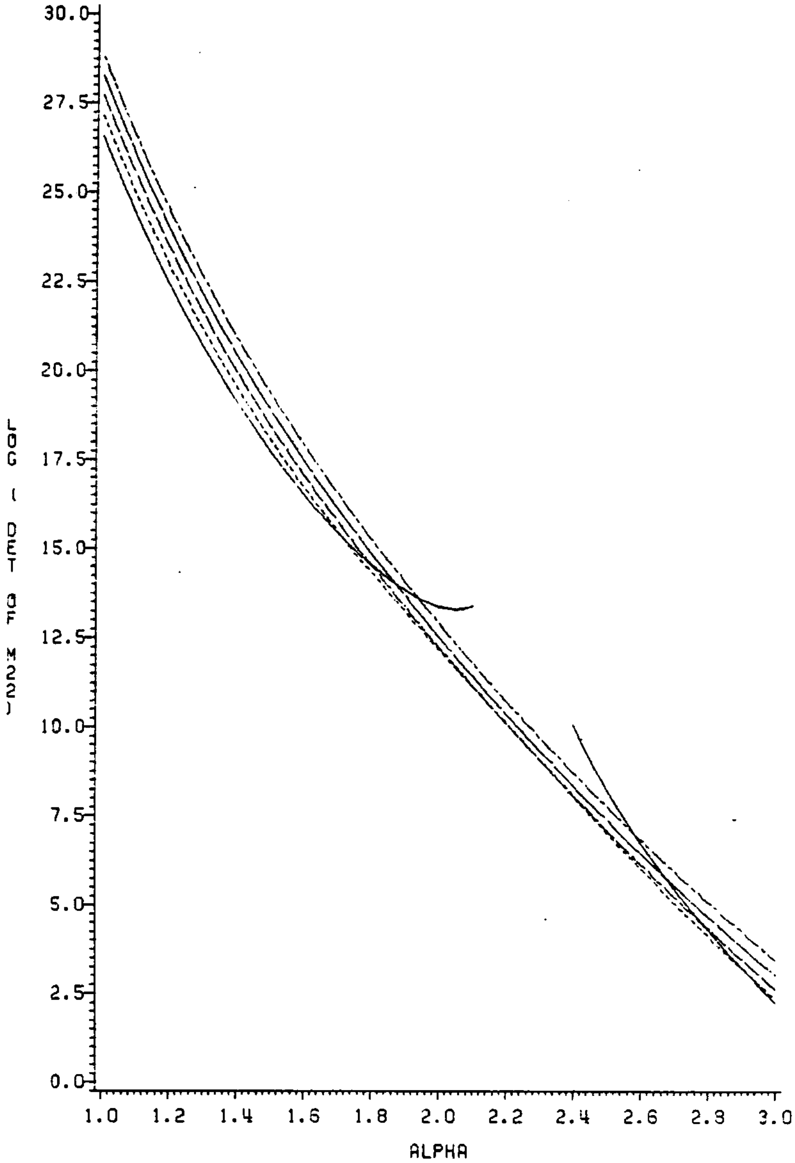

Figure 4.6

log(Det(M^{22}) Westlake #2 k = 5

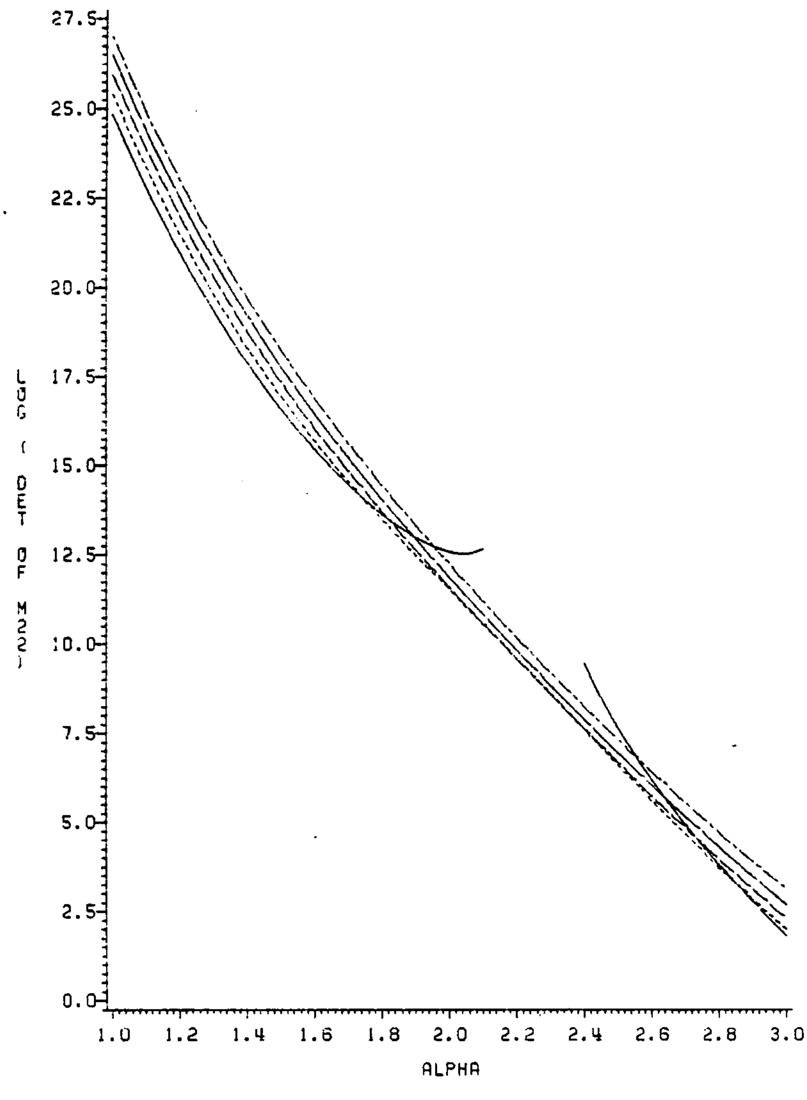

Figure 4.7

log(Det(M^{22})) Westlake #3 k = 5

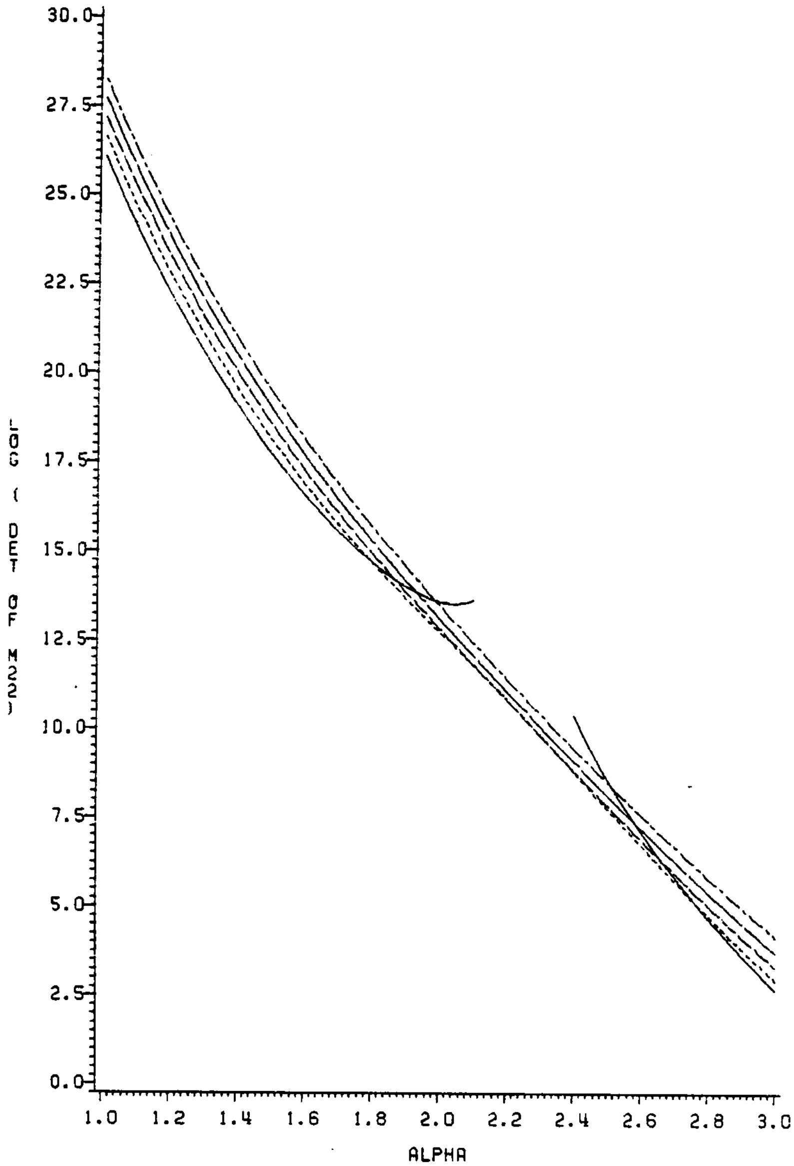

Figure 4.8

$\log(\mathrm{Det}(M^{22}))$ Draper $k = 5$

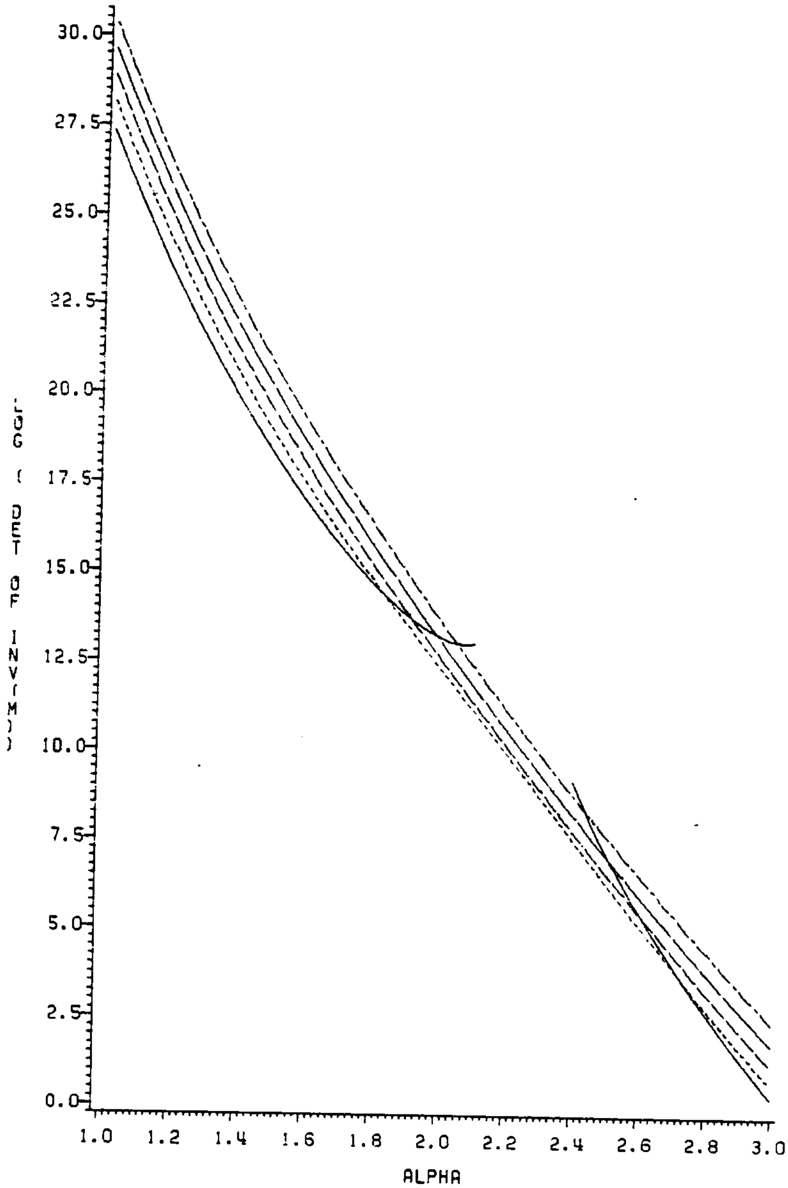

Figure 4.9

log(Det(M^{-1})) Westlake #1 k = 5

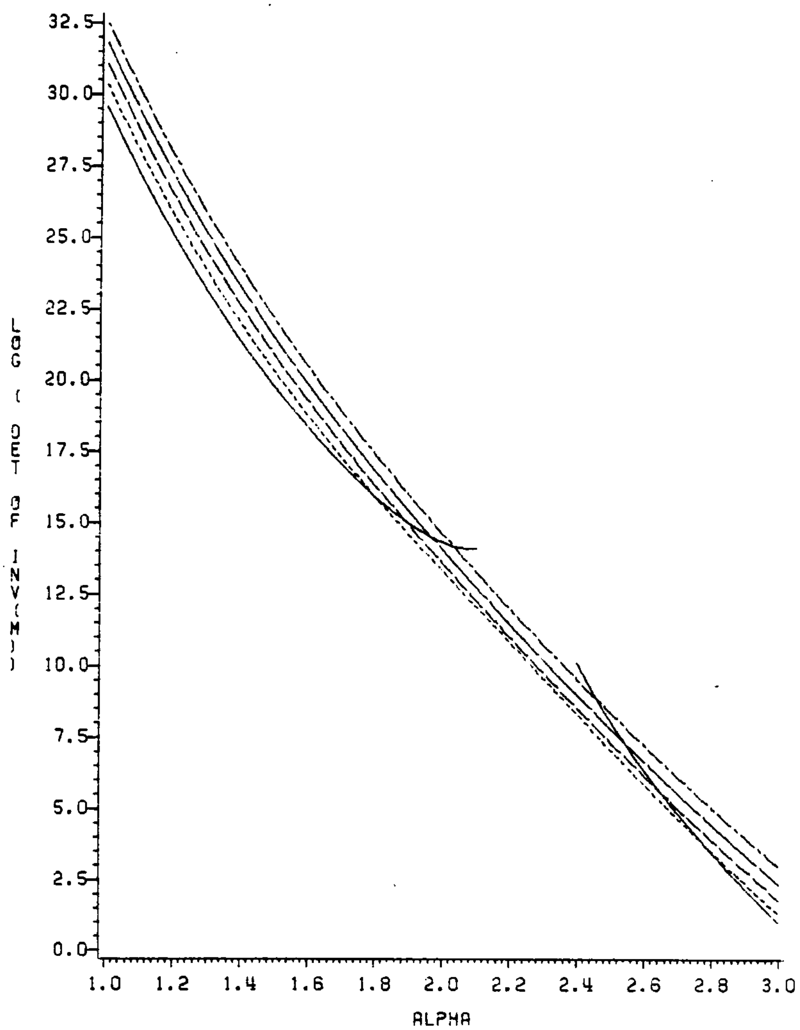

Figure 4.10

log(Det(M^{-1})) Westlake #2 k = 5

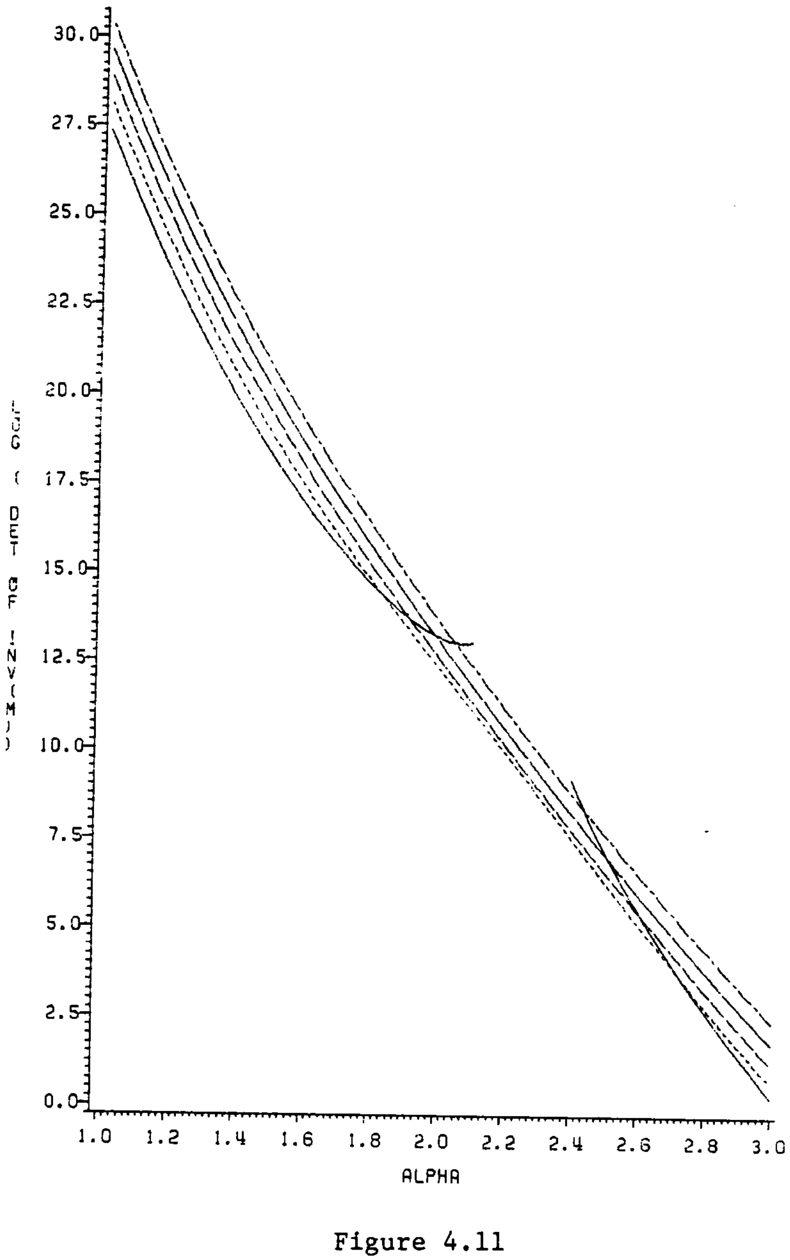

Figure 4.11

log(Det(M^{-1})) Westlake #3 k = 5

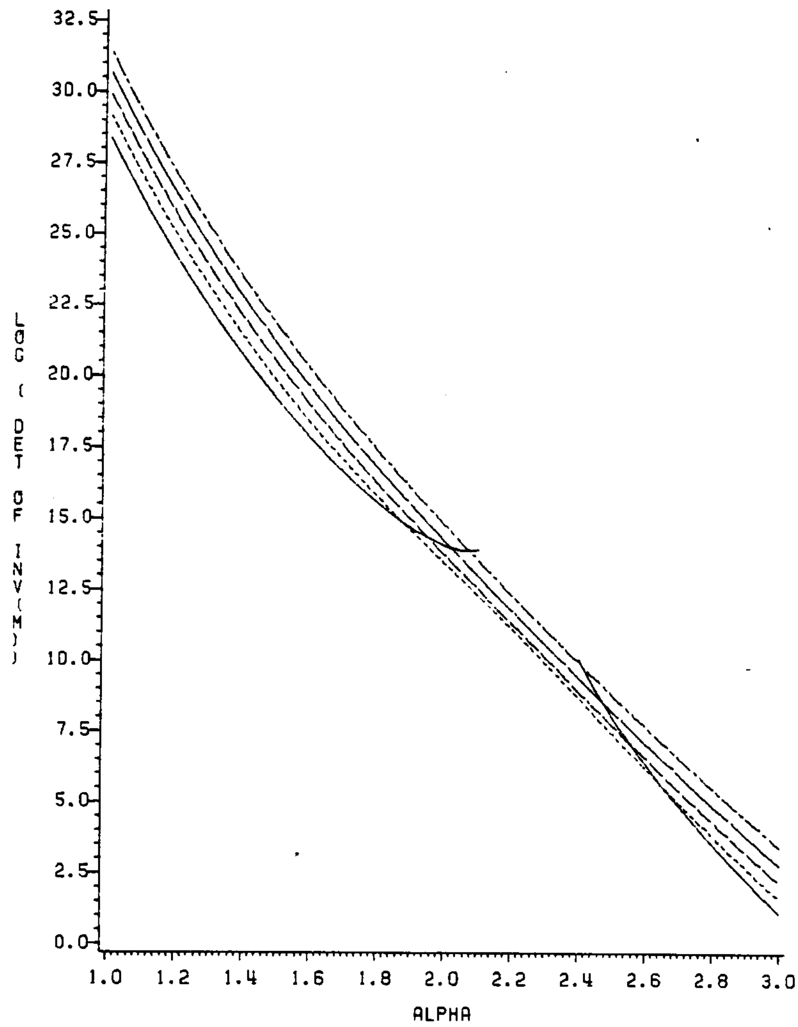

Figure 4.12

$\log(\mathrm{Det}(M^{-1}))$ Draper $k = 5$

(ii) Small numbers of center points are best. Zero center points is best for large or small values of α. As α approaches $\sqrt{k}$, a single center point becomes best.

(iii) The ordering of the designs with respect to the D-criterion is:

1. Westlake's #1
2. Westlake's #3
3. Westlake's #2
4. Draper's .

The reader will notice that the conclusions for the D_s- and D-criterion are exactly the same. This results from the large number of coefficients the D_s criterion takes into account. The majority of coefficients are quadratic or interaction coefficients when $k = 5$. Hence, as we saw in the case of the Box-Behnken designs for large k, the designs, in terms of center points especially, appear similar for each criterion.

CHAPTER V

INTEGRATED VARIANCE CRITERIA

5.1 Introduction

As described in Section 2.13, the Integrated Variance (IV) criterion is another method of selecting or ranking response surface designs. The IV-criterion is a portion of a more general criterion due to Box and Draper (1959) called Integrated Mean Squared Error (IMSE). This more general criterion is to minimize the form (5.1.1),

$$\mathrm{IMSE} = \frac{NK}{\sigma^2} \int_R E(y(\underline{x}) - \hat{y}(\underline{x}))^2 d\underline{x}, \; K^{-1} = \int_R d\underline{x} \; . \tag{5.1.1}$$

This form, (5.1.1), may be written as

$$\mathrm{IMSE} = \frac{NK}{\sigma^2} \{\int_R E(y(\underline{x}) - E(\hat{y}(\underline{x})))^2 d\underline{x} + \int_R E(\hat{y}(\underline{x}) - E(\hat{y}(\underline{x})))^2 d\underline{x}\} \; , \tag{5.1.2}$$

and is typically written symbolically as

$$\mathrm{IMSE} = \mathrm{IB}^2 + \mathrm{IV} \quad . \tag{5.1.3}$$

The IB^2 is the squared bias of $\hat{y}(\underline{x})$, integrated as a function of $\underline{x}$ over the region R. Our interest will center on the second term in (5.1.2), IV. This term represents the prediction variance of the model, $\hat{y}(\underline{x})$, integrated as a function of $\underline{x}$ over the region R. A design with small IV will be best with respect to this criterion. The IV criterion will be used to select designs. It is our intention here to not only determine optimal design parameters in terms of IV but also to compare the results with those obtained for the D_s-criterion.

This chapter will consist of several parts. A discussion of the choice of the integrating region R will be given first. Next, a general formula for calculating IV over a symmetric region, R, will be given. Following this, a general formulation of the IV criterion, first suggested in a paper by Myers and Lahoda (1975), will be discussed. This formulation will be applied to measuring the variance of $\partial\hat{y}(\underline{x})/\partial\underline{x}$ integrated over R. Finally, each of the design classes previously studied in terms of the D_s-criterion will be examined with respect to IV and the extended IV criterion of Myers and Lahoda, hereafter called IV*. This discussion will include a comparison of the designs suggested by the two integrated variance criteria and those designs suggested by the determinant criteria, particularly D_s-optimality.

5.2 Regions of Integration

Two possible regions for integration have been illustrated in previous examples in Chapter III. These regions were spherical. One possible choice of an integrating region is to integrate out to the outermost design point. In the case of a central composite design, this gives rise to the region

$$R_2 = \{\underline{x}: \underline{x}'\underline{x} \leq \max(\alpha^2,k)\} \quad . \tag{5.2.1}$$

This region will only be reasonable for composite designs. R_2 suggests the experimenter is interested in predicting within the whole region in which he believes the model is appropriate.

Often the experimenter has a region of interest smaller than the region in which the model is thought to be appropriate. This is the situation described in Example 2 of Chapter III. In that example, the experimenter is interested in prediction in medium-sized communities, but he is willing to extend the model, and hence the design, outside of the boundaries describing this class of communities. The region of integration to describe this situation is given by

$$R_1 = \{x: \underline{x}'\underline{x} \le k\} \quad . \tag{5.2.2}$$

Note that the factorial points lie on this sphere, and the axial points may or may not lie inside of the sphere, depending on the choice of α.

A final region of integration may be seen best by illustration.

Example 1:

Refer to Example 1 of Chapter III. Suppose the experimenter decided that it was now reasonable to consider the extremes of the two independent factors occurring together. That is, assume the points

$$(1\text{ cm},\ 0.1\text{ g/cm}^3),\ (1\text{ cm},\ 1.0\text{ g/cm}^3),$$
$$(5\text{ cm},\ 0.1\text{ g/cm}^3),\ (5\text{ cm},\ 1.0\text{ g/cm}^3)$$

are reasonable according to the model. Assume further that he is still willing to extend observations along the axes. It thus seems reasonable to redefine the design variables as

$$x_1 = \frac{w_1 - 3}{2}$$
$$x_2 = \frac{w_1 - 0.55}{0.45} \quad . \tag{5.2.3}$$

Using (5.2.3), the region of integration most reasonable for this situation is

$$R_3 = \{\underline{x}: -1 \le x_i \le 1, \ i=1,2,\ldots,k\} \quad . \tag{5.2.4}$$

Region R_3 defines a k-dimensional hypercube with sides of length 2.

Of the three regions of integration just described, it is interesting to note that only R_2, given by (5.2.1), contains all design points. The other two regions, R_1 and R_3, allow design points to be taken from outside of the region of integration. This is reasonable because the region of integration should correspond to the experimenter's region of interest. In the description of each of the regions, two regions have been implicitly assumed. One assumed region is the region of interest to the experimenter. The other assumed region is the region in which the model operates correctly. As mentioned previously, only in region R_2 do these two regions agree. The regions R_1, R_2 and R_3 are probably not the only possible regions of integration. They are the regions that seemed most reasonable to this author.

5.3 A General Formula for IV

It will be convenient to have a general formula for IV over a symmetric region of integration. First, a definition of the notion of region moments will be useful. The region moments will be used to define the concept of symmetry used here. Region moments will also be used in the general formula for IV.

Definition 5.1:

The $(i,j,k,\ell)^{th}$ region moment of region R is given by

$$\mu_{ijk\ell} = K \int_R x_i x_j x_k x_\ell d\underline{x}, \quad K^{-1} = \int_R d\underline{x} \ . \tag{5.3.1}$$

If any i, j, k or ℓ is zero, that subscript is dropped in the naming of the moment. If $i = j$, for example, then the moment is $\mu_{iik\ell}$ and is given by

$$\mu_{iik\ell} = K \int_R x_i^2 x_k x_\ell d\underline{x} \quad .$$

Definition 5.2:

A region, R, is symmetric if

$$\mu_{\delta_1 \delta_2 \dots \delta_k} = K \int_R x_1^{\delta_1} x_2^{\delta_2} \dots x_k^{\delta_k} d\underline{x} = 0,$$

whenever at least one δ_i is odd.

Using Definition 5.1 and Definition 5.2, for a symmetric region R, the region moments may be written as

$$\mu_1 = K \int_R x_i d\underline{x} = 0$$

(*) $$\mu_2 = K \int_R x_i^2 d\underline{x}$$

$$\mu_{12} = K \int_R x_i x_j d\underline{x} = 0$$

$$\mu_{112} = K \int_R x_i^2 x_j d\underline{x} = 0$$

$$\mu_{123} = K \int_R x_i x_j x_k d\underline{x} = 0$$

$$\mu_{1234} = K \int_R x_i x_j x_k x_\ell d\underline{x} = 0$$

$$\mu_{1123} = K \int_R x_i^2 x_j x_k d\underline{x} = 0$$

$$\mu_{1113} = K \int_R x_i^3 x_k d\underline{x} = 0$$

(*) $$\mu_4 = K \int_R x_i^4 d\underline{x}$$

(*) $$\mu_{22} = K \int_R x_i^2 x_j^2 d\underline{x} \quad , \text{ for any } i,j,k,\ell \ . \qquad (5.3.2)$$

Only the region moments designated with a (*) are non-zero for a symmetric region R.

Using (5.1.2), the IV-criterion for a model with model matrix X may be written as

$$IV = K \int_R \underline{x}' M^{-1} \underline{x} d\underline{x} \quad . \tag{5.3.3}$$

Manipulating,

$$IV = K \int_R \mathrm{tr}(\underline{x}\underline{x}' M^{-1}) d\underline{x} \tag{5.3.4}$$

or

$$IV = \mathrm{tr}\{K \int_R \underline{x}\underline{x}' d\underline{x} M^{-1}\} \quad . \tag{5.3.5}$$

Letting

$$\Gamma = \begin{bmatrix} 1 & \underline{0}' & \mu_2 \underline{1}_k' & \underline{0}' \\ \underline{0} & \mu_2 I_k & \phi & \phi \\ \mu_2 \underline{1}_k & \phi & (\mu_4 - \mu_{22}) I_k + \mu_{22} J_k & \phi \\ \underline{0} & \phi & \phi & \mu_{22} I_\ell \end{bmatrix} , \tag{5.3.6}$$

equation (5.3.5) may be written as

$$IV = \mathrm{tr}(\Gamma M^{-1}) \quad . \tag{5.3.7}$$

Finally, using (5.3.7)

$$IV = m^{11} + \mu_2\left(\sum_{i=1}^{k} m^{i+1,i+1} + 2\sum_{i=1}^{k} m^{1,i+k+1}\right)$$

$$+ \mu_4 \cdot \sum_{i=1}^{k} m^{i+k+1,i+k+1} + \mu_{22} \cdot \left(\sum_{i=1}^{\ell} m^{2k+i+1,2k+i+1}\right.$$

$$\left. + 2 \cdot \sum_{i<j}^{k}\sum m^{i+k+1,j+k+1}\right) , \qquad (5.3.8)$$

where m^{ij} is the $(i,j)^{th}$ element of M^{-1}. Equation (5.3.8) allows IV to be calculated for any design and any symmetric region by merely calculating region moments. The region moments for each of the regions, R_1, R_2 and R_3, are included in Appendix III.

5.4 A More General IV-Criterion

In a paper in 1975, Myers and Lahoda generalized the concept of IMSE (see Myers and Lahoda (1975)). In this paper, Myers and Lahoda assumed that r parametric functions of the coefficient vector were of interest. Denote this r-vector by

$$\underline{\gamma}(\underline{x}) = \Lambda(x)\underline{\beta} \quad . \qquad (5.4.1)$$

The IMSE-criterion is now generalized to

$$IMSE* = \frac{NK}{\sigma^2}\int_R E\{(\underline{\beta}-\hat{\underline{\beta}})'\Lambda'(\underline{x})\Lambda(\underline{x})(\underline{\beta}-\hat{\underline{\beta}})\}d\underline{x} \; , \qquad (5.4.2)$$

where $\hat{\beta}$ is the least squares estimator of $\underline{\beta}$ and $K^{-1} = \int_R d\underline{x}$. Using the same sort of manipulation as in (5.1.2) and (5.1.3) the generalized IV-criterion is

$$IV^* = \frac{NK}{\sigma^2}\int_R E\{(\hat{\underline{\beta}}-E(\hat{\underline{\beta}}))'\Lambda'(\underline{x})\Lambda(\underline{x})(\hat{\underline{\beta}}-E(\hat{\underline{\beta}}))\}d\underline{x} \ . \qquad (5.4.3)$$

For a linear model with moment matrix M, the form (5.4.3) becomes

$$IV^* = tr(\Gamma^* M^{-1}) \ , \qquad (5.4.4)$$

where $\Gamma^* = K\int_R \Lambda'(\underline{x})\Lambda(\underline{x})d\underline{x}$.

In a particular case of interest in RSM, the prediction variance of the k slopes of the prediction function, $\hat{y}(\underline{x})$, may be of interest. That is, the $k \times 1$ vector

$$\frac{\partial\hat{y}(\underline{x})}{\partial\underline{x}} = \underline{\gamma}(\underline{x}) \ . \qquad (5.4.5)$$

In this case, Myers and Lahoda showed that the matrix Γ^* is a diagonal matrix of the form

$$\Gamma^* = \begin{bmatrix} 0 & \underline{0}' & \underline{0}' & \underline{0}' \\ \underline{0} & I_k & \phi & \phi \\ \underline{0} & \phi & 4\mu_2 I_k & \phi \\ \underline{0} & \phi & \phi & 2\mu I_\ell \end{bmatrix} , \ \mu_2 = K\int_R x_i^2 d\underline{x} \ . \qquad (5.4.6)$$

Using (5.4.4) and (5.4.6) the IV*-criterion for the slopes may be written as

$$IV^* = \sum_{i=1}^{k} m^{i+1,i+1} + 4\mu_2 \sum_{i=1}^{k} m^{i+k+1,i+k+1} + 2\mu_2 \sum_{i=1}^{\ell} m^{2k+i+1,2k+i+1} . \tag{5.4.7}$$

As with the IV-criterion, it is a simple calculation using (5.4.7) to find IV* for any symmetric region. This calculation, again as with IV, involves substituting the value of the appropriate region moment into (5.4.7). IV* will be calculated in this way for each of the design classes and appropriate regions.

5.5 IV and IV* for Central Composite Designs

The IV and IV* criteria can be written in a very general way using equations (5.3.8) and (5.4.7). This can be done easily since the inverse of the moment matrix of a central composite design can be calculated in general. The forms for the two criteria are

$$IV = N\{a + \mu_2(kc + 2kb) + k\mu_4 d + \binom{k}{2}\mu_{22}(f + 2e)\} , \tag{5.5.1}$$

and

$$IV^* = N\{kc + 4k\mu_2 d + 2\binom{k}{2}\mu_2 f\} , \tag{5.5.2}$$

where

$$a = (kF+2\alpha^2)/D$$

$$b = -(F+2\alpha^2)/D$$

$$c = 1/(F+2\alpha^2)$$

$$d = (D+J)/(2\alpha^4 D)$$

$$e = J/(2\alpha^4 D)$$

$$f = 1/F$$

$$D = N(kF+2\alpha^4) - k(F+2\alpha^2)^2$$

$$J = (F+2\alpha^2)^2 - NF \quad . \qquad (5.5.3)$$

From equations (5.5.1), (5.5.2) and (5.5.3) it seems clear that it would be a very complicated task to directly minimize IV and IV* with respect to the design parameters. We will instead allow the computer to calculate the IV and IV* for various choices of the design parameters and choose the best set of parameters.

Figures 5.1 through 5.6 are plots of IV for the three regions against α for n_0 = 0, 1, 2, 3, or 4. Only k = 2 and 4 are presented. Plots for k = 2, 3, 4, 5, $5(\frac{1}{2})$, 6, $6(\frac{1}{2})$, where $5(\frac{1}{2})$ and $6(\frac{1}{2})$ denote half-fractions in the factorial portion of the design, were generated. In each case, the plots were very similar to the plots presented.

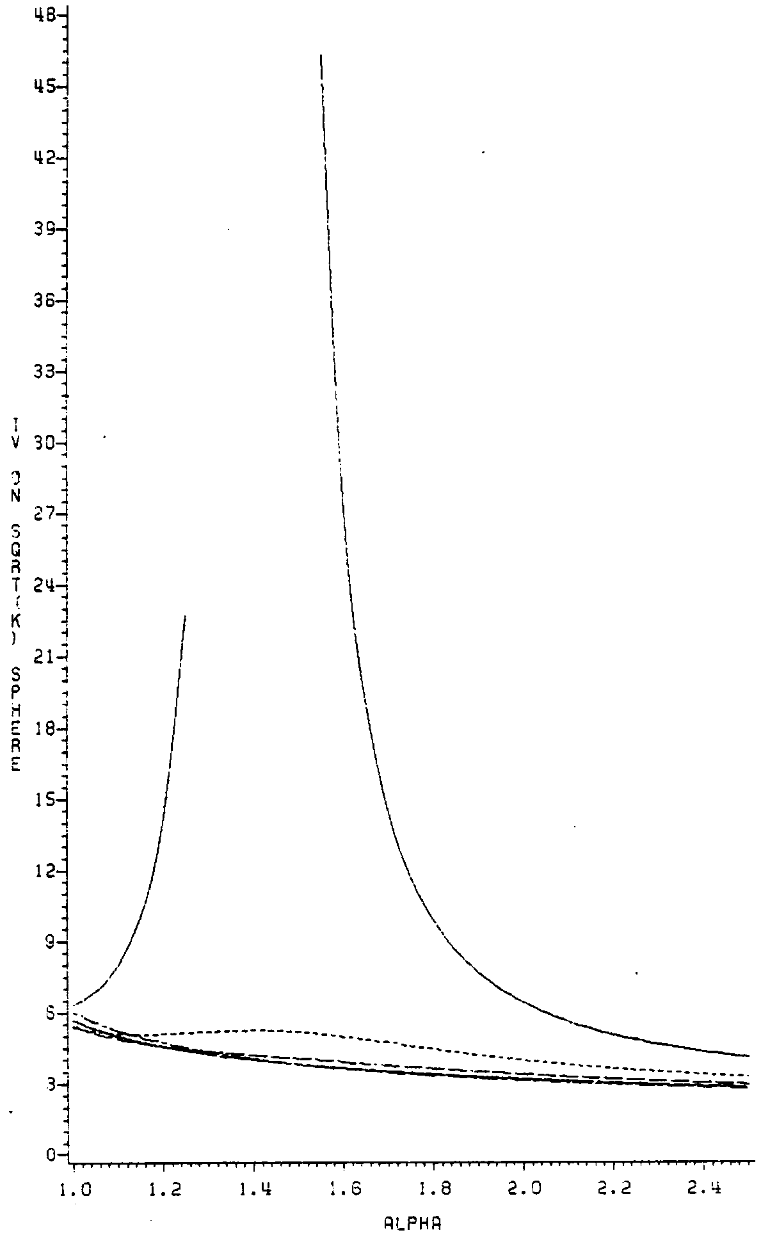

Figure 5.1

IV on Region R_1, $k = 2$ ccd

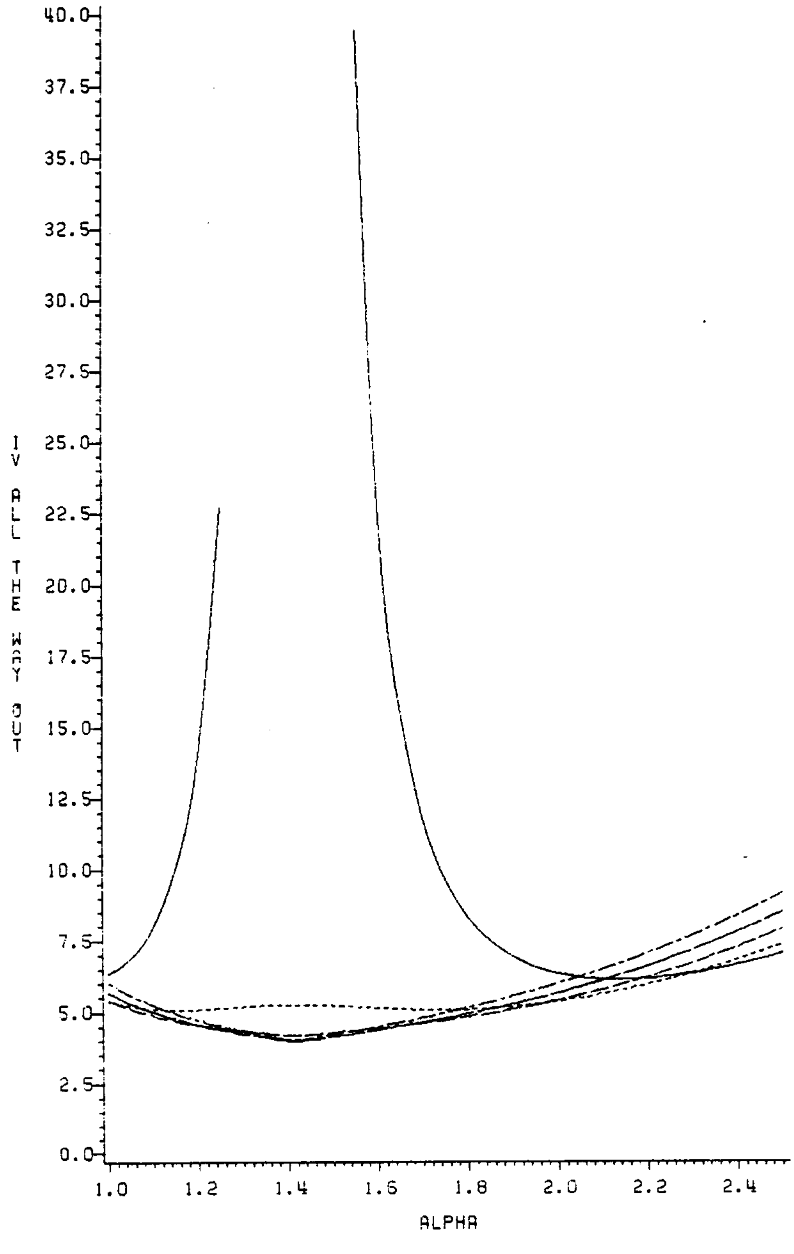

Figure 5.2

IV on Region R_2, $k = 2$ ccd

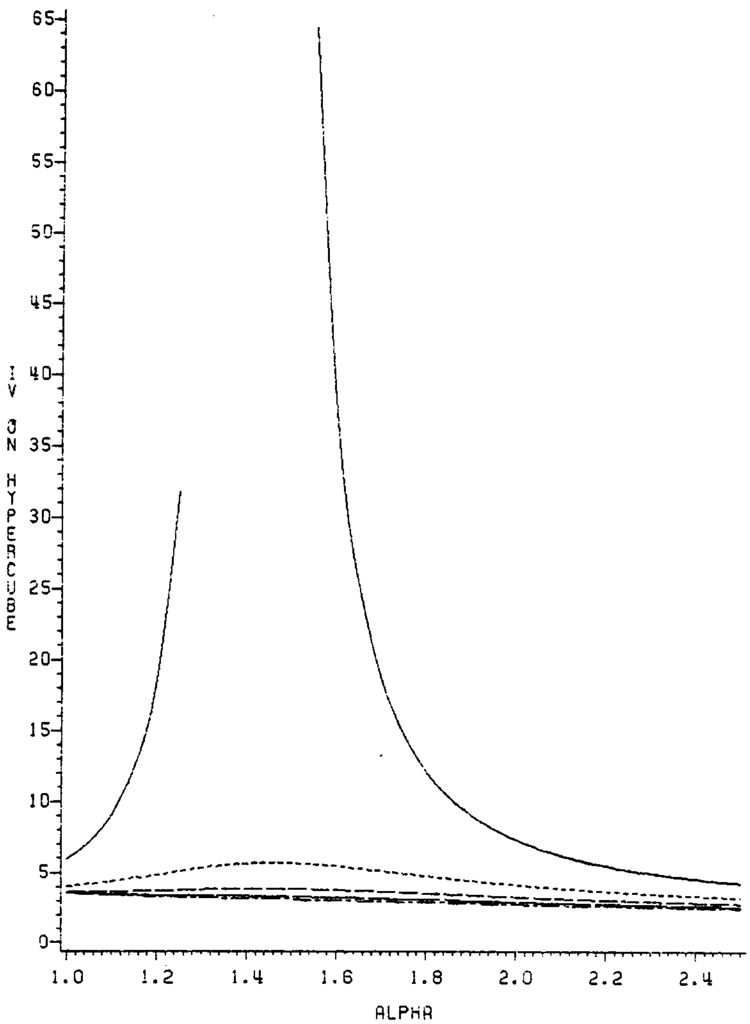

Figure 5.3

IV on Region R_3, $k = 2$ ccd

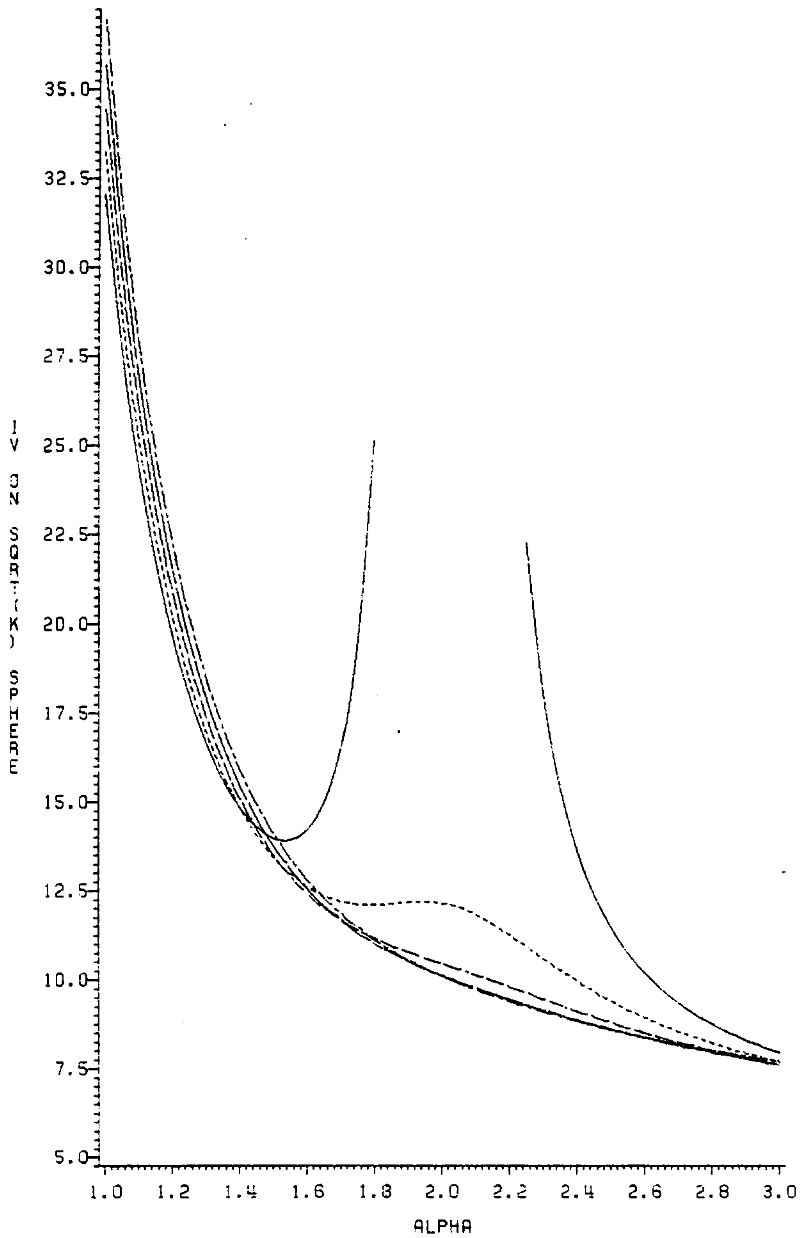

Figure 5.4

IV on Region R_1, $k = 4$ ccd

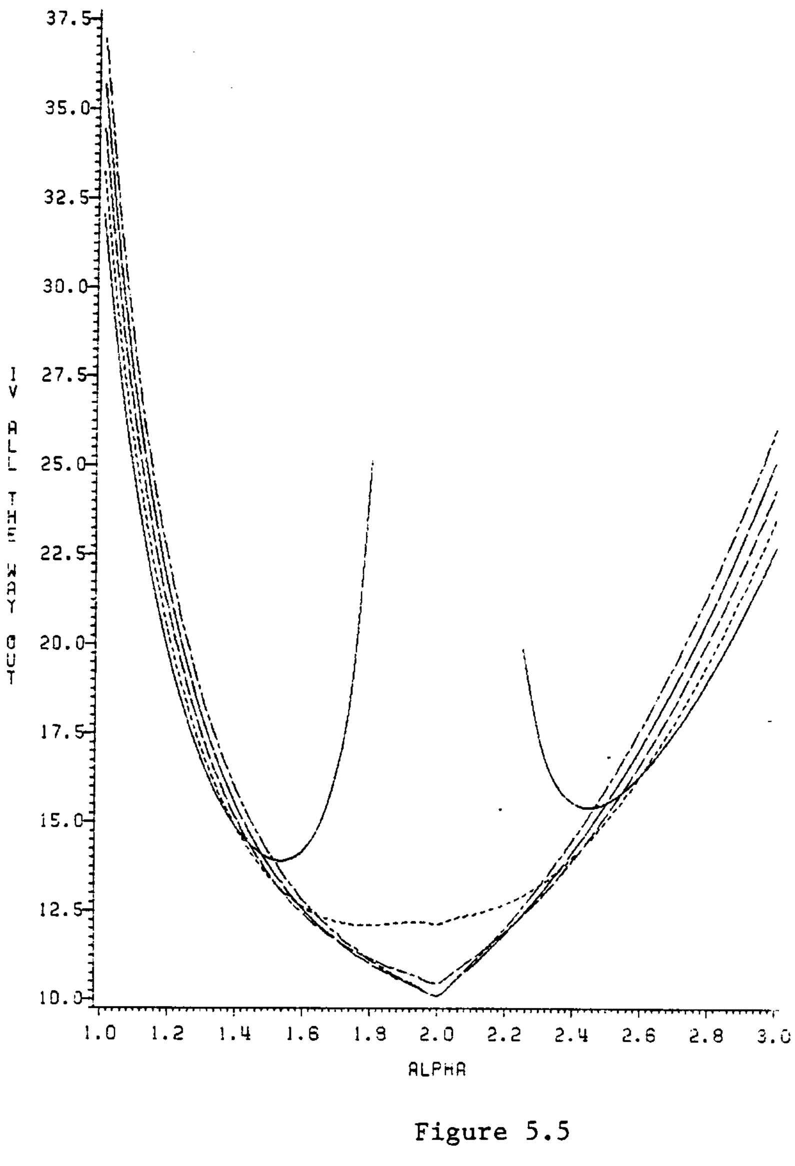

Figure 5.5

IV on Region R_2, $k = 4$ ccd

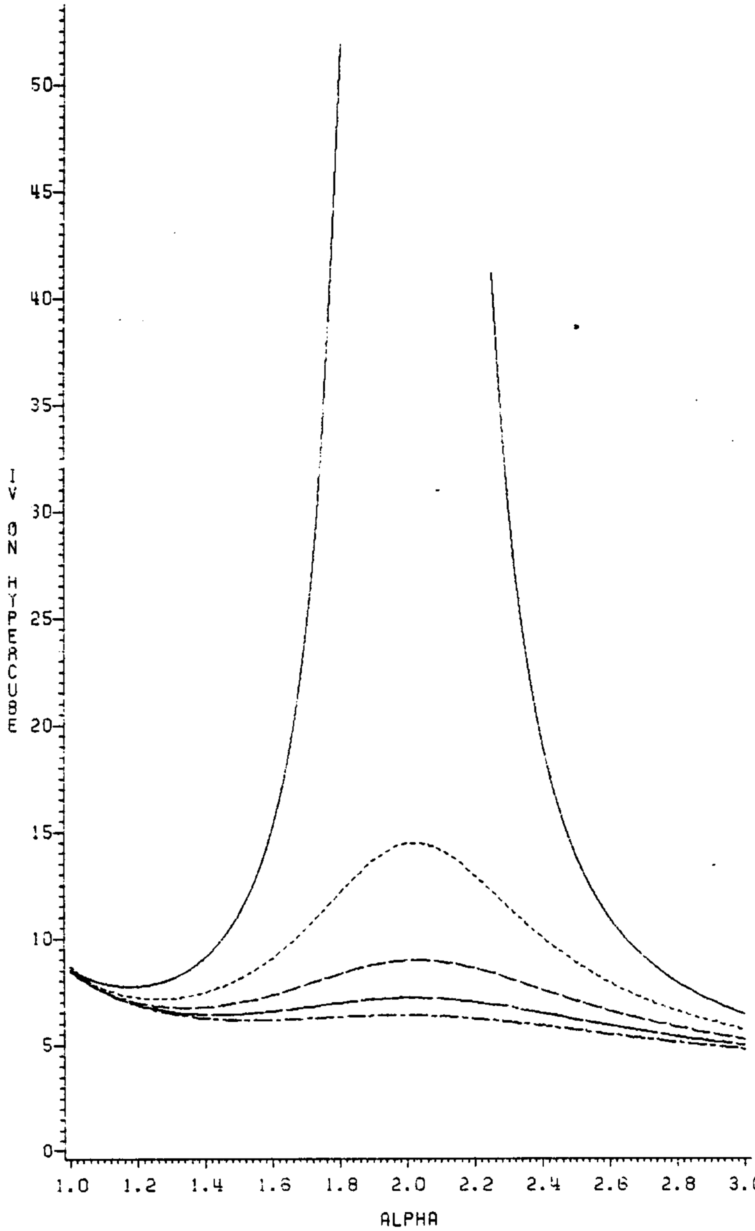

Figure 5.6

IV on Region R_3, $k = 4$ ccd

Hence, only k = 2 and 4 are presented for clarity and economy. Conclusions will be made for all values of k, however.

For clarity and succinctness, the conclusions which may be drawn from the plots will be listed.

(i) For each k when $n_0 = 0$, the IV becomes very large as α approaches $\alpha = \sqrt{k}$. This was the case with $\text{Det}(M^{22})^{-1}$ also. Again, this is caused by the singularity or near singularity of the design for this choice of α and n_0.

(ii) For $n_0 \geq 1$, the IV is decreasing in α for region R_1, when $k \geq 3$. When k = 2 and $n_0 = 1$, the IV curve shows a slight "hump" at $\alpha = \sqrt{k}$. This is again due to the near singularity of the design for this small k.

(iii) The rate at which the IV curve decreases with increasing α is smaller as α becomes larger for region R_1.

(iv) The number of center points required for small α is small for region R_1. As α increases, the number of center points required increases.

(v) The shape of the plots for region R_2 is bowl shaped for $n_0 \geq 1$, with a minimum at $\alpha = \sqrt{k}$.

(vi) The optimal number of center points for small or large α is $n_0 = 0$ for region R_2. As α approaches $\alpha = \sqrt{k}$, the number of center points needed becomes larger.

(vii) The shape of the plots for R_3 are different from either of the preceding regions. For large numbers of center points, the curves are essentially flat.

(viii) For region R_3, large numbers of center points appear to be preferable. This can be seen most clearly for $k = 4$.

Each of the eight observations made above can be explained by examining the three regions of integration. Region R_1 integrates out to the factorial points. The decrease in IV is very large until α increases to the radius of these points. After that, the increase in effectiveness that is experienced by moving the axial points further out becomes less dramatic.

Region R_2 integrates out to the furthest possible design point. As α goes beyond $\alpha = \sqrt{k}$, an increase in α is counterproductive as far as IV is concerned. This can be explained by noting that with the axial points being far away from the origin, many regions will be sparsely populated with design points. These regions will likely have large prediction variance.

Finally, region R_3 is essentially region R_1 with portions trimmed. That is, the hypercube is formed by trimming off portions of the hypersphere. From the plots, we can infer that these trimmed portions have prediction variances that vary greatly with α.

The reason for considering the IV criterion in this thesis was to compare the suggested designs with those suggested by the D_s-criterion. From the discussion above, it seems reasonable to say that this comparison depends on the experimenter's region of interest. If the region of interest is R_1, D_s-optimality and IV agree on the choice of α for the central composite design. In the choice of center points, the two criteria do not agree for this region. The IV criterion requires more center points than the D_s-criterion. If either of the other two regions, R_2 or R_3, are the experimenter's region of interest, it is clear that the IV criterion and the D_s-criterion suggest very different designs in terms of choice of α and of the number of center points required.

Figures 5.7 through 5.12 are plots of IV* against α for k = 2 and 4. Again, the plots for k = 2, 3, 4, 5, $5(\frac{1}{2})$, 6, $6(\frac{1}{2})$ were obtained. The plots presented are representative, and can be examined to understand the basis for the conclusions drawn about IV* in the case of the central composite design. Again, the conclusions for this criterion will be listed for clarity and conciseness.

(i) For each k and each region, when $n_0 = 0$, the IV* is large for $\alpha = \sqrt{k}$. Again, this is due to the singularity or near singularity of this design.

(ii) The plots for R_1 and R_3 are exactly the same except the plots for R_1 are shifted upward. In both cases, small numbers of center points are best for large or small α. Again, as α approaches $\sqrt{k}$, the number of center points needed becomes greater.

(iii) The curves for R_2 are again bowl-shaped for IV* with a minimum at $\alpha = \sqrt{k}$. Also, $n_0 = 0$ is the optimal choice if α is large or small. Larger numbers of center points are required for α near $\sqrt{k}$.

The conclusions reached in terms of IV* can be explained again by comparing the regions of integration. As α becomes very large in region R_2, the slopes of the prediction function become difficult to estimate in the outer portions of the hypersphere. This explains

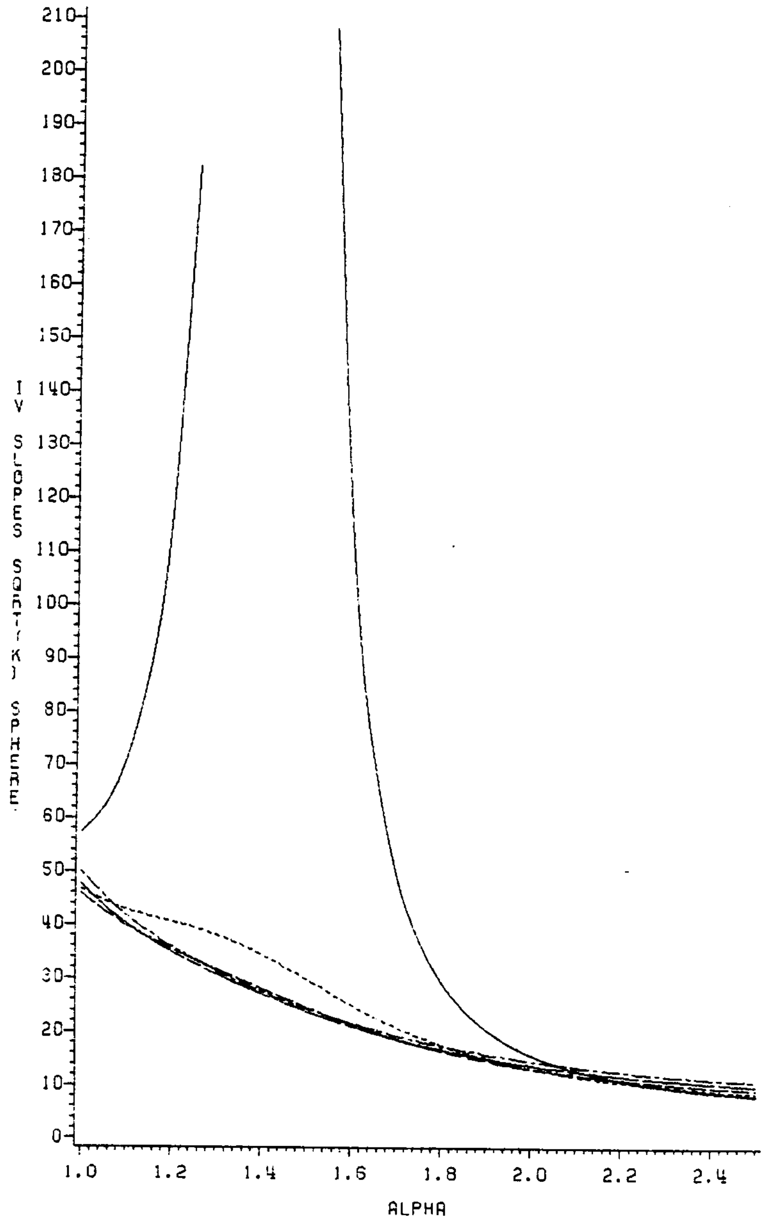

Figure 5.7

IV* on Region R_1, $k = 2$ ccd

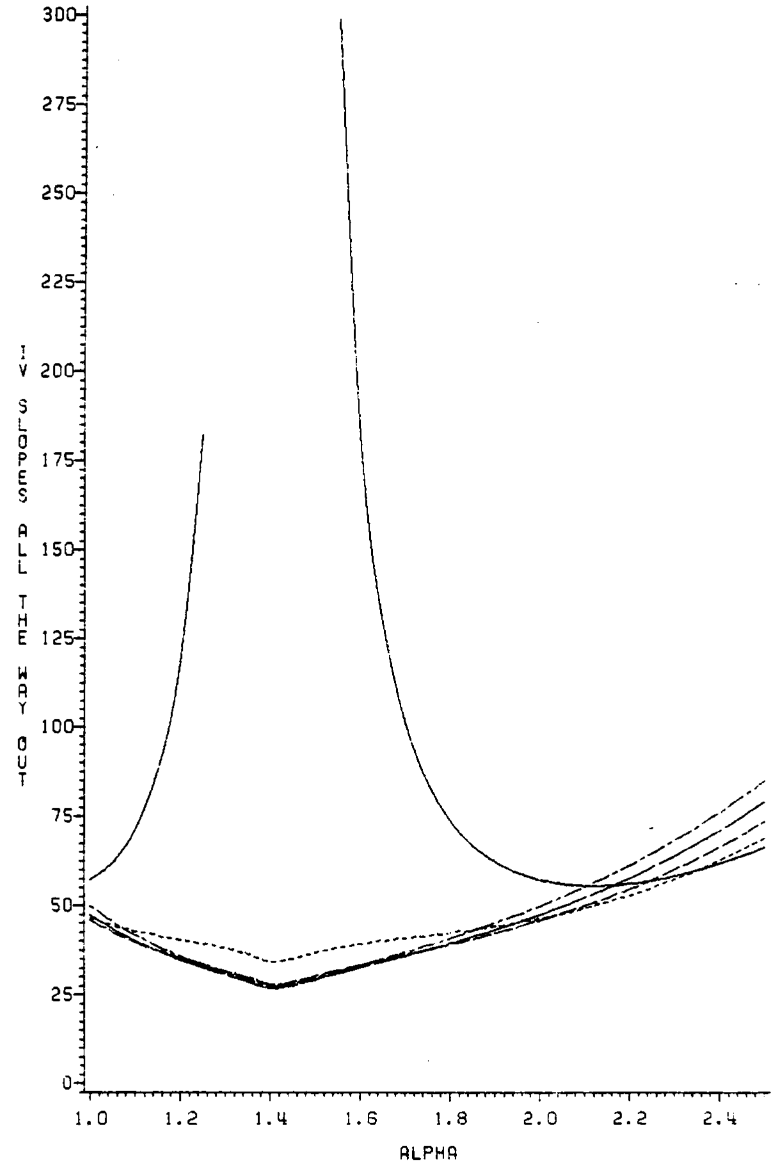

Figure 5.8

IV* on Region R_2, $k = 2$ ccd

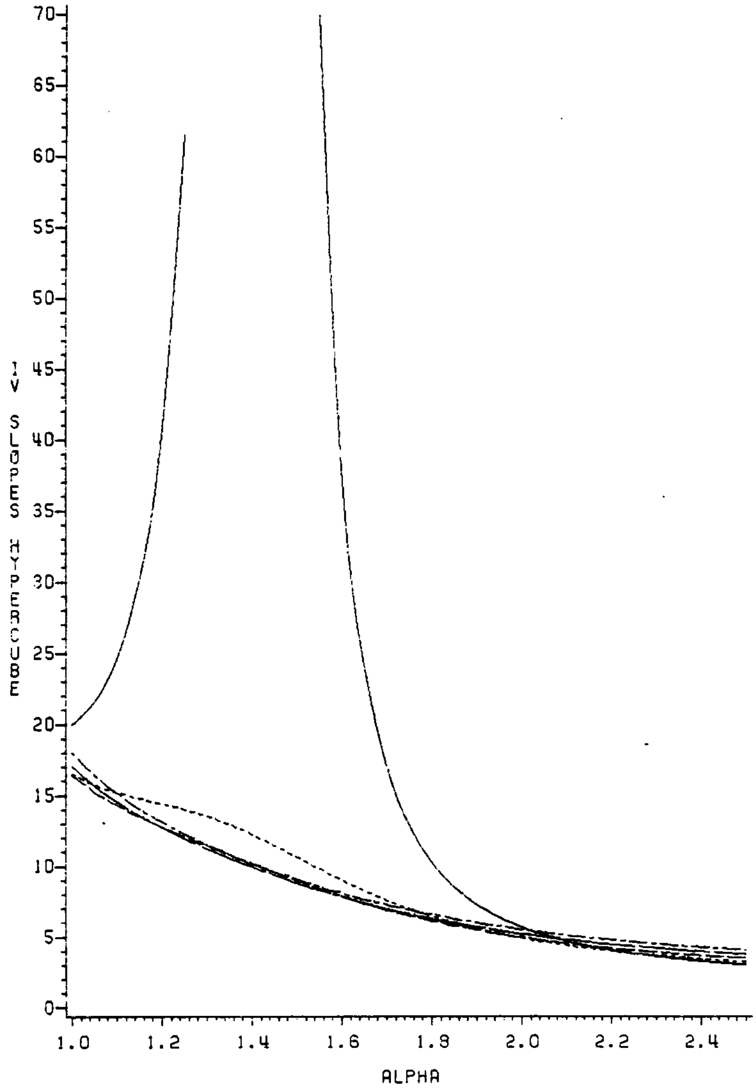

Figure 5.9

IV* on Region R_3, k = 2 ccd

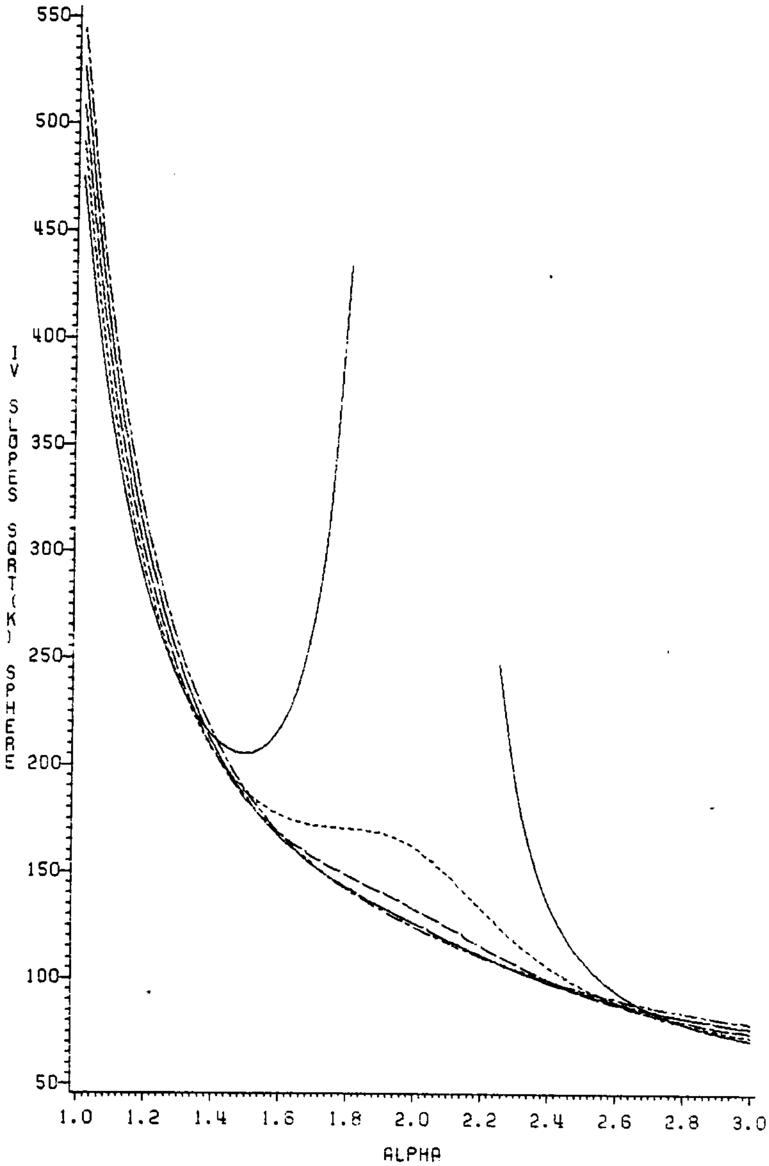

Figure 5.10

IV* on Region R_1, $k = 4$ ccd

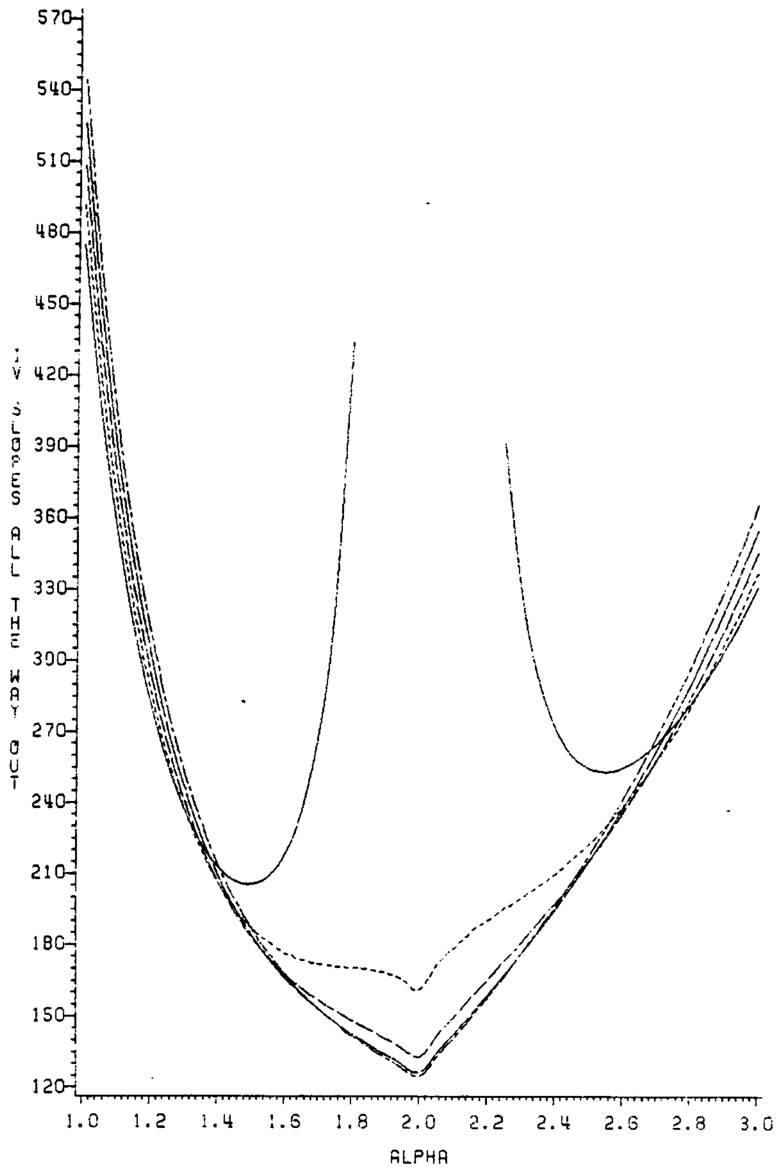

Figure 5.11

IV* on Region R_2, $k = 4$ ccd

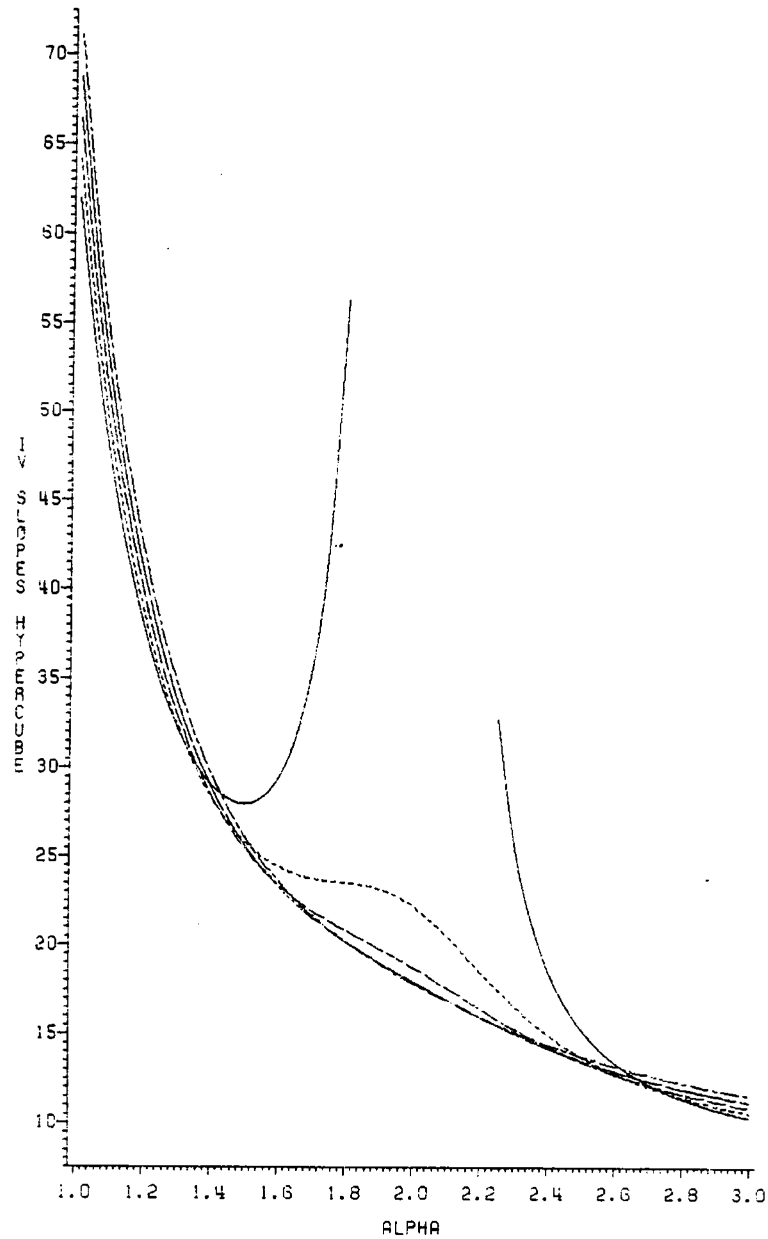

Figure 5.12

IV* on Region R_3, $k = 4$ ccd

Figures 5.8 and 5.11. This conclusion agrees with the conclusion reached for the IV-criterion.

Again, comparing the designs suggested by the D_s-criterion to those suggested by the IV*-criterion, we see a very nice agreement for regions R_1 and R_3. Both criteria suggest large α and with the large α, small numbers of center points. This agreement is not startling when we note that the IV*-criterion has slopes as its functions of interest. These slopes contain cross-product and quadratic terms; just those coefficients about which the D_s-criterion is concerned.

5.6 IV and IV* in Equiradial Design

The equiradial design was presented previously in Section 2.10. This k = 2 design places n_1 points on a circle of radius ρ and n_0 points at the center of the design. The design matrix was given in Section 2.10, and the moment matrix in Section 4.1.

In this section we discuss the choice of n_1, n_0 to optimize the IV and IV* criteria, for regions R_1 and R_3. Region R_2 is not reasonable here as the experimenter does not have an axial distance parameter to choose. All outer points must lie on the same circle. Also, because of the scale-invariance of the IV and IV* criteria, ρ will be fixed at $\rho = 1$.

Using the moment matrix given in equation (4.1.2) the M^{-1} can be found by applying results found in Graybill (1976) on partitioned matrices.

$$M^{-1} = \begin{bmatrix} (b^2-c^2)/D & 0 & 0 & -a(b-c)/D & -a(b-c)/D & 0 \\ 0 & \frac{1}{a} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{a} & 0 & 0 & 0 \\ -a(b-c)/D & 0 & 0 & (b-a^2)/D & -(c-a^2)/D & 0 \\ -a(b-c)/D & 0 & 0 & -(c-a^2)/D & (b-a^2)/D & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{c} \end{bmatrix}, \quad (5.6.1)$$

where

$$a = \frac{\rho^2 n_1}{2N}$$

$$b = \frac{3\rho^4 n_1}{8N}$$

$$c = \frac{\rho^4 n_1}{8N}$$

$$D = (b-c)(b+c-2a^2) \quad . \qquad (5.6.2)$$

Using (5.6.1), (5.3.8), and (5.4.7), the integrated variance criteria may be written

$$IV = \frac{b^2-c^2}{D} + \mu_2\left(\frac{2}{a} - \frac{2a(b-c)}{D}\right) + \mu_4 \cdot \frac{2(b-a^2)}{D}$$

$$+ \mu_{22}\left(\frac{1}{c} + \frac{2(a^2-c)}{D}\right) \ , \qquad (5.6.3)$$

and

$$IV^* = \frac{2}{a} + \mu_2\left(\frac{4(b-a\ )}{D} + \frac{2}{c}\right) \quad .$$

Table 5.1 presents the IV and IV* criteria for each of the two regions for n_0 = 1, 2, 3, 4, 5 and n_1 = 6, 7, 8, 9, 10, 11, 12, and regions R_1 and R_3.

For region R_1, there are several choices of (n_1,n_0) pairs which give best or almost best values of IV. The best pair of (n_1,n_0) is (11,5), giving IV = 6.4970. Each of the three pairs (6,3), (8,4) and (9,4) give IV = 6.5. The pair (11,5) has ratio of center points to outer points of 5:11. The D_s-best ratio from Chapter IV is 1:3 while the D-best ratio is 1:5. This suggests that the IV-criterion for R_1 requires more center points to achieve optimality than do either of the determinant criteria.

The cuboidal region R_3 has a different optimal pair. The pair producing the lowest IV for R_3 is (10,3). This ratio of center points to exterior points is much closer to that given by the D_s-criterion than that given in R_1. This is likely due to the portion of region R_3 that lies outside of $\{\underline{x}: x'x \le 1\}$. More emphasis is placed on the outer points to aid in the estimation of the response in these regions.

The IV* has the same optimal pair of (n_1,n_0) for both regions. This pair is (10,4). Here, the ratio of center points to exterior points is 2:5 or $1:2\frac{1}{2}$. Again, more center points are required by the IV* criterion for both regions than for the determinant-criteria.

Table 5.1

Integrated Variance Criterion for Equiradial

n_0	n_1	IV,R_1	IV,R_3	IV*,R_1	IV*,R_3
1	6	8.1667	5.7556	56.0000	38.8889
1	7	8.7619	5.9683	59.4286	41.1429
1	8	9.3750	6.2000	63.0000	43.5000
1	9	10.0000	6.4444	66.6667	45.9259
1	10	10.6333	6.6978	70.4000	48.4000
1	11	11.2727	6.9576	74.1818	50.9091
1	12	11.9167	7.2222	78.0000	53.4444
2	6	6.6667	5.4222	48.0000	33.7778
2	7	6.8571	5.4143	48.8571	34.2857
2	8	7.0833	5.4444	50.0000	35.0000
2	9	7.3333	5.5000	51.3333	35.8519
2	10	7.6000	5.5733	52.8000	36.8000
2	11	7.8788	5.6596	54.3636	37.8182
2	12	8.1667	5.7556	56.0000	38.8889
3	6	6.5000	5.6667	48.0000	34.0000
3	7	6.5079	5.5344	47.6190	33.6508
3	8	6.5694	5.4593	47.6667	33.6111
3	9	6.6667	5.4222	48.0000	33.7778
3	10	6.7889	**5.4119**	48.5333	34.0889
3	11	6.9293	5.4209	49.2121	34.5051
3	12	7.0833	5.4444	50.0000	35.0000
4	6	6.6667	6.0556	50.0000	35.5556
4	7	6.5476	5.8230	48.7143	34.5714
4	8	6.5000	5.6667	48.0000	34.0000
4	9	6.5000	5.5611	47.6667	33.7037
4	10	6.5333	5.4911	**47.6000**	**33.6000**
4	11	6.5909	5.4470	47.7273	33.6364
4	12	6.6667	5.4222	48.0000	33.7778
5	6	6.9667	6.5022	52.8000	37.6444
5	7	6.7429	6.1790	50.7429	36.1143
5	8	6.6083	5.9511	49.4000	35.1000
5	9	6.5333	5.7867	48.5333	34.4296
5	10	6.5000	5.6667	48.0000	34.0000
5	11	**6.4970**	5.5790	47.7091	33.7455
5	12	6.5167	5.5156	**47.6000**	33.6222

However, the D_s-criterion's suggested design is closer to that suggested by IV* than the design suggested by the D-criterion.

5.7 IV and IV* in k-factor Box-Behnken Designs

In a k-factor Box-Behnken design the experimenter is left to choose the number of center points to be used in the design. The objective in this section is to find numbers of center points to minimize the IV and IV* of a k-factor Box-Behnken design for k = 3, 4, 5 and 6. The regions of integration used are R_1 and R_3. Again, R_2 is unreasonable as the experimenter does not have an axial distance to choose.

When k = 3, 4, or 5, the usual Box-Behnken design, as given in the original 1960 paper, is constructed using a balanced incomplete block design. Because of this, the form of the IV and IV* may be written in general for these designs.

Using equation (5.3.8) and a general form for $(X'X)^{-1}$ found in Hussey (1983) for k = 3, 4, 5 Box-Behnken design, the general form of IV and IV* may be written as (5.7.1) and (5.7.2).

$$IV = N[a + \mu_2 \cdot (kc+2kb) + \mu_4 \cdot k \cdot d$$

$$+ \mu_{22} \cdot \frac{k(k-1)}{2} \cdot (2e+f)] \; , \qquad (5.7.1)$$

where

$$a = \frac{(A + (k-1)B)}{D}$$

$$b = -\frac{A}{D}$$

$$c = \frac{N}{A}$$

$$d = \frac{D + (A^2 - NB)}{D(A-B)}$$

$$e = \frac{A^2 - NB}{D(A-B)}$$

$$f = \frac{1}{B}$$

$$D = N(A + (k-1)B) - kA^2 \quad , \qquad (5.7.2)$$

(See Hussey (1983) for the elements of $(X'X)^{-1}$.) The IV* can be written as

$$IV^* = N \cdot \{k \cdot c + 4 \cdot k \cdot \mu_2 \cdot d + k(k-1)\mu_2 f\} \quad , \qquad (5.7.3)$$

where c, d, and f are defined above. The form of each of the criteria is much more complicated for the k = 6 Box-Behnken design. Because of this, the general forms given by (5.3.8) and (5.4.7) will instead be used to calculate the IV and IV* for this design.

Table 5.2 presents the IV and IV* for each of the two regions of interest, R_1 and R_3, and for k = 3, 4, 5 and 6. In each case, the

Table 5.2

Integrated Variance Criteria for Box-Behnken Designs

n_0	IV, R_1	IV, R_3	IV^*, R_1	IV^*, R_3
		K=3		
1	11.9554	7.7458	172.57	34.1250
2	**11.7250**	6.1250	148.05	29.7500
3	12.1518	5.7708	**145.12**	**29.3750**
4	12.7429	**5.7333**	147.60	30.0000
5	13.3996	5.8225	152.23	31.0250
6	14.0893	5.9750	157.95	32.2500
7	14.7977	6.1637	164.28	33.5893
8	15.5179	6.3750	171.00	35.0000
9	16.2458	6.6014	177.97	36.4583
10	16.9793	6.8383	185.13	37.9500
		K=4		
1	34.7222	13.3333	611.1111	80.5556
2	31.7778	11.2667	496.8889	66.4444
3	**31.5000**	10.8000	468.0000	63.0000
4	31.8889	**10.7333**	**460.4444**	**62.2222**
5	32.5444	10.8267	461.4222	62.5111
6	33.3333	11.0000	466.6667	63.3333
7	34.1984	11.2190	474.3492	64.4603
8	35.1111	11.4667	483.5556	65.7778
9	36.0556	11.7333	493.7778	67.2222
10	37.0222	12.0133	504.7111	68.7556
		K=5		
1	101.1645	23.3947	1741.89	169.4097
2	84.7153	21.0486	1409.37	138.5417
3	80.2766	**20.5544**	1314.96	129.8958
4	**78.8406**	20.5231	**1280.06**	**126.8056**
5	78.6057	20.6771	1268.97	125.9375
6	78.9712	20.9236	1269.79	126.1806
7	79.6800	21.2230	1277.41	127.0585
8	80.6032	21.5556	1289.29	128.3333
9	81.6694	21.9101	1303.99	129.8727
10	82.8356	22.2801	1320.68	131.5972
		K=6		
1	90.5263	24.3715	1858.81	144.3977
2	82.3738	20.6096	1596.75	125.1224
3	80.6213	19.5736	1526.69	120.0693
4	**80.4688**	19.2191	1504.63	118.5718
5	80.9562	**19.1373**	**1501.76**	**118.4964**
6	81.7637	19.1917	1508.50	119.1322
7	82.7540	19.3240	1520.72	120.1743
8	83.8587	19.5049	1536.37	121.4704
9	85.0395	19.7184	1554.30	122.9359
10	86.2736	19.9545	1573.84	124.5198

value of the IV or IV* that is smallest is highlighted.

A general pattern noticeable in Table 5.2 is that as k increases, the number of center points required by each of the criteria, for each of the regions increases. Also, for each region, the IV* requires the same number of center points for a fixed value of k. This indicates the slopes are estimated with nearly the same precision in both regions. This can be explained by noting that for both regions, the points of the k-factor Box-Behnken design lie totally within the regions of interest. The regions, R_1 and R_3, will most surely contain areas where the slope and in fact the response function are poorly estimated, i.e. estimated with large variance. With respect to estimation of slopes these two regions must not be substantially different according to Table 5.2.

Comparing the number of center points required by the prediction variance criteria, IV and IV*, with the number required by the determinant criteria D- and D_s-optimality, we see that the IV and IV* criteria require more center points for each region and value of k. The results of Chapter IV summarized in Table 4.1 and Table 4.2 for the Box-Behnken designs show that both determinant criteria require no more than three center points. Table 5.2 shows the IV and IV* criteria require three or more center points, except for region R_1, $k = 3$ when two center points are required.

5.8 IV and IV* for Small Composite Designs

The small composite designs of Westlake, Hartley and Draper were introduced in Section 2.8. These designs are typically used when observations are expensive and the number of observations must be kept to a minimum. As mentioned before, in each of the three types of small composite designs under study, the number of points is reduced by extensive aliasing in the factorial portion of the composite design. This aliasing causes a covariance structure to exist between the linear and cross-product coefficient. Because of this covariance structure, two things result in our study of these designs. First, the general forms (5.3.8) and (5.4.7) must be used to calculate IV and IV*. Second, we would expect the IV and IV* criteria to suffer due to this covariance structure. This will be demonstrated in what follows.

As we are again studying composite designs, each of the three regions will be reasonable regions of interest to the experimenter. We will look first at Hartley's designs for $k = 4$ and 6 for each of the three regions. We will then study the four designs for the $k = 5$ case, Westlake's three designs and Draper's design, again for each region.

Figures 5.13 through 5.18 are the plots of IV and IV* against α for Hartley's $k = 4$ design. From these plots, a pattern very much like the central composite design emerges. That is

(i) When $n_0 = 0$, IV and IV* are extremely large at $\alpha = \sqrt{k}$.

(ii) For $n_0 \geq 1$, the curves for IV in R_1 are decreasing with increasing α. As α approaches $\alpha = \sqrt{k}$, the number of center points needed becomes larger.

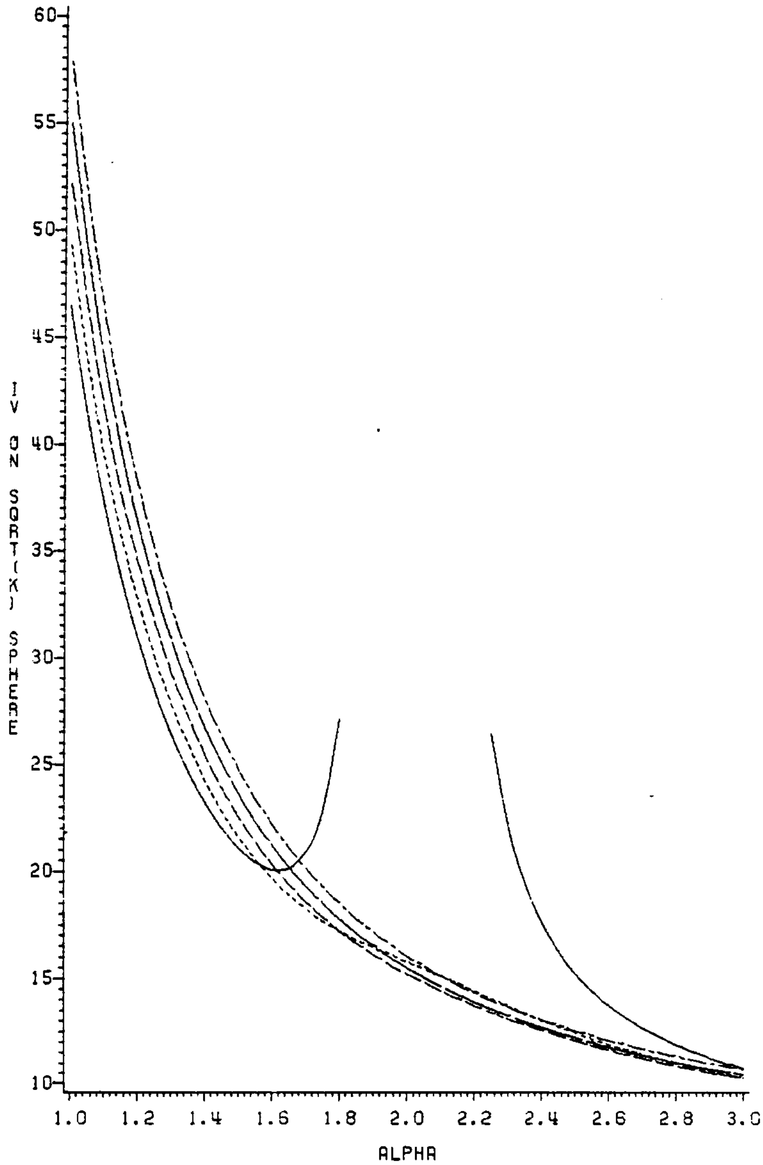

Figure 5.13

IV on Region R_1, Hartley $k = 4$

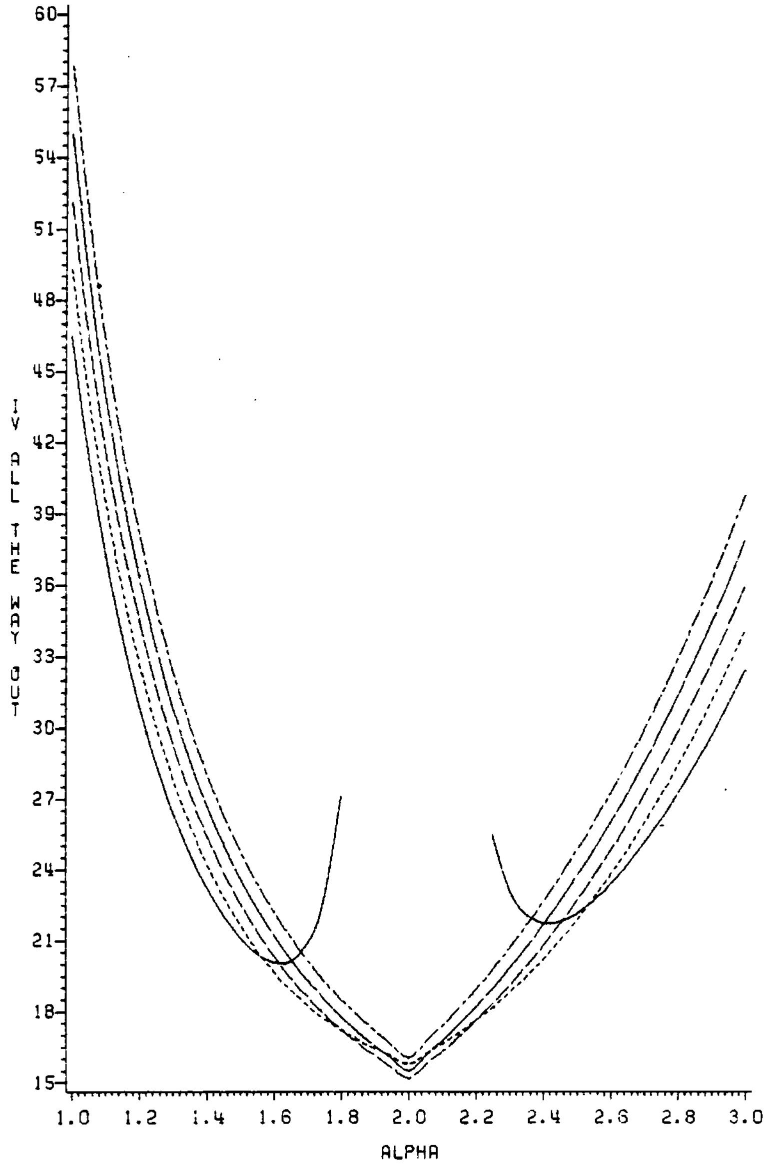

Figure 5.14

IV on Region R_2, Hartley $k = 4$

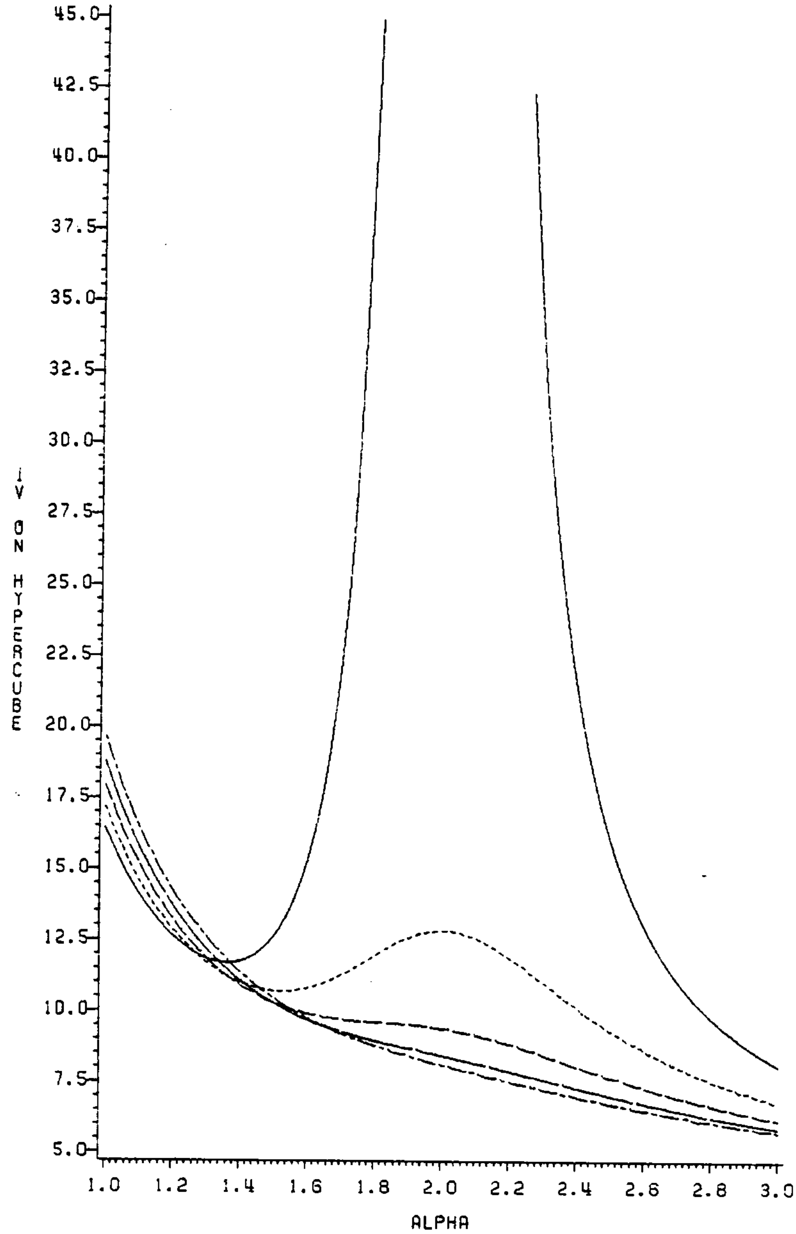

Figure 5.15

IV on Region R_3, Hartley $k = 4$

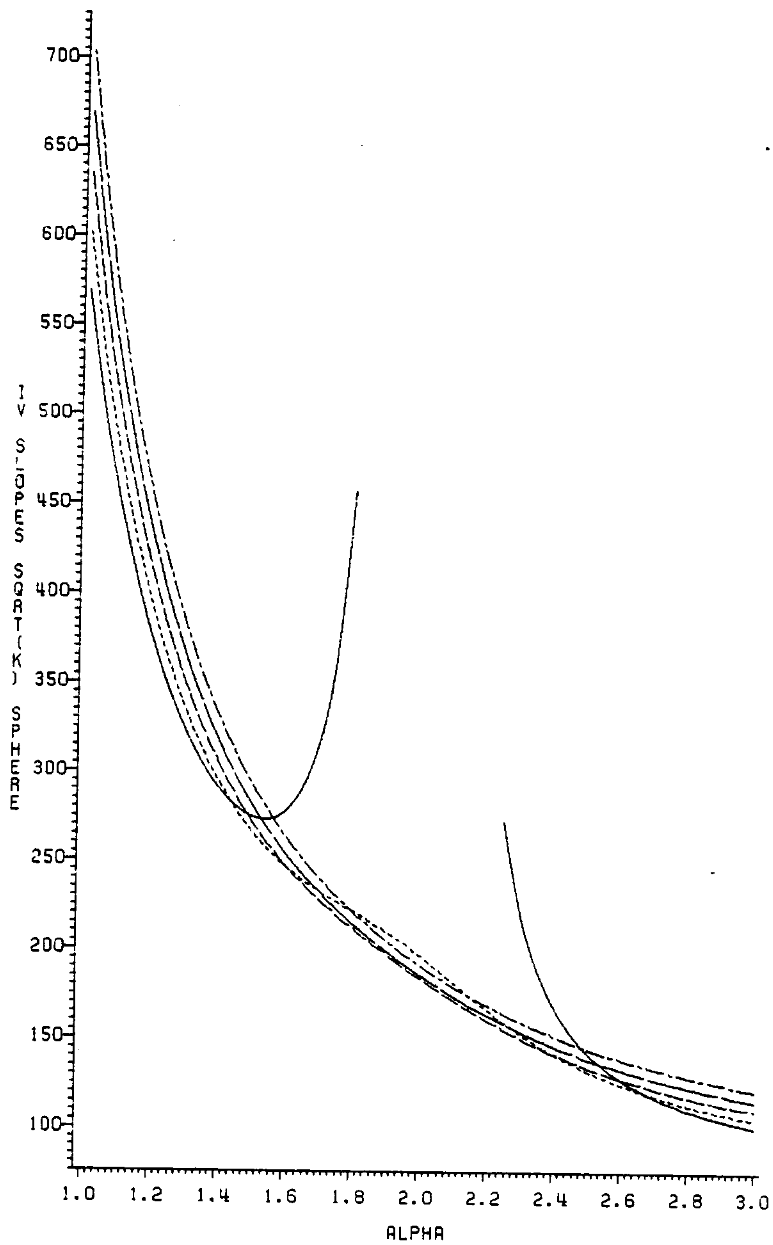

Figure 5.16

IV* on Region R_1, Hartley $k = 4$

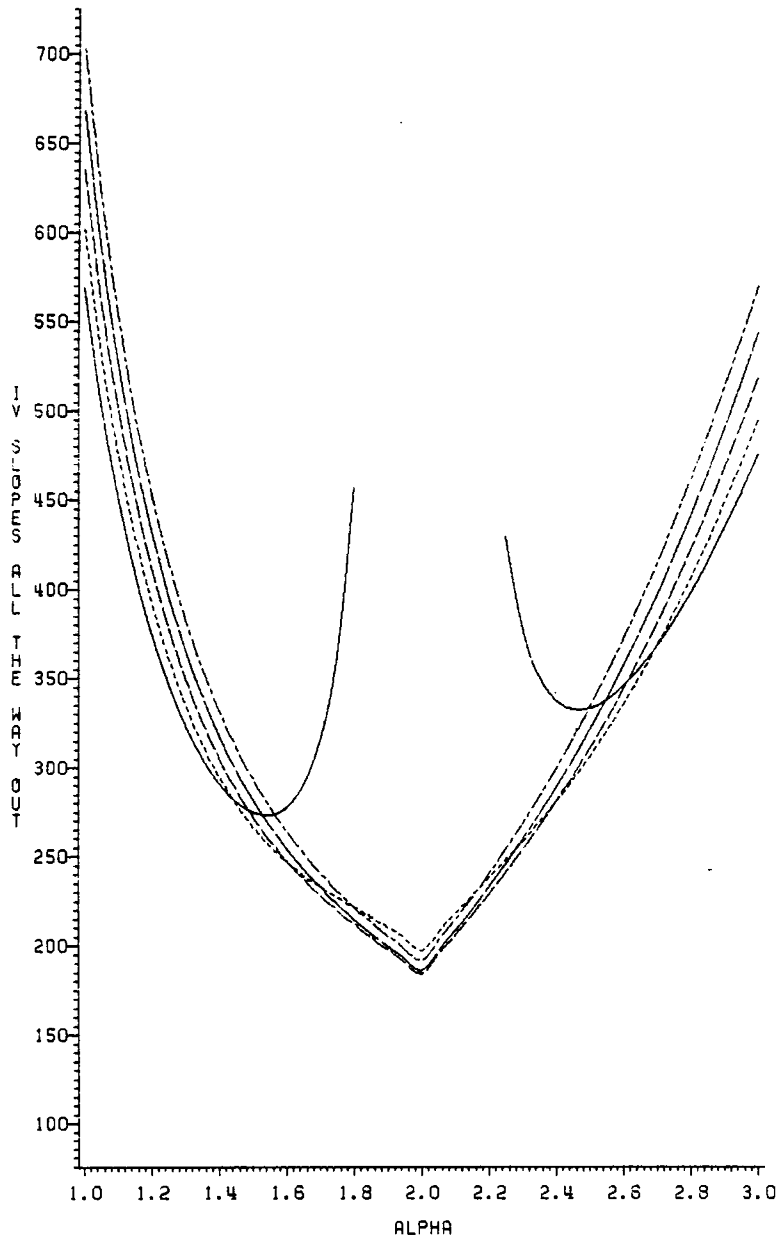

Figure 5.17

IV* on Region R_2, Hartley $k=4$

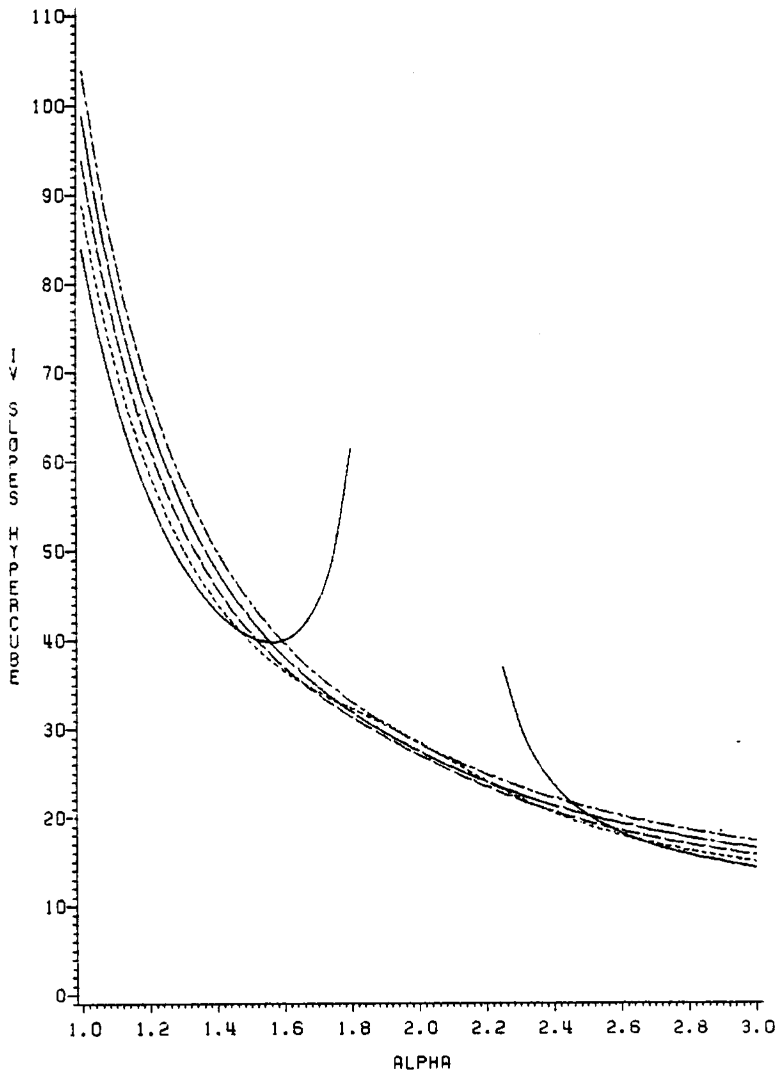

Figure 5.18

IV* on Region R_3, Hartley $k = 4$

(iii) The plots of IV against α, for $n_0 \geq 1$, are bowl-shaped with a minimum at $\alpha = \sqrt{k}$. Here, for large or small values of α, $n_0 = 0$ is the optimal number of center points.

(iv) The curves for IV against α in R_3 are relatively flat. However, they decrease more than they do for the k = 4 central composite design. For moderately large α, (say, $\alpha > 1.6$) large numbers of center points is optimal.

(v) Again the plots of IV* against α are similar for R_1 and R_3. In these plots, $n_0 \geq 1$, the curves are decreasing with increasing α. If α is large or small, $n_0 = 0$ is the optimal choice. For moderate α, larger numbers of center points are required.

(vi) The plots for IV* against α for R_2 show the same bowl-shape as the plots of IV against for R_2. The same conclusion on choice of center points for IV holds.

Figures 5.19 through 5.24 are plots of IV and IV* against α for Hartley's k = 6 design. As the reader can see, the plots are very similar to those for the k = 4 case. Because of this, the same conclusions as those reached for the k = 4 case will be reached here. For conciseness, these conclusions will not be repeated.

Plots of IV and IV* against α were generated from each of the four five-factor small composite designs: Westlake #1, Westlake #2, Westlake #3 and Draper. The general shape of the plots is the same as for the other composite designs. The conclusions which can be reached concerning parameter choices are similar, also. Because of

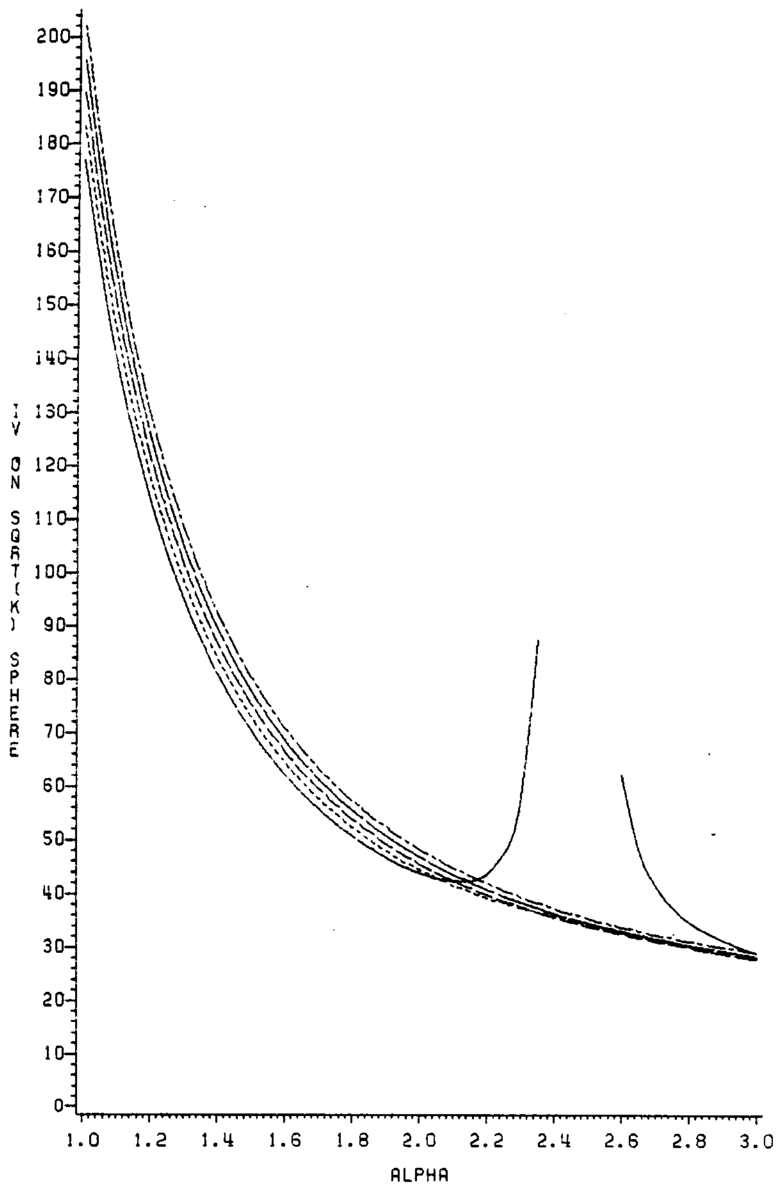

Figure 5.19

IV on Region R_1, Hartley $k = 6$

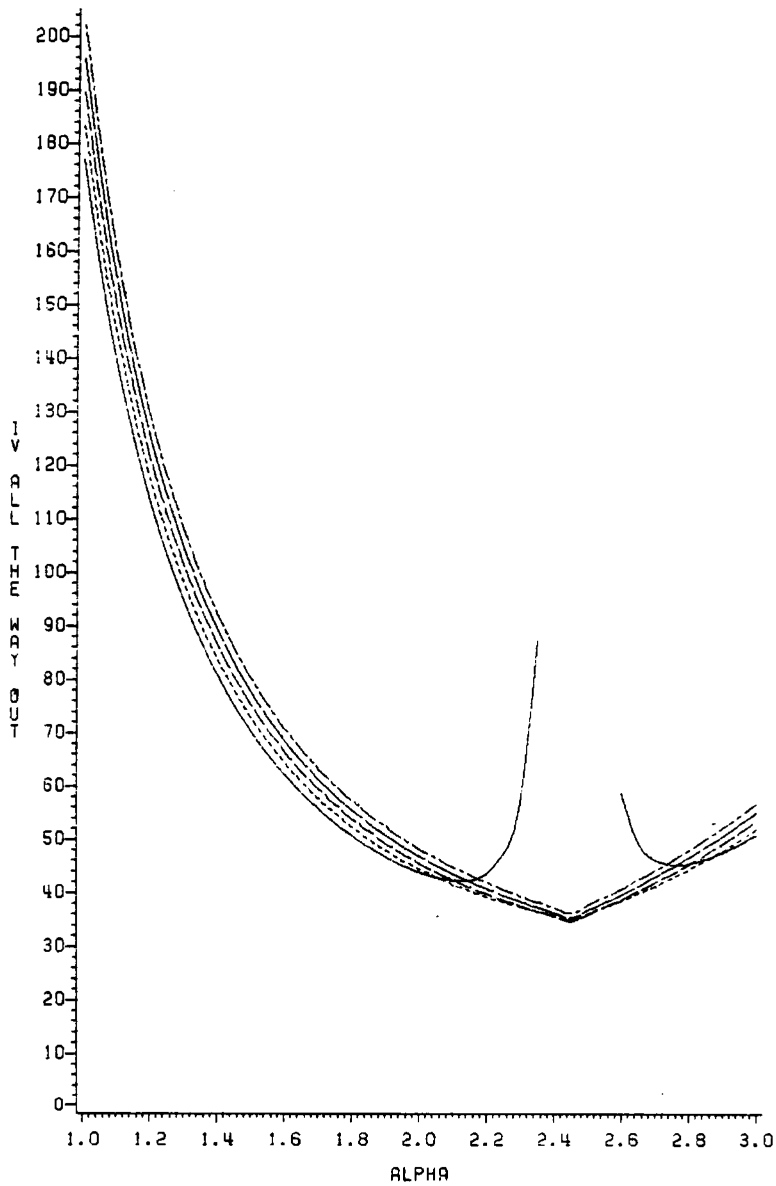

Figure 5.20

IV on Region R_2, Hartley $k = 6$

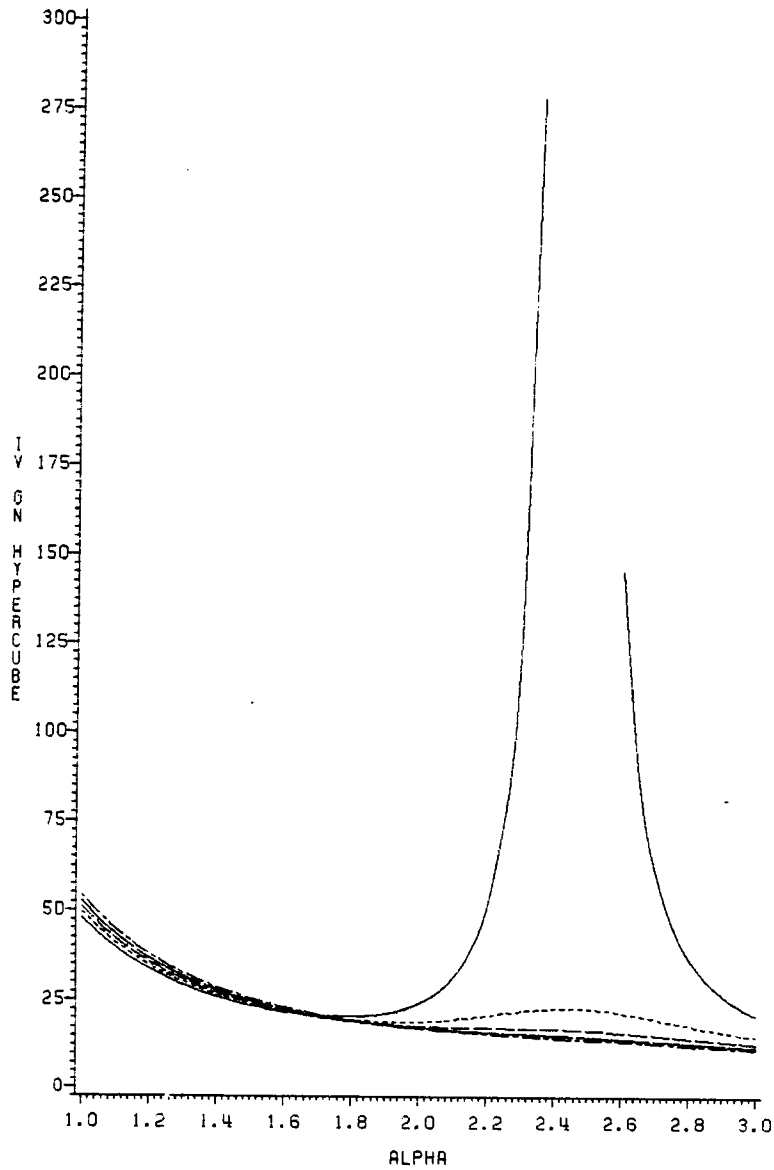

Figure 5.21

IV on Region R_3, Hartley $k = 6$

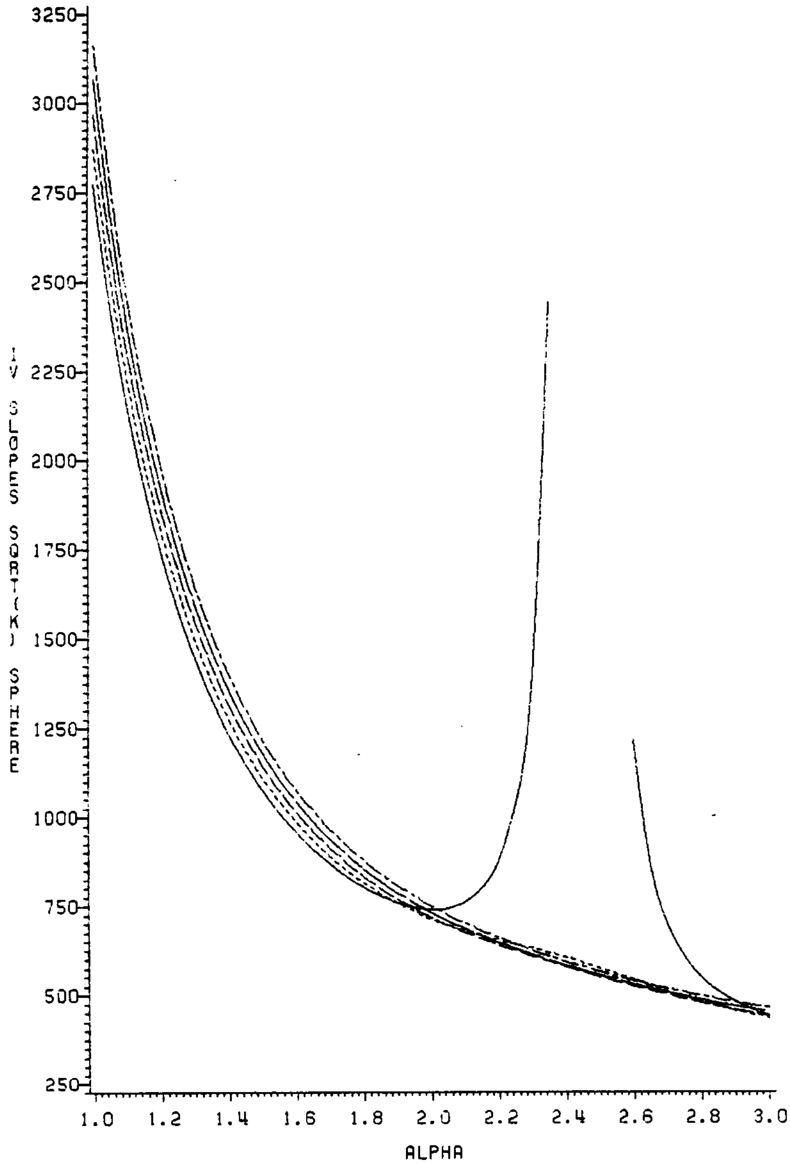

Figure 5.22

IV* on Region R_1, Hartley $k = 6$

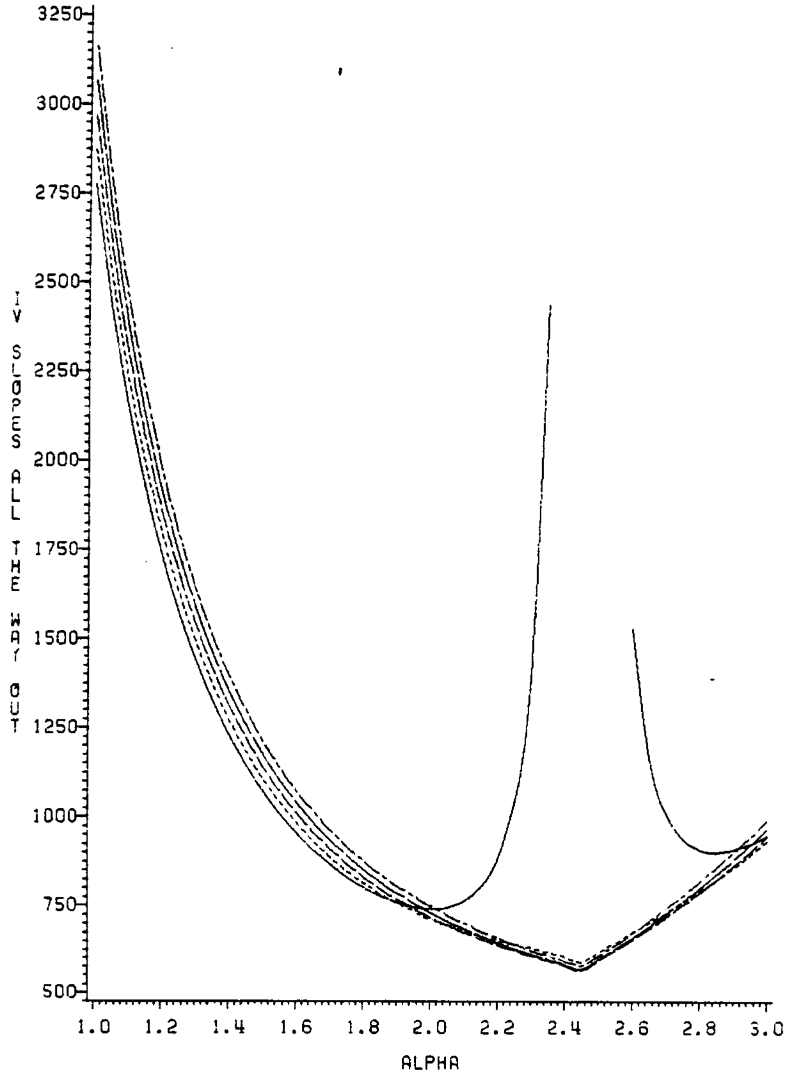

Figure 5.23

IV* on Region R_2, Hartley $k = 6$

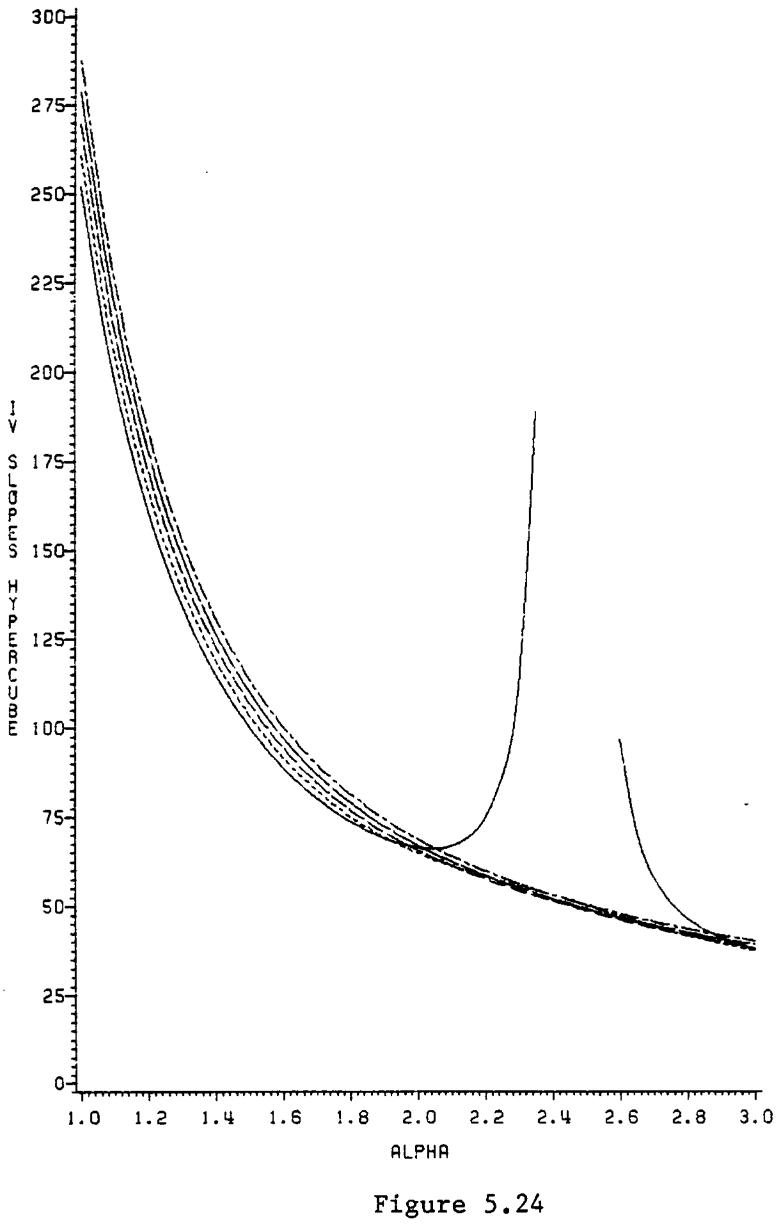

Figure 5.24

IV* on Region R_3, Hartley $k = 6$

this similarity, the plots are not included. Since our interest here is on the ordering of the designs with respect to IV and IV*, this ordering is reported.

The ordering for both criteria is

$$\text{Essentially tied}\left\{\begin{array}{ll}1. & \text{Draper's}\\ 2. & \text{Westlake's \#3}\end{array}\right.$$

3. Westlake's #2

4. Westlake's #1

The design of Draper yields essentially the same plot as Westlake's #3. The other rankings are very clear. We should note that this ordering is opposite from the ordering obtained by the D_s- and D-criteria. The covariance structure in the variance-covariance matrix of the least squares estimator will certainly play a large role in the integrated variance criteria. This fact accounts for the difference in the orderings between the two types of criteria; integrated variance and determinants.

CHAPTER VI

SUMMARY, RECOMMENDATIONS, AND FURTHER RESEARCH

The purpose of this thesis was to apply a design criteria, D_s-optimality, to several classes of response surface designs with the goal of constructing designs that are the best according to this criterion. Justification for the use of this criterion was provided by a modest statistical experiment as well as other considerations. Further, this thesis extended the results of previous work on D-optimal response surface designs. Finally, the classes of designs studied by the D_s-criterion were also studied using integrated variance criteria to assess the quality of D_s-best response surface designs from the standpoint of prediction.

This chapter will summarize the results obtained from both types of optimality criteria, D_s-optimality, IV and IV*. This will be done by collecting the recommended designs for each class and then comparing between these designs for fixed k.

6.1 D_s-Best Response Surface Designs

The D_s-criterion has been used in this thesis as a selection criterion to choose between the response surface designs in a particular class. The selection of the designs using D_s-optimality has generated rules for constructing designs. These rules are collected here as a summary of the results of the study of the D_s-criterion.

- Central Composite Design, $k = 2, 3, 4, 5, 6$
  - α as large as practicable,
  - if α is close to $\sqrt{k}$, use some center points (see Figures 3.3 through 3.9, and Theorem 3.3),
  - if all points may be replicated, use weights given by Theorem 3.3 or in Tables 3.10 - 3.14,
  - if only a small number of points may be replicated, use Tables 3.10 - 3.14 as a guide to which points to replicate.
- Equiradial Design, $k = 2$
  - choose ρ as large as practicable,
  - choose n_0 according to Theorem 4.2.
- Box-Behnken Design, $k = 3, 4, 5, 6$
  - choose n_0 as in Table 4.1 or 4.2, depending on value of k,
  - usually 2 or 3 center points.
- Small Composite Design, $k = 4, 5, 6$
  - choose α as large as practicable,
  - choose n_0 using plots in Figures 4.1 through 4.6.

For a fixed k, the composite designs may be compared. This can be done by comparing plots of $\log(\det(M^{22}))$ against α for each design. From this comparison, the central composite designs with a full factorial portion are better in terms of D_s-optimality than the other composite designs for fixed α. This seems reasonable as we would expect the small composite designs to suffer because of the covariance structure caused by aliasing. Also, for fixed k and a reasonable choice of α (say, α near $\sqrt{k}$), the composite designs are substantially better in terms of D_s-optimality than the Box-Behnken designs.

(See, for example, the k = 6 Box-Behnken and Hartley's k = 6 small composite design.) The fact that the Box-Behnken designs do not perform well is probably due to their lack of flexibility achieved in the composite designs by the choice of the axial point.

6.2 IV- and IV*-Best Designs

The classes studied using the D_s-criterion were also studied by two integrated variance criteria for three regions of interest. The results of this study are summarized below and compared with the results from D_s-optimality.

- Central Composite Design
  - IV
    - R_1: α as large as practicable, several center points
    - R_2: $\alpha = \sqrt{k}$, several center points
    - R_3: many center points, α makes little difference
  - IV*
    - R_1: α as large as practicable, no center points
    - R_2: $\alpha = \sqrt{k}$, several center points
    - R_3: same as IV* for R_1.
- Equiradial Design
  - IV
    - R_1: $n_1 = 11$, $n_0 = 5$
    - R_3: $n_1 = 10$, $n_0 = 3$
  - IV*
    - R_1: $n_1 = 12$, $n_0 = 5$ or $n_1 = 10$, $n_0 = 4$
    - R_3: $n_1 = 10$, $n_0 = 4$

- Box-Behnken
  - IV
    - R_1: $k = 3$, $n_0 = 2$; $k = 4$, $n_0 = 3$; $k = 5$ or 6, $n_0 = 4$
    - R_3: $k = 3$, $n_0 = 4$; $k = 4$, $n_0 = 4$; $k = 5$, $n_0 = 3$;
      $k = 6$, $n_0 = 5$
  - IV*
    - R_1: $k = 3$, $n_0 = 3$; $k = 4$, $n_0 = 4$; $k = 5$, $n_0 = 4$;
      $k = 6$, $n_0 = 5$
    - R_3: same as IV* for R_1 .
- Small Composite Design
  - The results are essentially identical to those of the central composite designs.

As was mentioned in Chapter V, the designs suggested by the IV*-criterion and those suggested by D_s-optimality agree for the composite designs. For the other classes, equiradial and Box-Behnken, the IV* criterion requires more center points. This is probably due again to the lack of flexibility of the latter two classes of designs.

6.3 Further Research

As is the case with most research projects of this type, this investigation has raised questions which merit further study. Some of these questions are:

- There are less widely used design classes (e.g. hybrid) that should be studied with respect to the D_s-, IV- and IV*-criteria.

- In studying the plots of IV and IV* against α for central composite designs with the various regions, the notion of regions of large integrated variance was mentioned. This notion suggests that designs that appear good in other respects may be bad for even slight extrapolations.
- Other regions of interest might be suggested. A study of IV and IV* with these new regions for the composite designs would be interesting.
- The effect of aliasing on the four criteria studied in this thesis is very evident in the small composite design. A characterization of this effect would be useful.

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Appendix I

```
PROC MATRIX FUZZ;
FETCH XYY DATA=ONE;

*--------------------------------------------------------*
* THE FOLLOWING LINES SET-UP THE VARIABLES NEEDED TO    *
* DO THE LOOPING. THEY ARE Y VALUE INDEPENDENT.          *
*                                                        *
*  N=NUMBER OF DESIGN POINTS.                            *
*  P=NUMBER OF VARIABLES=(K+2)*(K+1)/2                   *
*  CRITVAL=F-VALUE FOR CONSTRUCTING A (1-ALPHA)*100%     *
*          CONFIDENCE ELLIPSOID FOR BETA.                *
*  PORIG=MATRIX TO TRANSFORM TO PRINCIPAL COMPONENTS.    *
*--------------------------------------------------------*;

N=NROW(XYY);P=NCOL(XYY);
X=J(N,1,1)||XYY(,1:P-1);
PRINT X; PIFOUR=ARCOS(0)#/2;XPX=X'*X;
EIGEN D PP XPX; DI=DIAG(1#/SQRT(D)); PORIG=PP*DI;
CRITVAL=FINV(.90,P,N-P);

*--------------------------------------------------------*
*  THE LOOP INDEXED BY NTIMES IS THE LOOP TO CREATE      *
*  Y-DATA. BEFORE DOING THE LOOPS FOR FINDING THE        *
*  CONFIDENCE INTERVALS, WE FIND BETAHAT ALSO.           *
*--------------------------------------------------------*;

DO NTIMES=1 TO 250;
Y=XYY(,P)+RANNOR(J(N,1,5647479979696972));
XY=X||Y;XYPXY=XY'*XY;
SOLN=SWEEP(XYPXY,1:P);BETA=SOLN(1:P,P+1);
SIGMA2=SOLN(P+1,P+1)#/(N-P);CC=SQRT(CRITVAL*P*SIGMA2);

 DISCRIM=SQRT((BETA(4,)-BETA(5,))*(BETA(4,)-
          BETA(5,))+BETA(6,)*BETA(6,));
 LNOW=((BETA(4,)+BETA(5,))+DISCRIM)#/2;

 DETBETA=BETA(4,)*BETA(5,)-BETA(6,)*BETA(6,)#/4;

 XONOW=-BETA(2,)*BETA(5,)+BETA(6,)*BETA(3,)#/(2*DETBETA)//
       -BETA(3,)*BETA(4,)+BETA(6,)*BETA(2,)#/(2*DETBETA);

 YNOW=BETA(1,)-(BETA(2,)*BETA(2,)*BETA(5,)+BETA(3,)*BETA(3,)*
      BETA(4,)-BETA(2,)*BETA(3,)*BETA(6,))#/(4*DETBETA);
```

```
*     SET THE VARIABLES TO START THE LOOP                    *;

LSMALP=100000000;LLARGP=-10000000;
LSMALM=100000000;LLARGM=-10000000;
YSMALL=100000000;YLARGE=-10000000;
X01SMA=100000000;X01LAR=-10000000;
X02SMA=100000000;X02LAR=-10000000;
PTCOUNT=0;

PAGE;

*-----------------------------------------------------*
* START THE DO-LOOPS TO DO THE SEARCH. THE Z-I S ARE  *
* GENERALIZED POLAR COORDINATES.                      *
*-----------------------------------------------------*;

DO T1=-PIFOUR TO PIFOUR BY 2*PIFOUR;
 Z1=SIN(T1);
  DO T2=-PIFOUR TO PIFOUR BY 2*PIFOUR;
   Z2=Z1*SIN(T2)#/TAN(T1);
    DO T3=-PIFOUR TO PIFOUR BY 2*PIFOUR;
     Z3=Z2*SIN(T3)#/TAN(T2);
      DO T4=-PIFOUR TO PIFOUR BY 2*PIFOUR;
       Z4=Z3*SIN(T4)#/TAN(T3);
        DO T5=-3*PIFOUR TO 3*PIFOUR BY 2*PIFOUR;
         Z5=Z4*SIN(T5)#/TAN(T4);
         Z6=Z5#/TAN(T5);
          Z=Z1//Z2//Z3//Z4//Z5//Z6;
          PROD=PORIG*Z;

*      THE VALUE OF CC IS THE F*SIGMA CUTOFF                  ;

          DO R=.1*CC TO CC BY .1*CC;
           ZZ=R*PROD;ZZZ=ZZ';
           PTCOUNT=PTCOUNT+1;

           BNEW=BETA-ZZ;

           DISCRIM=SQRT((BNEW(4,)-BNEW(5,))*
           (BNEW(4,)-BNEW(5,))+BNEW(6,)*BNEW(6,));

           LTESTP=((BNEW(4,)+BNEW(5,))+DISCRIM)#/2;
           LTESTM=((BNEW(4,)+BNEW(5,))-DISCRIM)#/2;

           DETBNEW=BNEW(4,)*BNEW(5,)-BNEW(6,)*BNEW(6,)#/4;
```

```
           XOTEST=-BNEW(2,)*BNEW(5,)+BNEW(6,)*BNEW(3,)
                  #/(2*DETBNEW)//-BNEW(3,)*BNEW(4,)+BNEW(6,)
                  *BNEW(2,)#/(2*DETBNEW);

           YTEST=BNEW(1,)-(BNEW(2,)*BNEW(2,)*
                 BNEW(5,)+BNEW(3,)*BNEW(3,)*BNEW(4,)-
                 BNEW(2,)*BNEW(3,)*BNEW(6,))#/(4*DETBNEW);

*         TEST THE VALUES OBTAINED                      ;

           IF LTESTP<LSMALP THEN LSMALP=LTESTP;
           IF LTESTP>LLARGP THEN LLARGP=LTESTP;
           IF LTESTM<LSMALM THEN LSMALM=LTESTM;
           IF LTESTM>LLARGM THEN LLARGM=LTESTM;
           IF YTEST<YSMALL THEN YSMALL=YTEST;
           IF YTEST>YLARGE THEN YLARGE=YTEST;
           IF XOTEST(1,)>X01LAR THEN X01LAR=XOTEST(1,);
           IF XOTEST(1,)<X01SMA THEN X01SMA=XOTEST(1,);
           IF XOTEST(2,)>X02LAR THEN X02LAR=XOTEST(2,);
           IF XOTEST(2,)<X02SMA THEN X02SMA=XOTEST(2,);

         END;
       END;
     END;
   END;
 END;
END;
PAGE;

OUTMAT=NTIMES||YSMALL||YLARGE||LSMALP||LLARGP||LSMALM||LLARGM||
       BETA'||YNOW||LNOW||XONOW'||X01SMA||X01LAR||X02SMA||X02LAR;
OUTPUT OUTMAT DATA=SIMUL(RENAME=(COL1=NTIMES COL2=YSMALL
                  COL3=YLARGE COL4=LSMALP COL5=LLARGP
                  COL6=LSMALM COL7=LLARGM COL8=BETA0
                  COL9=BETA1 COL10=BETA2 COL11=BETA11
                  COL12=BETA22 COL13=BETA12 COL14=YNOW
                  COL15=LNOW COL16=X01 COL17=X02 COL18=X01SMA
                  COL19=X01LAR COL20=X02SMA COL21=X02LAR));

END;
```

Appendix II

The following are the factorial portions of the small composite designs used in Chapter 4.

HARTLEY DESIGN, K=4;

$$D = \begin{matrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{matrix}$$

DRAPERS DESIGN, K=5;

$$D = \begin{matrix} 1 & 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 \end{matrix}$$

WESTLAKE DESIGN NUMBER ONE, K=5

$$D = \begin{matrix} -1 & 1 & 1 & -1 & -1 \\ -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 \\ -1 & -1 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & -1 & 1 \end{matrix}$$

WESTLAKE DESIGN NUMBER TWO, K=5

$$
D = \begin{matrix}
-1 & -1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 \\
-1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 \\
-1 & 1 & 1 & -1 & 1 \\
-1 & 1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & -1 & 1 \\
-1 & -1 & 1 & -1 & 1 \\
-1 & -1 & -1 & 1 & 1 \\
1 & -1 & 1 & 1 & 1
\end{matrix}
$$

WESTLAKE DESIGN NUMBER THREE, K=5

$$
D = \begin{matrix}
-1 & -1 & 1 & 1 & -1 \\
1 & -1 & 1 & -1 & -1 \\
1 & -1 & -1 & 1 & -1 \\
-1 & -1 & -1 & -1 & -1 \\
-1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 \\
1 & 1 & -1 & 1 & 1 \\
-1 & 1 & -1 & -1 & 1 \\
-1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 \\
-1 & -1 & -1 & -1 & 1
\end{matrix}
$$

HARTLEY DESIGN, K=6

$$
D = \begin{matrix}
1 & -1 & -1 & 1 & -1 & -1 \\
-1 & 1 & -1 & 1 & -1 & -1 \\
-1 & -1 & 1 & 1 & -1 & -1 \\
1 & 1 & 1 & 1 & -1 & -1 \\
1 & -1 & -1 & -1 & 1 & -1 \\
-1 & 1 & -1 & -1 & 1 & -1 \\
-1 & -1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & -1 & 1 & -1 \\
1 & -1 & -1 & -1 & -1 & 1 \\
-1 & 1 & -1 & -1 & -1 & 1 \\
-1 & -1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 \\
-1 & 1 & -1 & 1 & 1 & 1 \\
-1 & -1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1
\end{matrix}
$$

APPENDIX III

The following are the region moments needed in the calculation of IV and IV* of Chapter V.

R_1:

$$\mu_2 = k/(k+2)$$

$$\mu_4 = 3k^2/[(k+2)(k+4)]$$

$$\mu_{22} = 3k^2/[(k+2)(k+4)]$$

R_2: Let $m = \max\{\alpha^2, k\}$.

$$\mu_2 = m/(k+2)$$

$$\mu_4 = 3m^2/[(k+2)(k+4)]$$

$$\mu_{22} = m^2/[(k+2)(k+4)]$$

R_3:

$$\mu_2 = 1/3$$

$$\mu_4 = 1/5$$

$$\mu_{22} = 1/9$$

See Hussey (1983) or Myers (1976) for details.

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