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.

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

Approved:

Richard E. Lund
Chairperson, Graduate Committee

K Tiahrt
Head, Major Department

Henry L Parsons
Graduate Dean

MONTANA STATE UNIVERSITY
Bozeman, Montana

June, 1978

ACKNOWLEDGMENT

The author wishes to express his gratitude to his thesis advisor, Dr. Richard E. Lund, for his guidance and helpful suggestions made during the preparation of this dissertation.

Appreciation is also extended to Professors Kenneth Tiahrt, Martin Hamilton, Warren Esty, Norman Eggert, and Eric Strohmeyer for serving on his graduate committee. Dr. Richard Schwaller is thanked for sitting in for Dr. Hamilton while he was on leave.

Finally, appreciation is extended to my wife, Virginia, for her encouragement and understanding during the writing of the dissertation and for her help in preparing the manuscript.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

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.

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 $(\pm1,\pm1,\ldots,\pm1)$. 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 $(\pm1,\pm1,\ldots,\pm1)$.
2. Inner cube - coordinates $(\pm\frac{1}{2},\pm\frac{1}{2},\ldots,\pm\frac{1}{2})$.
3. Star points - coordinates $(\pm1,0,\ldots,0)$, $(0,\pm1,0,\ldots,0)$, 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

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

Experimental Factors: X_1–X_5

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:

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

$$\eta_2(X) = \beta_0 + \sum_{i=1}^{K} x_i\beta_i + \sum_{i=1}^{K}\sum_{j\geq i}^{K} x_i x_j \beta_{ij} + \sum_{i=1}^{K}\sum_{j\geq i}^{K}\sum_{k\geq j}^{K} x_i x_j x_k \beta_{ijk}. \quad (3.2)$$

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

$$X' = (x_1,\ldots,x_K). \quad (3.3)$$

If the vectors β_1, β_2, X_1 and X_2 are defined by:

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

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

$$X_1' = (1,x_1,\ldots,x_K,x_1^2,\ldots,x_K^2,x_1x_2,\ldots,x_{K-1}x_K) \quad (3.6)$$

$$X_2' = (x_1^3,\ldots,x_K^3,x_1x_2^2,\ldots,x_Kx_{K-1}^2,x_1x_2x_3,\ldots,x_{K-2,K-1,K}) \quad (3.7)$$

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

The two models may be written as:

$$\eta_1(X) = X_1'\beta_1 \quad (3.1a)$$

$$\eta_2(X) = X_1'\beta_1 + X_2'\beta_2 \text{ .} \quad (3.2a)$$

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:

1. $N > 0$
2. $[400] \neq [220]$ (3.19)
3. $N([400]-[220]) + (K-1)(N\cdot[220]-[200]^2) \neq 0$,

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

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:

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

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:

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

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	Model 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.

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

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

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

Figure 3.2 General Form of X'X

$X'X =$

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													
							8.5												
								8.5											
									8.5										
	10.5									10.125			8.125	8.125					
		10.5									10.125				8.125	8.125			
			10.5									10.125					8.125	8.125	
	8.5									8.125			8.125	8.125					
	8.5									8.125			8.125	8.125					
		8.5									8.125				8.125	8.125			
		8.5									8.125				8.125	8.125			
			8.5									8.125					8.125	8.125	
			8.5									8.125					8.125	8.125	
																			8.125

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

$$X^{*'} = (1, x^2, \ldots, x_K^2, x_1 x_2, \ldots, x_{K-1} x_K, x_1, x_1^3, x_1 x_2^2, \ldots, x_1 x_K^2,$$
$$x_2, x_2^3, x_2 x_1^2, \ldots, x_K x_{K-1}^2, x_1 x_2 x_3, \ldots, x_{K-2} x_{K-1} x_K) \qquad (3.22)$$

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 $(x_i, x_i^3, x_i x_j^2)$, $j \neq i$, 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

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

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

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

Figure 3.3a $X^{*'}X^{*}$ 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:

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

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 $A_{33} = A_{44} = A_{55}$.

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

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 $H^{*} = (X^{*'}X^{*})^{-} X^{*'} X^{*}$ 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 $q^{*'}H^{*} = q^{*'}$ where $q^{*'}$ is the rearrangement of q in the same manner as $X^{*'}$ 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).

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

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:

$$\tilde{b}_1 = T'Y \tag{3.35}$$

where T' is such that:

$$T'X = A \tag{3.36}$$

where A is defined by:

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

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:

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

which gives:

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

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

$$A = \begin{bmatrix}
1 &&&&&&&&&&&&&&&&&&& \\
& 1 &&&&&&&&& .6 &&& 1/3 & 1/3 &&&&& \\
&& 1 &&&&&&&&& .6 &&&& 1/3 & 1/3 &&& \\
&&& 1 &&&&&&&&& .6 &&&&& 1/3 & 1/3 & 0 \\
&&&& 1 &&&&&&&&&&&&&&& \\
&&&&& 1 &&&&&&&&&&&&&& \\
&&&&&& 1 &&&&&&&&&&&&& \\
&&&&&&& 1 &&&&&&&&&&&& \\
&&&&&&&& 1 &&&&&&&&&&& \\
&&&&&&&&& 1 &&&&&&&&&&
\end{bmatrix}$$

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:

$$H^*_{33} = A^-_{33}A_{33} \qquad (3.42)$$

The rows of H^*_{33} will represent a basis for the linear combinations of $(\beta_i, \beta_{iii}, \beta_{ijj})_{j\neq i}$ 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] ≠ [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:

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

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:

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

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:

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

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:

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

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

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

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:

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

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

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

which when evaluated gives:

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

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.