Efficiency evaluation for the nested cube response surface design
by Melvin Gail Linnell

A thesis submitted in partial fulfillment of the requirements for the degree of DOCTOR OF PHILOSOPHY in Mathematics
Montana State University

Abstract:
The nested cube response surface design is defined and its attributes described. Variance, bias and potential estimators are evaluated for the nested cube design. The standard least-squares estimator is examined for the quadratic and cubic models. Estimable parameters in the cubic model are derived for the nested cube design as well as a set of select designs. A minimum bias estimator is examined where the true model is cubic and the fitted model is quadratic. The nested cube design was the only design of the set examined for which the estimator existed. Two measures of bias efficiency are introduced and used to compare the nested cube design to a set of selected designs. Variance efficiency is evaluated in terms of A-, V-, and D-efficiencies. A calculation formula for the determinant of the sum of squares matrix is derived for symetric designs with zero odd moments. Profiles of the variance are shown on selected vectors in the region of interest.

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ABSTRACT

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1. INTRODUCTION

Response surface methodology is a collection of statistical and mathematical techniques used by researchers to aid in the study of relations between quantitative, continuous variables. Applications usually involve some system in which a feature of the system is influenced by one or more variables. This feature is termed the response. Examples of this are: (1) crop yield, (2) proportion of a population responding to a stimulus, (3) textile strength, and (4) proportion of end products meeting quality standards. Variables that influence the response are termed input variables or independent variables. These are subject to control by the researcher. Examples of independent variables corresponding to the previously mentioned responses are: (1) amounts of various fertilizers applied, (2) doses of the stimulus, (3) types of weave or mixture of fiber content, and (4) temperature of reaction, method of cleaning or time to cool. The activities included in response surface methodology entail the design of the experiment, development of the model and data analysis.

1.1 Literature Review

The use and study of response surface methodology has gained a high level of use since the Box and Wilson (1951) paper. Mead and Pike (1975) examined 412 papers in fifteen journals in the biological sciences. One-fourth utilized response surface techniques.

The goal associated with many response surface studies is the optimization of the response. This goal was behind many of the early papers by Box. Box and Wilson (1951) discuss the method of steepest ascent in the search for an optimum or near optimum setting for the independent variables. This technique and other sequential techniques have been applied extensively in the fields of chemistry and chemical engineering.

In the same paper, Box and Wilson (1951) introduced the concept of a composite design. This concept involved a balanced addition of experimental points to the standard factorial designs in order to obtain desirable properties. Some of the properties for which they strived are rotatability, uniform precision and estimability of second order terms. Designs are rotatable when the variance of an estimate of the response is equal at points of equal distance from the center of the settings for the independent variables. Many of the designs used today are composite designs of one form or another.

Box and Draper (1959) examined the criteria for selecting a design. They demonstrate that different designs should be used for different objectives. One of the criteria that they consider is bias in estimation due to fitting an inappropriate model. Karson, Manson, and Hader (1969) and Karson (1970) expanded on this by considering the alternative of using the form of the estimator rather than design construction to minimize bias for designs satisfying certain criteria.

Beginning with Keifer (1959) the concepts of optimal designs and design efficiency have influenced statistical literature and practice. Some of the design criteria proposed are D-optimality, G-optimality, A-optimality, and V-optimality. D-optimality seeks to minimize $|(X'X)^{-1}|$ or equivalently seeks to maximize $|X'X|$ where X is the design matrix defined explicitly in Chapter 2. G-optimality seeks to minimize the maximum variance of the estimator in the region of interest. Keifer (1974) shows that when using standard least-squares estimation a design is G-optimal if and only if it is D-optimal thus the two criteria are equivalent. A-optimality considers minimizing the trace of the variance-covariance matrix of the parameters of the model. V-optimality considers the integrated variance of the estimator and seeks to minimize this quantity. Efficiency measures corresponding to these have been developed and are used to compare designs.

1.2 Dissertation Objective

As Box and Draper (1959) demonstrated, the objective of an experiment is a determining factor in deciding which design is best suited for an experiment. A particular situation of interest was agricultural field trials. Review of papers and interviews with researchers in this field indicated that a quadratic polynomial is generally an adequate model. In some instances, however, higher order terms may be present. A design that has equal spacing and is easily expanded to include another independent factor or reduced when a factor is abandoned is more desirable than one without such features. The deletion of a factor may result from a factor being included initially when setting up the experiment, but eliminated during analysis after deciding the information on that factor is nil.

Thus four qualities to consider in evaluating a design are:

1. precision of estimation in a specified region of interest;
2. ability to detect departure from quadratic model and expand model if departure is detected;
3. equal spacing of factor levels;
4. number of factors can be expanded or reduced easily.

Initial work indicated that the nested cube design, to be described in detail in Chapter 2, has the four qualities. The objective of the dissertation can be given in four parts:

1. show that the nested cube design has qualities three and four but that not all designs in use do;
2. examine the estimability of quadratic and cubic models for the nested cube design;
3. examine the variance structure of estimates using the nested cube design and compare it to other selected designs;
4. examine the bias resulting from using a quadratic model when the true model is cubic for the nested cube design and compare it to other selected designs.

2. DESCRIPTION OF THE NESTED CUBE DESIGN

An experimental design may be defined as a specification of factors, a selection of levels and combinations of levels of factors, and a determination of structure and extent of replication. A response surface problem starts with the selection of factors. If too many factors are selected, the experimental runs necessary to provide adequate information become too large. If too few factors are selected, the researcher misses some potentially important agents influencing the response.

The combinations of levels of factors utilized for a specific experimental unit or trial of the basic experiment is often called an experimental setting or design point. In an experiment having K factors, an experimental setting consists of a K-tuple such as $\Lambda' = (\lambda_1, \lambda_2, \ldots, \lambda_K)$ where λ_i = level of factor i. The region of interest to be considered is of the form $(\gamma_1 \pm \delta_1, \ldots, \gamma_K \pm \delta_K)$, that is, a hyper-rectangular region.

Investigation of a design in terms of the original space gives the impression that each design is unique. It is convenient to standardize the analysis by transforming the experimental settings and the region of interest to a unit hypercube. The required linear transformation is:

$$x_u = (\lambda_u - \gamma_u)/\delta_u \qquad u = 1, \ldots, K. \tag{2.1}$$

The result is a transformed setting

$$X' = (x_1, \ldots, x_K), \tag{2.2}$$

where $-1 \leq x_i \leq 1$ for $i = 1,\ldots,K$. A specific example of this transformation is given in the example later in the chapter.

Choice of an experimental design consists of selecting a specific set of K-tuples from the unit hypercube. The most elementary design in common use contains the set $(\pm 1,\pm 1,\ldots,\pm 1)$. This is called a 2^K design. It allows for the fitting of polynomial models containing linear terms and cross products for all variables. Additional experimental settings are necessary to fit higher order polynomials or other more complicated models.

2.1 The Nested Cube Design

A variate of the nested cube design was used by Fuller (1969). He used three half replicates of a 2^3 design at unequal distances from the origin plus center and star points. The levels were spaced to make the linear and quadratic effects orthogonal.

The nested cube design in its basic form has two full replicates of a 2^K design at distances ½ and 1 from the origin, star points and one or more center points. The K-tuples utilized are:

1. Outer cube - coordinates $(\pm 1,\pm 1,\ldots,\pm 1)$.
2. Inner cube - coordinates $(\pm\frac{1}{2},\pm\frac{1}{2},\ldots,\pm\frac{1}{2})$.
3. Star points - coordinates $(\pm 1,0,\ldots,0)$, $(0,\pm 1,0,\ldots,0)$, etc.
4. Center points - coordinates $(0,0,\ldots,0)$.

The nested cube design may not always be used in its most basic form. The number of replications for each part will be designated by n_1, n_2, n_3 and n_4 respectively.

It is easy to verify that the nested cube design has the third and fourth qualities of a good design specified in chapter 1. Quality three (equal spacing) is seen to be satisfied by observing that within each factor the experimental settings lie at one of five levels: -1, $-\frac{1}{2}$, 0, $\frac{1}{2}$, 1. Quality four is checked by examining the ability to retain structure when adding or deleting a factor.

To expand from K factors to K+1 factors, the K-dimensional cubes are used for each of the two levels for the new factor (± 1 for the outer cube and $\pm\frac{1}{2}$ for the inner cube). The star points in the original design are used at the center of the new factor. Two new points are added with zero levels for the original K factors and ± 1 for the new factor. These procedures are illustrated in Table 2.1. Table 2.1 shows the experimental settings corresponding to the outer cube and star points for between two and five independent variables.

The deletion of a factor may occur either before the experiment begins or after the data have been collected and an analysis started. If deletion precedes experimentation, the number of design points can be reduced by using the equivalent design for one less factor. If the factor is deleted or abandoned in the analysis after the experiment has been performed, the result is two replications of the cube portions of the design and an addition of two center points when

TABLE 2.1 Outer Cube and Star Points for Nested Cube Design

for K = 2 to 5 Factors

	Experimental Factors				
K	X_1	X_2	X_3	X_4	X_5
	1	1	1	1	1
	-1	1	1	1	1
	1	-1	1	1	1
	-1	-1	1	1	1
	1	0	0	0	0
	-1	0	0	0	0
	0	1	0	0	0
2	0	-1	0	0	0
	1	1	-1	1	1
	-1	1	-1	1	1
	1	-1	-1	1	1
	-1	-1	-1	1	1
	0	0	1	0	0
3	0	0	-1	0	0
	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
	0	0	0	1	0
4	0	0	0	-1	0
	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
	0	0	0	0	1
5	0	0	0	0	-1

compared to the basic nested cube design for K-1 factors. The star points associated with the abandoned factor become the two center points for the collapsed design and star points associated with the remaining factors stay as such.

An advantage of this design over some of the other designs is that it retains the same form and factor levels when the number of factors change. This is not true for the rotatable central composite design. A rotatable central composite design contained within the unit hypercube locates star points on the faces of the cube and includes a $2^K \cdot \alpha$ design where $\alpha = 2^{-K/4}$ (i.e., includes K-tuples of the form $(\pm\alpha, \pm\alpha, \ldots, \pm\alpha)$). Thus if the number of factors is changed it becomes necessary to change the factor levels.

2.2 Example

A current experiment being conducted by Vincent Haby of the Montana State University Plant and Soil Department is using the nested cube design. Use of the design resulted from cooperative efforts of Haby and Richard Lund of the Montana State University Statistical Laboratory. Aspects of the design were discussed at the 1977 and 1978 Soils Conference held at Montana State University.

The experiment considers yield of winter wheat to applications of potassium, phosphorous and nitrogen fertilizers. There are three factors and an experimental setting would be an ordered triplet such as $(\lambda_1,\lambda_2,\lambda_3)$ where:

1. λ_1 = level of potassium fertilizer,
2. λ_2 = level of phosphorous fertilizer,
3. λ_3 = level of nitrogen fertilizer.

The researcher wants to measure yield associated with application of:

1. potassium from 0 to 96 pounds per acre,
2. phosphorous from 0 to 40 pounds per acre,
3. nitrogen from 0 to 100 pounds per acre.

The transformation constants are $\gamma_1 = 48$, $\gamma_2 = 20$, $\gamma_3 = 50$, $\delta_1 = 48$, $\delta_2 = 20$ and $\delta_3 = 50$. After applying the transformation, each of the factors has -1 to 1 as the range of interest.

3. THE MODEL AND ITS ESTIMATION

The problem of estimation can be discussed only after a suitable model to explain the expected response as a function of experimental settings has been chosen. As was noted in Chapter 1, a polynomial model will be considered. The linear model is bypassed because there exist simpler designs that provide adequate information with considerably fewer design points. Treatment will be restricted to quadratic and cubic models.

The appropriate model can be represented by:

$$\eta_1(x) = \beta_0 + \sum_{i=1}^{K} x_i\beta_i + \sum_{i=1}^{K}\sum_{j\geq i}^{K} x_ix_j\beta_{ij} \text{ ,or} \tag{3.1}$$

$$\eta_2(x) = \beta_0 + \sum_{i=1}^{K} x_i\beta_i + \sum_{i=1}^{K}\sum_{j\geq i}^{K} x_ix_j\beta_{ij} + \sum_{i=1}^{K}\sum_{j\geq i}^{K}\sum_{k\geq j}^{K} x_ix_jx_k\beta_{ijk}. \tag{3.2}$$

The vector x containing the experimental settings is defined in (2.2) by:

$$x' = (x_1,\ldots,x_K). \tag{3.3}$$

If the vectors β_1, β_2, x_1 and x_2 are defined by:

$$\beta_1' = (\beta_0,\beta_1,\ldots,\beta_K,\beta_{11},\ldots,\beta_{KK},\beta_{12},\ldots,\beta_{K-1,K}) \tag{3.4}$$

$$\beta_2' = (\beta_{111},\ldots,\beta_{KKK},\beta_{122},\ldots,\beta_{1KK},\ldots,\beta_{123},\ldots,\beta_{K-2,K-1,K}) \tag{3.5}$$

$$x_1' = (1,x_1,\ldots,x_K,x_1^2,\ldots,x_K^2,x_1x_2,\ldots,x_{K-1}x_K) \tag{3.6}$$

$$x_2' = (x_1^3,\ldots,x_K^3,x_1x_2^2,\ldots,x_Kx_{K-1}^2,x_1x_2x_3,\ldots,x_{K-2,K-1,K}) \tag{3.7}$$

Note that β is used both as an element and a vector.

The two models may be written as:

$$\eta_1(x) = x_1'\beta_1 \tag{3.1a}$$

$$\eta_2(x) = x_1'\beta_1 + x_2'\beta_2 . \tag{3.2a}$$

The vectors x_1 and β_1 have dimension

$$p_1 = 1 + 2K + \binom{K}{2} \tag{3.8}$$

and the vectors x_2 and β_2 have dimension

$$p_2 = K + 2\binom{K}{2} + \binom{K}{3} . \tag{3.9}$$

Observed data can be expressed as

$$y(x) = \eta_i(x) + \varepsilon \tag{3.10}$$

where $\eta_i(x)$ is the appropriate model for expected response and ε is a random variable with mean zero and variance σ^2. One uses the observed values of y to construct estimates of the parameter vector.

The vectors β_1, β_2, x_1 and x_2 for K = 3 are as follows:

$$\beta_1' = (\beta_0,\beta_1,\beta_2,\beta_3,\beta_{11},\beta_{22},\beta_{33},\beta_{12},\beta_{13},\beta_{23}) \tag{3.4a}$$

$$\beta_2' = (\beta_{111},\beta_{222},\beta_{333},\beta_{122},\beta_{133},\beta_{211},\beta_{233},\beta_{311},\beta_{322},\beta_{123}) \tag{3.5a}$$

$$x_1' = (1,x_1,x_2,x_3,x_1^2,x_2^2,x_3^2,x_1x_2,x_1x_3,x_2x_3) \tag{3.6a}$$

$$x_2' = (x_1^3,x_2^3,x_3^3,x_1x_2^2,x_1x_3^2,x_2x_1^2,x_2x_3^2,x_3x_1^2,x_3x_2^2,x_1x_2x_3) \tag{3.7a}$$

The values of p_1 and p_2 are both ten for K = 3.

Responses are measured at each of N experimental settings. Define the matrix X_1 (N x p_1) and X_2 (N x p_2) as:

$$X_1 = ((x_1')) \tag{3.11}$$

$$X_2 = ((x_2')) . \tag{3.12}$$

That is, the rows of X_1 and X_2 are the N vectors x_1 and x_2 for the various experimental settings. The vector of observed values Y (N x 1) can be represented as:

$$Y = X_1\beta_1 + e \text{ , or} \tag{3.13}$$

$$Y = X_1\beta_1 + X_2\beta_2 + e \tag{3.14}$$

depending on whether the true model is given by (3.1a) or (3.2a). The vector e is assumed to be a vector of independent, identically distributed random variables with mean zero and variance σ^2.

3.1 Estimating the Quadratic Model

If η_1 represents the appropriate model, the standard least-squares estimator will provide a minimum variance, unbiased estimate of the parameter vector β_1. The standard least-squares estimator,

$$\hat{\beta} = (X_1'X_1)^{-1}X_1'Y \text{ ,} \tag{3.15}$$

can be used provided the matrix $X_1'X_1$ is nonsingular.

In order to study conditions under which the matrix is nonsingular, certain notation is needed. The moments for independent variables (design moments) are defined by:

$$[ijk\ldots m] = \sum_{u=1}^{N} x_{1u}^{i} x_{2u}^{j} x_{3u}^{k} \ldots x_{Ku}^{m} . \tag{3.16}$$

The designs that are commonly used and those that are considered herein have the properties of symmetry and zero odd moments. That is:

$$[ijk\ldots] = 0 \text{ if } i, j, k \text{ or } \ldots, \text{ is odd, and} \tag{3.17}$$

$$[ijk\ldots] = [ikj\ldots] = [\text{any permutation of powers}]. \tag{3.18}$$

When considering at most a cubic model, the non-zero design moments are equivalent in value to the moments: (1) [200...0], (2) [400...0], (3) [220...0], (4) [600...0], (5) [420...0], and (6) [2220...0]. To simplify notation, only the first three values will be given when there are three or more values and the non-zero exponents will be written first. That is: [0200] or [0002] become [200] and [42000] or [20400] become [420]. This simplification is possible because each moment of interest is equal to one of the six moments listed and at most three exponents are non-zero.

The form of $X_1'X_1$ is displayed in Figure 3.1 using this notation. It can be seen that the conditions for $X_1'X_1$ to be nonsingular are:

1. $[200] \neq 0$,
2. $[220] \neq 0$, and
3. the matrix $\begin{bmatrix} N & [200]\cdot j' \\ [200]\cdot j & [400]\cdot I + [220]\cdot(J-I) \end{bmatrix}$ (K+1 x K+1)

   be nonsingular.

Conditions one and two are satisfied for most experimental designs. Condition three is satisfied when the design moments involved satisfy certain restrictions. Roy and Sarhan (1956) determine the inverse of a matrix of this type and Graybill (1969) gives a technique for inverting a family of matrices including this one. Using either the results of Roy and Sarhan or Graybill gives the following restrictions on the moments in order for the inverse to exist:

$$\begin{aligned}
&1.\ N > 0 \\
&2.\ [400] \neq [220] \qquad\qquad (3.19) \\
&3.\ N([400]-[220]) + (K-1)(N\cdot[220]-[200]^2) \neq 0\ ,
\end{aligned}$$

$$X_1'X_1 = \begin{array}{c} 1 \\ K \\ K \\ \binom{K}{2} \end{array} \begin{bmatrix} N & 0 & [200]\cdot j' & 0 \\ 0 & [200]\cdot I & 0 & 0 \\ [200]\cdot j & 0 & [400]\cdot I + [220](J-I) & 0 \\ 0 & 0 & 0 & [220]\cdot I \end{bmatrix} .$$

Figure 3.1 $X_1'X_1$ for Symmetric Designs with Zero Odd Moments

The first restriction in (3.19) is satisfied for any experimental design. Restrictions two and three are characterizations of a second order design. Restriction two is satisfied by inclusion of star points. When the number of replications of the four parts of the design are designated by n_1, n_2, n_3 and n_4 as in Chapter 2, the quantity in restriction 3 is for the nested cube design:

$$2n_3\{(n_1+n_2)2^K+2Kn_3+n_4\}+(K-1)\{n_1n_2(2^{2K-1}+2^{2K-4})+n_1n_3(K2^{K+1}-2^{K+2})+ n_1n_4 2^K+n_2n_3(K2^{K-3}-2^K)+n_2n_4 2^{K-4}-4n_3^2\} \quad (3.20)$$

which is non-zero for any reasonable choice of n_1, n_2, n_3 and n_4. In particular, if all are one, the quantity equals:

$$2(2^{K+1}+2K+1)+(K-1)\{2^{2K-1}+2^{2K+1}+K(2^{K+1}+2^{K-3})+2^{K-4}-2^{K+2}-4\} \quad (3.21)$$

This is 149 for K = 3.

Thus, if the true model is given by (3.1a), it is possible to use the standard least-squares estimator which is minimum variance unbiased.

The case in which (3.2a) represents the true model is now considered. As can be seen in Table 3.1, the number of parameters in the cubic model (η_2) increases much more rapidly with increasing K than the number of parameters in the quadratic model (η_1). For this reason it is preferable to use the quadratic model when it is adequate. A large number of parameters requires a large number of experimental settings.

Table 3.1 Number of Parameters in Models η_1 and η_2

K	Model η_1	η_2
1	3	4
2	6	10
3	10	20
4	15	35
5	21	56
6	28	84

The nested cube design is such that not all of the parameters in the full cubic model (η_2) are estimable. Thus, if η_2 is the true model, there are three alternatives:

1. estimate as many parameters as possible in η_2 and accept some bias introduced by the confounding of parameters,
2. use model η_1 and accept the bias introduced by omission of cubic terms, or
3. use model η_1 and minimize the bias by use of an appropriate estimator.

The three alternatives will be examined in their order of occurence.

3.2 Estimating the Cubic Model

In order to consider alternative number one, the linear combinations of parameters that are estimable need to be determined. Theorem 3.1 gives a list of these combinations.

Theorem 3.1: For the nested cube design, the following parameters and linear combinations of parameters are estimable:

1. β_i $i = 0,1,\ldots,K$
2. β_{ij} $i = 1,\ldots,K$ $j = i,\ldots,K$
3. β_{iii} $i = 1,\ldots,K$
4. β_{ijk} $i \neq j \neq k \neq i$
5. $\sum_{j \neq i} \beta_{ijj}$ $i = 1,\ldots,K$ (Summation is over j)

Proof of Theorem 3.1:

Let $X = [X_1\ X_2]$

then for symmetric designs with zero odd moments, such as the cube square design, figure 3.2 shows the form of $X'X$. If the order of the terms is rearranged so as to group the first and third order terms together and the second order terms with the mean, the rank and generalized inverse of $X'X$ can be recognized more easily. The new order will be:

$$
X'X = \begin{array}{c} 1 \\ K \\ K \\ \binom{K}{2} \\ K \\ 2\binom{K}{2} \\ \binom{K}{3} \end{array}
\begin{bmatrix}
N & 0 & [200]\cdot j' & 0 & 0 & 0 & 0 \\
0 & [200]\cdot I & 0 & 0 & [400]\cdot I & [220]\cdot j'\boxtimes I & 0 \\
[200]\cdot j & 0 & [400]\cdot I + [220]\cdot(J-I) & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & [220]\cdot I & 0 & 0 & 0 \\
0 & [400]\cdot I & 0 & 0 & [600]\cdot I & [420]\cdot j'\boxtimes I & 0 \\
0 & [220]\cdot j\boxtimes I & 0 & 0 & [420]\cdot j\boxtimes I & \{[420]\cdot I + [222]\cdot(J-I)\}\boxtimes I & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & [222]\cdot I
\end{bmatrix}
$$

Figure 3.2 General Form of X'X

$$
X'X = \left[\begin{array}{cccccccccccccccccccc}
23 & & & & 12 & 12 & 12 & & & & & & & & & & & & & \\
 & 12 & & & & & & & & & 10.5 & & & 8.5 & 8.5 & & & & & \\
 & & 12 & & & & & & & & & 10.5 & & & & 8.5 & 8.5 & & & \\
 & & & 12 & & & & & & & & & 10.5 & & & & & 8.5 & 8.5 & \\
12 & & & & 10.5 & 8.5 & 8.5 & & & & & & & & & & & & & \\
12 & & & & 8.5 & 10.5 & 8.5 & & & & & & & & & & & & & \\
12 & & & & 8.5 & 8.5 & 10.5 & & & & & & & & & & & & & \\
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 & 10.5 & & & & & & & & & 10.125 & & & 8.125 & 8.125 & & & & & \\
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 & & & 8.5 & & & & & & & & & 8.125 & & & & & 8.125 & 8.125 & \\
 & & & 8.5 & & & & & & & & & 8.125 & & & & & 8.125 & 8.125 & \\
 & & & & & & & & & & & & & & & & & & & 8.125
\end{array}\right]
$$

Figure 3.2a X'X for Nested Cube Design K = 3 $n_1 = n_2 = n_3 = n_4 = 1$

$$X^{*'} = (1,x^2,\ldots,x_K^2,x_1x_2,\ldots,x_{K-1}x_K,x_1,x_1^3,x_1x_2^2,\ldots,x_1x_K^2,$$
$$x_2,x_2^3,x_2x_1^2,\ldots,x_Kx_{K-1}^2,x_1x_2x_3,\ldots,x_{K-2}x_{K-1}x_K) \qquad (3.22)$$

The matrix X becomes X^* when using this order and $X^{*'}X^*$ is shown in figure 3.3. $X^{*'}X^*$ for K = 3 can be denoted as:

$$X^{*'}X^* = \begin{bmatrix} A_{11} & & & & & \\ & A_{22} & & & & \\ & & A_{33} & & & \\ & & & A_{44} & & \\ & & & & A_{55} & \\ & & & & & A_{66} \end{bmatrix} \qquad (3.23)$$

A_{11} was shown earlier to be non-singular. A_{22} and A_{66} are diagonal matrices and of full rank. Next observe that $A_{33} = A_{44} = A_{55}$. Thus the rank of $X^{*'}X^*$ and consequently of $X'X$ will be determined by the rank of A_{33}. This can be generalized for $K \geq 3$ by noting the following:

1. A_{11} of order and rank K+1 is associated with the mean and pure second order terms,
2. A_{22} of order and rank $\binom{K}{2}$ is associated with the linear by linear interaction terms,
3. A_{ii} for i = 3,...,K+2 are of order K+1 and associated with segments of $X^{*'}$ that contain $(x_i,x_i^3,x_ix_j^2)$, $j \neq i$, and
4. $A_{K+3,K+3}$ of rank and order $\binom{K}{3}$ is associated with the linear by linear by linear interactions.

The matrix $A_{K+3,K+3}$ has no elements for K = 2 since there can be no

$$X^{*'}X^{*} = \begin{array}{c} 1 \\ K \\ \binom{K}{2} \\ K^2+K \\ \binom{K}{3} \end{array} \begin{bmatrix} N & [200]\cdot j' & 0 & 0 & 0 \\ [200]\cdot j & [400]\cdot I + [220]\cdot(J-I) & 0 & 0 & 0 \\ 0 & 0 & [220]\cdot I & 0 & 0 \\ 0 & 0 & 0 & \begin{bmatrix} [200] & [400] & [220]\cdot j' \\ [400] & [600] & [420]\cdot j' \\ [220]\cdot j & [420]\cdot j & [420]\cdot I + [222]\cdot(J-I) \end{bmatrix} \otimes I_K & 0 \\ 0 & 0 & 0 & 0 & [222]\cdot I \end{bmatrix}$$

Figure 3.3 General Form of $X^{*'}X^{*}$

$$
X^{*\prime}X^{*} = \begin{bmatrix}
23 & 12 & 12 & 12 &&&&&&&&&&&&&&&& \\
12 & 10.5 & 8.5 & 8.5 &&&&&&&&&&&&&&&& \\
12 & 8.5 & 10.5 & 8.5 &&&&&&&&&&&&&&&& \\
12 & 8.5 & 8.5 & 10.5 &&&&&&&&&&&&&&&& \\
&&&& 8.5 &&&&&&&&&&&&&&& \\
&&&&& 8.5 &&&&&&&&&&&&&& \\
&&&&&& 8.5 &&&&&&&&&&&&& \\
&&&&&&& 12 & 10.5 & 8.5 & 8.5 &&&&&&&&& \\
&&&&&&& 10.5 & 10.125 & 8.125 & 8.125 &&&&&&&&& \\
&&&&&&& 8.5 & 8.125 & 8.125 & 8.125 &&&&&&&&& \\
&&&&&&& 8.5 & 8.125 & 8.125 & 8.125 &&&&&&&&& \\
&&&&&&&&&&& 12 & 10.5 & 8.5 & 8.5 &&&&& \\
&&&&&&&&&&& 10.5 & 10.125 & 8.125 & 8.125 &&&&& \\
&&&&&&&&&&& 8.5 & 8.125 & 8.125 & 8.125 &&&&& \\
&&&&&&&&&&& 8.5 & 8.125 & 8.125 & 8.125 &&&&& \\
&&&&&&&&&&&&&&& 12 & 10.5 & 8.5 & 8.5 & \\
&&&&&&&&&&&&&&& 10.5 & 10.125 & 8.125 & 8.125 & \\
&&&&&&&&&&&&&&& 8.5 & 8.125 & 8.125 & 8.125 & \\
&&&&&&&&&&&&&&& 8.5 & 8.125 & 8.125 & 8.125 & \\
&&&&&&&&&&&&&&&&&&& 8.125
\end{bmatrix}
$$

Figure 3.3a $X^{*\prime}X^{*}$ for Nested Cube Design $K = 3$ $n_1 = n_2 = n_3 = n_4 = 1$

three factor interactions.

The form of A_{33} and hence A_{ii}, i=3,...,K+2, is:

$$A_{33} = \begin{array}{c} 1 \\ 1 \\ K-1 \\ \\ \end{array} \begin{bmatrix} [200] & [400] & [220]\cdot j' \\ [400] & [600] & [420]\cdot j' \\ [220]\cdot j & [420]\cdot j & [420]\cdot I + \\ & & [222]\cdot(J-I) \end{bmatrix} \qquad (3.24)$$

For the nested cube design [222] = [420] and thus the last K-1 rows of the matrix A_{33} are identical. Consequently the rank of A_{33} cannot exceed the dimension of A_{33} (K+1) minus K-2 for the duplicate rows. This gives rank$(A_{33}) \leq 3$. To show that rank$(A_{33}) = 3$, it is sufficient to show that the leading principal minor of order three is nonsingular. For K = 3 and one replication of each part of the design ($n_1= n_2= n_3= n_4=1$), the determinant of the three by three leading principal minor is eighteen and it can be shown that for any reasonable number of replications of the four parts (all $n_i \geq 1$) will result in a positive determinant. Thus, rank $(A_{33}) = 3$.

From this, it is seen that for $K \geq 3$, the matrix $X'X$ is not of full rank. For K = 2, the matrix $X'X$ is nonsingular. To find what linear combinations of the parameters are estimable, a generalized inverse of $X'X$ is sought. To do this we find a generalized inverse of $X^{*'}X^*$ then rearrange to get the generalized inverse of $X'X$. For K = 3 the form of the generalized inverse is shown in (3.25). The form includes A_{11}^{-1}, A_{22}^{-1} and A_{66}^{-1} since each is of full rank. It is only necessary to find one generalized inverse because $A_{33} = A_{44} = A_{55}$.

$$(X^{*\prime}X^{*})^{-} = \begin{bmatrix} A_{11}^{-1} & & & & & \\ & A_{22}^{-1} & & & & \\ & & A_{33}^{-} & & & \\ & & & A_{44}^{-} & & \\ & & & & A_{55}^{-} & \\ & & & & & A_{66}^{-1} \end{bmatrix} \qquad (3.25)$$

This is found using the method described by Searle (1971) which involves finding the inverse of the leading principal minor of order three and filling the remainder of the matrix with zeroes.

Either the matrix $H^{*} = (X'X)^{-} X'X$ or $H^{*} = (X^{*\prime}X^{*})^{-} X^{*\prime} X^{*}$ is examined to find the estimable linear combinations of the parameters. All linear combinations $q'\beta$ that are estimable are such that $q'H = q'$ or $q^{*\prime}H^{*} = q^{*\prime}$ where $q^{*\prime}$ is the rearrangement of q in the same manner as $X^{*\prime}$ is the rearrangement of X'.

From (3.23) and (3.25) it is seen that:

$$H^{*} = \begin{bmatrix} I_{K+1} & & & \\ & I_{\binom{K}{2}} & & \\ & & (A_{33}^{-}A_{33})\otimes I_{K} & \\ & & & I_{\binom{K}{3}} \end{bmatrix} \qquad (3.26)$$

The form of $A_{33}^{-}A_{33}$ for the nested cube design is shown in (3,27).

$$A_{33}^{-}A_{33} = \begin{array}{c} 1 \\ 1 \\ 1 \\ K-2 \end{array} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \cdot j' \\ 0 & 0 & 0 \end{bmatrix}_{K+1 \times K+1} \qquad (3.27)$$

Using (3.26) and (3.27) the results of Theorem 3.1 follow immediately completing the proof.

Theorem 3.1 indicates confounding will occur when attempting to estimate all coefficients in the cubic model (η_2). It is possible to estimate $\beta_{i..} = \sum_{j \neq i} \beta_{ijj}$ but not the individual β_{ijj}'s.

3.3 Use of Quadratic Model when True Model is Cubic

Alternatives two and three involve using a quadratic model to estimate the cubic surface. Bias in the estimate results if the true model is

$$Y = X_1\beta_1 + X_2\,\beta_2 + e \qquad (3.28)$$

and the used model is

$$Y = X_1 b_1 + e. \qquad (3.29)$$

The resulting estimate is

$$\hat{Y}(x) = x_1'(X_1'X_1)^{-1}X_1'Y. \qquad (3.30)$$

A choice exists between (1) using an unbiased minimum variance estimator for the used quadratic model and (2) using an estimator that is unbiased for the used model, minimum bias under the true model (for linear estimators based on the used model) but with a slightly larger variance.

The minimum variance estimator is the standard least-squares estimator for the model used. The contribution of the bias to the integrated mean square error was derived by Box and Draper (1959) and Karson, Manson and Hader (1969) and is given by:

$$B = (N\, 2^K/\sigma^2) \int \cdots_R \int (E(Y(X)) - \eta(X))^2 dX \qquad (3.31)$$

A further discussion of bias is given in Chapter 4.

3.4 Minimum Bias Estimator

Karson, Manson and Hader (1969) introduced the concept of minimizing the bias of an estimate by use of the estimator rather than the design. The description of the estimator and its properties requires certain notation which will be developed using symbols similiar to Karson, Manson and Hader.

The moment matrices of a uniform design over the region of interest are defined as:

$$W_{11} = 2^{-K} \int \cdots_R \int X_1 X_1' \, dX \qquad (3.32)$$

$$W_{12} = 2^{-K} \int \cdots_R \int X_1 X_2' \, dX \qquad (3.33)$$

$$W_{22} = 2^{-K} \int \cdots_R \int X_2 X_2' \, dX \qquad (3.34)$$

Figure 3.4 shows the three matrices for K=3.

The linear estimator that will minimize the bias contribution

$$W_{11} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 \\ 0 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 & 1/5 & 1/9 & 1/9 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 & 1/9 & 1/5 & 1/9 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 & 1/9 & 1/9 & 1/5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/9 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/9 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/9 \end{bmatrix}$$

$$W_{12} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/5 & 0 & 0 & 1/9 & 1/9 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/5 & 0 & 0 & 0 & 1/9 & 1/9 & 0 & 0 & 0 \\ 0 & 0 & 1/5 & 0 & 0 & 0 & 0 & 1/9 & 1/9 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$W_{22} = \begin{bmatrix} 1/7 & 0 & 0 & 1/15 & 1/15 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/7 & 0 & 0 & 0 & 1/15 & 1/15 & 0 & 0 & 0 \\ 0 & 0 & 1/7 & 0 & 0 & 0 & 0 & 1/15 & 1/15 & 0 \\ 1/15 & 0 & 0 & 1/15 & 1/27 & 0 & 0 & 0 & 0 & 0 \\ 1/15 & 0 & 0 & 1/27 & 1/15 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/15 & 0 & 0 & 0 & 1/15 & 1/27 & 0 & 0 & 0 \\ 0 & 1/15 & 0 & 0 & 0 & 1/27 & 1/15 & 0 & 0 & 0 \\ 0 & 0 & 1/15 & 0 & 0 & 0 & 0 & 1/15 & 1/27 & 0 \\ 0 & 0 & 1/15 & 0 & 0 & 0 & 0 & 1/27 & 1/15 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/27 \end{bmatrix}$$

Figure 3.4 W_{11}, W_{12} and W_{22} for $K = 3$

to integrated mean square error uses:

$$\tilde{b}_1 = T'Y \qquad (3.35)$$

where T' is such that:

$$T'X = A \qquad (3.36)$$

where A is defined by:

$$A = (I \quad W_{11}^{-1}W_{12}) \qquad (3.37)$$

A matrix T' exists if and only if $A\beta$ is estimable. A is not design dependent. The general form of A and an example for K = 3 are shown in figure 3.5.

Theorem 3.2: $A\beta$ is estimable for the nested cube design.

Proof of Theorem 3.2:

From Figure 3.5 it is seen that the following linear combinations of parameters need be estimable:

1. β_0

2. $\beta_i + .6 \ _{iii} + 1/3 \sum_{j \neq i} \beta_{ijj}$ $\qquad i = 1,\ldots,K$

3. β_{ij} $\qquad i = 1,\ldots,K \quad j \geq i \qquad (3.38)$

But theorem 3.1 indicates these are estimable, completing the proof.

The matrix T' is not unique and thus there exists an entire family of estimators. Karson, Manson and Hader show that the matrix T' within this family provides the estimate with minimum variance when:

$$T' = A(X'X)^{-}X' \qquad (3.39)$$

which gives:

$$\text{Var}\ (\tilde{Y}(x)) = \sigma^2 . x_1'T'T\ x_1 \qquad (3.40)$$

$$A = \begin{array}{c} 1 \\ K \\ K+\binom{K}{2} \end{array} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & I & 0 & .6\ I & 1/3\ j'\otimes I & 0 \\ 0 & 0 & I & 0 & 0 & 0 \end{bmatrix}$$

$$A = \left[\begin{array}{cccccccccccccccccccc}
1 &&&&&&&&&&&&&&&&&&& \\
& 1 &&&&&&&&& .6 &&& 1/3 & 1/3 &&&&& \\
&& 1 &&&&&&&&& .6 &&&& 1/3 & 1/3 &&& \\
&&& 1 &&&&&&&&& .6 &&&&& 1/3 & 1/3 & 0 \\
&&&& 1 &&&&&&&&&&&&&&& \\
&&&&& 1 &&&&&&&&&&&&&& \\
&&&&&& 1 &&&&&&&&&&&&& \\
&&&&&&& 1 &&&&&&&&&&&& \\
&&&&&&&& 1 &&&&&&&&&&& \\
&&&&&&&&& 1 &&&&&&&&&&
\end{array}\right]$$

Figure 3.5 General Form of A and Example when K = 3

Theorem 3.2 verifies that it is possible to use this type of estimator with the nested cube design. In order to compare the nested cube design to other designs, it is necessary to determine for which designs the minimum bias estimator exists.

<u>Theorem 3.3</u>: For symmetric experimental designs with zero odd moments, $A\beta$ is estimable if the following conditions hold:

1. $[220] \neq 0$

2. $N > 0$

3. $[400] \neq [220]$

4. $N([440]-[220]) + (K-1)(N[220]-[220]^2) \neq 0$

5. $[200][600]\{(K-2)[222]+[420]\}+2(K-1)[220][400][420]-(K-1)[420]^2$
$[200]-(K-1)[600][220]^2-[400]^2\{(K-2)[222]+[420]\} \neq 0$

6. and either $[420]=[222]$ or $[400][420] \neq [600][220]$ (3.41)

Proof of Theorem 3.3:

In order for $A\beta$ to be estimable, the linear combinations of parameters shown in (3.38) must be estimable. For parts one and three of (3.38) A_{11} and A_{22} of (3.23) must be nonsingular. Condition one of Theorem 3.3 is a necessary and sufficient condition for A_{22} to be nonsingular because A_{22} = diagonal([220]). Conditions two, three and four are the same as those of (3.19) which were shown to be necessary and sufficient for A_{11} to be nonsingular.

Part two of (3.38) is $\beta_i + .6\beta_{iii} + 1/3 \sum_{j\neq i} \beta ijj$. Sufficient conditions for this to be estimable are examined in two cases:

1. $[222] = [420]$

2. $[222] \neq [420]$

Define H^*_{33} by:

$$H^*_{33} = A^-_{33}A_{33} \tag{3.42}$$

The rows of H^*_{33} will represent a basis for the linear combinations of $(\beta_i, \beta_{iii}, \beta_{\substack{ijj \\ j\neq i}})$ that are estimable.

Case 1 ([420] = [222]):

If condition five of Theorem 3.3 holds then A_{33} is of rank three and H_{33}^* has the form shown in (3.27). This shows that β_i, β_{iii} and $\sum_{j \neq i} \beta_{ijj}$ are estimable and thus $\beta_i + .6\beta_{iii} + 1/3 \sum_{j \neq i} \beta_{ijj}$ is also.

Case 2 ([420] $\neq$ [222]):

If condition five and part two of condition six hold, A_{33} is nonsingular and all parameters are estimable. If all parameters are estimable, the desired linear combination is also estimable. This completes the proof of Theorem 3.3.

Theorem 3.3 gives sufficient conditions for the estimability of $A\beta$. In order to prove that a design may not estimate $A\beta$, it is necessary to examine $H = (X'X)^{-}X'X$. Ten frequently used, standard designs were chosen for comparison with the nested cube design.

The designs are:

1. Factorial with three levels (3K),
2. Factorial with two levels plus star points plus center (KS),
3. Factorial with two levels plus two star points plus center (KS+),
4. Factorial with two levels replicated twice plus star points plus center (K+S),
5. Factorial with two levels plus edge points plus center (KE),
6. Factorial with two levels plus two edge points plus center (KE+),

7. Factorial with two levels replicated twice plus edge points plus center (K+E),

8. Rotatable central composite (RC),

9. Rotatable central composite with two star points (RC+),

10. Rotatable icosahedron (RI).

H_{33}^* for these designs is shown in Appendix B. A summary of the results is given in Table 3.2. Appendix A provides a description of each of the designs.

Table 3.2 shows that $A\beta$ is estimable only for the nested cube design among the designs considered. It should be noted that the designs that include edge points (3K, KE, KE+ and K+E) have most of the parameters estimable but not the proper linear combination of β_i and β_{iii}.

Table 3.2 Estimable Linear Combinations of $(\beta_i, \beta_{iii}, \beta_{ijj})_{i \neq j}$ for Selected Designs

Design	$A\beta$ Estimable	Estimable Combinations
NC	Yes	β_i, β_{iii}, $\sum_{j \neq i} \beta_{ijj}$
NC+	Yes	β_i, β_{iii}, $\sum_{j \neq i} \beta_{ijj}$
3K	No	$\beta_i+\beta_{iii}$, β_{ijj} $j \neq i$
KS	No	$\beta_i+\beta_{iii}$, $\sum_{j \neq i} \beta_{ijj}$
KS+	No	$\beta_i+\beta_{iii}$, $\sum_{j \neq i} \beta_{ijj}$
K+S	No	$\beta_i+\beta_{iii}$, $\sum_{j \neq i} \beta_{ijj}$
KE	No	$\beta_i+\beta_{iii}$, β_{ijj} $j \neq i$
KE+	No	$\beta_i+\beta_{iii}$, β_{ijj} $j \neq i$
K+E	No	$\beta_i+\beta_{iii}$, β_{ijj} $j \neq i$
RC	No	$\beta_i+a_1 \sum_{j \neq i} \beta_{ijj}$, $\beta_{iii}+b_1 \sum_{j \neq i} \beta_{ijj}$ *
RC+	No	$\beta_i+a_2 \sum_{j \neq i} \beta_{ijj}$, $\beta_{iii}+b_2 \sum_{j \neq i} \beta_{ijj}$ *
RI	No	$\beta_i+a_3\beta_{ij_1j_1}+a_4\beta_{ij_2j_2}$, $\beta_{iii}+c$ *

* See Appendix B for values of a_1, a_2, a_3, a_4, b_1, b_2 and c.

4. BIAS AND BIAS COMPARISONS

When a polynomial model of a degree less than the degree of the true model is used, bias in estimation of $\eta(X)$ will occur. The amount of bias can be reduced by selection of design and/or estimator. In Chapter 3 it was shown that of the designs examined only the nested cube design was able to use the minimum bias estimator. The efficiency in terms of bias will be compared for the designs examined in order to determine if choice of design or choice of estimator is preferred.

It is necessary to have a method of comparing bias for two designs or two estimators. If the true model and values of the parameters are known, it is an easy task to derive the expected bias. But of course, there would be no point in estimation. The more common situation is when the parameters and sometimes even the model are unknown. If no assumption can be made concerning the model then it is not possible to compare the bias because the bias can not be derived. However, if a model can be assumed, then the bias can be derived in terms of the unknown parameters.

Box and Draper (1959) show that the contribution of the bias to the integrated mean square error is as given in (3.31). Karson, Manson and Hader (1969) show that the minimum bias attainable by either the use of estimator or the choice of design is:

$$B_{min} = (N/\sigma^2)\ \beta_2'(W_{22} - W_{12}'W_{11}^{-1}W_{12})\beta_2 \tag{4.1}$$

where β_2, W_{11}, W_{12} and W_{22} are defined in Chapter 3. If standard least-squares estimation is used, Karson, Manson and Hader show that:

$$B = (N/\sigma^2)\ \beta_2'\{W_{22} - X_2'X_1(X_1'X_1)^{-1}W_{12} - W_{12}'(X_1'X_1)^{-1}X_1'X_2 + X_2'X_1(X_1'X_1)^{-1}W_{11}(X_1'X_1)^{-1}X_1'X_2\}\beta_2 \tag{4.2}$$

Two methods for comparing these biases will be considered. The first involves considering an average over all vectors β_2 having the same norm. That is, $B^{\#}$ is defined by:

$$B^{\#} = \int_{\beta_2'\beta_2=t}\cdots\int B\ d\beta_2 \Big/ \int_{\beta_2'\beta_2=t}\cdots\int d\beta_2 \tag{4.3}$$

and relative sizes of $B^{\#}$ are compared. The second involves considering a subjectively chosen set of β_2's and comparing B for each of the vectors β_2.

4.1 Bias Efficiency for Averaged β_2:

The evaluation of $B^{\#}$ is made easier by the following theorem.

Theorem 4.1: For any real, symmetric matrix C,

$$\int_{\alpha'\alpha=t}\cdots\int \alpha' C\alpha\ d\alpha \Big/ \int_{\alpha'\alpha=t}\cdots\int d\alpha = \frac{t}{n}\ \text{trace } C$$

where α is n x 1 and C is n x n.

Proof of Theorem 4.1:

$$\int_{\alpha'\alpha=t}\cdots\int \alpha' C\alpha\ d\alpha = \int_{\alpha'\alpha=t}\cdots\int \operatorname{tr}(\alpha' C\alpha)\ d\alpha$$

$$= \int_{\alpha'\alpha=t}\cdots\int \operatorname{tr}(C\alpha\alpha')\ d\alpha$$

$$= \operatorname{tr}\{C\cdot\int_{\alpha'\alpha=t}\cdots\int \alpha\alpha'\ d\alpha\}$$

If $\alpha' = (\alpha_1,\ldots,\alpha_n)$, the ijth element of $\alpha\alpha'$ is $\alpha_i\alpha_j$. Searle (1976) shows that:

$$\int_{\alpha'\alpha=t}\cdots\int \alpha_i\alpha_j \, d\alpha = 0 \qquad i \neq j$$

$$= \pi^{n/2} t^{n/2} \,/\, (n\Gamma(\tfrac{n}{2}))\, dt \qquad i = j$$

and

$$\int_{\alpha'\alpha=t}\cdots\int d\alpha = \pi^{n/2} t^{n/2-1} \,/\, \Gamma(\tfrac{n}{2})\, dt$$

From this it is seen that:

$$\int_{\alpha'\alpha=t}\cdots\int \alpha'C\alpha \, d\alpha \,/ \int_{\alpha'\alpha=t}\cdots\int d\alpha = \mathrm{tr}\{C\cdot \mathrm{diagonal}(\pi^{n/2} t^{n/2} \,/\, (n\Gamma(n/2))\, dt)\} \,/$$

$$(\pi^{n/2} t^{n/2-1} \,/\, \Gamma(\tfrac{n}{2})\, dt$$

$$= \mathrm{tr}\{C\cdot \mathrm{diagonal}(\tfrac{t}{n})\}$$

$$= \mathrm{tr}\ \{\tfrac{t}{n}\ C\}$$

$$= \tfrac{t}{n}\cdot \mathrm{tr}(C)$$

This completes the proof of Theorem 4.1.

Theorem 4.1 is used in the calculation of $B^{\#}$ of (4.4). The theorem is applied using $\alpha = \beta_2$ and $C = W_{22} - X_2'X_1(X_1'X_1)^{-1} W_{12} - W_{12}'(X_1'X_1)^{-1} X_1'X_2 + X_2'X_1(X_1'X_1)^{-1} W_{11}(X_1'X_1)^{-1} X_1'X_2$.

It is possible to derive the form of the matrix C in terms of the design moments under mild regularity conditions when the true model is a cubic polynomial and the used model is a quadratic model. The conditions are: (1) odd design moments zero, (2) design moments symmetric and, (3) $X_1'X_1$ of full rank. These conditions are met for all of the designs under consideration. Condition one can be relaxed but the general form of the matrix C becomes much more complicated. When the conditions are satisfied, the form is:

$$C = \begin{bmatrix} a\cdot I & b\cdot j'\otimes I & 0 \\ b\cdot j\otimes I & \{c\cdot I + d\cdot(J-I)\}\otimes I & 0 \\ 0 & 0 & e\cdot I \end{bmatrix} \tag{4.4}$$

where:

$a = ([400]/[200])^2/3 - 2\cdot[400]/(5\cdot[200]) + 1/7$

$b = [400]\cdot[220]/(3\cdot[200]^2) - [220]/(5\cdot[200]) - [400]/(9\cdot[200]) + 1/5$

$c = ([220]/[200])^2/3 - 2\cdot[220]/(9\cdot[200]) + 1/15$

$d = ([220]/[200])^2/3 - 2\cdot[220]/(9\cdot[200]) + 1/27$

$e = 1/27$

Trace C for the nested cube design is found to be:

$$\mathrm{Tr}(C) = K\cdot a + 2\cdot\binom{K}{2}\cdot c + \binom{K}{3}\cdot e \tag{4.5}$$

The smallest bias obtainable for either design construction or estimator choice is:

$$B^{\#}_{min} = \left(\frac{Nt}{\sigma^2 p_2}\right) \mathrm{tr}\left(W_{22} - W'_{12}W_{11}^{-1}W_{12}\right) \tag{4.6}$$

which when evaluated gives:

$$B^{\#}_{min} = \left(\frac{Nt}{\sigma^2 p_2}\right)\cdot\left(4K/175 + 8\binom{K}{2}/135 + \binom{K}{3}/27\right) \tag{4.7}$$

As an example this is $.283386(Nt/\sigma^2 p_2)$ for $K = 3$. Values of $B^{\#}$ for the selected designs are compared with $B^{\#}_{min}$ in Table 4.1.

Table 4.1 Bias Efficiency for Selected Designs

for K = 2,...,7

	$B^{\#}_{min}/B^{\#}$					
Design	K = 2	3	4	5	6	7
NC	.495	.443	.408	.399	.406	.420
NC+	.568	.546	.473	.434	.424	.429
3K	.207	.213	.230	.250	.271	.291
KS	.367	.322	.291	.183	.288	.300
KS+	.456	.426	.354	.317	.306	.309
K+S	.294	.267	.260	.266	.279	.295
KE	.367	.358	.354	.358	.366	.376
KE+	.456	.426	.396	.385	.385	.391
K+E	.294	.300	.312	.326	.342	.357
RC	.842	.898	.827	.757	.709	.682
RC+	.273	.639	.900	.901	.823	.759
RI		.828				

To illustrate the entries, $B^{\#}$ for the nested cube design with K = 3 is .519095$(Nt/\sigma^2 p_2)$ which gives $B^{\#}_{min}/B^{\#}$ = .443. This means that the minimum bias attainable for a design with the same sample size as the nested cube design is .443 times the bias actually attained. Thus the entries are a measure of bias efficiency of the design-estimator combination. The measure has eliminated the influence of the sample sizes for the different designs. The general form of the entries in Table 4.1 is given by:

$$B^{\#}_{min}/B^{\#} = \{4K/175 + 4K(K-1)/135 + \binom{K}{3}/27\} \;/\; \{K(R_1^2/3 - 2R_1/5 + 1/7) + K(K-1)(R_2^2/3 - 2R_2/9 + 1/15) + \binom{K}{3}/27\} \quad (4.8)$$

where R1 = [400]/[200] and R2 = [220]/[200]. It will be noted that $B^{\#}_{min}/B^{\#} \leq 1$.

Two important comparisons can be made using Table 4.1: (1) least squares estimation versus minimum bias estimation and (2) one design versus another design. The first comparison is useful mainly for the nested cube design because with it the minimum bias estimator may be used. In making comparisons of the second type, it should be noted that there is no adjustment for sample size. An illustration of the second type of comparison is:

1. NC for K = 4 has $B^{\#}_{min}/B^{\#} = .408$
2. KS+ for K = 4 has $B^{\#}_{min}/B^{\#} = .354$

This means that the nested cube has a smaller bias than the KS+ design. In this case both designs contain twenty-three experimental settings and so no adjustment is necessary.

4.2 Bias Efficiency for Select β_2's

If prior information concerning the relative importance of the components of β_2 is available, use of it in the bias comparison would improve the results. This is the basis for a second set of comparisons of the bias among the selected set of designs.

The components of the vector β_2 are the unknown parameters for the omitted part of the model. These are the cubic terms in a polynomial in the case being studied. The matrix C of (4.4) makes evident two possible subdivisions of the parameters:

1. groups are:
   a. pure cubic
   b. quadratic by linear interactions
   c. linear by linear by linear interactions.
2. groups are:
   a. $(\beta_{iii}, \underset{j\neq i}{\beta_{ijj}})$ $\quad i = 1,\ldots,K$
   b. (β_{ijk}) $\quad i \neq j \neq k \neq i$

In some situations the relative sizes of parameters within these groups may be the same while different relative sizes for the parameters in different groups. Other situations will result in each parameter being considered separately. Ten β_2 vectors were subjectively chosen and normalized $(\beta_2'\beta_2 = 1)$ in order to illustrate comparisons of this type when K = 3. The β_2 vectors were normalized to allow comparisons between vectors as well a between designs. Table 4.2 contains the β_2 vectors before normalizing and Table 4.3 contains $E_b = B_{min}/B$ where B_{min} is the smallest attainable bias for the β_2 vector being examined.

Some observations may be made concerning the entries in Table 4.3. First and perhaps most important is that none of the selected

Table 4.2 Selected β_2 Vectors for Bias Comparisons for K = 3

β_2^i	β_{111}	β_{222}	β_{333}	β_{122}	β_{133}	β_{211}	β_{233}	β_{311}	β_{322}	β_{123}
β_2^1	1	1	1	1	1	1	1	1	1	1
β_2^2	1	1	1	0	0	0	0	0	0	0
β_2^3	0	0	0	1	1	0	0	0	0	0
β_2^4	1	0	0	-1	-1	0	0	0	0	0
β_2^5	1	0	0	0	0	-1	0	-1	0	0
β_2^6	1	0	0	-.5	-.5	0	0	0	0	0
β_2^7	1	0	0	-.3	-.3	0	0	0	0	0
β_2^8	1	0	0	0	0	-.3	0	-.3	0	0
β_2^9	1	1	1	-.3	-.3	-.3	-.3	-.3	-.3	0
β_2^{10}	.3	.3	.3	-1	-1	-1	-1	-1	-1	0

designs is best for every situation. The rotatable designs are best among the selected designs for several selected β_2's but are among the poorest for other β_2's.

4.3 Optimum Designs for Fixed β_2 and β_2's for which a Fixed Design is Efficient

In order to consider the circumstances that lead to high bias efficiency for the nested cube design, the bias component of the integrated mean square error will be written as:

$$B = \frac{N2^{-K}}{\sigma^2}\{\sum_{i=1}^{K}\beta_{iii}^2(R_1^2/3 - 2R_1/5 + 1/7) + \sum_{i=1}^{K}\beta_{iii}\sum_{j\neq i}\beta_{ijj}(R_1R_2/3 - R_1/9 -$$

$$R_2/5 + 1/15) + \sum_{i=1}^{K}\sum_{j\neq i}\beta_{ijj}^2(R_2^2/3 - 2R_2/9 + 1/15) +$$

$$\sum_{i=1}^{K}\sum_{j\neq i}\sum_{k\neq i,j}\beta_{ijj}\beta_{ikk}(R_2/3 - 2R_2/9 + 1/27) +$$

$$\sum_{i=1}^{K}\sum_{j>i}\sum_{k>j}\beta_{ijk}^2/27\} \qquad (4.9)$$

where R_1 = [400]/[200] and R_2 = [220]/[200]. Each component of B involves a parameter dependent factor and a design dependent factor. Table 4.4 contains the values of R_1 and R_2 for selected designs.

Table 4.3 Bias Efficiency of Selected Designs

for Selected β_2 Vectors K = 3

	β_2^i									
Design	i = 1	2	3	4	5	6	7	8	9	10
NC	.212	.476	.240	.522	.408	.919	.971	.456	.971	.292
NC+	.286	.444	.372	.791	.511	.997	.836	.460	.836	.465
3K	.199	.300	.286	.776	.392	.962	.679	.320	.679	.381
KS	.137	.300	.169	.464	.293	.962	.855	.298	.855	.218
KS+	.199	.300	.372	.776	.392	.962	.679	.320	.679	.381
K+S	.110	.300	.126	.328	.241	.821	.950	.282	.950	.158
KE	.157	.300	.204	.567	.327	.998	.790	.307	.790	.266
KE+	.199	.300	.286	.776	.392	.962	.679	.320	.679	.381
K+E	.126	.300	.151	.406	.272	.919	.894	.292	.894	.192
RC	.841	.993	.736	.766	.884	.838	.900	.962	.900	.733
RC+	.999	.753	.865	.711	.871	.675	.679	.781	.679	.804
RI	.956	.567	.932	.677	.807	.580	.550	.615	.550	.846

Table 4.4 R_1 and R_2 for Selected Designs

Design	R_1	R_2
NC	.875	.7083
NC+	.893	.6070
3K	1.000	.6666
KS	1.000	.8000
KS+	1.000	.6666
K+S	1.000	.8888
KE	1.000	.7500
KE+	1.000	.6667
K+E	1.000	.8333
RC	.621	.2070
RC+	.750	.2500
RI	.829	.2760

By considering the β's as fixed values and taking partial derivatives with respect to R_1 and R_2 and setting the partial derivatives equal to zero, the optimum values of R_1 and R_2 may be obtained. The partial derivatives set to zero result in the equations:

$$\left(2\sum_{i=1}^{K}\beta_{iii}^2/3\right)R_1 + \left(\sum_{i=1}^{K}\sum_{j\neq i}\beta_{iii}\beta_{ijj}/3\right)R_2 = 2\sum_{i=1}^{K}\beta_{iii}^2/5 + \sum_{i=1}^{K}\sum_{j\neq i}\beta_{iii}\beta_{ijj}/9 \qquad (4.10)$$

$$\left(\sum_{i=1}^{K}\sum_{j\neq i}\beta_{iii}\beta_{ijj}/3\right)R_1 + \left(\sum_{i=1}^{K}\sum_{j\neq i}\left(2\beta_{ijj}^2 + \sum_{k\neq i,j}2\beta_{ijj}\beta_{ikk}\right)/3\right)R_2 =$$

$$\sum_{i=1}^{K}\sum_{j\neq i}\left(\beta_{iii}\beta_{ijj}/5 + 2\beta_{ijj}^2/9 + \sum_{k\neq i,j}2\beta_{ijj}\beta_{ikk}/9\right) \qquad (4.11)$$

<u>Theorem 4.2</u> A solution to (4.10) and (4.11) is $R_1 = .6$ and $R_2 = 1/3$.

Proof of Theorem 4.2:

Let: $$a = \sum_{i=1}^{K}\beta_{iii}^2$$

$$b = \sum_{i=1}^{K}\sum_{j\neq i}\beta_{iii}\beta_{ijj}$$

$$c = \sum_{i=1}^{K}\sum_{j\neq i}\beta_{ijj}^2$$

$$d = \sum_{i=1}^{K}\sum_{j\neq i}\sum_{k\neq i,j}\beta_{ijj}\beta_{ikk}$$

then (4.10) and (4.11) become:

$$(2a/3)R_1 + (b/3)R_2 = 2a/5 + b/9 \tag{4.10a}$$

$$(b/3)R_1 + (2c+2d)R_2/3 = b/5 + 2c/9 + 2d/9 \tag{4.11a}$$

Substitution of $R_1 = .6$ and $R_2 = 1/3$ verifies the theorem. The solution is unique only if a and c from the proof are both non-zero.

One may also wish to consider R_1 and R_2 as fixed and determine the set of β_2 vectors for which B attains a local minimum. The β_2 vectors under consideration will be restricted to vectors of unit length. Minimization is accomplished using a lagrangian multiplier and consider the matrix derivatives of the equation:

$$B = \frac{N}{\sigma^2}\beta_2'C\beta_2 + \theta(\beta_2'\beta_2-1) \tag{4.12}$$

Setting the derivative with respect to θ equal to zero gives the restriction of unit vectors. Setting the matrix derivative with respect to β_2 equal to zero and letting $\lambda = -\theta\sigma^2/N$ results in:

$$(C-\lambda I)\beta_2 = 0 \tag{4.13}$$

<u>Theorem 4.3</u>: The set of β_2 vectors which provide extreme values of B for a fixed design are among the eigen-vectors of the matrix C.

Proof of Theorem 4.3:

From (4.13) it is seen that for a non-trivial solution it is necessary that λ be an eigen value of C and β_2 be the corresponding eigen vector. This completes the proof.

Theorem 4.3 is applied to the nested cube design with K = 3 and $n_1 = n_2 = n_3 = n_4 = 1$ resulting in the eigen vectors displayed in Table 4.5. Table 4.6 compares the actual bias for these β_2 vectors to the minimum bias for the selected set of designs. Sets of eigen vectors associated with the same eigen value form bases for all possible local extremes.

The entries of Table 4.6 indicate that the space spanned by the eigen vectors associated with the eigen value of .219572 is where the maximum bias exists for the nested cube design. Similarly the space spanned by the eigen vectors associated with the eigen value of .029630 is where the minimum bias is for the nested cube design.

Table 4.5 Eigen Vectors for the Nested Cube Design

$K = 3 \quad n_1 = n_2 = n_3 = n_4 = 1$

$i =$	1	2	3	4	5	6	7	8	9	10
$\lambda_i =$	.219572	.219572	.219572	.037037	.029630	.029630	.029630	.029630	.029630	.029630
β_{111}	.775663	0	0	0	0	0	−.000004	−.631147	0	0
β_{222}	0	.775663	0	0	0	−.000004	0	0	−.631147	0
β_{333}	0	0	.775663	0	−.000004	0	0	0	0	−.631147
β_{122}	.446288	0	0	0	0	0	−.707103	.548481	0	0
β_{133}	.446288	0	0	0	0	0	.707110	.548481	0	0
β_{211}	0	.446288	0	0	0	−.707103	0	0	.548481	0
β_{233}	0	.446288	0	0	0	.707110	0	0	.548481	0
β_{311}	0	0	.446288	0	−.707103	0	0	0	0	.548481
β_{322}	0	0	.446288	0	.707110	0	0	0	0	.548481
β_{123}	0	0	0	1.0	0	0	0	0	0	0

Table 4.6 Bias Efficiencies for β_2 = Eigen Vectors for the Nested Cube Design

	$E_b = B_{min}/B$									
Design	i = 1	2	3	4	5	6	7	8	9	10
NC	.203	.203	.203	1.00	1.00	1.00	1.00	.588	.588	.588
NC+	.256	.256	.256	1.00	1.00	1.00	1.00	.858	.858	.858
3K	.172	.172	.172	1.00	1.00	1.00	1.00	.863	.863	.863
KS	.127	.127	.127	1.00	1.00	1.00	1.00	.546	.546	.546
KS+	.172	.172	.172	1.00	1.00	1.00	1.00	.863	.863	.863
K+S	.106	.106	.106	1.00	1.00	1.00	1.00	.388	.388	.388
KE	.141	.141	.141	1.00	1.00	1.00	1.00	.659	.659	.659
KE+	.172	.172	.172	1.00	1.00	1.00	1.00	.863	.863	.863
K+E	.118	.118	.118	1.00	1.00	1.00	1.00	.480	.480	.480
RC	.892	.892	.892	1.00	1.00	1.00	1.00	.778	.778	.778
RC+	.978	.978	.978	1.00	1.00	1.00	1.00	.700	.700	.700
RI	.827	.827	.827	1.00	1.00	1.00	1.00	.654	.654	.654

5. VARIANCE AND VARIANCE COMPARISONS

A major consideration in choosing an experimental design is the variance of the estimator. Many papers have been written concerning choice of designs based on some aspect of the variance. Some characteristics studied are D-optimality, G-optimality, V-optimality, A-optimality and related measures of efficiency.

The measure of D-efficiency proposed by Keifer (1959) considers the extent to which the determinant of the information matrix ($1/N\ X'X$) is maximized. Further works are reviewed in St. John and Draper (1975). In one of the papers, Kono (1962) derives a set of D-optimal designs for which integer approximations are available. Some of the practical aspects of D-optimality are examined by Nalimov, Galinkova and Mikeshina (1970). A recent paper by Lucas (1976) examines D-efficiency and G-efficiency for a select set of designs.

G-efficiency emphasizes minimization of the maximum variance over a region of interest. Keifer (1974) showed that D-efficiency and G-efficiency were equivalent and so only D-efficiency is examined.

V-efficiency examines the integrated variance over the region of interest. A-efficiency examines the trace of the variance-covariance matrix. V- and A-efficiencies are different in that V-efficiency considers both variance and covariance of parameters while A-efficiency considers only the variance of the parameters.

Since no single measure of variance efficiency is uniformly accepted as best, a variety of measures will be used and the results compared. The measures that will be used are:

1. D-efficiency - $|1/N\ X'X|^{1/p}$
2. A-efficiency - $N \cdot tr(X'X)^{-1}$
3. V-efficiency - $N \cdot tr\{(X'X)^{-1}W_{11}\}$
4. Profiles of variance for selected values of independent variables.

As was discussed in previous chapters, there are several situations of interest concerning possible true populations and the model used. Situations to be considered are:

1. Population model cubic and cubic model used.
2. Population model cubic and quadratic model used with minimum bias estimation.
3. Population model cubic and quadratic model used with standard estimator.
4. Population model quadratic and quadratic model used with standard estimator.

It was shown in Chapter 3 that of the designs examined only for the nested cube design did the minimum bias estimator exist. The variance for the nested cube design using the cubic model and using the minimum bias estimator will be derived and compared with the standard estimator for the quadratic model.

5.1 Population Model Cubic and Cubic Model Used

As was demonstrated in Chapter 3, not all of the parameters of the cubic model are estimable with the nested cube design. In order to use the full model it is necessary to define some constraints. Theorem 3.1 indicates which parameters and linear combinations of parameters are estimable for the nested cube design. $\sum_{j \neq i} \beta_{ijj}$ is estimable but the individual parameters are not. Using the constraint that:

$$\beta_{ijj} = 1/(K-1) \sum_{j \neq i} \beta_{ijj} = \bar{\beta}_{i..} \tag{5.1}$$

enables the use of the full model. Using the matrix Q to specify the constraints, the estimate of β is:

$$\hat{\beta}_c = Q(X'X)^- X'Y \tag{5.2}$$

where

$$Q = \begin{bmatrix} I & & \\ & 1/(K-1)\cdot J \otimes I & \\ & & I \end{bmatrix} \tag{5.3}$$

From this, the estimate of the response is seen to be:

$$\hat{Y}_c(x) = x'\hat{\beta}_c \tag{5.4}$$

It is easily seen that:

$$\mathrm{Var}(\hat{Y}_c(x)) = \sigma^2 \; x'Q(X'X)^- Q'x \tag{5.5}$$

and

$$\int_R \cdots \int \mathrm{Bias}^2(\hat{Y}_c(x)) \, dx \Big/ \int_R \cdots \int dx = \beta_b'\{(\tfrac{1}{15}\cdot I + \tfrac{1}{27}(J-I)) \otimes I\}\beta_b \tag{5.6}$$

where $\beta_b' = (\beta_{122}-\bar{\beta}_{1..}, \beta_{133}-\bar{\beta}_{1..}, \ldots, \beta_{K,K-1,K-1} - \bar{\beta}_{K..})$ (5.7)

Thus, if the model is cubic and a cubic model is used, the variance of the estimate depends on the matrix $Q(X'X)^- Q'$ and the bias depends on the variability of β_{ijj} for a fixed value of i. Figure 5.1 shows the general form of the matrix $Q(X'X)^-Q'$.

The determinant of $Q(X'X)^-Q'$ being equal to zero follows from $\det(Q) = 0$. Thus, comparisons of efficiency involving the determinant (D-efficiency) would be meaningless. The other efficiency measures will be examined. From Figure 5.1, the trace of $Q(X'X)^-Q'$ is seen to be (for use in A-efficiency measure):

$$\mathrm{tr}(Q(X'X)^-Q') = a_1 + Ka_2 + Ka_6 + \binom{K}{2}/[220] + Ka_8 + K(K-1)a_{10} + \binom{K}{3}/[222] \qquad (5.8)$$

where the a_i's are specified in Figure 5.1. The values of $\mathrm{tr}(Q(X'X)^-Q'$ for the nested cube design with one or two replicates of star points and three independent factors are 5.33247 and 2.20945. These values will be compared with other designs using the quadratic model later in this chapter. It should be noted, however, that more parameters are estimated here than with the quadratic model.

The other efficiency measure that is to be used is V-efficiency. For this the integrated variance is examined.

$$\int_R \cdots \int \mathrm{Var}(\hat{Y}_c(x))\, dx = \sigma^2 \int_R \cdots \int x'Q(X'X)^-Q'x\, dx$$

$$Q(X'X)^{-}Q' = \begin{bmatrix} a_1 & 0 & a_2 \cdot j' & 0 & 0 & 0 & 0 \\ 0 & a_3 \cdot I & 0 & 0 & a_4 \cdot I & \varepsilon \cdot a_5 \cdot j' \otimes I & 0 \\ a_2 \cdot j & 0 & a_6 \cdot I + a_7 \cdot (J-I) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/[220]\ I & 0 & 0 & 0 \\ 0 & a_4 \cdot I & 0 & 0 & a_8 \cdot I & \varepsilon \cdot a_9 \cdot j' \otimes I & 0 \\ 0 & \varepsilon \cdot a_5 \cdot j \otimes I & 0 & 0 & \varepsilon \cdot a_9 \cdot j \otimes I & \varepsilon \cdot a_{10} \cdot J \otimes I & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/[222]\ I \end{bmatrix}$$

$\varepsilon = 1/(K-1)$

$\lambda = 1/(N([400]-[220]) + (K-1)(N[220]-[200]^2))$

$\delta = [200][600][222] + 2[400][220][420] - [600][220]^2 - [222][400]^2 - [200][420]^2$

$a_1 = (1 + \lambda[200]^2(K-1))/N$

$a_2 = -\lambda[200]$

$a_3 = ([600][222] - [420]^2)/\delta$

$a_4 = ([420][220] - [400][222])/\delta$

$a_5 = ([400][420] - [600][220])/\delta$

$a_6 = (1 - \lambda(N[220] - [200]^2))/([400] - [220])$

$a_7 = \lambda([200]^2 - N[220])/([400] - [220])$

$a_8 = ([200][222] - [220]^2)/\delta$

$a_9 = ([400][220] - [200][420])/\delta$

$a_{10} = ([200][600] - [400]^2)/\delta$

Figure 5.1 Form of $Q(X'X)^{-}Q'$ for the Nested Cube Design

$$= \sigma^2 \int_R \cdots \int \mathrm{tr}(x' Q(X'X)^- Q' x \; dx$$

$$= \sigma^2 \int_R \cdots \int \mathrm{tr}(Q(X'X)^- Q' xx') \; dx$$

$$= \sigma^2 \; \mathrm{tr}(Q(X'X)^- Q' W)/2^K \tag{5.9}$$

where $W = \begin{bmatrix} W_{11} & W_{12} \\ W_{12}' & W_{22} \end{bmatrix}$

and W_{11}, W_{12}, and W_{22} are defined in (3.32)-(3.34). Completing the matrix multiplication and evaluating the trace results in

$$\mathrm{tr}(Q(X'X)^- Q' W) = a_1 + 2Ka_2/3 + K\{a_3/3 + 2a_4/5 + 2a_5/9 + a_8/7 + 2a_9/15 + a_6/5 + (K-1)a_7/9 + a_{10}((K-2)/27(K-1) + 1/15(K-1))\} + \binom{K}{2}/9[220] + \binom{K}{3}/27[222] \tag{5.10}$$

The values of this quantity for the nested cube design with one and two replicates of star points are .9299 and .335.

5.2 Population Model Cubic and Quadratic Model Used with Minimum Bias Estimator

It was shown in Chapter 3 that the minimum bias estimator proposed by Karson, Manson and Hader (1969) exists for the nested cube design. Karson, Manson, and Hader show that

$$\mathrm{Var}\,(\tilde{Y}(x)) = \sigma^2 x' A(X'X)^- A' x \tag{5.11}$$

where $\tilde{Y}(x)$ is the minimum bias estimator. The general form of the matrix $A(X'X)^- A'$ is shown in Figure 5.2. This matrix will be used in the same manner as $Q(X'X)^{-}Q'$ for the efficiency comparisons.

$$A(X'X)^{-}A' = \begin{bmatrix} a_1 & 0 & a_2 \cdot j' & 0 \\ 0 & z \cdot I & 0 & 0 \\ a_2 \cdot j & 0 & a_6 \cdot I + a_7 \cdot (J-I) & 0 \\ 0 & 0 & 0 & 1/[220] \cdot I \end{bmatrix}$$

$z = a_3 + 6a_4/5 + 2a_5/3 + 9a_8/25 + 2a_9/5 + a_{10}/9$

a_i's are defined in Figure 5.1.

Figure 5.2 $A(X'X)^{-}A'$ for the Nested Cube Design

5.3 Standard Estimator for Quadratic Model Used with either Cubic or Quadratic Model

The variance of the estimator depends on the model used and not upon the underlying model. When a quadratic model is used, the standard least-squares estimator is:

$$\hat{Y}(x) = x_1'(X_1'X_1)^{-1}X_1'Y \tag{5.12}$$

with variance given by

$$\mathrm{Var}\ (\hat{Y}(x)) = \sigma^2 x_1'(X_1'X_1)^{-1}x_1 \tag{5.13}$$

It was demonstrated in Chapter 3 that $(X_1'X_1)^{-1}$ exists. The form of $(X_1'X_1)^{-1}$ is shown in Figure 5.3.

In order to make D-efficiency comparisons it is necessary to evaluate the determinant of $(X_1'X_1)^{-1}$ for the selected designs. Theorem 5.1 gives a computational formula for the inverse of these determinants in terms of the design moments.

$$(X_1'X_1)^{-1} = \begin{bmatrix} a_1 & 0 & a_2\cdot j' & 0 \\ 0 & 1/[200]\cdot I & 0 & 0 \\ a_2\cdot j & 0 & a_6\cdot I + a_7\cdot(J-I) & 0 \\ 0 & 0 & 0 & 1/[220]\cdot I \end{bmatrix}$$

a_i's are defined in Figure 5.1.

Figure 5.3 $(X_1'X_1)^{-1}$ for Symmetric Second Order Designs with Zero Odd Moments

Theorem 5.1 For $X_1'X_1$ as shown in Figure 3.1

$$|X_1'X_1| = [200]^K[220]^{\binom{K}{2}} \{N - K[200]^2/([400] - [220]) + K^2[200]^2[220]/(([400] - [220])([400] + (K-1)[220]))\}\cdot ([400] + (K-1)[220])([400] - [220])^{K-1}$$

Proof of Theorem 5.1:

By partitioning $X_1'X_1$ it is seen that the determinant can be found as the product of three matrices A_1, A_2 and A_3, where

$$A_1 = \begin{bmatrix} N & [200]\cdot j' \\ [200]\cdot j & [400]\cdot I + [220]\cdot(J-I) \end{bmatrix}_{K+1 \times K+1} \tag{5.14}$$

$$A_2 = [200]\cdot I_K \tag{5.15}$$

$$A_3 = [220]\cdot I_{\binom{K}{2}} \tag{5.16}$$

The determinant of a diagonal matrix is the product of the diagonal elements and thus

$$|A_2| \cdot |A_3| = [200]^K [220]^{\binom{K}{2}} \qquad (5.17)$$

Showing that $|A_1|$ is the remaining factor in Theorem 5.1 involves three theorems found in Graybill (1969). The results of the theorem will be stated without proof.

The first result that will be used is for a partitioned matrix :

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

where B_{ij} has dimension $n_i \times n_j$, if B_{22} is nonsingular then

$$|B| = |B_{22}| \cdot |B_{11} - B_{12}B_{22}^{-1}B_{21}|.$$

This is applied by partitioning A_1 as in (5.14) which gives

$$|A_1| = |([400]-[220]) \cdot I + [220] \cdot J| \cdot |N-[200]^2 j' B_{22}^{-1} j| \qquad (5.18)$$

for $\beta_{22} = ([400]-[220]) \cdot I + [220] \cdot J$.

The next result to be applied concerns a matrix with a particular form. For a square matrix $C = D + \alpha ab'$ where D is a nonsingular diagonal, a and b are $K \times 1$ vectors and α is a scalar such that $\alpha \neq -\{\sum_{i=1}^{K} a_i b_i / d_{ii}\}^{-1}$, the inverse of C is given by:

$$C^{-1} = D^{-1} + \gamma a^* b^{*\prime},$$

where $\gamma = -\alpha(1 + \alpha \sum_{i=1}^{K} a_i b_i / d_i)^{-1}$; $a_i^* = a_i/d_{ii}$ and $b_i^* = b_i/d_{ii}$.

This result is applied to find the inverse of B_{22} by making the following associations:

$$d_{ii} = [400]-[220] \qquad i=1,\dots,K$$

$$a_i = b_i = 1 \qquad i=1,\dots,K$$

$$\alpha = [220]$$

This gives:

$$B_{22}^{-1} = 1/([400]-[220])\cdot I - ([220]-[400])/([220]([400]+(K-1)[220]))\cdot J \tag{5.19}$$

The last of the three theorems from Graybill gives the determinant of the matrix C of the previous result. The result is:

$$|C| = \{1 + \alpha \sum_{j=1}^{K} a_j b_j / d_{jj}\} \prod_i d_{ii} \tag{5.20}$$

Application of this result gives:

$$|B_{22}| = ([400] + (K-1)[220])([400]-[220])^{K-1}$$

Combining all of the results gives:

$$|A_1| = ([400]+(K-1)[220])([400]-[220])^{K-1}\{N - [200]^2(K/([400]-[220]) - K^2[220]/(([400]-[220])([400] + (K-1)[220])))\} \tag{5.21}$$

This completes the proof of Theorem 5.1.

The result of this theorem makes calculations of relative D-efficiencies easier. The rationale behind the D-efficiency is that the volume of the dispersion ellipsoid of concentration of parameter estimates is inversely proportional to the square root of the determinant of the information matrix (Nalimov, Golikova, and

Mikeshina 1970). The measure of efficiency associated with D-efficiency considers the p^{th} root of the determinant of the matrix $X'X$ where p is the number of parameters involved. Table 5.1 contains information for making comparisons of D-efficiency for K = 3. The column labeled R_D gives the relative D-efficiency as compared to the nested cube design.

The A- and V-efficiencies are examined next. In section 5.1 it was shown that the integrated variance is directly proportional to the trace of $(X_1'X_1)^{-1}W$ when the model is cubic. A similar argument shows that when the model is quadratic, the value of interest is the trace of $(X_1'X_1)^{-1}W_{11}$. For A-efficiency, the value of interest is the trace of $(X_1'X_1)$. Both of these traces are shown in Table 5.2. In order to account for different sample sizes required for different designs, the values of $N \cdot tr(X_1'X_1)^{-1}$ and $N \cdot tr(X_1'X_1)^{-1}W_{11}$ are also given. The columns labeled R_A and R_V give the relative A- and V-efficiencies as compared to the nested cube design with sample size taken into consideration.

In examining Table 5.2 it is noticed that the measures rank the nested cube design and other designs differently. The difference arises from A-efficiency accounting only for the variance of the parameters and V-efficiency accounting for both variance and covariance. When covariance is taken into consideration, the nested design is ranked third among the designs considered. While, when

Table 5.1 D-efficiency Comparisons

Design	$\lvert X'X \rvert$	$\lvert 1/N \cdot X'X \rvert$	R_D
NC	8.51078×10^{8}	2.0545×10^{-5}	1.000
NC+	7.21238×10^{9}	1.7144×10^{-5}	.982
3K	5.87720×10^{10}	2.8546×10^{-4}	1.301
KS	1.84318×10^{8}	3.1964×10^{-4}	1.316
KS+	2.20828×10^{9}	1.3239×10^{-4}	1.205
K+S	1.70079×10^{10}	4.1057×10^{-4}	1.349
KE	8.15359×10^{9}	4.8883×10^{-4}	1.373
KE+	4.34859×10^{11}	2.8394×10^{-4}	1.300
K+E	2.26489×10^{11}	5.3837×10^{-4}	1.386
RC	2277.89	3.9502×10^{-9}	.426
RC+	304126	4.9604×10^{-8}	.547
RI	4.1201	6.5877×10^{-11}	.289
NC_b *	4.0300×10^{7}	9.7280×10^{-7}	.737
$NC+_b$ *	1.9796×10^{8}	4.7054×10^{-7}	.685

* involves use of minimum bias estimator.

Table 5.2 A- and V-efficiency Comparisons

Design	$tr(X_1'X_1)^{-1}$	$N\cdot tr(X_1'X_1)^{-1}$	R_A	$tr(X_1'X_1)^{-1}W_{11}$	$N\cdot tr(X_1'X_1)^{-1}W_{11}$	R_V
NC	1.712	39.376	1.00	.170	3.912	1.00
NC+	1.239	35.944	1.10	.155	4.486	.87
3K	1.102	29.750	1.32	.146	3.950	.99
KS	2.004	30.054	1.31	.232	3.482	1.12
KS+	1.390	29.193	1.35	.187	3.930	.996
K+S	1.615	37.153	1.06	.154	3.531	1.11
KE	1.595	33.503	1.18	.204	4.291	.91
KE+	1.033	34.080	1.16	.135	4.459	.88
K+E	1.356	39.314	1.00	.166	4.810	.81
RC	6.353	95.295	.41	.811	12.167	.32
RC+	3.571	67.857	.58	.460	8.746	.45
RI	4.968	59.612	.66	.605	7.261	.54
NC_b *	2.010	46.238	.85	.269	6.199	.63
$NC+_b$ *	1.520	44.085	.89	.248	7.20	.54
NC_c @	5.330	122.647	.32	.930	21.388	.18
$NC+_c$ @	2.210	64.074	.61	.335	9.705	.40

* involves use of minimum bias estimator.

@ involves use of cubic model.

only variance of parameters is considered, it ranks eighth. Observing the last four rows of Table 5.2 shows that use of the minimum bias estimator or the full cubic model reduce the variance efficiency in terms of A- and V-efficiency. It should be noted that in using the full cubic model more parameters are estimated. It may be noted that use of two replications of star points on the nested cube design gives approximately twice as much efficiency as use of one replication when the full cubic model is used.

The three comparisons thus far indicate efficiencies averaged in some sense over the entire region of interest. Profiles of the variance for a select set of the designs when K = 3 are presented in Figures 5.4 - 5.9 in order to show the behavior of the variance for the designs over a subjectively selected set of vectors. The vectors are chosen to be representative of the region. By reason of symmetry the vectors are able to be in one quadrant of the cube. In five of the six figures, two variables are considered fixed and the third varied. In the other figure all three variables vary at the same rate. For clarity only four other designs are shown in the profiles with the variations of the nested cube design.

Examination of the profiles of the variance shows the relative goodness of the designs varying with location in the cube. Thus, if a particular subregion is of interest, the choice of design should account for this. The variance of the nested cube design appears

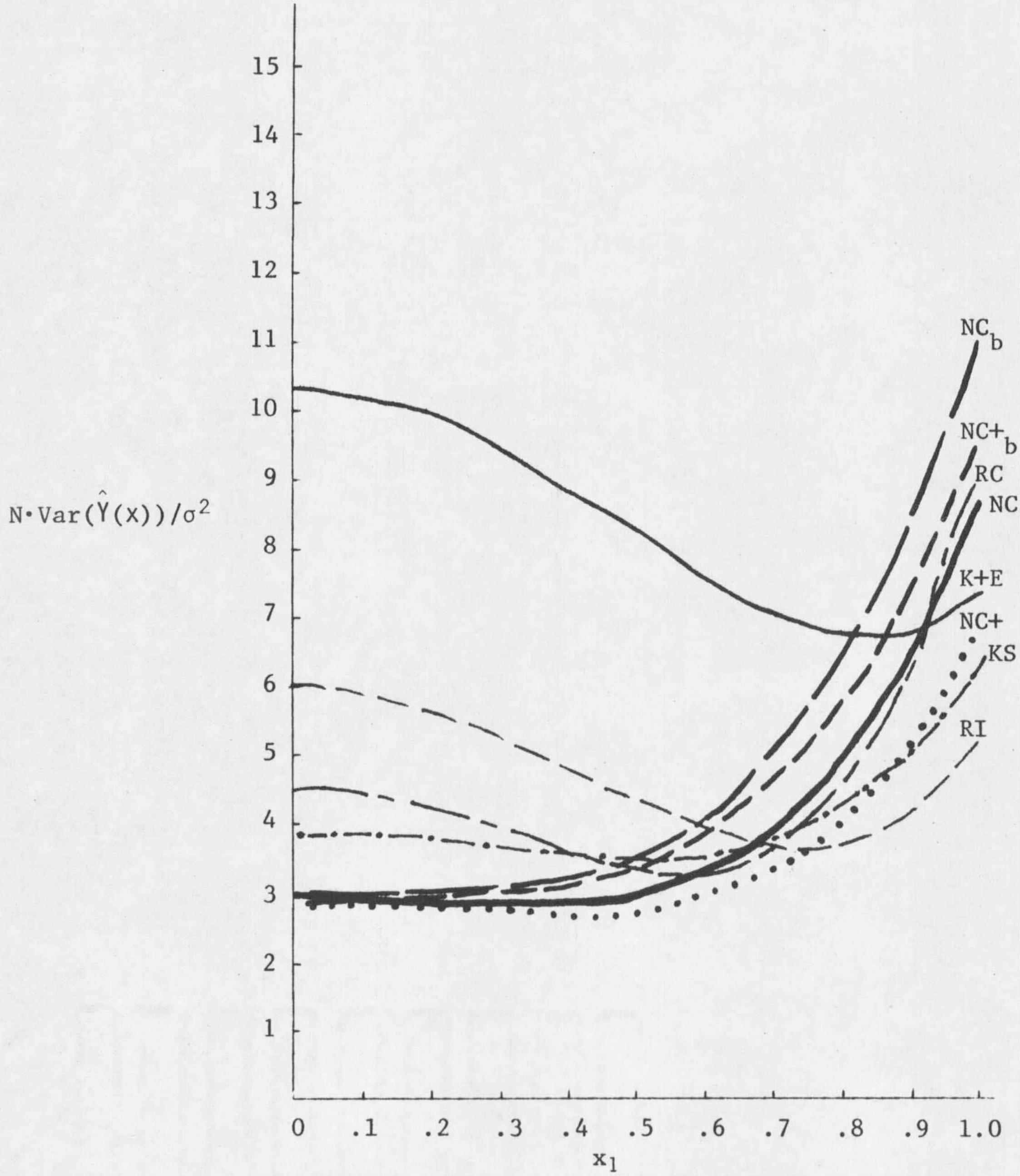


Figure 5.4 N Var($\hat{Y}$(X))/σ^2 when $x_2 = x_3 = 0$

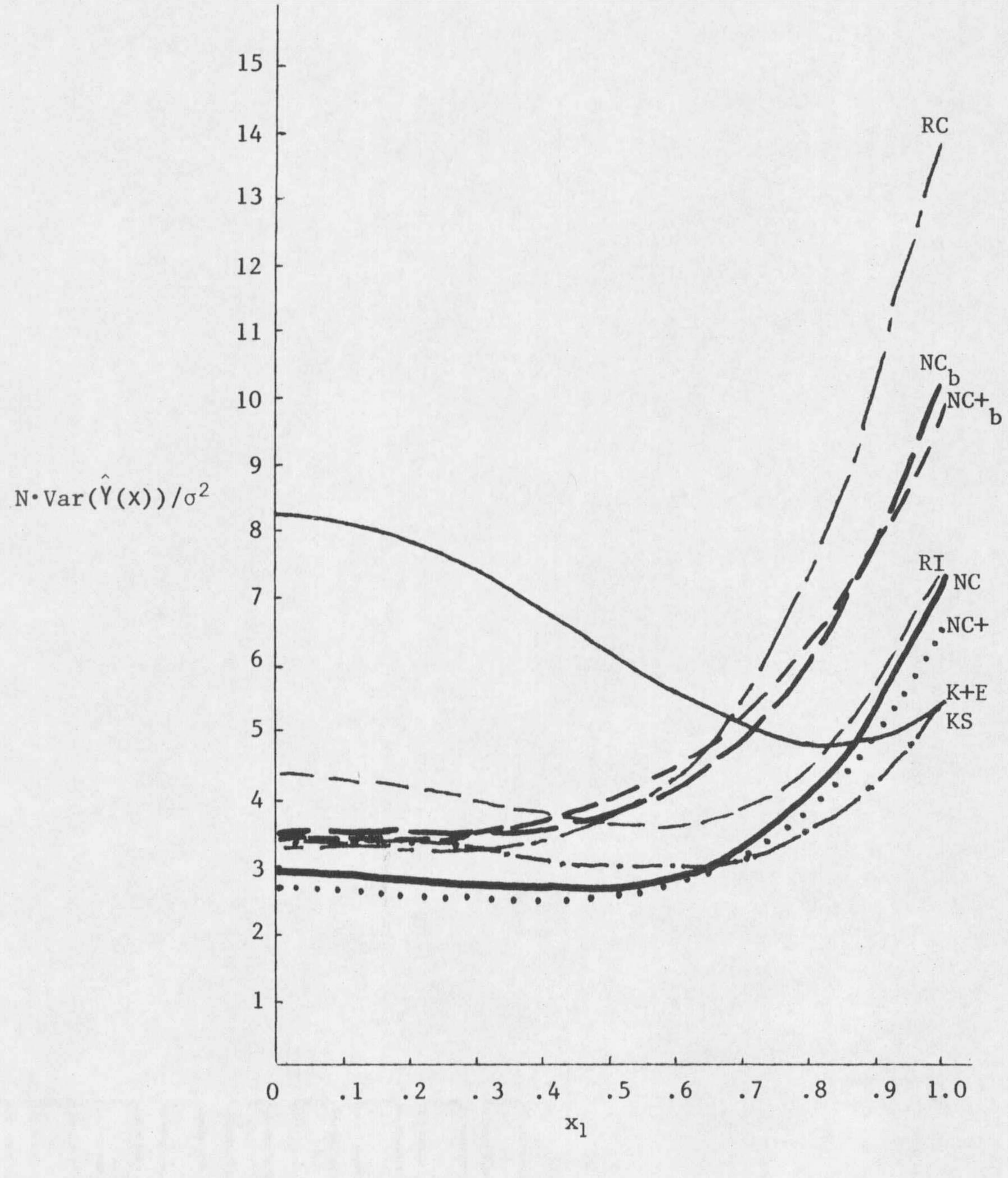


Figure 5.5 $N \cdot Var(\hat{Y}(X))/\sigma^2$ when x_2 = .5 & x_3 = 0

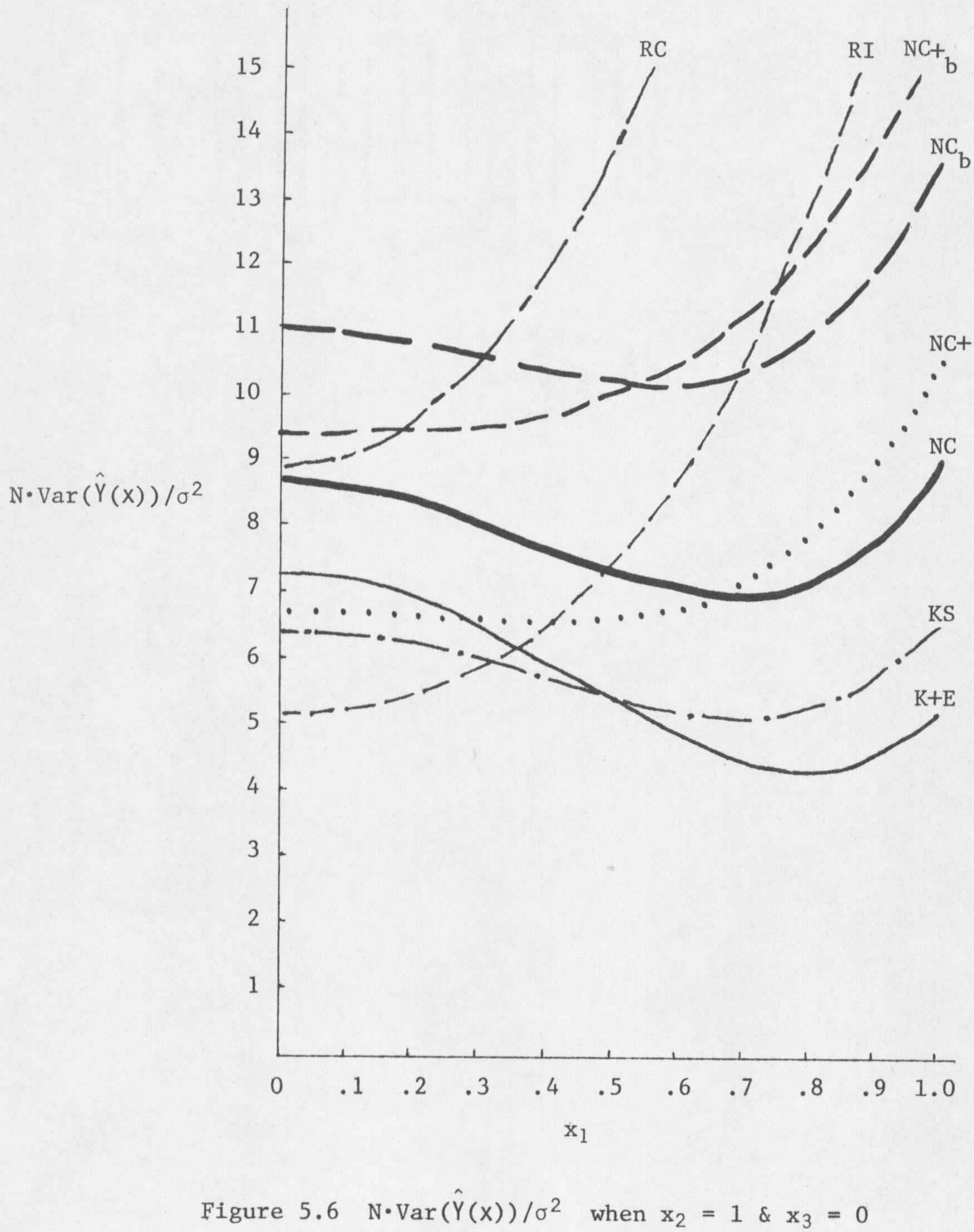


Figure 5.6 $N \cdot Var(\hat{Y}(X))/\sigma^2$ when $x_2 = 1$ & $x_3 = 0$

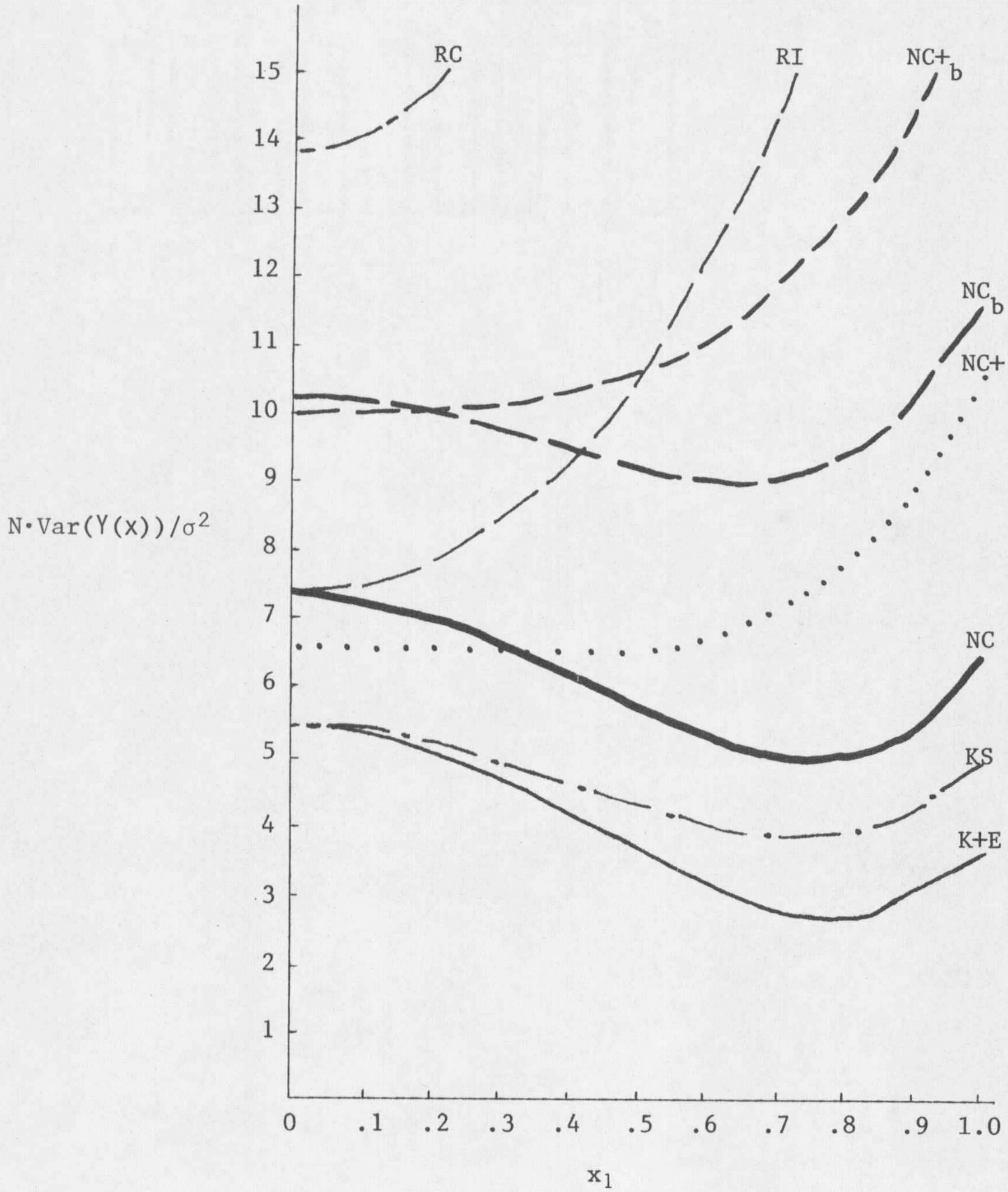
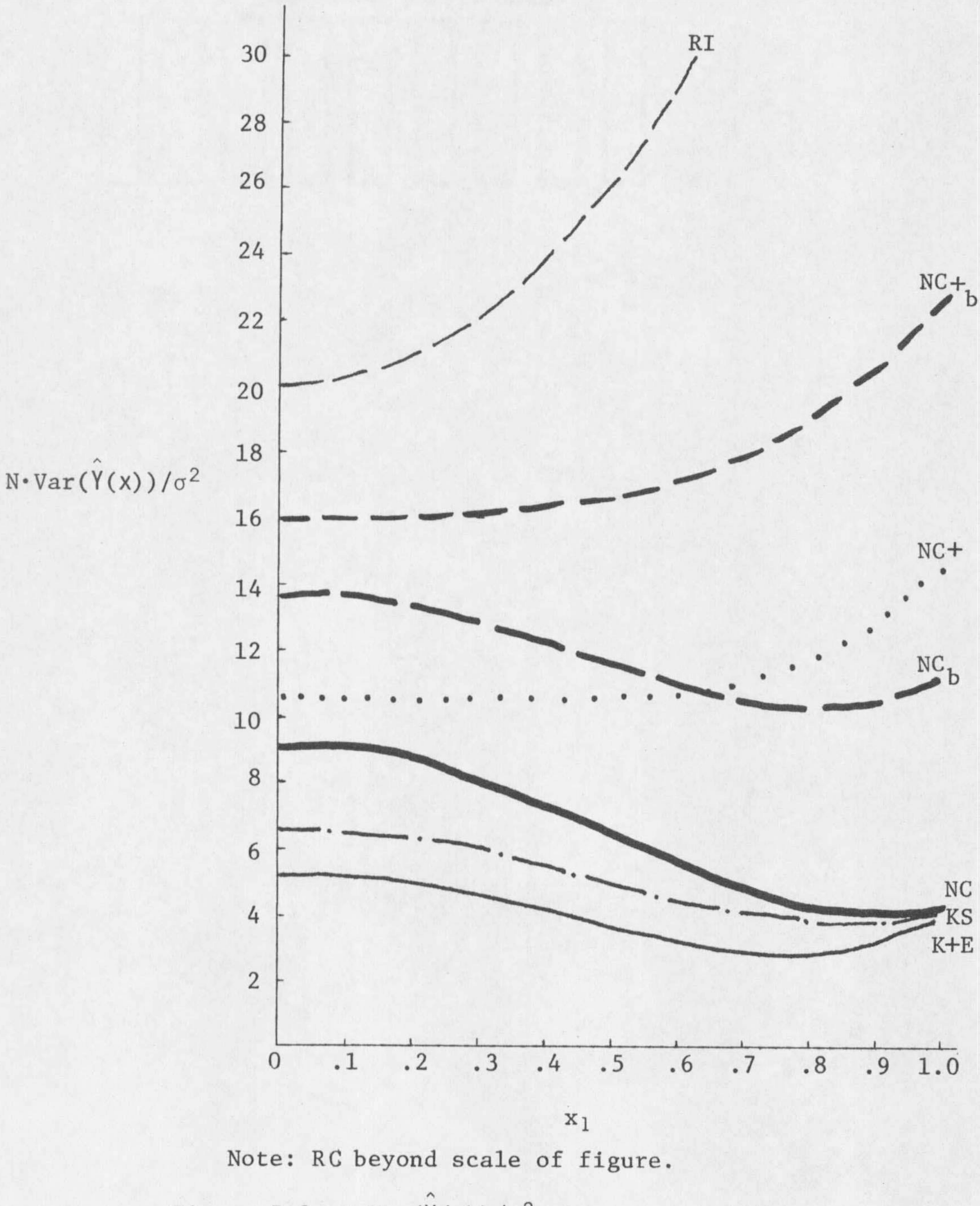


Figure 5.7 $N \cdot Var(\hat{Y}(x))/\sigma^2$ when $x_2 = 1$ & $x_3 = .5$



Note: RC beyond scale of figure.

Figure 5.8 $N \cdot Var(\hat{Y}(x))/\sigma^2$ when $x_2 = x_3 = 1$

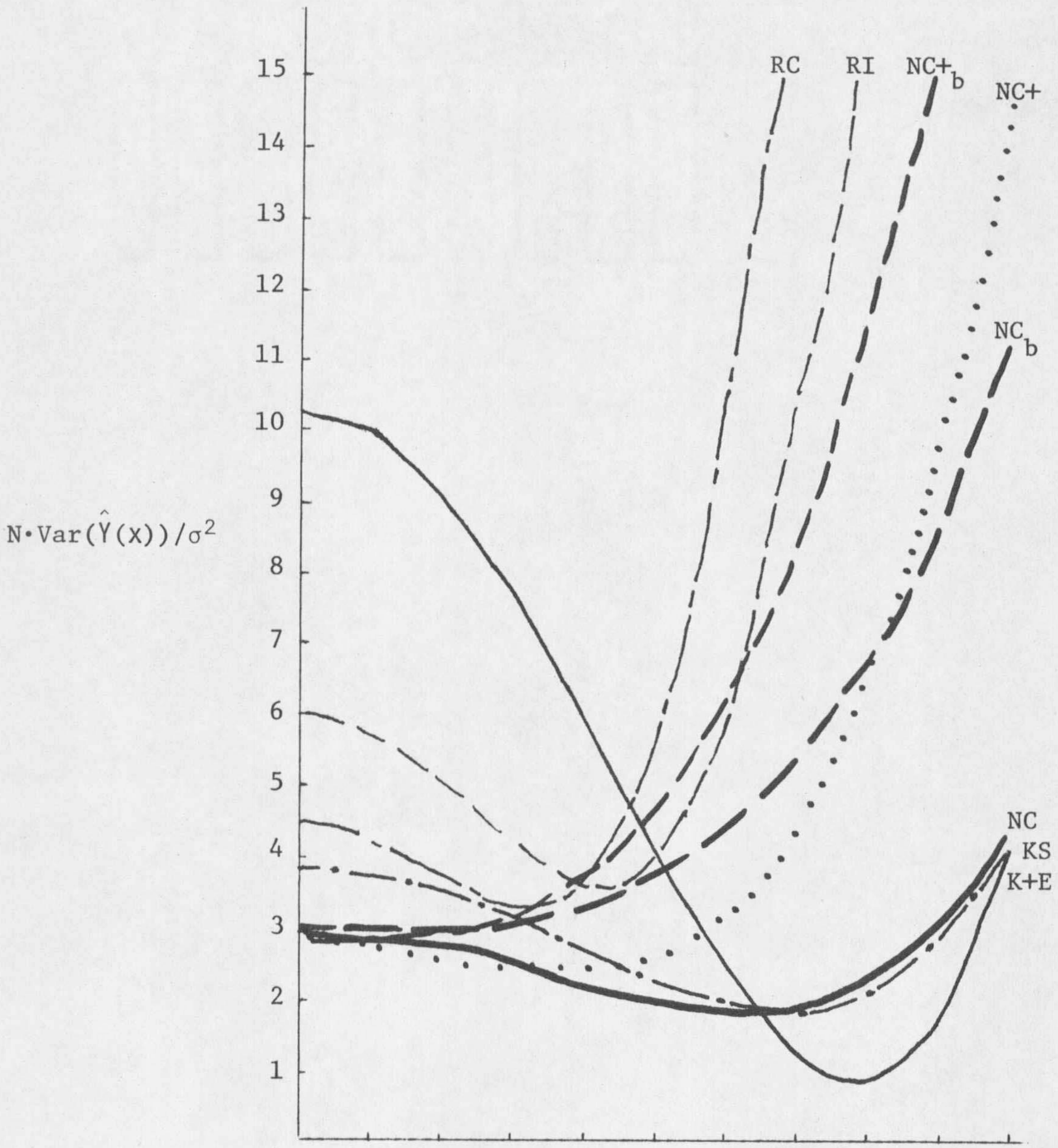


Figure 5.9 $N \cdot Var(\hat{Y}(x))/\sigma^2$ when $x_1 = x_2 = x_3$

quite stable. From examination of the profiles, the V-efficiency measure of relative efficiency for variance appears to be most satisfactory.

5.4 Combining Variance and Bias Comparisons

The bias comparisons of Table 4.1 are made in terms of integrated bias. Consequently, the most appropriate variance comparison to combine with it would be the integrated variance (R_V) of Table 5.2. Some type of mean would be deemed appropriate in order to combine the two kinds of efficiency. Choices to be considered are weighted or unweighted arithmetic or geometric means.

In defining a relative efficiency measure of bias efficiency, the number of experimental settings will be taken into consideration. Define: $R_B = (N \cdot B^{\#} \text{ for Nested Cube}) / (N_i \cdot B^{\#} \text{ for Design } i)$ (5.22)

The weighted arithmetic and geometric means would be:

$$E_A = pR_B + qR_V \qquad (5.23)$$

$$E_G = R_B^p \; R_V^q \qquad (5.24)$$

where $p + q = 1$. The unweighted means occur when $p = q = 1/2$. The unweighted means are shown in Table 5.3. The columns of R_B and R_V show that most of the designs that perform better in terms of E_A do so because of good performance with bias. The high efficiency of the KS design is chiefly due to the small number of experimental settings. The small number of experimental settings gives smaller degrees of freedom for detecting lack of fit and restricts the number of estimable linear combinations of parameters.

Table 5.3 Combined Variance and Bias Comparisons

Design	N	R_B	R_V	E_A	E_G
NC	23	1.00	1.00	1.000	1.000
NC+	29	.98	.87	.925	.923
3K	27	.41	.99	.700	.637
KS	15	1.11	1.12	1.115	1.115
KS+	21	1.05	.996	1.023	1.023
K+S	23	.60	1.11	.855	.816
KE	21	.89	.91	.900	.900
KE+	33	.67	.88	.775	.768
K+E	29	.53	.81	.670	.655
RC	15	3.11	.32	1.715	.998
RC+	21	1.58	.45	1.015	.843
RI	12	3.58	.54	2.060	1.390
NC_b *	23	1.88	.63	1.255	1.090
$NC+_b$ *	29	1.49	.54	1.015	.900

* involves use of minimum bias estimator.

6. SUMMARY AND CONCLUSION

The objectives of the dissertaition as stated in Chapter 1 were to:

1. Show that the nested cube design has the use of equal spacing of factors and is easily expanded or reduced.
2. Examine the estimability of quadratic and cubic models for the nested cube design.
3. Examine the variance structure of estimates using the nested cube design and compare it to other selected designs.
4. Examine the bias resulting from using a quadratic model when the true model is cubic for the nested cube design and compare it to other selected designs.

The nested cube design is described in detail in Chapter 2. It is verified that the nested cube design makes use of equally spaced factors and is easily expanded or reduced to change the number of factors.

The estimability of the quadratic and cubic models is examined for the nested cube design in Chapter 3. It was found that the nested cube design enables estimation of all parameters in the quadratic model and a specific set of linear combinations of parameters in the cubic model. The minimum bias estimator of Karson, Manson, and Hader (1969) is examined and conditions are given for the use of the minimum bias estimator. It is shown that the nested cube design satisfies the specific conditions and other selected designs do not. The estimable linear combinations for the other selected designs are given.

The bias resulting from fitting a quadratic model when the true model is cubic is examined in Chapter 4. Comparisons are made with the selected designs. The comparisons are made using two measures of efficiency introduced in the chapter. The first involves comparing expected bias averaged over parameter vectors of the same length. The basis for the comparison comes from the paper Karson, Manson, and Hader (1969). The second measure used involves subjectively chosen parameter vectors where the relative sizes of the parameters are specified. This idea may be able to be expanded upon at a future date by considering an a priori distribution for the β_2 vectors and using Bayesian techniques to derive expected bias.

The first type of comparison on bias shows the nested cube design has more bias than the rotatable designs but less than any of the other designs examined. From Table 4.1 it appears that the rotatable designs have their peak bias efficiency when there are a small number of factors, while the remaining designs examined have a low in bias efficiency for K small. Examination of the bias efficiency for specific β_2 vectors shows that none of the selected designs are uniformly better than the remaining. The selected vectors depict situations for which the nested cube design has both smaller and larger bias.

The variance for the standard estimator for the quadratic model, the minimum bias estimator and the estimator for the cubic model are examined in Chapter 5. Comparisons of efficiencies are made in terms of D-efficiency, A-efficiency and V-efficiency. Also examined are profiles of variance for selected levels of independent factors. Utilization of these various measures does not show one design to be superior to all others. The rotatable designs are less efficient in terms of variance due to the designs being constructed for use on a spherical independent variable space rather than on a cube. However, among the remaining designs, the different measures of efficiency indicate different orderings. The D-efficiency measure ranked the K+E design as best which agrees with Kono (1962) who showed that an integer approximation to a D-optimal design was a variation of the KE design. Both A-efficiency and V-efficiency rank variations of the KS design slightly higher than the nested cube design.

Examination of the profiles of variance for selected designs on selected sets of factor values suggest the preferable efficiency measure to be V-efficiency. The average bias measure of efficiency and the V-efficiency for variance are combined because they are both related to contributions to the integrated mean square error. The resulting measure is a combined bias and variance measure of relative efficiency. The nested cube design ranks high among the designs with the minimum bias estimator ranking higher than the standard estimator.

APPENDIX A

DESCRIPTION OF DESIGNS USED FOR COMPARISONS

1. Nested Cube (NC) - this design is made up of four parts:

    a) Outer cube - all combinations of points where factors take on values ±1.

    b) Inner cube - all combinations of points where factors take on values ± .5.

    c) Star points - set of 2K points where ith factor takes on values ±1 and all other factors are 0 for $i=1,\cdots,K$.

    d) Center point - all factors at 0 level.

Example: $K = 3$ $(N = 2^{K+1}+2K+1 = 23)$

X_1	X_2	X_3	
1	1	1	Outer cube
1	1	-1	
1	-1	1	
1	-1	-1	
-1	1	1	
-1	1	-1	
-1	-1	1	
-1	-1	-1	
.5	.5	.5	
.5	.5	-.5	
.5	-.5	.5	

$$[200] = 2^K+2^{K-2}+2 = 12$$

$$[400] = 2^K+2^{K-4}+2 = 10.5$$

$$[600] = 2^K+2^{K-6}+2 = 10.125$$

$$[220] = 2^K+2^{K-4} = 8.5$$

$$[420] = 2^K+2^{K-6} = 8.125$$

$$[222] = 2^K+2^{K-6} = 8.125$$

X_1	X_2	X_3	
.5	-.5	-.5	Inner cube
-.5	-.5	-.5	
-.5	-.5	.5	
-.5	.5	-.5	
-.5	.5	.5	
1	0	0	Star points
-1	0	0	
0	1	0	
0	-1	0	
0	0	1	
0	0	-1	
0	0	0	Center point

2. Nested Cube with two replications of star points (NC+) - this design is a variation of design 1. The difference is the use of two replications of the star points.

For K = 3 $(N = 2^{K+1}+4K+1 = 29)$

$[200] = 2^K+2^{K-2}+4 = 14$

$[400] = 2^K+2^{K-4}+4 = 12.5$

$[600] = 2^K+2^{K-6}+4 = 12.125$

$[220] = 2^K+2^{K-4} = 8.5$

$[420] = 2^K+2^{K-6} = 8.125$

$[222] = 2^K+2^{K-6} = 8.125$

3. Factorial with three levels (3K) - this design includes all combinations of design points where factors are -1, 0 or 1.

Example: K = 3 ($N = 3^K = 27$)

X_1	X_2	X_3
1	1	1
1	1	0
1	1	-1
1	0	1
1	0	0
1	0	-1
1	-1	1
1	-1	0
1	-1	-1
0	1	1
0	1	0
0	1	-1
0	0	1
0	0	0
0	0	-1
0	-1	1
0	-1	0
0	-1	-1
-1	1	1

X_1	X_2	X_3
-1	1	0
-1	1	-1
-1	0	1
-1	0	0
-1	0	-1
-1	-1	1
-1	-1	0
-1	-1	-1

$[200] = 2 \cdot 3^{K-1} = 18$

$[400] = 2 \cdot 3^{K-1} = 18$

$[600] = 2 \cdot 3^{K-1} = 18$

$[220] = 4 \cdot 3^{K-2} = 12$

$[420] = 4 \cdot 3^{K-2} = 12$

$[222] = 8 \cdot 3^{K-3} = 8$

4. Factorial with two levels plus star points plus center (KS) - this design as seen in the name consists of three parts:

   a) 2^K - same as outer cube in nested cube design.

   b) Star points - same as star points in nested cube design.

   c) Center point - all factors at 0 level.

Example: K = 3 ($N = 2^K+2K+1 = 15$)

X_1	X_2	X_3	
1	1	1	2^K
1	1	-1	
1	-1	1	
1	-1	-1	
-1	1	1	
-1	1	-1	
-1	-1	1	
-1	-1	-1	
1	0	0	Star points
-1	0	0	
0	1	0	
0	-1	0	
0	0	1	
0	0	-1	
0	0	0	Center point

[200] = 2^K+2 = 10

[400] = 2^K+2 = 10

[600] = 2^K+2 = 10

[220] = 2^K = 8

[420] = 2^K = 8

[222] = 2^K = 8

5. Factorial with two levels plus two star points plus center (KS+) - this design is the same as design number 4 except for use of two replications of the star points.

For K = 3 $(N = 2^K+4K+1 = 21)$

$[200] = 2^K+4 = 12$

$[400] = 2^K+4 = 12$

$[600] = 2^K+4 = 12$

$[220] = 2^K = 8$

$[420] = 2^K = 8$

$[222] = 2^K = 8$

6. Factorial with two levels replicated twice plus star points plus center (K+S) - this design is the same as design number 4 except for use of two replications of the 2^K part.

For K = 3 $(N = 2^{K+1}+2K+1 = 23)$

$[200] = 2^{K+1}+2 = 18$

$[400] = 2^{K+1}+2 = 18$

$[600] = 2^{K+1}+2 = 18$

$[220] = 2^{K+1} = 16$

$[420] = 2^{K+1} = 16$

$[222] = 2^{K+1} = 16$

7. Factorial with two levels plus edge points plus center (KE) - this design like design 4 is divided into three parts:

a) 2^K - same as design 4.

b) Edge points - set of $K \cdot 2^{K-1}$ points in which one of the factors has a value of zero and the remaining form a 2^{K-1} design.

c) Center - same as design 4.

Example: $K = 3$ $(N = 2^K + K \cdot 2^{K-1} + 1 = 21)$

X_1	X_2	X_3	
1	1	0	Edge points
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	
0	0	0	Center point

X_1	X_2	X_3	
1	1	1	2^K
1	1	-1	
1	-1	1	
1	-1	-1	
-1	1	1	
-1	1	-1	
-1	-1	1	
-1	-1	-1	

$[200] = 2^K+(K-1)2^{K-1} = 16$

$[400] = 2^K+(K-1)2^{K-1} = 16$

$[600] = 2^K+(K-1)2^{K-1} = 16$

$[220] = 2^K+(K-2)2^{K-1} = 12$

$[420] = 2^K+(K-2)2^{K-1} = 12$

$[222] = 2^K+(K-3)2^{K-1} = 8$

8. Factorial with two levels plus two edge points plus center (KE+) - this design is the same as design 7 except for use of two replications of the edge points.

For $K = 3$ $(N = (K+1)2^K+1 = 33)$

$[200] = K2^K = 24$

$[400] = K2^K = 24$

$[600] = K2^K = 24$

$[220] = (K-1)2^K = 16$

$[420] = (K-1)2^K = 16$

$[222] = (K-2)2^K = 8$

9. Factorial with two levels replicated twice plus edge points plus center (K+E) - this design is the same as design 7 except for use of two replications of the 2^K part.

For $K = 3$ $(N = 2^{K+1}+K2^{K-1}+1 = 29)$

$[200] = 2^{K+1}+(K-1)2^{K-1} = 24$

$[400] = 2^{K+1}+(K-1)2^{K-1} = 24$

$[600] = 2^{K+1}+(K-1)2^{K-1} = 24$

$[220] = 2^{K+1}+(K-2)2^{K-1} = 20$

$[420] = 2^{K+1}+(K-2)2^{K-1} = 20$

$[222] = 2^{K+1}+(K-3)2^{K-1} = 16$

10. Rotatable central composite (RC) - this design like many of the previous designs can be separated into three parts:

a) Star points - same as before.

b) $\alpha \cdot 2^K$ - these points are like a 2^K except at a distance α from the center.

c) Center point - same as before.

α is chosen so that the design satisfies rotatability criteria of $[400] = 3 \cdot [220]$.

Example: $K = 3$ $(N = 2^K+2K+1 = 15)$

X_1	X_2	X_3	
α	α	α	$\alpha \cdot 2^K$
α	α	$-\alpha$	
α	$-\alpha$	α	
α	$-\alpha$	$-\alpha$	
$-\alpha$	α	α	
$-\alpha$	α	$-\alpha$	
$-\alpha$	$-\alpha$	α	
$-\alpha$	$-\alpha$	$-\alpha$	
1	0	0	Star points
-1	0	0	
0	1	0	
0	-1	0	
0	0	1	
0	0	-1	
0	0	0	Center point

$\alpha = 2^{-K/4}$

$[200] = 2^{K/2}+2 = 4.828427$

$[400] = 3$

$[600] = 2^{-K/2}+2 = 2.35355$

$[220] = 1$

$[420] = 2^{-K/2} = .35355$

$[222] = 2^{-K/2} = .35355$

11. Rotatable central composite with 2 star points (RC+) - this design is like design 10 except that it has two replications of the star points. Rotatability requires a different α.

For $K = 3$ $(N = 2^K+4K+1 = 21)$ $\alpha = 2^{(-K+1)/4}$

$[200] = 2^{(K+1)/2}+4 = 8$

$[400] = 6$

$[600] = 2^{(-K+3)/2}+4 = 5$

$[220] = 2$

$[420] = 2^{(-K+3)/2} = 1$

$[222] = 2^{(-K+3)/2} = 1$

12. Rotatable icosahedron (RI) - this a design specifically for three factors given in Meyers (1976). This design differs from the others by not being symmetric in the mixed sixth moment. The design has the following design points.

X_1	X_2	X_3	X_1	X_2	X_3
0	1	a	a	0	-1
0	1	-a	-a	0	-1
0	-1	a	1	a	0
0	-1	-a	1	-a	0
a	0	1	-1	a	0
-a	0	1	-1	-a	0

$N = 12$

$a = .61843$

$[200] = 5.5298$

$[400] = 4.585$

$[600] = 4.224$

$[220] = 1.530$

$[420] = 1.530$

$[240] = .5851$

$[222] = 0$

APPENDIX B

ESTIMABLE PARAMETERS IN CUBIC MODEL FOR OTHER DESIGNS

All of the designs considered in this paper are symmetric which leads to odd design moments equal zero. The general form of $X'X$ is given in figure 3.2 and which becomes figure 3.3 upon rearrangement. As was noted in equation 3.32, the rearranged version of $X'X$ (ie. $X^{*\prime}X^{*}$) can be denoted by the direct sum of matrices A_{ii} where:

1. A_{11} is associated with the mean and pure second order terms,
2. A_{22} is associated with the linear by linear interactions,
3. A_{ii} for i = 3,•••,K+2 are each of order K+1 and are associated with segments of $X^{*\prime}$ which contain elements $(x_i, x_i^3, x_i x_j^2)$, $j \neq i$

and 4. $A_{K+3,K+3}$ is associated with linear by linear by linear interactions for $K \geq 3$ and nonexistant for $K < 3$.

A_{11} and A_{22} are nonsingular for the designs considered. Hence the parameters associated with corresponding terms are estimable. This follows from the estimability criteria of $q^{*\prime}H^{*} = q^{*\prime}$ as stated in the proof of theorem 3.1. For all except the rotatable icosahedron the matrix H^{*} will have the form of equation 3.36. The rotatable icosahedron is similar but with the identity in the lower right hand corner replaced by a matrix of zeros because [222] = 0. Thus the only variation in the designs studied is in the form of $A_{33}^{-}A_{33}$. Define H_{33}^{*} by:

$$H_{33}^{*} = A_{33}^{-}A_{33} \qquad \text{(B.1)}$$

The rows of H^*_{33} indicate which linear combinations of the parameters $(\beta_i, \beta_{iii}, \underset{j\neq i}{\beta_{ijj}})$ are estimable because:

$$\begin{aligned} H^*_{33}H^*_{33} &= A^-_{33}A_{33}A^-_{33}A_{33} \\ &= A^-_{33}A_{33} \\ &= H^*_{33} \end{aligned} \tag{B.2}$$

For all designs:

$$A_{33} = \begin{bmatrix} [200] & [400] & [220]\cdot j' \\ [400] & [600] & [420]\cdot j' \\ [220]\cdot j & [420]\cdot j & [420]\cdot I + [222]\cdot(J-I) \end{bmatrix}$$

H^*_{33} and the estimable combinations of $(\beta_i, \beta_{iii}, \underset{j\neq i}{\beta_{ijj}})$ are now given for all designs considered herein except the nested cube design.

3. Factorial with three levels (3K) -

$$H^*_{33} = \begin{bmatrix} 0 & 0 & 0\cdot j' \\ 1 & 1 & 0\cdot j' \\ 0\cdot j & 0\cdot j & I \end{bmatrix}$$

β_{ijj} for $j\neq i$ and $\beta_i+\beta_{iii}$ are estimable.

4. Factorial with two levels plus star points plus center (KS) -

$$H^*_{33} = \begin{bmatrix} 0 & 0 & 0\cdot j' \\ 1 & 1 & 0\cdot j' \\ 0 & 0 & 1\cdot j' \\ 0\cdot j & 0\cdot j & 0\cdot I \end{bmatrix}$$

$\sum_{j \neq i} \beta_{ijj}$ and $\beta_i+\beta_{iii}$ are estimable.

5. Factorial with two levels plus two star points plus center (K+S) - same as design 4.
6. Factorial with two levels replicated twice plus star points and center (K+S) - same as design 4.
7. Factorial with two levels plus edge points plus center (KE) -

$$H^*_{33} = \begin{bmatrix} 0 & 0 & 0 \cdot j' \\ 1 & 1 & 0 \cdot j' \\ 0 \cdot j & 0 \cdot j & I \end{bmatrix}$$

β_{ijj} for $j \neq i$ and $\beta_i+\beta_{iii}$ are estimable.

8. Factorial with two levels plus two edge points plus center (KE+) - same as design 7.
9. Factorial with two levels replicated twice plus edge points plus center (K+E) - same as design 7.
10. Rotatable central composite (RC) -

$$H^*_{33} = \begin{bmatrix} 1 & 0 & a \cdot j' \\ 0 & 1 & b \cdot j' \\ 0 \cdot j & 0 \cdot j & 0 \cdot I \end{bmatrix} \qquad \begin{aligned} a &= (2-2^{-K/2+1})/(2^{K/2+1}+2^{-K/2+1}-4) \\ b &= -a \end{aligned}$$

$\beta_i+a \cdot \sum_{j \neq i} \beta_{ijj}$ and $\beta_{iii}+b \cdot \sum_{j \neq i} \beta_{ijj}$ are estimable.

11. Rotatable central composite with 2 star points (RC+) - same as design 10 except values of a and b as follow:

$a = (-2^{(-K+7)/2})/(2^{(K+5)/2}+2^{(-K+7)/2}-20)$

$b = -8/(2^{(K+5)/2}+2^{(-K+7)/2}-20)$

12. Rotatable icosahedron (RI) -

$$H_{33}^{*} = \begin{bmatrix} 1 & 0 & -.2369 & 1.619 \\ 0 & 1 & .6193 & -1.619 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$\beta_i - .2369 \cdot \beta_{ij_1j_1} + 1.619 \cdot \beta_{ij_2j_2}$ and

$\beta_{iii} + .6193 \cdot \beta_{ij_1j_1} - 1.619 \cdot \beta_{ij_2j_2}$ are estimable.

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