OPTIMUM SYMMETRIC DESIGNS FOR MIXTURES OF THREE COMPONENTS

By

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CHAPTER I

INTRODUCTION

Mixture Experiments

Experiments are often encountered in research work in which the response depends upon the relative proportions of the components in a mixture. If the response depends only upon the proportions and not upon the total amounts then the experiment is called a mixture experiment. The factors in such an experiment are the fractions of the components in the mixture. The factors must therefore be non-negative and sum to unity.

Gasoline blending experiments in which the response is octane rating are examples of mixture experiments. In such experiments a gasoline is produced by blending a number of gasoline base stocks having various octane ratings. The octane rating of the blend depends only upon the relative proportions of the component base stocks.

A type of design which is commonly used with mixture experiments is the simplex-lattice design described by Sheffé (11). With the use of these designs the required computations for analysis are relatively simple when a polynomial approximation to the response is to be made. The simplex-lattice designs are indexed by two parameters: the number of mixture components, q, and an integer, m, where m denotes that each component can occur in a mixture in the proportions p:0, 1/m, 2/m, ..., m/m. An experimental point for q components is denoted by (p_1, p_2,

..., p_q), and the design points are all those for which the p_i are 0, 1/m, 2/m, ..., m/m and $\sum_i p_i = 1$.

A later development by Sheffe' (12) is the class of simplex-centroid designs. When the number of components is q there are $2^q - 1$ points in the design. These are the q pure components, the $\binom{q}{2}$ mixtures of two components in equal proportions, the $\binom{q}{3}$ mixtures of three components in equal proportions, ..., and the mixture with all components in the equal proportions of 1/q. In this work Sheffe' also considered experiments with both mixture and process variables as well as the problem of fractional designs.

Draper and Lawrence, (4) and (5), have derived designs for three and four component mixtures which, in the absence of random error, have the property of minimizing the average bias incurred when a polynomial of degree $d_1 < d_2$ is assumed when the true model is a polynomial of degree d_2. The cases investigated were for ($d_1 = 1$, $d_2 = 2$) and ($d_1 = 2$, $d_2 = 3$). The situation where both bias and variance occur was also considered and designs for this case were obtained by taking the so-called all-bias designs and expanding them while retaining their basic shape.

Optimal Designs

The work of Draper and Lawrence (4), described above, is an example of applying a specific criterion of excellence, namely average bias, to the problem of choosing an experimental design. Folks (6) has made a rather extensive survey of such criteria which are applicable to the general problem of choosing optimal designs. A review of the literature concerning response relationships and optimal designs in general has been made by Gillett (7) and Gurley (9).

Statement of the Problem

In Chapter II a class of designs termed symmetric designs will be defined for three component mixtures. This class includes as subclasses the simplex-lattice and simplex-centroid designs.

Also in Chapter II a one-to-one correspondence will be established between certain subclasses of the class of N-point symmetric designs and a factor space of dimension less than N. These factors will be referred to as design factors.

To aid in selecting an N-point symmetric design, a number of criteria of excellence are defined in Chapter III and it is shown that these criteria can be expressed as functions of the design factors.

In Chapter IV the criterion of minimum generalized variance is employed to find optimal or near optimal designs assuming either a first or second order polynomial model. The results of a computer-aided search in the factor space indicate optimal designs for each N to be of the same configuration as the simplex-lattice or simplex-centroid designs. However, with N greater than the number of points in the corresponding simplex design, there resulted some variation in the optimum allocation of replicates. Rules for the optimum allocation are given.

Chapter V deals with the selection of N-point symmetric designs (for second order polynomial models) which are optimal with respect to the average variance of the predicted response over a specified region of interest. Designs are found for triangular regions of interest and for regions of operability containing a region of interest.

Chapter VI discusses the effect on the average variance of assuming a model with too many terms.

Chapter VII summarizes the work done and gives some ideas relating to the extension of symmetric designs to the case of mixtures involving more than three components.

CHAPTER II

SYMMETRIC DESIGNS FOR MIXTURES OF THREE COMPONENTS

Introductory Remarks

This discussion will be concerned with mixtures of three components where the total content of the mixture is 1, and where the amount of each component in the mixture is expressed as a positive fraction. Thus the possible mixtures are restricted to a triangular region, R, of the three-dimensional space, (x_1, x_2, x_3). This region R lies on the plane $x_1+x_2+x_3=1$ and is bounded by the planes $X_1=0$, $x_2=0$ and $x_3=0$. In set notation:

$$R=\{(x_1, x_2, x_3) : x_1+x_2+x_3=1, x_i \geq 0\}.$$

Although R can be represented as an equilateral triangle in only two dimensions, it is helpful at first to represent points of R in terms of triangular coordinates. Thus, in Figure 1, the x_1 axis is along the line from a_0 to a_1, with $x_1=0$ at the point $a_0=(0, \frac{1}{2}, \frac{1}{2})$ and $x_1=1$ at the point $a_1=(1, 0, 0)$. The x_2 axis is along the line from $b_0=(\frac{1}{2}, 0, \frac{1}{2})$ to $b_1=(0, 1, 0)$ and the x_3 axis is along the line from $c_0=(\frac{1}{2}, \frac{1}{2}, 0)$ to $c_1=(0, 0, 1)$. The component x_1 is zero along the line from b_1 to c_1, $x_2=0$ along the line from a_1 to c_1, and $x_3=0$ along the line from a_1 to b_1. The intersection of the three axes is the point $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, the centroid of the triangle.

In considering various possible sets of experimental points to be

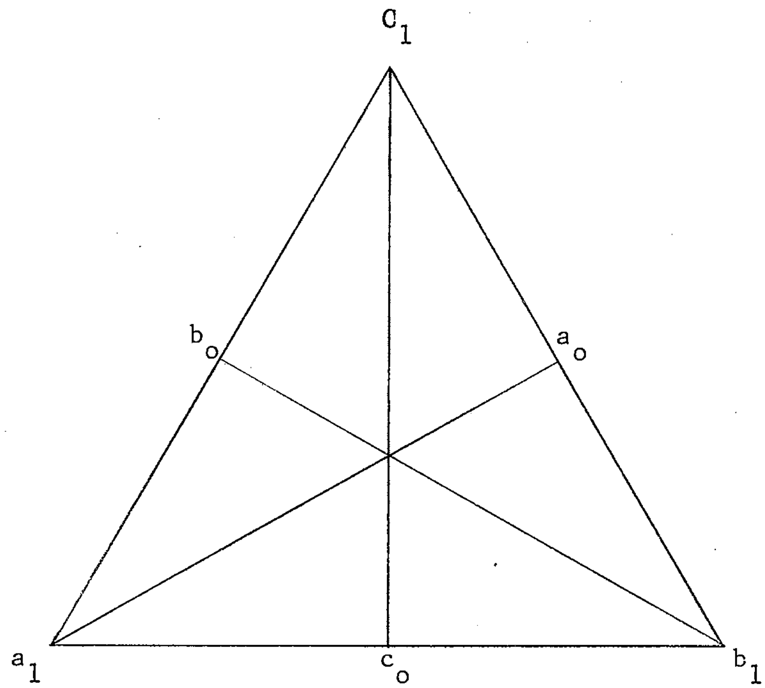

Figure 1. Illustration of Triangular Coordinates

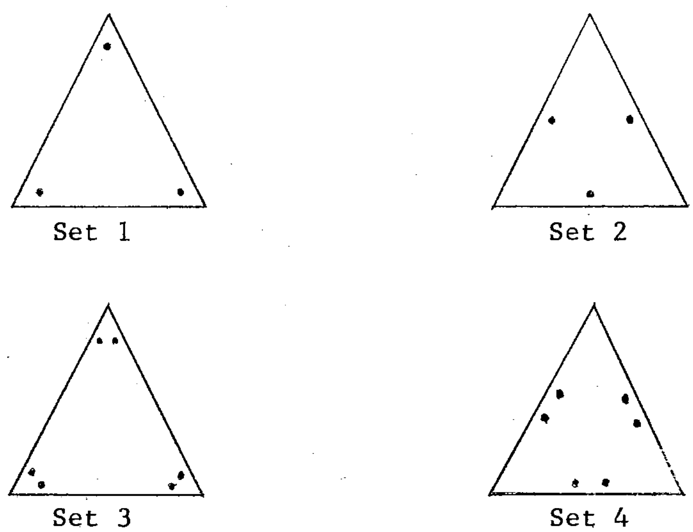

Figure 2. Examples of Symmetrical Sets of Points

run in R, those sets containing arrangements of the form shown in Figure 2 have considerable intutive appeal, especially if the experimenter is equally interested in all components of mixtures over R. Note that the points are arranged symmetrically with respect to all three axes. Sets of points such as those in Figure 2 can be constructed by choosing a single point, $r=(x_1, x_2, x_3)$, in R plus those additional points whose coordinates are some permutation of x_1, x_2, and x_3. It is clear that such sets will consist of one, three or six points depending on the number of distinct coordinate values. Thus, for sets 1 and 2 in Figure 2, each point has exactly two identical coordinate values. In sets 3 and 4 all coordinate values are distinct for each point. If $x_1=x_2=x_3$ one would have the center point or centroid, $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, for which there is only one distinct permutation.

Definition of Symmetry

The above are examples of symmetrical point sets which will be called permutation sets. It will be helpful, however, to require the point elements of a permutation set to be ordered. To define the ordering it is necessary to first define the following subsets of R:

$$R_0 = \{(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3})\}$$
$$R_1 = \{(x_1, x_2, x_3) : x_2=x_3\neq x_1\}$$
$$R_2 = \{(x_1, x_2, x_3) : x_1=x_3\neq x_2\}$$
$$R_3 = \{(x_1, x_2, x_3) : x_1=x_2\neq x_3\}$$
$$R_{123}= \{(x_1, x_2, x_3) : x_1<x_2<x_3\}$$
$$R_{132}= \{(x_1, x_2, x_3) : x_1<x_3<x_2\}$$
$$R_{213}= \{(x_1, x_2, x_3) : x_2<x_1<x_3\}$$
$$R_{231}= \{(x_1, x_2, x_3) : x_2<x_3<x_1\}$$

$$R_{312}= \{(x_1, x_2, x_3) : x_3<x_1<x_2\}$$
$$R_{321}= \{(x_1, x_2, x_3) : x_3<x_2<x_1\},$$

where (x_1, x_2, x_3) is in each case an element of R. Thus R is the union of the above sets. In Figure 3, R_0 is the center point or centroid; R_1 is the set of points on the line a_0 to a_1, with the exception of the center point; similarly R_2 is the set of points along the line from b_0 to b_1 and R_3 is the set from c_0 to c_1. The subregions defined by the remaining subsets are indicated in Figure 3.

Let

$$R_I =R_1xR_2xR_3= \{(r_1, r_2, r_3) : r_1\epsilon R_1, r_2\epsilon R_2, r_3\epsilon R_3\}$$

and

$$R_{II}=R_{123}xR_{132}x\cdots xR_{321}.$$

Then R_I consists of ordered sets of three points and R_{II} consists of ordered sets of six points.

<u>Definition 2-1</u>. A set P whose elements are triples, (x_1, x_2, x_3), from R is a <u>permutation set</u> if and only if

(1) the elements of P are identical up to a permutation of coordinate values, and

(2) either $P\epsilon R_I$, $P\epsilon R_{II}$, or $P=R_0$.

Condition (2) in the above definition orders the elements of P and insures that the elements are distinct.

In order to construct combinations of permutation sets it is desirable to define a set operation which will be called the adjunction of ordered sets.

<u>Definition 2-2</u>. Let $A=(a_1, a_2, \ldots, a_k)$ and $B=(b_1, \ldots, b_m)$ be

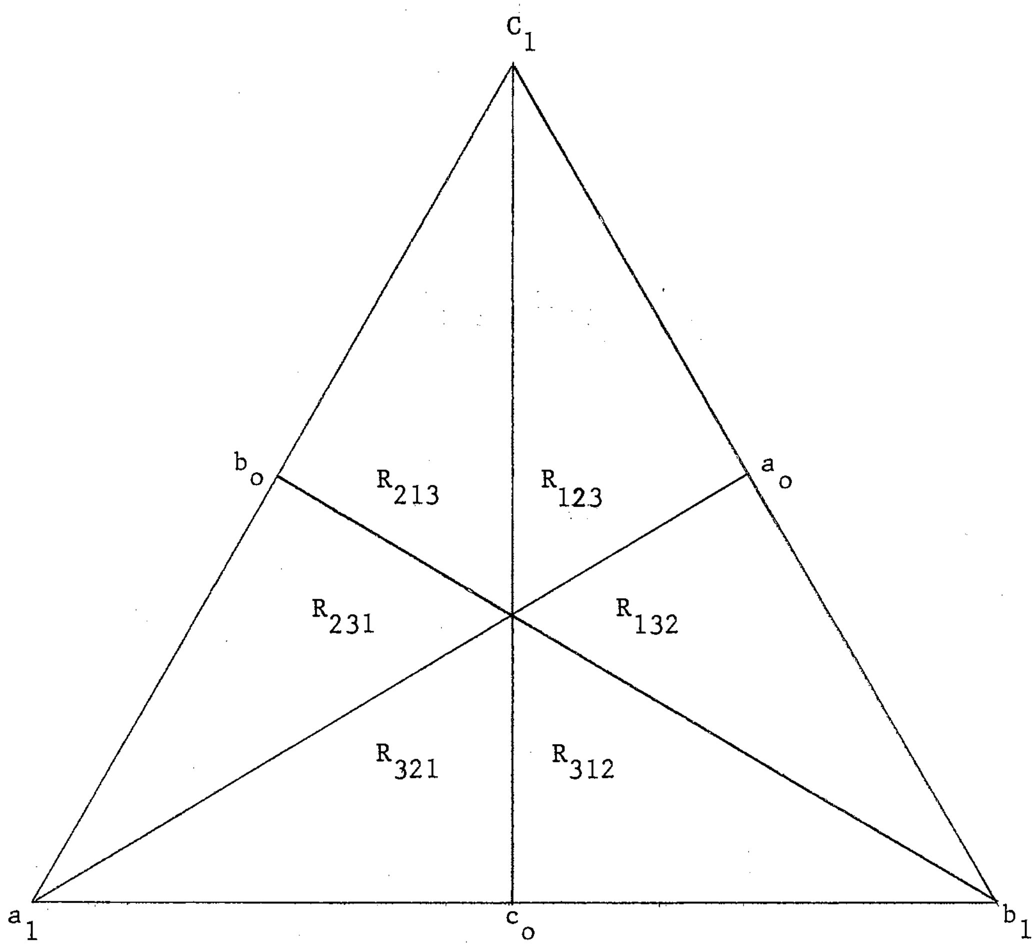

Figure 3. Subregions of R

ordered sets. Define

$$A+B= (a_1, \ldots, a_k, b_1, \ldots, b_m)$$

and $$B+A= (b_1, \ldots, b_m, a_1, \ldots, a_k)$$

Let $A_i=(a_{1i}, \ldots, a_{n_i i})$, $i=1, \ldots, m$, be a sequence of ordered sets, denoted by $\langle A_i \rangle_1^m$ and define

$\sum_i A_i=(a_{11}, \ldots, a_{n_1 1}, \ldots, a_{1m}, \ldots, a_{n_m m})$.

The noncommutative set operation, +, or Σ, will be called the <u>adjunction operation for ordered sets</u>.

Since permutation sets were defined to be ordered sets, the adjunction operation can be used for the summation of the sequences defined below.

<u>Definition 2-3</u>. Let $\langle P_i \rangle_1^k$ be a finite sequence of permutation sets with the following properties:

(1) the first u permutation sets of the sequence are elements of R_0, i.e., 1-point sets,

(2) the next t permutation sets are elements of R_I, i.e., 3-point sets,

(3) the remaining $s=k-u-t$ permutation sets are elements of R_{II}, i.e., 6-point sets.

Then the <u>class of all sequences of permutation sets</u> having properties (1), (2) and (3) with k, u, t and s fixed integers, will be denoted by [u, t, s].

Let D be a set with N elements each of which is a triple, (x_1, x_2, x_3), from R. Then D can be considered an element of R^N, where:

$$R^N=\{(r_1, r_2, \ldots, r_N) : r_i \epsilon R\}.$$

Such sets will be called N-point designs.

Definition 2-4. A design $D \epsilon R^N$ is a symmetric design of N points if and only if there exists a sequence of permutation sets $\langle P_i \rangle_1^k$ from a class [u, t, s] such that $N=u+3+6s$ and $D=\sum_i P_i$.

The class of all N-point symmetric designs is denoted by S^N. For a given N there are, in general, several classes, [u, t, s], of sequences of permutation sets such that $N=u+3t+6s$. Corresponding to each such class with given u, t, and s, there exists a subset of S^N which will be denoted by S[u, t, s]. Such subsets of S^N are mutually disjoint and S^N is the union of all such subsets. For example:

$$S^6=S[6, 0, 0] \cup S[3, 1, 0] \cup S[0, 2, 0] \cup S[0, 0, 1].$$

Thus for any $D \epsilon S^N$, D is an element of exactly one subset, S[u, t, s], of S^N.

Definition of Design Factors

The remainder of this chapter will be devoted to showing the existence of, and defining a one-to-one mapping between the subclass, S[u, t, s], of N-point symmetric designs and a "factor space," F, of dimension t+2s. This will be accomplished by means of the following lemmas and theorem.

Lemma 2-5. Given integers u, t and s with $N=u+3t+6s$, there exists a one-to-one mapping between S[u, t, s] and [u, t, s], where $S[u, t, s] \subset S^N$, and where [u, t, s] is a class of sequences of permutation sets.

Proof of Lemma 2-5. Define φ_1: S[u, t, s] → [u, t, s] such that for every D∈S[u, t, s], $\varphi_1(D) = \langle P_i\rangle_1^k \in [u, t, s]$, where $\langle P_i\rangle_1^k$ is a sequence such that $D = \sum_i P_i$. Thus, the definition of a symmetric design of N points establishes φ_1 as a one-to-one mapping.

Lemma 2-6. There exists a one-to-one mapping between [u, t, s] and $R_1^t R_{123}^s$ where

$R_1^t R_{123}^s = \{(p_1, \ldots, p_{t+s}) : p_i \in R_1,\ i \le t \text{ and } p_i \in R_{123},\ i > t\}$.

Proof of Lemma 2-6. Define φ_2:[u, t, t] → $R_1^t R_{123}^s$ such that for every $\langle P_i\rangle_1^k$ ∈[u, t, s]

$$\varphi_2(\langle P_i\rangle_1^k) = (p_1, \ldots, p_{t+s})$$

where $p_i \in P_{u+i}$ is the first element of the ordered set:

$$P_{u+i} \quad (i=1, 2, \ldots, t+s).$$

Now

$$P_{u+i} \in R_I = R_1 x R_2 x R_3 \text{ for } i \le t$$

and

$$P_{u+i} \in R_{II} = R_{123} x \ldots x R_{321} \text{ for } i > t.$$

Therefore

$$\varphi_2(\langle P_i\rangle_1^k) = (p_1, \ldots, p_{t+s}) \in R_1^t R_{123}^s$$

and

$$\varphi_2([u, t, s]) \subset R_1^t R_{123}^s.$$

On the other hand, let

$$(p_1, \ldots, p_{t+s}) \in R_1^t R_{123}^s,$$

then

$$p_i \in R_1,\ i \leq t,$$

which implies that p_i is an element, (x_1, x_2, x_3), such that $x_1 \neq x_2 = x_3$. Thus, there exists a permutation set, say $P_{u+1} \in R_I$, such that p_i is its first element. Similarly, $p_i \in R_{123}$ for $i > t$ implies the existence of a permutation set, $P_{u+i} \in R_{II}$, such that p_i is its first element. Therefore, there exists a $\langle P_i \rangle_1^k \in [u, t, s]$ such that

$$\varphi_2(\langle P_i \rangle_1^k) = (p_1, \ldots, p_{t+s}).$$

Hence:

$$\varphi_2([u, t, s]) \supset R_1^t R_{123}^s$$

which implies

$$\varphi_2([u, t, s]) = R_1^t R_{123}^s.$$

Let $\langle P_i \rangle_1^k$, $\langle P'_i \rangle_1^k \in [u,t,s]$ and $\langle P_i \rangle_1^k = \langle P'_i \rangle_1^k$.

Then, since these are ordered sequences of ordered sets, each element of each set is identical. Thus, $p_i = p'_i$, $i = 1, \ldots, t+s$, and $\varphi_2(\langle P_i \rangle_1^k) = \varphi_2(\langle P'_i \rangle_1^k)$. Therefore, φ_2 is a mapping.

Let

$$(p_1, \ldots, p_{t+s}) = \varphi_2(\langle P_i \rangle_1^k)$$

and

$$(p'_1, \ldots, p'_{t+s}) = \varphi_2(\langle P'_i \rangle_1^k)$$

be elements of $R_1^t R_{123}^s$ such that

$$(p_1, \ldots, p_{t+s}) = (p'_1, \ldots, p'_{t+s}).$$

Then $p_i = p'_i$, $i=1, \ldots, t+s$, which implies:

$$P_{u+i} = P'_{u+i}, \quad i=1, \ldots, t+s.$$

But $P_i = R_0$ for $i \leq u$ for every $\langle P_i \rangle_1^k \in [u, t, s]$.

Therefore,

$$\langle P_i \rangle_1^k = \langle P'_i \rangle_1^k .$$

Thus, φ_2 is an injective mapping and since it is also surjective it is a one-to-one mapping.

<u>Lemma 2-7</u>. There exists a one-to-one mapping between $R_1^t R_{123}^s$ and a (t+2s)-dimensional factor space, F.

<u>Proof of Lemma 2-7</u>. This lemma is clearly true since R_1 is a one-dimensional space and R_{123} is a two-dimensional space. Hence, the identity transformation

$$i : R_1^t R_{i23}^s \rightarrow R_1^t R_{123}^s = F$$

or any other nonsingular transformation which maps p_i into F_1 for $i \leq t$ and p_i into F_{123} for $i > t$ will be a one-to-one transformation from $R_1^t R_{123}^s$ to $F = F_1^t F_{123}^s$.

It will, however, simplify some later computations to use the particular transformation, φ_3, defined as follows:

for every $(p_i, \ldots, P_{t+s}) \in R_1^t R_{123}^s$

$$\varphi_3(p_1, \ldots, p_{t+s}) = [y_1, \ldots, y_{t,\ t+1}, y_{2,\ t+1}), \ldots,$$
$$(y_{1,\ t+s}, y_{2,\ t+s})]$$

where, for

$$p_i = (x_1, x_2, x_3) \in R_1, \quad i \leq t$$
$$y_i = x_1 - 2x_2 + x_3 = 1 - 3x_2$$

$$y_i = x_1 + x_2 + 2x_3 = 1-3x_3$$
$$1 = x_1 + x_2 + x_3$$

and for $p_i = (x_1, x_2, x_3) \in R_{123},\ i>t$

$$y_{1i} = -\frac{3}{\sqrt{2}} x_1 + \frac{3}{\sqrt{2}} x_2 = \frac{1}{\sqrt{2}}[(1-3x_1) - (1-3x_2)]$$

$$y_{2i} = -\frac{1}{\sqrt{2}} x_1 - \frac{1}{\sqrt{2}} x_2 + \frac{2}{\sqrt{2}} x_3 = \frac{1}{\sqrt{2}}[(1-3x_1) + (1-3x_2)]$$

$$1 = x_1 + x_2 + x_3.$$

Then

$$F_1 = \{y : -\tfrac{1}{2} \le y < 0 \text{ or } 0 < y \le 1\}$$

and

$$F_{123} = \{(y_1, y_2) : y_1 > 0;\ y_2 > \frac{\sqrt{2}}{4} y_1;\ y_1 + y_2 \le \frac{2}{\sqrt{2}}\}.$$

The inverse transformations are such that

for $p_i = (x_1, x_2, x_3),\ i \le t$

$$x_1 = (2y_i+1)/3$$
$$x_2 = (1-y_i)/3$$
$$x_3 = (1-y_i)/3$$

and for $p_i = (x_1, x_2, x_3),\ i>t$

$$x_1 = (2 - \sqrt{2}\, y_{1i} - \sqrt{2}\, y_{2i})/6$$
$$x_2 = (2 + \sqrt{2}\, y_{1i} - \sqrt{2}\, y_{2i})/6$$
$$x_3 = (2 + 2\sqrt{2}\, y_{2i})/6$$

Now the composition $\varphi = \varphi_3\varphi_2\varphi_1$ is a one-to-one mapping; therefore, the following theorem has been proved.

Theorem 2-8. There exists a one-to-one mapping, φ, between the subclass $S[u, t, s]$ of N-point symmetric designs and a t+2s dimensional factor space, F. The mapping, φ, is the composition of the mapping φ_1, φ_2 and φ_3 defined in Lemmas 2-5, 2-6 and 2-7. The factor space $F = F_1^t F_{123}^s$ is as defined in Lemma 2-7.

In Lemma 2-6 the mapping φ_2 was from S[u, t, s] onto $R_1^t R_{123}^s$. Clearly, one could define a similar mapping onto $R_1^t R_{132}^s$, $R_1^t R_{213}^s$, ..., or $R_1^t R_{321}^s$, or indeed onto a number of various products of the subsets R_1, R_2, R_3, R_{123}, ..., R_{321} of R. If, for instance, one defined $\varphi_2 : S[u, t, s] \rightarrow R_1^t R_{321}^s$ then, the mapping, φ_3, in Lemma 2-7 would be defined the same as before except for its range, which would be $F_1^t F_{321}^s$. Thus, φ, in effect, maps R_1 onto F_1 as previously defined, and maps R_{123} onto F_{123}, R_{132} onto F_{132}, ..., and R_{321} onto F_{321}. The subsets R_{123}, ..., R_{321} and their respective images under φ are graphically depicted in Figure 4.

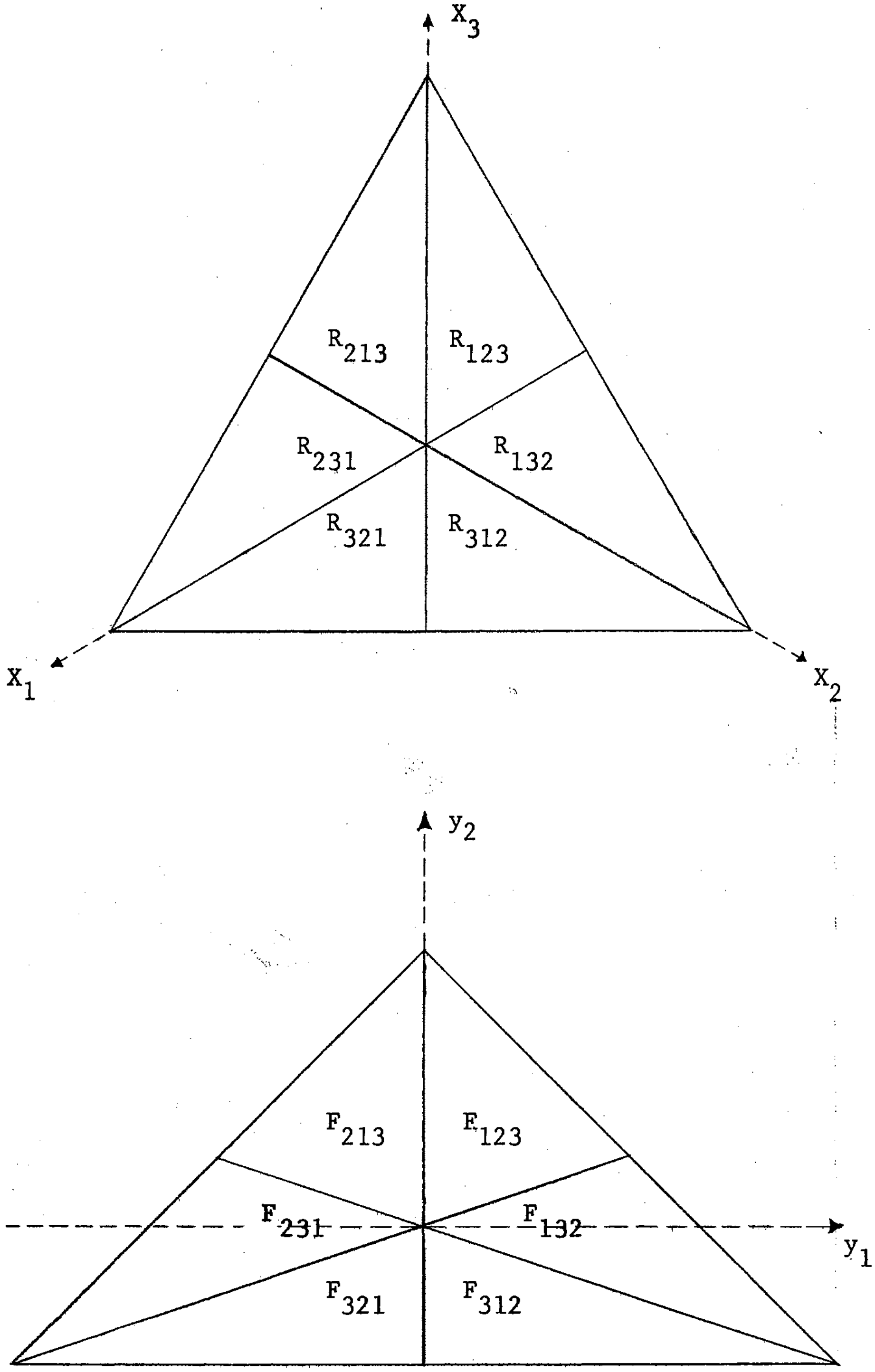

Figure 4. Corresponding Subregions of R and F

CHAPTER III

CRITERIA FOR THE SELECTION OF A SYMMETRIC DESIGN

Introductory Remarks

In Chapter II a class of designs termed symmetric designs was defined for the three component mixture problem. Given the possibility of running N experimental points, one would like to choose from the class S^N a design (or designs) which is best in the sense of some criterion. The criteria to be used in this thesis are defined in this chapter, and formulas are developed for implementing the criteria in searching for the best N-point symmetric design.

Models to be Used

In this chapter, it will be assumed that the response, y, is given by one of the following models:

either

$$y(x_1, x_2, x_3) = \alpha_0 x_0 + \alpha_1 x_1 + \alpha_2 x_2 + \epsilon$$

or

$$y(x_1, x_2, x_3) = \alpha_0 x_o + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_{12} x_1 x_2 + \alpha_{11} x_1^2 + \alpha_{22} x_2^2 + \epsilon$$

where $x_0 = x_1 + x_2 + x_3 = 1$, $(x_1, x_2, x_3) \epsilon R$ and $\epsilon \sim NID(0, \sigma^2)$.

It will be convenient to use the matrix notation,

$$Y = X\alpha + E$$

to denote the Nx1 vector of responses, Y, corresponding to the matrix, X, of design points.

In the case of the second order model, for example, one has:

$Y' = [y_1, y_2, \ldots, y_N]$

$E' = [\epsilon_1, \epsilon_2, \ldots, \epsilon_N]$

$\alpha' = [\alpha_0, \alpha_1, \alpha_2, \alpha_{12}, \alpha_{11}, \alpha_{22}]$

and

$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & x_{11}x_{12} & x_{11}^2 & x_{12}^2 \\ 1 & x_{21} & x_{22} & x_{21}x_{22} & x_{21}^2 & x_{22}^2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & x_{N1} & x_{N2} & X_{N1}x_{N2} & x_{N1}^2 & x_{N2}^2 \end{bmatrix} .$$

In terms of the above notation, the least squares and maximum likelihood estimates of α are given by

$$\hat{\alpha} = (X'X)^{-1} X'Y.$$

If $u = (u_1, u_2, u_3)$ is a point in R,

let

$U' = [1, u_1, u_2, u_1u_2, u_1^2, u_2^2]$,

then the estimated response at u is given by

$$\hat{y}\ (u) = U'\hat{\alpha} .$$

Transformation of the Space R

Each criterion to be considered in this thesis will involve in some manner, the matrix X'X. It was found that computations could be simplified by working in a transformed space with the matrix Z'Z obtained by employing a transformation used by Draper and Lawrence (4). The transformation effects a nonsingular linear transformation from the

space R, or (x_1, x_2, x_3), to the space R', or (z_1, z_2, z_3).
The transformation is given by:

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} -1/2 & 1/2 & 0 \\ -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{2\sqrt{3}}{6} \\ 1 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

and its inverse by

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -1 & -\frac{\sqrt{3}}{3} & 1/3 \\ 1 & -\frac{\sqrt{3}}{3} & 1/3 \\ 0 & \frac{2\sqrt{3}}{3} & 1/3 \end{pmatrix} \cdot \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}.$$

The above transformation takes the triangular region R into an equilateral triangle in the plane $z_3 = 1$, with the centroid at $(z_1, z_2) = (0, 0)$. One vertex of the triangle lies on $z_1 = 0$ and the other vertices are symmetrical about $z_1 = 0$. The length of each side of the triangle is unity. This triangular region will be referred to as R'.

For a design point from a one-point permutation set, that is, $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, one finds the corresponding point in R; to be

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1/2 & 1/2 & 0 \\ -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{2\sqrt{3}}{6} \\ 1 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \end{pmatrix}.$$

Suppose $(x_1, x_2, x_3) = (a, a, 1-2a)$ is one of the design points, then the points (a, 1-2a, a) and (1-2a, a, a) are also design points. The correspondence between the coordinates of these points and those under the transformation are given in Table I.

TABLE I

COORDINATES OF POINTS IN R AND THEIR CORRESPONDING TRANSFORMED VALUES IN R' FOR THE CASE OF A THREE-POINT PERMUTATION SET

Coordinates in R			Coordinates in R'		
x_1	x_2	x_3	z_1	z_2	z_3
a	a	1-2a	0	$\frac{2\sqrt{3}}{6}(1-3a)$	1
a	1-2a	a	(1-3a)/2	$-\frac{\sqrt{3}}{6}(1-3a)$	1
1-2a	a	a	-(1-3a)/2	$-\frac{\sqrt{3}}{6}(1-3a)$	1

If $(x_1, x_2, x_3) = (a, b, 1-a-b)$ is a design point and $a \neq b$, $a \neq 1-a-b$ and $b \neq 1-a-b$, then the five points obtained by permuting x_1, x_2 and x_3 are also design points. The coordinates of all six points and the corresponding coordinates under the transformation are listed in Table II.

Working in the space (z_1, z_2, z_3), the second order polynomial will be:

$$y(z_1, z_2, z_3) = \beta_0 z_3 + \beta_1 z_1 + \beta_2 z_2 + \beta_{12} z_1 z_2 + \beta_{11} z_1^2 + \beta_{22} z_2^2 + \epsilon$$

where $z_3 = 1$, $(z_1, z_2, z_3) \epsilon R'$ and $\epsilon \sim NID(0, \sigma^2)$.

The least squares and maximum likelihood estimates of β are given by

$$\hat{\beta} = (Z'Z)^{-1} Z'Y$$

and if $u = (u_1, u_2, 1) \epsilon R'$ and $U' = [1, u_1, u_2, u_1 u_2, u_1^2, u_2^2]$

then

$$\hat{y}(u) = U'\hat{\beta}$$

is the estimated response at u.

By inspection of the point coordinates in R' given in Table I and Table II, one can deduce that the matrix Z'Z for the second order model has the form:

$$Z'Z = \begin{bmatrix} N & 0 & 0 & 0 & c & c \\ 0 & c & 0 & -d & 0 & 0 \\ 0 & 0 & c & 0 & -d & d \\ 0 & -d & 0 & f & 0 & 0 \\ c & 0 & -d & 0 & 3f & f \\ c & 0 & d & o & f & 3f \end{bmatrix}.$$

TABLE II

COORDINATES OF POINTS IN R AND THEIR CORRESPONDING TRANSFORMED VALUES IN R'
FOR THE CASE OF A SIX POINT PERMUTATION SET

Coordinates in R			Coordinates in R'		
x_1	x_2	x_3	z_1	z_2	z_3
a	b	1-a-b	$\frac{1}{2}(b-a)$	$\frac{\sqrt{3}}{6}(2-3a-3b)$	1
a	1-a-b	b	$\frac{1}{2}(1-2a-b)$	$\frac{\sqrt{3}}{6}(3b-1)$	1
b	a	1-a-b	$-\frac{1}{2}(b-a)$	$\frac{\sqrt{3}}{6}(2-3a-3b)$	1
b	1-a-b	a	$\frac{1}{2}(1-a-2b)$	$\frac{\sqrt{3}}{6}(3a-1)$	1
1-a-b	a	b	$-\frac{1}{2}(1-2a-b)$	$\frac{\sqrt{3}}{6}(3b-1)$	1
1-a-b	b	a	$-\frac{1}{2}(1-a-2b)$	$\frac{\sqrt{3}}{6}(3a-1)$	1

where

$$c = \sum_{i=1}^{N} z_{i1}^2 = \sum_{i=1}^{N} z_{i2}^2$$

$$d = \sum_{i=1}^{N} z_{i2}^3 = -\sum_{i=1}^{N} x_{i1}^2 z_{i2}$$

$$f = \sum_{i=1}^{N} z_{i1}^2 z_{i2}^2 = (1/3)\sum_{i=1}^{N} z_{i1}^4 = (1/3)\sum_{i=1}^{N} z_{i2}^4 .$$

Correspondence Between Z'Z and the Design Factor Space, F

It will be shown that Z'Z is a function of the design factors defined in Theorem 2-8. Having done this it will be possible to move between the subclass of N-point symmetric designs, $S[u,t,s] \subset S^N$, the design factor space, F, and the class of matrices, {Z'Z}, as indicated diagramatically by the arrows in Figure 5, below.

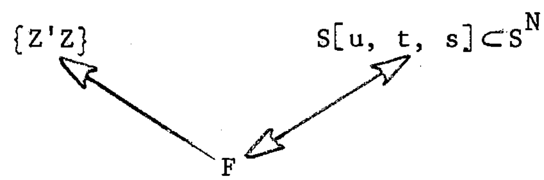

Figure 5. Diagram of Correspondence Between {Z'Z}, F, and S[u, t, s]

Each arrow in Figure 5 represents a function with the domain of the function being the set at the tail of the arrow and the range being the set at the head of the arrow.

Now each permutation set of points in a symmetric design contributes either one, three or six terms to the sums c, d and f of Z'Z. Using the values of z_1 and z_2 in Tables I and II, the respective "sum-of-squares" contribution of a one-point, three-point and six-point set were computed in terms of the original coordinate values. These are listed in Table III, where, for convenience,

$$w = 1-3a$$

for the three point set and

$$w_1 = 1-3a$$

$$w_2 = 1-3b$$

for the six point permutation set.

TABLE III

CONTRIBUTIONS OF k-POINT PERMUTATION SETS TO THE ELEMENTS

N, c, d AND f OF Z'Z

k	N	c	d	f
1	1	0	0	0
3	3	$\frac{1}{2}w^2$	$\frac{\sqrt{3}}{12}w^3$	$w^4/24$
6	6	$(1/3)(w_1^2 + w_2^2 + w_1w_2)$	$\frac{\sqrt{3}}{12}(w_1^2w^2 + w_1w_1^2)$	$\frac{1}{108}(w_1^2 + w_2^2 + w_1w_2)^2$

Referring to the definition of the design factors in terms of the original triangular coordinates on page 14 of Chapter II, one finds that

$$y = 1-3a = w$$

for the three-point case and

$$y_1 = \frac{1}{\sqrt{2}}[(1-3a) - (1-3b)] = \frac{1}{\sqrt{2}}(w_1-w_2)$$

$$y_2 = \frac{1}{\sqrt{2}}[(1-3a) + (1-3b)] = \frac{1}{\sqrt{2}}(w_1+w_2)$$

for the six-point permutation set.

Thus

$$w_1 = \frac{1}{\sqrt{2}}(y_1 + y_2)$$

and

$$w_2 = \frac{1}{\sqrt{2}}(y_2 - y_1),$$

and making these substitutions in Table III, one obtains the results given in Table IV.

TABLE IV

CONTRIBUTIONS OF k-POINT PERMUTATION SETS IN TERMS OF THE DESIGN FACTORS TO THE ELEMENTS N, c, d AND f OF Z'Z

k	N	c	d	f
1	1	0	0	0
3	3	$y^2/2$	$\frac{\sqrt{3}}{12}y^3$	$y^4/24$
6	6	$(y_1^2 + 3y_2^2)/6$	$(y_2^2 - y_1^2)y_2/4\sqrt{6}$	$(y_1^2 + 3y_2^2)^2/432$

From the above developments, one sees that the elements c, d and f are functions of the design factors and hence, so is Z'Z.

An Induced Transformation of the Space of Independent Variables in the Quadratic Model

<u>Theorem 3-1</u>. A nonsingular linear transformation from $(1, x_1, x_2)$ to $(1, z_1, z_2)$ induces a nonsingular linear transformation from $(1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$ to $(1, z_1, z_2, z_1z_2, z_1^2, z_2^2)$. If A is the matrix for the transformation from $(1, x_1, x_2)$ to $(1, z_1, z_2)$ and B is the matrix for the induced transformation, then $|B| = |A|^4$.

The fact that $x_0 = x_1 + x_2 + x_3 = 1$ may be used to rewrite the transformation matrix on page 20 as follows:

$$\begin{pmatrix} z_3 \\ z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} \\ \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} \end{pmatrix} \cdot \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix}$$

Now consider an arbitrary nonsingular transformation:

$$\begin{pmatrix} z_3 \\ z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \cdot \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix},$$

from the space (x_0, x_1, x_2) to the space (z_3, z_1, z_2), where $z_3=x_0=1$. That is, $a_{11} + a_{12}x_1 + a_{13}x_2 = 1$ for all x_1 and x_2. Then $a_{11}=1$ and $a_{12} = a_{13} = 0$.

Then for the second order polynomial model in the space of (z_1, z_2, z_3), one can write

$$V_z = \begin{pmatrix} 1 & 0 & 0 \\ A_1 & A_2 & 0 \\ B_1 & B_2 & B_3 \end{pmatrix} V_x \quad ,$$

where

$$V'_z = (z_3, z_1, z_2, z_1z_2, z_1^2, z_2^2)$$

$$V'_x = (x_0, x_1, x_2, x_1x_2, x_1^2, x_2^2)$$

$$A_1 = \begin{pmatrix} a_{21} \\ a_{31} \end{pmatrix} , \qquad A_2 = \begin{pmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{pmatrix}$$

$$B_1 = \begin{pmatrix} a_{21}a_{31} \\ a_{21}^2 \\ a_{31}^2 \end{pmatrix}, \qquad B_2 = \begin{pmatrix} a_{21}a_{32} + a_{31}a_{22} & a_{21}a_{33} + a_{31}a_{23} \\ 2a_{21}a_{22} & 2a_{21}a_{23} \\ 2a_{31}a_{32} & 2a_{31}a_{33} \end{pmatrix}$$

and

$$B_3 = \begin{pmatrix} a_{22}a_{33} + a_{32}a_{23} & a_{22}a_{32} & a_{23}a_{33} \\ 2a_{22}a_{23} & a_{22}^2 & a_{23}^2 \\ 2a_{32}a_{33} & a_{32}^2 & a_{33}^2 \end{pmatrix}.$$

The above transformation from X to Z is clearly linear. It is also nonsingular as will be shown below. Consider the determinant:

$$\begin{vmatrix} 1 & 0 & 0 \\ A_1 & A_2 & 0 \\ B_1 & B_2 & B_3 \end{vmatrix} = \begin{vmatrix} A_2 & 0 \\ B_2 & B_3 \end{vmatrix} = \begin{vmatrix} A_2 & 0 \\ 0 & B_3 \end{vmatrix} = \left|A_2\right| \cdot \left|B_3\right| .$$

The above equalities are due to the fact that the rows of B_2 are linear combinations of the rows of A_2.

Furthermore, the determinant $|A_2|$ is nonzero by definition, and for the determinant, $|B_3|$ one has:

$$\begin{aligned} |B_3| &= (a_{22}a_{33} + a_{32}a_{23})\, a_{22}^2a_{33}^2 + 2a_{22}a_{23}^2a_{32}^2a_{33} + 2a_{22}a_{23}^2a_{32}^2a_{33} \\ &\quad -2a_{22}^2a_{23}a_{32}a_{33}^2 - (a_{22}a_{33} + a_{32}a_{23})a_{23}^2a_{32}^2 - 2a_{22}^2a_{23}a_{32}a_{33}^2 \\ &= (a_{22}a_{33})^3 + (a_{22}a_{33})^2(a_{32}a_{23}) + 2(a_{22}a_{33})(a_{32}a_{23})^2 \\ &\quad + 2(a_{22}a_{33})(a_{32}a_{23})^2 - 2(a_{22}a_{33})^2(a_{32}a_{23}) - (a_{22}a_{33})(a_{32}a_{23})^2 \\ &\quad - (a_{32}a_{23})^3 - 2(a_{22}a_{33})^2(a_{32}a_{23}) \end{aligned}$$

$$= (a_{22}a_{33})^3 - 3(a_{22}a_{33})^2(a_{32}a_{23}) + 3(a_{22}a_{33})(a_{32}a_{23})^2 - (a_{32}a_{23})^3$$

$$= (a_{22}a_{33} - a_{32}a_{23})^3$$

$$= |A_2|^3 .$$

Therefore $|B_3| \neq 0$, and the theorem has been proved.

Minimum Generalized Variance of $\hat{\beta}$

The least squares and maximum likelihood estimates of β are given by

$$\hat{\beta} = (Z'Z)^{-1} Z'Y.$$

Also $\hat{\beta}$ is distributed as

$$N[\beta, \sigma^2 (Z'Z)^{-1}] .$$

The generalized variance of the distribution of $\hat{\beta}$ is

$$\sigma^2 |(Z'Z)^{-1}| = \sigma^2 / |Z'Z| .$$

Definition 3-2. Let Z_1 and Z_2 be the matrices of design points for the designs D_1 and D_2 from the class S^N. Then D_1 is better than D_2 in the sense of generalized variance if and only if

$\sigma^2 / |Z'_1 Z_1| < \sigma^2 / |Z'_2 Z_2|$, or equivalently

$$|Z'_1 Z_1| > |Z'_2 Z_2| .$$

Definition 3-3. Let D^* be a design from S^N. If the generalized variance for the design D^* is finite then D^* is optimum with respect to generalized variance if and only if there exists no design in S^N which is better in the sense of generalized variance.

Now taking the determinant of the matrix Z'Z as given on page 22 one finds:

$$| Z'Z | = 4(2Nf - c^2)(cf - d^2)^2.$$

Folks (6) proved that the optimum generalized variance design (or designs) is invariant under nonsingular linear transformations on the space of independent variables. The argument is reproduced in this context for completeness.

Let

$$Z = XB'$$

represent the transformation which takes each row vector of the design matrix X into the corresponding row vector of Z.

Then

$$| Z'Z | = | BX'XB' | = | B | \cdot | X'X | \cdot | B | = | B |^2 \cdot | X'X | .$$

If B is the matrix of Theorem 3-1, then

$$| Z'Z | = | A |^8 \cdot | X'X | ,$$

so that the optimum generalized variance design for the quadratic model is invariant under transformations from $(1, x_1, x_2)$ to $(1, z_1, z_2)$. In particular for the transformation introduced on page 20 of this chapter, one has:

$$| Z'Z | = \left(\frac{\sqrt{3}}{8}\right)^8 | X'X | = \frac{81}{256} | X'X | .$$

Minimum Average Variance of the Predicted Response

Let $\hat{y}(u)$ be the estimated response at the point u in a region of interest I. The region of interest, I, will quite often correspond exactly to the triangular region R or R'. Let p(u) be a density function defined on I.

<u>Definition 3-4</u>. The <u>average variance</u> with respect to the region of interest, I, for the design, D, with design matrix, Z is given by

$$\sigma^2 \int_I p(u)\ U'(Z'Z)^{-1}\ U\ du\ ,$$

where $\sigma^2 U'(Z'Z)^{-1}$ U is the variance of $\hat{y}(u)$.

<u>Definition 3-5</u>. Let Z_1 and Z_2 be the matrices of design points for the designs D_1 and D_2 from S^N. Then D_1 is <u>better</u> than D_2 in the sense of <u>average variance</u> if and only if

$$\int_I p(u)\ U'(Z'_1 Z_1)^{-1}\ U\ du < \int_I p(u)\ U'\ (Z'_2 Z_2)^{-1}\ U\ du\ .$$

<u>Definition 3-6</u>. Let D^* be a design from S^N. If the average variance for the design D^* is finite then D^* is <u>optimum with respect to average variance</u> if and only if there exists no design in S^N which is better in the sense of average variance.

In this thesis it will be assumed that p(u) is a uniform density over the region of interest and unless otherwise stated the region of interest will be R', the triangular region in the space of $(z_1,\ z_2,\ z_3)$. With this region of interest one has:

$$p(u_1,\ u_2) = \int_{-a}^{2a} \int_{-b}^{b} du_1\ du_2 = \frac{\sqrt{3}}{4}\ ,$$

where $a = \frac{\sqrt{3}}{6}$ and $b = (1/3)(1 - u_2/\sqrt{3})$.

For the second order polynomial model,

let

$$U' = (1,\ u_1,\ u_2,\ u_1u_2,\ u_1^2,\ u_2^2)\ .$$

Then for a design D with matrix of design points Z one has

$$\frac{4}{\sqrt{3}} \int_{-a}^{2a} \int_{-b}^{b} U'\ (Z'Z)^{-1}\ U\ du_1\ du_2$$

$$= \frac{4}{\sqrt{3}} \int_{-a}^{2a} \int_{-b}^{b} \text{trace}\ [UU'\ (Z'Z)^{-1}] du_1 du_2$$

$$= \text{trace}\ \left[(Z'Z)^{-1} \frac{4}{\sqrt{3}} \int_{-a}^{2a} \int_{-b}^{b} UU'\ du_1 du_2\right]$$

$$= \text{trace}\ \ [(Z'Z)^{-1}\ M]\ ,$$

where M, the matrix of design moments was found by Draper and Lawrence (4) to be:

$$M = \begin{bmatrix} 1 & 0 & 0 & 0 & \frac{1}{24} & \frac{1}{24} \\ 0 & \frac{1}{24} & 0 & -\frac{\sqrt{3}}{360} & 0 & 0 \\ 0 & 0 & \frac{1}{24} & 0 & -\frac{\sqrt{3}}{360} & \frac{\sqrt{3}}{360} \\ 0 & -\frac{\sqrt{3}}{360} & 0 & \frac{1}{720} & 0 & 0 \\ \frac{1}{24} & 0 & -\frac{\sqrt{3}}{360} & 0 & \frac{1}{240} & \frac{1}{720} \\ \frac{1}{24} & 0 & \frac{\sqrt{3}}{360} & 0 & \frac{1}{720} & \frac{1}{240} \end{bmatrix}$$

The matrix $(Z'Z)^{-1}$ is listed in Table V.

Thus, in terms of the element c, d and f of Z'Z, the average

TABLE V

ELEMENTS OF THE MATRIX $(Z'Z)^{-1}$ FOR THE SECOND ORDER MODEL

1	z_1	z_2	$z_1 z_2$	z_1^2	z_2^2
$\frac{2f}{2Nf-c^2}$	0	0	0	$\frac{-2c}{4(2Nf-c^2)}$	$\frac{-2c}{4(2Nf-c^2)}$
0	$\frac{f}{cf-d^2}$	0	$\frac{d}{cf-d^2}$	0	0
0	0	$\frac{f}{cf-d^2}$	0	$\frac{2d}{4(cf-d^2)}$	$\frac{-2d}{4(cf-d^2)}$
0	$\frac{d}{cf-d^2}$	0	$\frac{c}{cf-d^2}$	0	0
$\frac{-2c}{4(2Nf-c^2)}$	0	$\frac{2d}{4(cf-d^2)}$	0	$\frac{N}{4(2Nf-c^2)} + \frac{c}{4(cf-d^2)}$	$\frac{N}{4(2Nf-c^2)} - \frac{c}{4(cf-d^2)}$
$\frac{-2c}{4(2Nf-c^2)}$	0	$\frac{-2d}{4(cf-d^2)}$	0	$\frac{N}{4(2Nf-c^2)} - \frac{c}{4(cf-d^2)}$	$\frac{N}{4(2Nf-c^2)} + \frac{c}{4(cf-d^2)}$

variance for the corresponding N-point symmetric design, D, is found to be

$$\frac{720f - 30c + N}{360\ (2Nf - c^2)} + \frac{30f - 4\sqrt{3}\,d + c}{360\ (cf - d^2)} .$$

As in the case of the generalized variance, Folks (6), showed the average variance to be invariant under nonsingular linear transformations of the independent variables. Thus, by Theorem 3-1, the average variance for the quadratic model is also invariant under the transformation from the space R to the space R'.

The argument for invariance of the average variance goes as follows. Using the symbols defined in the proof of Theorem 3-1 let $Z = XB$ and $V_z' = V_x'B$, then since B is nonsingular $X = ZB^{-1}$ and $V_x' = V_z'B^{-1}$. The average variance in the X space is given by

$$\sigma^2 \int_I q(x)V_x'(X'X)^{-1}V_x\, d(x)$$

$$= \sigma^2 \int_{I'} q(z)V_z'B^{-1}\,[B'^{-1}Z'ZB^{-1}]^{-1}\,B'^{-1}\,V_z\,|J|\,dz$$

$$= \sigma^2 \int_{I'} q(z)V_z'(Z'Z)^{-1}V_z\,|J|\,dz$$

$$= \sigma^2 \int_{I'} p(z)V_z'(Z'Z)^{-1}V_z\, dz ,$$

where J is the Jacobian of the transformation.

The last expression is the average variance in the Z space.

Other Criteria

A criterion which has received some attention in the literature is that of the minimum characteristic root of the matrix Z'Z, say η_{min}. The object is to choose the design, D^*, (or designs) which maximizes η_{min}. That is: $D^* = \max_{D \epsilon S^N} \eta_{min}$

or equivalently: $D^* = \min_{D \epsilon S^N} \lambda_{max}$

where λ_{max} is the maximum characteristic root of $(Z'Z)^{-1}$, and in fact, $\lambda_{max} = 1/\eta_{min}$.

The appeal of this criterion is due, in part at least, to the fact that it relates to the variance of linear combinations of the parameters in the model. However, Folks (6) has shown that this criterion is not invariant under linear transformation, and it is due to this that this criterion will not be used. The characteristic roots of Z'Z and $(Z'Z)^{-1}$ are, however, listed in Tables VI and VII.

TABLE VI

CHARACTERISTIC ROOTS OF Z'Z

η_1	$= \frac{1}{2}\,[f+c - \sqrt{(f-c)^2 + 4d^2}]$	$= \frac{1}{2}\,[f+c + \sqrt{(f+c)^2 - 4(cf-d^2)}]$
η_2	$= \frac{1}{2}\,[f+c - \sqrt{(f-c)^2 + 4d^2}]$	$= \frac{1}{2}\,[f+c - \sqrt{(f+c)^2 - 4(cf-d^2)}]$
η_3	$= \frac{1}{2}\,[4f+N + \sqrt{(4f-N)^2 + 8c^2}]$	$= \frac{1}{2}\,[4f+N + \sqrt{(4f+N)^2 - 8(2Nf-c^2)}]$
η_4	$= \frac{1}{2}\,[4f+N - \sqrt{(4f-N)^2 + 8d^2}]$	$= \frac{1}{2}\,[4f+N - \sqrt{(4f+N)^2 - 8(2Nf-c^2)}]$
η_5	$= \frac{1}{2}\,[2f+c + \sqrt{(2f-c)^2 + 8d^2}]$	$= \frac{1}{2}\,[2f+c + \sqrt{(2f+c)^2 - 8(cf-d^2)}]$
η_6	$= \frac{1}{2}\,[2f+c - \sqrt{(2f-c)^2 + 8d^2}]$	$= \frac{1}{2}\,[2f+c - \sqrt{(2f+c)^2 - 8(cf-d^2)}]$

Another criterion suggested by Folks (6) is that of the minimum average bias of $\hat{y}(u)$, where the bias is incurred when the true model is a polynomial of higher degree than that which is assumed by the experimenter. This criterion has been applied in the context of three

TABLE VII

CHARACTERISTIC ROOTS OF $(Z'Z)^{-1}$

$$\lambda_1 = \frac{c + f + [(c-f)^2 + 4d^2]^{\frac{1}{2}}}{2(cf-d^2)}$$

$$\lambda_2 = \frac{c + f - [(c-f)^2 + 4d^2]^{\frac{1}{2}}}{2(cf-d^2)}$$

$$\lambda_3 = \frac{4f + N + [(4f-N)^2 + 8c^2]^{\frac{1}{2}}}{4(2Nf-c^2)}$$

$$\lambda_4 = \frac{4f + N - [(4f-N)^2 + 8c^2]^{\frac{1}{2}}}{4(2Nf-c^2)}$$

$$\lambda_5 = \frac{c + 2f + [(c-2f)^2 + 8d^2]^{\frac{1}{2}}}{3(cf-d^2)}$$

$$\lambda_6 = \frac{c + 2f - [(c-2f)^2 + 8d^2]^{\frac{1}{2}}}{4(cf-d^2)}$$

and four-component mixture problems by Draper and Lawrence, (4) and (5). Although the class of designs considered by Draper and Lawrence neither includes, nor is included in, the class of symmetric designs, the two classes overlap to the extent that it is felt that further consideration of the criterion is not warranted in this thesis.

Several other criteria have been suggested in the literature. It is not the purpose of this work, however, to make a survey of these criteria, but rather to employ some of those which have been suggested. It is felt that either the criterion of minimum generalized vaiance or of minimum average variance will appeal to the experimenter in most instances and the following chapters will be devoted to employing these criteria in the search for optimum N-point symmetric designs.

CHAPTER IV

OPTIMUM GENERALIZED VARIANCE DESIGNS

This chapter will be concerned with the problem of selecting designs from the class S^N which are optimal in the sense of minimizing the generalized variance of the $\hat{\beta}$s. The definition of optimal with respect to this criterion is given by Definition 3-3. Also in Chapter III it was seen that the criterion measure, $|Z'Z|$, is a function of the design factors. Consequently, $|Z'Z|$ will be regarded as a response over the space, F, of design factors rather than over the space, R^N, of design points. This will result in reducing the dimensionality of the search by two-thirds since a separate search can be made for each subclass, S[u, t, s], of S^N. The corresponding factor space has dimensionality t+2s compared to 3t + 6s for the search in R^N.

If the optimal design or designs are found for each subclass of S^N, it will be easy to select from among these the optimal designs for S^N. This is the approach that will be taken.

The problem in the case of the first order polynomial model is relatively simple and can be handled analytically. For the second order model a computer-aided search will be conducted in the space F. As mentioned above the dimension of F for the subclass S[u, t, s] is t + 2s. However, the dimensionality of the search can be reduced even more by virtue of Theorem 4-1. This theorem will allow the search in F to be limited to those points in F which correspond to designs having three or more points on the boundary of R.

Theorem 4-1. If any symmetric design which is optimum with respect to generalized variance is plotted as an arrangement of points in R, then at least three points will lie on the boundary of R.

Proof of Theorem 4-1. Let D be a design in S^N. Then there exists integers u, t, and s such that D is an element of the subclass, S[u, t, s], of S^N.

Let B(R) be the subclass of all designs in S[u, t, s] which have some points on the boundary of R. Since these are symmetric designs, if one point is on the boundary all points in the corresponding permutation set will lie on the boundary. Therefore, all designs in B(R) have at least three points on the boundary of R.

Let F be the factor space corresponding to S[u, t, s] and let B(F) be the subset of F which maps into B(R).

Now from Chapter III:

$$|Z'Z|_D = (2Nf-c^2)(cf-d^2)^2$$

where, in terms of the t + 2s design factors, c is a sum of terms of the form

$$y^2/2 \qquad \text{or} \qquad (y_1^2 + 3y_2^2)/6,$$

d is a sum of terms of the form

$$\sqrt{3}y^3/12 \qquad \text{or} \qquad (y_2^2 - y_1^2)\, y_2/4\sqrt{6}$$

and f is a sum of terms of the form

$$y^4/24 \qquad \text{or} \qquad (y_1^2 + 3y_2^2)^2/432 \,.$$

For convenience denote the t + 2s factors by $w_1, w_2, \ldots, w_{t+2s}$ and let

$$r = \left(\sum_{1}^{t+2s} w_i^2\right)^{\frac{1}{2}}$$

and

$$\theta_i = \text{arc cos } (w_i/r)$$

so that

$$w_i = r \cos \theta_i, \quad i = 1, \ldots, t+2s$$

Then

$$c = r^2 c'$$

$$d = r^3 d'$$

$$f = r^4 f'$$

where c', d' and f' are functions of $\theta = (\theta_1, \theta_2, \ldots, \theta_{t+2s})$ alone. Then making these substitutions it is seen that $| Z'Z |_D$ can be written as

$$| Z'Z |_D = r^{16} f(\theta).$$

Since Z'Z is positive semidefinite, $| Z'Z |_D \geq 0$. Also $r \geq 0$ so that $f(\theta) \geq 0$. Therefore, considering θ fixed, the partial derivative below is nonnegative, i.e.,

$$\frac{\partial | Z'Z |_D}{\partial r} = 16 \, r^{15} \, f(\theta_1, \ldots, \theta_{t+s}) \geq 0.$$

If $| Z'Z |_D = 0$ for all D in the subclass S[u, t, s], then by definition there exists no optimum design in the subclass. If $| Z'Z |_D > 0$, then $r > 0$ so that

$$\frac{\partial | Z'Z |_D}{\partial r} > 0 .$$

Therefore, let (r_1, θ) correspond to D_1 and (r_2, θ) correspond to D_2 with $r_2 > r_1$. Then

$$|Z'Z|_{D_2} > |Z'Z|_{D_1}$$

so that if (r_2, θ) is a point in F then D_2 is better than D_1 and D_1 is not optimal.

Now the set of points (r, θ) in F with θ fixed and r variable has a maximum element, (r_m, θ), which belongs to B(F). Furthermore, if D_m corresponds to (r_m, θ) and D corresponds to (r, θ) with $r < r_m$, then

$$|Z'Z|_{D_m} > |Z'Z|_{D}$$

and D_m belongs to B(R).

This completes the proof of Theorem 4-1.

As was stated previously, the above theorem will be useful in the search for optimum designs when the second order model is assumed. A similar theorem could be proved for first order models but this case is easily handled in the manner given below.

First Order Model

For the linear model:

$$y = \beta_0 + \beta_1 Z_1 + \beta_2 Z_2 + \epsilon$$

with matrix Z'Z has the form:

$$Z'Z = \begin{pmatrix} N & 0 & 0 \\ 0 & c & 0 \\ 0 & 0 & c \end{pmatrix}$$

so that

$$|Z'Z| = Nc^2$$

Thus to maximize $|Z'Z|$ for fixed N it is necessary to maximize c. But

$$c = \sum_{i=1}^{N} z_{1i}^2 = \sum_{i=1}^{N} z_{2i}^2 .$$

Thus c, as a measure of the "spread" of the design points, indicates that the optimum symmetric design is one in which the design points are distributed evenly on the three corners of the triangular region R', with any of the possible one or two remaining points being allocated to the center.

An Example for the Case of the Second Order Model

To illustrate some of the procedures to be used with larger values of N consider the search for optimum designs in S^6. A separate search will be conducted in each of the subclasses, S[6, 0, 0], S[3, 1, 0], S[0, 0, 1] and S[0, 2, 0]; then the best design or designs from among those found in each case will be selected for the optimum in S^N.

Clearly $|Z'Z| = 0$ for all designs in the subclasses S[6, 0, 0] and S[3, 1, 0], and hence no optimum designs exist in these subclasses.

Consider the subclass S[0, 0, 1]. From Table IV one finds:

$$c = \frac{1}{6}(y_1^2 + 3y_2^2)$$

$$d = \frac{1}{4\sqrt{6}}(y_2^2 - y_1^2)\, y_2$$

and

$$f = \frac{1}{432}(y_1^2 + 3y_2^2)^2 = \frac{1}{12} c^2 .$$

Thus

$$|Z'Z| = 4(12 \cdot \frac{1}{12} c^2 - c^2)(\frac{1}{12} c^3 - d^2)^2$$

$$= 4(c^2 - c^2)(\frac{1}{12} c^3 - d^2)^2$$

$$= 0$$

for any design in S[0, 0, 1]. Hence, there exist no optimum designs in this subclass.

For the subclass S[0, 2, 0] one finds:

$$c = \frac{1}{2}(y_1^2 + y_2^2)$$

$$d = \frac{\sqrt{3}}{12}(y_1^3 + y_2^3)$$

and $$f = \frac{1}{24}(y_1^4 + y_2^4)$$

where $$-\frac{1}{2} \leq y_1 \leq 1$$

and $$-\frac{1}{2} \leq y_2 \leq 1 .$$

Substituting these values of c, d and f into the formula for $|Z'Z|$ one has:

$$|Z'Z| = \frac{1}{48} y_1^2 y_2^2 (y_2^2 - y_1^2)^2 (y_2 - y_1)^2 .$$

This formula is symmetric in the factors y_1 and y_2 so that one need consider only those cases for which $y_1 < y_2$. Furthermore, due to Theorem 4-1, one need consider only those points in the factor space which lie in B(F), that is, the sets

$$\{(-\tfrac{1}{2}, y_2) : -\tfrac{1}{2} < y_2 \leq 1\}$$

and

$$\{(y_1, 1) : -\tfrac{1}{2} \leq y_1 < 1\} .$$

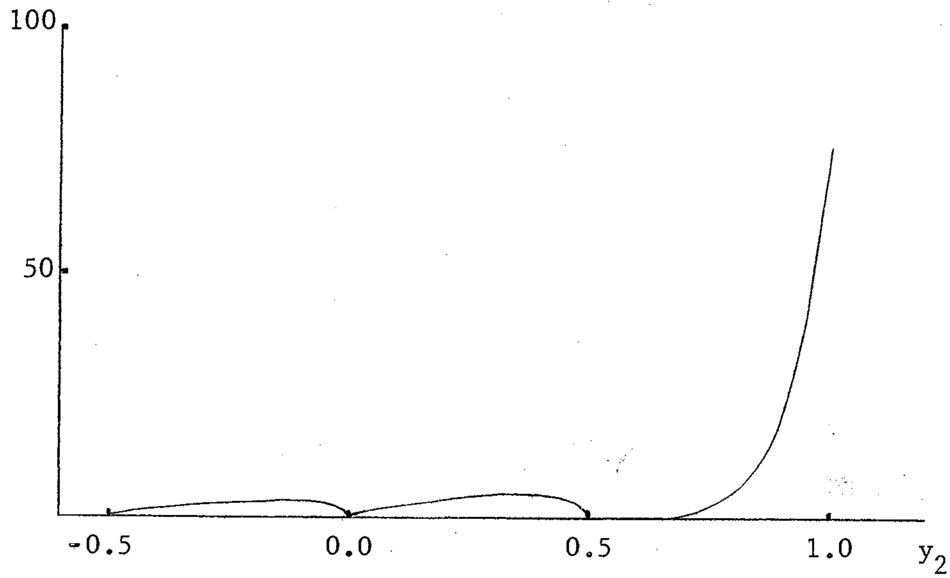

Figure 6. $10^6 \mid Z'Z \mid$ versus y_2 With $y_1 = -0.5$

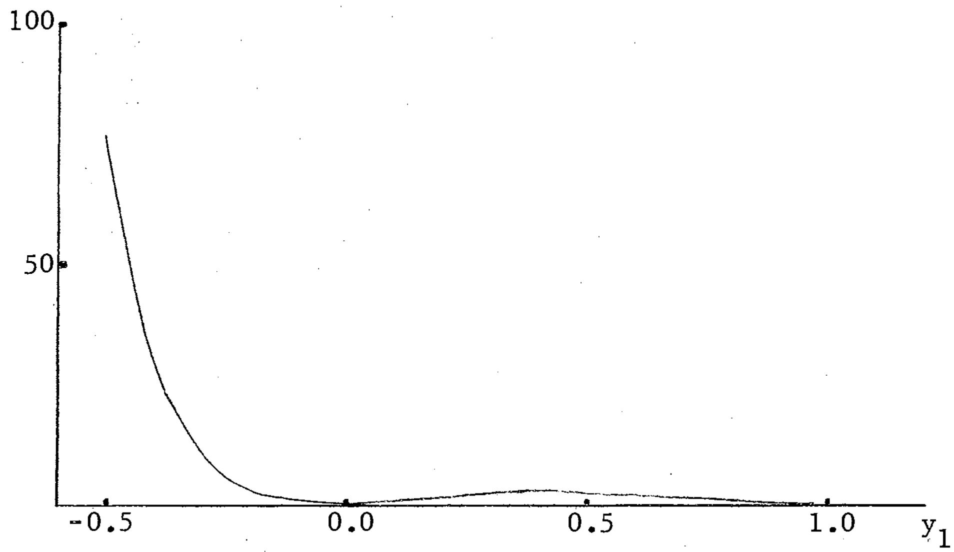

Figure 7. $10^6 \mid Z'Z \mid$ Versus y_1 With $y_2 = 1.0$

The graph of $|Z'Z|$ versus y_2 with $y_1 = -\frac{1}{2}$ is given in Figure 6. The height of the curve is exaggerated for y_2 between $-\frac{1}{2}$ and $\frac{1}{2}$ in order to show its shape. The graph of $|Z'Z|$ as a function of y_1 with $y_2 = 1$ is given in Figure 7, and again the height of the curve is exaggerated for y_1 between 0 and 1. From these two graphs it can be deduced that the optimum 6-point design corresponds to the point $(-\frac{1}{2}, 1)$ in the factor space. The corresponding design plotted as an arrangement of points in R is illustrated in Figure 8 below. This design is Sheffe's (11) 6-point design for the second order model.

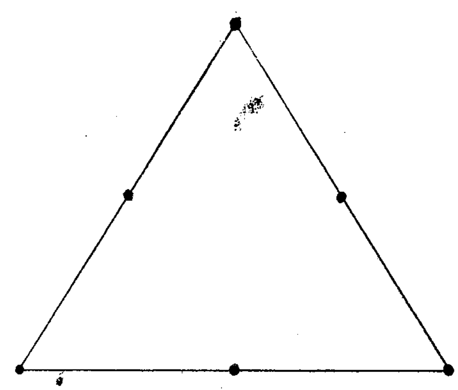

Figure 8. Optimum 6-Point Design

Computer Usage and Results for the Second Order Model

The above developments for the 6-point design were given in detail to illustrate the use of the design factors in the search. For larger values of N a computer program was written in the FORTRAN IV language for the IBM 7040 computer at Oklahoma State University. This program is listed in Appendix A. The program conducts a lattice search in the subspace B(F) of the factor space, making use of any symmetries in the factors to reduce the number of points to be investigated. The program can be instructed to search a given subclass, S[u, t, s], at points on a grid of specified fineness, and to output the k best designs found.

For N up to and including N = 17 the above program was employed with a grid of 0.1 increments in the design factors. In terms of triangular coordinates an increment of 0.1 in the design factors amounts to a maximum increment of 6.7 percent in any one mixture component. The 20 best designs were obtained as output in each case. For N up to and including N = 9 a finer grid was employed which amounted to increments as small as 0.1 percent in some components. Use of the finer grid did not result in the choice of any design other than those already found.

Results of the above search indicate that the minimum generalized variance design for each N has the same configuration as that for the 6-point design illustrated in Figure 8, except for some variation in the number of replicated points at the center, midpoints and corners of the triangular region. The following rules for allocation of the points were deduced from the computer output.

Case 1: N divisible by 6. Allocate N/6 points to each corner and to each midpoint.

Case 2: N-1 (or N-2) divisible by 6. Allocate (N-1)/6 (or (N-2)/6) points to each corner and to each midpoint and allocate the remaining one (or two) points to the center.

Case 3: N divisible by 3 but not divisible by 6. There are two optimum designs. Allocate (N + 3)/6 points to each corner and (N-3)/6 points to each midpoint or vice versa.

Case 4: N-1 (or N-2) divisible by 3 but not divisible by 6. Allocate (N+2)/6 (or (N+1)/6) points to each corner and (N-4)/6 (or (N-5)/6) points to each midpoint and allocate the remaining one (or two) points to the center.

The above rules were verified for N up to 100 by assuming that for N greater than 17 the optimum designs would have the same configuration as that which was observed for smaller N, i.e., the simplex-lattice or simplex-centroid configuration. Then with this assumption the formula for $|Z'Z|$ was simplified and investigated in the manner outlined below.

From the results of the investigation for $N \leq 17$ it was found that optimum designs in S^N were elements of subclasses of the form:

$$S[u, t, 0] ,$$

that is, no optimum designs were found having 6-point permutation sets. Thus,

$$N = u + 3t .$$

Let $t = t_1 + t_2$, where t_1 is the number of 3-point permutation sets (replicates) located on the midpoints of the triangular boundary of R, and where t_2 is the number of 3-point sets (replicates) on the corners. Then for

$$0 \leq \theta \leq 1$$

let

$$t_1 = \theta t$$

and

$$t_2 = (1 - \theta)t .$$

Since in F, $-\frac{1}{2}$ corresponds to a 3-point permutation set on the mid-points of the triangular region, and 1 corresponds to a 3-point set on the corners of R, the elements c, d and f can then be written in terms of the design factors as

$$c = \tfrac{1}{2}\,(t_1(-\tfrac{1}{2})^2 + t_2(1)^2)$$

$$= (t/2)(1-3\theta/4)$$

$$d = \frac{\sqrt{3}}{12}\,(t_1(-\tfrac{1}{2})^3 + t_2(1)^3)$$

$$= (t\,\frac{\sqrt{3}}{12})(1-9\theta/8)$$

and

$$f = \frac{1}{24}\,(t_1(-\tfrac{1}{2})^4 + t_2(1)^4)$$

$$= (t/24)(1-15\theta/16)\;.$$

Then making these substitutions in

$$|\,Z'Z\,| = (2Nf - c^2)(cf - d^2)^2$$

one has

$$|\,Z'Z\,| = \frac{3t^5}{2^{20}}\;\theta^2\;(1-\theta)^2(16u + 3(9t-5u)\theta - 27t\theta^2)$$

Now in the case where there are no center points, i.e., u = 0, one has

$$|\,Z'Z\,| = \frac{3^4t^6}{2^{20}}\;\theta^3(1-\theta)^3$$

which is symmetric about $\theta = \frac{1}{2}$.

Taking the partial derivative of $|\,Z'Z\,|$ with respect to θ one finds

$$\frac{\partial\,|\,Z'Z\,|}{\partial\theta} = \frac{3t^5}{2^{20}}\;\theta(1-\theta)\;\{54t\theta(1-\theta)\;[\frac{9t-5u}{18t} - \theta]$$

$$+ (\tfrac{1}{2} - \theta)\;[16u + 3(9t - 5u)\theta - 27t\theta^2]\}\;,$$

and with u = 0 this reduces to

$$\frac{\partial |Z'Z|}{\partial \theta} = \frac{3^5 t^5}{2^{20}} \theta^2 (1-\theta)^2 (\tfrac{1}{2}-\theta)$$

which has, in the range of interest, a zero at $\theta = \frac{1}{2}$. Thus for u = 0, N = 3t and $t_1 = t_2 = \frac{1}{2}t$.

Now if N is divisible by 6 then t is divisible by 2 so that $t_1 = t_2$ is an integer. This corresponds to Case 1, above, and verifies the rule given there if u = 0 is assumed.

With u = 0, Case 2 and Case 4 above are not possible with symmetric designs. For Case 3, where N is not divisible by 6, the solution $t_1 = t_2 = \frac{1}{2}t$ is not an integer. The integer values for $t_1 = \theta t$ correspond to $\theta = 0, 1/t, 2/t, \ldots, 1$, and of these, the two nearest $\theta = \frac{1}{2}$ are

$$\theta_1 = \frac{t-1}{2t} = \frac{(N/3) - 1}{2N/3} = \frac{N - 3}{2N}$$

and

$$\theta_2 = \frac{t+1}{2t} = \frac{(N/3) + 1}{2N/3} = \frac{N + 3}{2N}$$

so that either

$$t_1 = \frac{N}{3} \left(\frac{N - 3}{2N}\right) = \frac{N - 3}{6}$$

or

$$t_1 = \frac{N}{3} \left(\frac{N + 3}{2N}\right) = \frac{N + 3}{6} \quad .$$

Both of these are valid solutions and each results in an optimal design since it was shown above that $|Z'Z|$ is symmetric about $\theta = \frac{1}{2}$. This verifies the rule given for Case 3 if u = 0 is assumed.

The optimum value for θ could be found for arbitrary values of u by solving

$$\frac{\partial |Z'Z|}{\partial \theta} = 0$$

for roots in the range: $0 < \theta < 1$. The general solution would be of little value however, since in general, it would not result in integer solutions for t_1 and t_2. Furthermore, for $u \neq 0$, the expression for $|Z'Z|$ is not symmetric about the root in question. On the other hand, it was relatively simple to program the computer to calculate for each N the value of $|Z'Z|$ for all possible combinations of u, t_1 and t_2. Results of these computations showed no exceptions to the above rules for N up to 100.

This completes the discussion on optimum generalized variance designs. Designs which are optimum with respect to average variance will be considered in the following chapter.

CHAPTER V

OPTIMUM AVERAGE VARIANCE DESIGNS

This chapter will be concerned with the problem of choosing optimal designs from the class S^N using as the criterion the average variance of the predicted response.

Optimum designs for the first order model can be readily obtained by the mechanisms already developed. The optimum designs for average variance are exactly those obtained for the criteria of generalized variance, i.e., those with all points, up to the largest multiple of three, distributed evenly on the corners of the triangular region and with the remaining points at the center. The rationale is essentially that given by Draper and Lawrence (4) and will not be discussed further here. Optimum designs from S^N in the case of the second order model, however, cannot be obtained from the above mentioned work of Draper and Lawrence; therefore, the remainder of this chapter will be devoted to this case.

The criterion of average variance presupposes a region of interest on which a density function is defined. As previously mentioned a uniform density will be assumed. Initially the region of interest will be the entire triangular region, R (or R'). It will be shown how the results obtained for this case can be used when the region of interest is any triangular region in R. Consideration will then be given to cases where the region of interest is a triangular subregion, T, of R, but where it is possible to run design-points in another subregion, Q, of R, which contains T and which has the same center point and orientation in R as the region T. The region Q will be called the region of operability.

A computer program similar to the one used with the generalized variance criterion was used in the search for optimum average variance designs. This program, however, incorporates some additional search features based on developments in the following section.

Preliminary Developments

Let the region of interest be R and let AV_D denote the average variance of the N-point design, $D \epsilon S[u, t, s]$. Then from Chapter III, page 34,

$$AV_D = \frac{720f - 30c + N}{360\ (2Nf - c^2)} + \frac{30f - 4\sqrt{3}d + c}{360\ (cf - d^2)} \quad ,$$

where, in terms of the factors in F corresponding to D, c is a sum of terms of the form

$$\frac{1}{2}\, y^2 \qquad \text{or} \qquad \frac{1}{6}\,(y_1^2 + 3y_2^2) \ ,$$

d is a sum of terms of the form

$$\frac{\sqrt{3}}{12}\, y^3 \qquad \text{or} \qquad \frac{1}{4\sqrt{6}}\,(y_2^2 - y_1^2)\, y_2 \quad ,$$

and f is a sum of terms of the form

$$\frac{1}{24}\, y^4 \qquad \text{or} \qquad \frac{1}{432}\,(y_1^2 + 3y_2^2)^2 \quad .$$

Let the t+2s factors be denoted by $w_1, w_2, \ldots, w_{t+s}$ and let

$$r = \left(\sum_i w_i^2\right)^{\frac{1}{2}}$$

and

$$\cos \theta_i = w_i/r$$

so that

$$w_i = r \cos \theta_i .$$

Let

$$\theta = (\theta_1, \ldots, \theta_{t+2s})$$

Then (r,θ) is the polar coordinate representation of the point in F corresponding to the design D.

Thus c, d and f can be expressed as:

$$c = r^2 c'$$

$$d = r^3 d'$$

$$f = r^4 f'$$

where c', d' and f' are functions of θ alone.

Substituting the above into the formula for AV_D, one obtains

$$AV_D = \frac{720r^4 f' - 30r^2 c' + N}{360r^4 \ (2Nf' - c'^2)} + \frac{30r^4 f' - 4\sqrt{3}\ r^3 d' + r^2 c'}{360\ r^6\ (c'f' - d'^2)} .$$

Letting $\rho = \frac{1}{r}$ and combining terms of like power in ρ, the above expression can be written in the form

$$AV_D = A_4\rho^4 + A_3\rho^3 + A_2\rho^2 + A_0$$

where

$$A_4 = \frac{N}{360\ (2Nf' - c'^2)} + \frac{c'}{360\ (c'f' - d'^2)}$$

$$A_3 = \frac{-\sqrt{3}}{120\ (c'f' - d'^2)}$$

$$A_2 = \frac{f'}{12\ (c'f' - d'^2)} + \frac{c'}{12\ (2Nf' - c'^2)}$$

and

$$A_0 = \frac{2f'}{2Nf' - c'^2} \quad .$$

Now taking the partial derivative of AV_D with respect to ρ one obtains

$$\frac{\partial AV_D}{\partial \rho} = 4A_4\rho^3 + 3A_3\rho^2 + 2A_2\rho \quad .$$

Setting the above equal to zero yields the roots:

$$\rho_1 = 0$$

$$\rho_2 = \frac{-3A_3 - [9A_3^2 - 32A_2A_4]^{\frac{1}{2}}}{8A_4}$$

and

$$\rho_3 = \frac{-3A_3 + [9A_3^2 - 32A_2A_4]^{\frac{1}{2}}}{8A_4} \quad .$$

Now considering AV_D as a function of (r, θ), with θ fixed, one is looking at a ray in F beginning at the origin $(0, \theta)$, and projecting through some point in B(F), corresponding to a design with at least three points on the boundary of R. The point at the origin with $r = 0$ (or $\rho = \infty$) corresponds to the design having all points concentrated at the center of the region R. Thus the average variance approaches infinity as r approaches zero (or ρ approaches infinity) along the ray. Therefore the largest positive root above, if such exists, represents a possible local minimum value of the average variance along the ray. When such a root exists it will be denoted by ρ^*, and the corresponding value of r by $r^* = 1/\rho^*$. The corresponding point coordinates in terms of the design factors are given by:

$$w_i^* = r^* \cos \theta_i .$$

If the point $(w_1^*, \ldots, w_{t+s}^*)$ is contained in F, it will be of interest to calculate AV_{D^*}. This is easily determined if the original design, D, corresponding to the point (r, θ), is an element of B(F), since in this case (r^*, θ) is in F if and only if $r^* \le r$ or $\rho^* \ge \rho$. The manner in which these results were found useful is discussed below.

Computer Usage and Results For the Region of Interest, R

The developments in the above section suggest a method for beginning the search for optimum designs in a subclass S[u, t, s]. Namely, calculate AV_D for designs D, corresponding to a grid in B(F) and for each D determine if there exists a D* corresponding to a point in F. If so, calculate AV_{D^*}. Note that D* is a design with no points on the boundary of the region R.

The program used in searching for optimum generalized variance designs searched a grid in B(F). This program was therefore modified to perform the above suggested operations. The program listing is given in Appendix B. The resulting program was instructed to output the 20 best designs of the type D* as well as the 20 best designs corresponding to points in B(F).

For N from 6 to 20 the program above was used with a grid of increments of 0.1 in the design factors.

The best designs resulting from this search were all from subclasses of the type S[u, t, 0], that is, these designs contained no 6-point permutation sets. Furthermore, these designs had all points on the boundary of R with the exception of one 3-point set in some cases.

The above search was followed by a sequential pattern search described by Hookes and Jeeves (10). The computer program for the pattern search is listed in Appendix C. Starting points in the case of each N corresponded to the best design found by the grid search. The program was instructed to continue the search until 1000 iterations had been completed or until no improvement was achieved with increments of the design factors as small as 0.001. The resulting designs differed very little in average variance from those already found, the reduction being in fractions of one percent. The resulting design points were also in the same neighborhood as those already found, however, for each N divisible by 3 the optimum design was found to have one permutation set which was not on the boundary of R.

Different starting points for the pattern search were also tried in several instances and convergence to approximately the same design was achieved. It is recognized that the average variance viewed as a response surface over F is multimodal and convergence to a local optimum point is possible. The grid search, with output of the 20 best points (or designs) effectively ensures that a global optimum or near optimum design has been found however.

The best designs found by the above searches may be obtained from Table VIII. In this table N is the number of points in the design and AV is the average variance given as a fraction of σ^2. Coordinates of a representative point are given for each distinct permutation set in

TABLE VIII

AVERAGE VARIANCE DESIGNS IN R

N	AV	r	x_1	x_2	x_3
6	.63305	1	0.000	0.000	1.000
		1	0.498	0.498	0.004
7	.49950	1	0.333	0.333	0.333
		1	0.000	0.000	1.000
		1	0.500	0.500	0.000
8	.44026	2	0.333	0.333	0.333
		1	0.000	0.000	1.000
		1	0.500	0.500	0.000
9	.36602	1	0.000	0.000	1.000
		1	0.500	0.500	0.000
		1	0.490	0.490	0.020
10	.32407	1	0.333	0.333	0.333
		1	0.000	0.000	1.000
		2	0.500	0.500	0.000
11	.29852	2	0.333	0.333	0.333
		1	0.000	0.000	1.000
		2	0.500	0.500	0.000
12	.27660	1	0.000	0.000	1.000
		2	0.500	0.500	0.000
		1	0.472	0.472	0.056
13	.25637	1	0.333	0.333	0.333
		1	0.000	0.000	0.000
		3	0.500	0.500	0.000
14	.24180	2	0.333	0.333	0.333
		1	0.000	0.000	1.000
		3	0.500	0.500	0.000
15	.22743	2	0.000	0.000	1.000
		2	0.500	0.500	0.000
		1	0.484	0.484	0.032
16	.20745	1	0.333	0.333	0.333
		2	0.000	0.000	1.000
		3	0.500	0.500	0.500

TABLE VIII (Continued)

N	AV	r	x_1	x_2	x_3
17	.19326	2	0.333	0.333	0.333
		2	0.000	0.000	1.000
		3	0.500	0.500	0.000
18	.18276	2	0.000	0.000	1.000
		3	0.500	0.500	0.000
		1	0.452	0.452	0.096
19	.17116	1	0.333	0.333	0.333
		2	0.000	0.000	1.000
		4	0.500	0.500	0.000
20	.16204	2	0.333	0.333	0.333
		2	0.000	0.000	1.000
		4	0.500	0.500	0.000

the design. These are listed under the headings x_1, x_2 and x_3. The remaining points of the set are found by taking all permutations of x_1, x_2 and x_3. The number, r, preceding each set of coordinates indicates that r such permutation sets occur in the design. Therefore, the points obtained from the permutations of x_1, x_2 and x_3 should be replicated r times.

A sample output from the lattice or grid search program is given in Appendix D. A sample of some of the "near optimum" designs obtained by use of this program are given in Appendix E.

Triangular Subregions of Interest

Suppose the region of interest is a triangular subregion, T, of R. Let the triangular coordinates of the corners of the region T be represented by the 3 x 1 vectors c_1, c_2 and c_3. And let C be a 3 x 3 matrix defined by

$$C = [c_1, c_2, c_3] .$$

Then R is transformed into T by

$$t = C x$$

where x is a 3 x 1 vector of coordinates in R and t is the corresponding vector of coordinates in T. If T is a nondegenerate triangle the matrix C is nonsingular. Therefore, a symmetric design in T can be defined as the image, under the above linear transformation, of a symmetric design in R. Since products of nonsingular linear transformations are again nonsingular and linear and since the average variance is invariant under such transformations, optimum designs for T can be found by applying the above transformations to all the points found from Table VIII for the optimum N-point designs in R.

Regions of Interest Contained in Regions of Operability

Suppose the region of interest is a triangular subregion, T, of R and that it is possible to operate in a larger subregion containing T. If T does not intersect the boundary of R it will often be possible to approximate the region of operability by drawing a larger triangle about T having the same centroid, shape and orientation in R as T. If it is assumed that the region of operability Q is such a triangular region, then T can be transformed into R with the result that Q is transformed into a proportionately larger triangle containing R. Such a transformation is linear and nonsingular so that the search can be conducted in the transformed space. The previous computer programs can be used by simply extending the limits of the design factor space, F, by a proportion, θ, relating to the relative size of the triangles T and Q.

The parameter θ is defined as

$$\theta = L_Q/L_T$$

where L_Q is the distance from the centroid of Q to the midpoint of one of its sides and L_T is the distance from the common centroid to the midpoint of the corresponding side of T.

The lattice search program was used with θ = 1.5, 2.0, 2.5, 3.0 and 4.0 for N up to 14. The results obtained with a grid of increments of $\theta/10$ in the design factors are given in Table IX. No follow-up search was made with the pattern search program.

The designs obtained from Table IX can be transformed to the original subregions T and Q in the same manner as described in the preceding section. Namely, by use of the coordinates of the corners of the region T to build the transformation matrix C. It is important that all N points be determined by permutations of the coordinates given in Table IX before the transformation is applied.

TABLE IX

AVERAGE VARIANCE DESIGNS IN Q

N	θ	AV	r	x_1	x_2	x_3
6	1.5	.55444	1	0.533	0.533	-0.066
			1	-0.167	-0.167	1.334
6	2.0	.52384	1	0.600	0.600	-0.200
			1	-0.333	-0.333	1.667
6	2.5	.50713	1	0.600	0.600	-0.200
			1	-0.500	-0.500	2.000
6	3.0	.47945	1	0.633	0.633	-0.266
			1	-0.667	-0.667	2.333
6	4.0	.44997	1	0.773	0.773	-0.446
			1	-1.000	-1.000	3.000
7	1.5	.40984	1	0.333	0.333	0.333
			1	0.583	0.583	-0.166
			1	-0.167	-0.167	1.334
7	2.0	.38681	1	0.333	0.333	0.333
			1	0.600	0.600	-0.200
			1	-0.333	-0.333	1.667
7	2.5	.36680	1	0.333	0.333	0.333
			1	0.667	0.667	-0.333
			1	-0.500	-0.500	2.000
7	3.0	.35565	1	0.333	0.333	0.333
			1	0.733	0.733	-0.466
			1	-0.667	-0.667	2.333
7	4.0	.33674	1	0.333	0.333	0.333
			1	0.733	0.733	-0.466
			1	-1.000	-1.000	3.000
8	1.5	.32737	2	0.333	0.333	0.333
			1	0.583	0.583	-0.166
			1	-0.167	-0.167	1.334
8	2.0	.30411	2	0.333	0.333	0.333
			1	0.667	0.667	-0.333
			1	-0.333	-0.333	1.667

TABLE IX (Continued)

N	θ	AV	r	x_1	x_2	x_3
8	2.5	.29349	2	0.333	0.333	0.333
			1	0.667	0.667	-0.333
			1	-0.500	-0.500	2.000
8	3.0	.28026	2	0.333	0.333	0.333
			1	0.733	0.733	-0.466
			1	-0.667	-0.667	2.333
8	4.0	.26643	2	0.333	0.333	0.333
			1	0.867	0.867	-0.734
			1	-1.000	-1.000	3.000
9	1.5	.28085	3	0.333	0.333	0.333
			1	0.583	0.583	-0.166
			1	-0.167	-0.167	1.334
9	2.0	.25178	3	0.333	0.333	0.333
			1	0.667	0.667	-0.333
			1	-0.333	-0.333	1.667
9	2.5	.23990	3	0.333	0.333	0.333
			1	0.750	0.750	-0.500
			1	-0.500	-0.500	2.000
9	3.0	.23359	3	0.333	0.333	0.333
			1	0.833	0.833	-0.666
			1	-0.667	-0.667	2.333
9	4.0	.21953	3	0.333	0.333	0.333
			1	0.867	0.867	-0.734
			1	-1.000	-1.000	3.000
10	1.5	.24634	1	0.333	0.333	0.333
			1	0.483	0.483	0.034
			1	0.583	0.583	-0.166
			1	-0.167	-0.167	1.334
10	2.0	.21818	4	0.333	0.333	0.333
			1	0.667	0.667	-0.333
			1	-0.333	-0.333	1.667
10	2.5	.20443	4	0.333	0.333	0.333
			1	0.750	0.750	-0.500
			1	-0.500	-0.500	2.000

TABLE IX (Continued)

N	θ	AV	r	x_1	x_2	x_3
10	3.0	.19707	4	0.333	0.333	0.333
			1	0.833	0.833	-0.666
			1	-0.667	-0.667	2.333
10	4.0	.18810	4	0.333	0.333	0.333
			1	0.867	0.867	-0.734
			1	-1.000	-1.000	3.000
11	1.5	.21767	2	0.333	0.333	0.333
			1	0.533	0.533	-0.066
			1	0.583	0.583	-0.166
			1	-0.167	-0.167	1.334
11	2.0	.19469	2	0.333	0.333	0.333
			1	0.467	0.467	0.066
			1	0.667	0.667	-0.333
			1	-0.333	-0.333	1.667
11	2.5	.17973	5	0.333	0.333	0.333
			1	0.750	0.750	-0.500
			1	-0.500	-0.500	2.000
11	3.0	.17164	5	0.333	0.333	0.333
			1	0.833	0.833	-0.666
			1	-0.667	-0.667	2.333
11	4.0	.16342	5	0.333	0.333	0.333
			1	1.000	1.000	-1.000
			1	-1.000	-1.000	3.000
12	1.5	.19428	3	0.333	0.333	0.333
			2	0.583	0.583	-0.166
			1	-0.167	-0.167	1.344
12	2.0	.17480	3	0.333	0.333	0.333
			1	0.533	0.533	-0.066
			1	0.667	0.667	-0.333
			1	-0.333	-0.333	1.667
12	.25	.16154	6	0.333	0.333	0.333
			1	0.750	0.750	-0.500
			1	-0.500	-0.500	2.000
12	3.0	.15291	6	0.333	0.333	0.333
			1	0.833	0.833	-0.666
			1	-0.667	-0.667	2.333

TABLE IX (Continued)

N	θ	AV	r	x_1	x_2	x_3
12	4.0	.14415	6	0.333	0.333	0.333
			1	1.000	1.000	-1.000
			1	-1.000	-1.000	3.000
13	1.5	.17669	4	0.333	0.333	0.333
			2	0.583	0.583	-0.166
			1	-0.167	-0.167	1.334
13	2.0	.15778	4	0.333	0.333	0.333
			1	0.600	0.600	-0.200
			1	0.667	0.667	-0.333
			1	-0.333	-0.333	1.667
13	2.5	.14721	4	0.333	0.333	0.333
			1	0.600	0.600	-0.200
			1	0.750	0.750	-0.500
			1	-0.500	-0.500	2.000
13	3.0	.13854	7	0.333	0.333	0.333
			1	0.833	0.833	-0.666
			1	-0.667	-0.667	2.333
13	4.0	.12936	7	0.333	0.333	0.333
			1	1.000	1.000	-1.000
			1	-1.000	-1.000	3.000
14	1.5	.16350	5	0.333	0.333	0.333
			2	0.583	0.583	-0.166
			1	-0.167	-0.167	1.334
14	2.0	.14352	5	0.333	0.333	0.333
			2	0.667	0.667	-0.333
			1	-0.333	-0.333	1.667
14	2.5	.13446	5	0.333	0.333	0.333
			1	0.667	0.667	-0.333
			1	0.750	0.750	-0.500
			1	-0.500	-0.500	2.000
14	3.0	.12717	8	0.333	0.333	0.333
			1	0.833	0.833	-0.666
			1	-0.667	-0.667	2.333
14	4.0	.11765	8	0.333	0.333	0.333
			1	1.000	1.000	-1.000
			1	-1.000	-1.000	3.000

CHAPTER VI

EFFECT ON THE AVERAGE VARIANCE OF INCLUDING TOO MANY TERMS IN THE MODEL

Another aspect of the problem of choosing a symmetric design, or any design for that matter, is the necessity of making a prior judgment as to the appropriate model. Even when polynomial models are assumed, there remains the problem of deciding on the degree or order of the polynomial.

Suppose two models are under consideration, one of which is the correct model. Let the predicted responses at the point u be denoted by

$$\hat{y}_1 = U'_1\hat{\beta}$$

and

$$\tilde{y}_2 = U'_1\tilde{\beta}_1 + U'_2\tilde{\beta}_2$$

where

$$\hat{\beta}_1 = (Z'_1Z_1)^{-1}\, Z'_1Y$$

and

$$\begin{pmatrix} \tilde{\beta}_1 \\ \tilde{\beta}_2 \end{pmatrix} = \begin{pmatrix} Z'_1Z_1 & Z'_1Z_2 \\ Z'_2Z_1 & Z'_2Z_2 \end{pmatrix}^{-1} \cdot \begin{pmatrix} Z'_1Y \\ Z'_2Y \end{pmatrix}$$

$$= \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \cdot \begin{pmatrix} Z'_1Y \\ Z'_2Y \end{pmatrix}$$

were obtained from the respective models

$$Y = Z_1\beta_1 + e$$

and

$$Y = Z_1\beta_1 + Z_2\beta_2 + e \ .$$

If the second model is correct but the first is chosen then the error incurred involves both bias and variance. Draper and Lawrence, (4) and (5), have considered this problem. On the other hand suppose the first model above is correct, that is, $\beta_2 = 0$, but that the second is chosen. The error in this case can be measured in terms of average variances as will be shown below.

Consider the squared difference:

$$\begin{aligned}(\tilde{y}_2 - \hat{y}_1)^2 &= [U'_1\ (\tilde{\beta}_1 - \hat{\beta}_1) + U'_2\tilde{\beta}_2]^2 \\ &= (\tilde{\beta}_1 - \hat{\beta}_1)'\ U_1U'_1\ (\tilde{\beta}_1 - \hat{\beta}_1) + \tilde{\beta}'_2U_2U'_2\tilde{\beta}_2 \\ &\qquad + 2\tilde{\beta}'_2U_2U'_1(\tilde{\beta}_1 - \hat{\beta}_1) \\ &= \text{trace}\ [(\tilde{\beta}_1 - \hat{\beta}_1)(\tilde{\beta}_1 - \hat{\beta}_1)'\ U_1U'_1 + \tilde{\beta}_2\tilde{\beta}'_2U_2U'_2 \\ &\qquad + 2(\tilde{\beta}_1 - \hat{\beta}_1)\tilde{\beta}'_2U_2U'_1] \ .\end{aligned}$$

Now it is desired to find the expected value of $(\tilde{y}_2 - \hat{y}_1)^2$, denoted by $E(\tilde{y}_2 - \hat{y}_1)^2$, over the population of $\tilde{y}_2$s and $\hat{y}_1$s at the point u. To accomplish this it is necessary to find:

$$E(\tilde{\beta}_1 - \hat{\beta}_1)(\tilde{\beta}_1 - \hat{\beta}_1)'$$

$$E(\tilde{\beta}_2\tilde{\beta}'_2)$$

and

$$E(\tilde{\beta}_1 - \hat{\beta}_1)\tilde{\beta}'_2 \ .$$

Lemma 6-1. $\frac{1}{\sigma^2} E(\tilde{\beta}_1 - \hat{\beta}_1)(\tilde{\beta}_1 - \hat{\beta}_1)' = C_{11} - (Z'_1Z_1)^{-1}$.

Proof of Lemma 6-1. From the definitions given above one finds

$$\tilde{\beta}_1 - \hat{\beta}_1 = [C_{11}Z'_1 + C_{12}Z'_2 - (Z'_1Z_1)^{-1} Z'_1] Y$$

so that

$$E(\tilde{\beta}_1 - \hat{\beta}_1) = [C_{11}Z'_1Z_1 + C_{12}Z'_2Z_1 - I] \beta_1$$

and using the fact that

$$C_{12} = -C_{11}(Z'_1Z_2)(Z'_2Z_2)^{-1}$$

one has

$$\begin{aligned} E(\tilde{\beta}_1 - \hat{\beta}_1) &= [C_{11}(Z'_1Z_1 - Z'_1Z_2(Z'_2Z_2)^{-1}Z'_2Z_1) - I] \beta_1 \\ &= [C_{11}C_{11}^{-1} - I] \beta_1 \\ &= \emptyset\beta_1 \\ &= \emptyset \ . \end{aligned}$$

Therefore,

$$\tilde{\beta}_1 - \hat{\beta}_1 = [C_{11}Z'_1 + C_{12}Z'_2 - (Z'_1Z_1)^{-1}Z'_1] e$$

so that

$$\begin{aligned} \frac{1}{\sigma^2} E(\tilde{\beta}_1 - \hat{\beta}_1)(\tilde{\beta}_1 - \hat{\beta}_1)' = [C_{11}Z'_1 + C_{12}Z'_2 - (Z'_1Z_1)^{-1}Z'_1] \cdot \\ [C_{11}Z'_1 + C_{12}Z'_2 - (Z'_1Z_1)^{-1}Z'_1]' . \end{aligned}$$

Expanding this expression and using the well known identies for inverses of partitioned matrices the above result is obtained.

Lemma 6-2. $\frac{1}{\sigma^2} E(\tilde{\beta}_2\tilde{\beta}'_2) = C_{22}$

Proof of Lemma 6-2. Now from the above definitions

$$\tilde{\beta}_2 = [C_{21}Z'_1 + C_{22}Z'_2] Y$$

so that

$$E(\tilde{\beta}_2) = [C_{21}Z'_1Z_1 + C_{22}Z'_2Z_1]\ \beta_1$$

and using the fact that

$$C_{21} = -C_{22}\ (Z'_2Z_1)(Z'_1Z_1)^{-1}$$

one finds

$$E(\tilde{\beta}_2) = [C_{22}\ (Z'_2Z_1 - Z'_2Z_1)]\ \beta_1$$

$$= \emptyset .$$

Therefore

$$\tilde{\beta}_2 = [C_{21}Z'_1 + C_{22}Z'_2]\ e$$

so that

$$\frac{1}{\sigma^2} E(\tilde{\beta}_2\tilde{\beta}'_2) = [C_{21}Z'_1 + C_{22}Z'_2]\cdot[C_{21}Z'_1 + C_{22}Z'_2]'.$$

Expansion of this expression results in the stated conclusion.

<u>Lemma 6-3</u>. $\frac{1}{\sigma^2} E(\tilde{\beta}_1 - \hat{\beta}_1)\tilde{\beta}'_2 = C_{12}$

<u>Proof of Lemma 6-3</u>. From the two lemmas above it is seen that

$$\frac{1}{\sigma^2} E(\tilde{\beta}_1 - \hat{\beta}_1)\tilde{\beta}'_2 = [C_{11}Z'_1 + C_{12}Z'_2 - (Z'_1Z_1)^{-1}Z'_1]\cdot[Z_1C_{12} + Z_2C_{22}].$$

Expansion of this expression results in the stated conclusion.

The above lemmas result in the theorem stated below.

<u>Theorem 6-4</u>. If the appropriate model is

$$Y = Z\beta_1 + e$$

but the model

$$Y = Z\beta_1 + Z\beta_2 + e$$

is assumed, then the variances of the predicted responses at the point u, denoted respectively by $\sigma^2 v_1(u)$ and $\sigma^2 v_2(u)$ are such that

$$\sigma^2 v_2(u) \geq \sigma^2 v_1(u) \ .$$

Proof of Theorem 6-4. From Lemmas 6-1, 6-2 and 6-3 one finds

$$\frac{1}{\sigma^2} E\,(\tilde{y}_2 - \hat{y}_1)^2 = \text{trace}\,(U_1U'_1\,[C_{11}-(Z'_1Z_1)^{-1}] + U_2U'_2C_{22} + 2U_2U'_1C_{12})$$

$$= (U'_1,\ U'_2)\begin{pmatrix} C_{11} - (Z'_1Z_1)^{-1} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}\begin{pmatrix} U_1 \\ U_2 \end{pmatrix}$$

$$= (U'_1,\ U'_2)\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}\begin{pmatrix} U_1 \\ U_2 \end{pmatrix} - (U'_1, U'_2)\begin{pmatrix} (Z'_1Z_1)^{-1} & \emptyset \\ \emptyset & \emptyset \end{pmatrix}\begin{pmatrix} U_1 \\ U_2 \end{pmatrix}$$

$$= v_2(u) - v_1(u).$$

Then since $\frac{1}{\sigma^2} E\,(\tilde{y}_2 - \hat{y}_1)^2$ is clearly nonnegative one has

$$v_2(u) \geq v_1(u)$$

and the theorem is proved.

The corollary stated below follows immediately.

Corollary 6-5. For the assumptions in Theorem 6-4 the average variances AV_2 and AV_1 corresponding to the two models are such that:

$$AV_2 > AV_1$$

over any specified region of interest and for any weighting density p(u).

One might refer to an error of the type above, i.e., including too many terms in the chosen model, as an error of the first kind, and to the opposite type of error, i.e., including too few terms in the model, as an error of the second kind. The corollary above points out the existence of errors of the first kind, however, one would guess that this type error would usually be far less serious than an error of the second kind.

CHAPTER VII

SUMMARY AND EXTENSIONS

The class of experimental designs defined in this thesis are appropriate for use in three component mixture experiments. This class of designs, called symmetric designs, includes as subclasses the simplex-lattice and simplex-centroid designs defined by Sheffe'.

When a polynomial model of degree one or two is assumed and N experimental points are to be run, designs can be found from tables presented in this thesis which are optimal in the sense of one or the other of two criteria. One criterion used is that of minimum generalized variance of the $\tilde{\beta}$'s in the model. The other criterion designates as optimal those designs for which the average variance of the predicted response is a minimum. In this case the average is taken over a region in which the experimenter is assumed to have equal interest in the response at all points of the region.

For the case of generalized variance the optimum designs for each N were found to have the same configuration as the simplex designs mentioned above. However, the number of replicates to be assigned to the points on the simplex vary with N. Rules for the allocation of replicates are given on page 43 of Chapter IV.

With the criterion of average variance, designs were obtained for two cases relating to regions of interest and regions of operability. In the first case it is assumed that the regions of interest and operability coincide and are some triangular subregion of the region of all possible mixtures. Optimum designs for such cases may be obtained from Table VIII for N up to 20. In the second case it is assumed that the region of interest is a triangular subregion contained in another triangular subregion termed the region of operability. Designs for this case may be obtained from Table IX for N up to 14.

The principal idea behind the method of search for optimum designs consists of regarding the criterion measure, i.e., generalized variance, or average variance, as a response over a factor space called the design factor space. Rather formal definitions of symmetric designs and design factors are given in Chapter II where it is also shown that a one-to-one correspondence exists between the class of symmetric design and the design factor space.

In Chapter III it is shown that the criterion measures are functions of the design factors. Also in this chapter most of the mathematical mechanisms needed for implementing the search are derived.

Computer usage and results are presented for the case of optimum generalized variance and average variance designs in Chapters IV and V respectively.

A development relating to the effect of the choice of the model on the average variance is presented in Chapter VI.

Extensions to More Than Three Components

By use of the concept of permutation sets it is evident how symmetric designs could be defined for mixtures of q components. The number of different types of permutation sets is given by the number of nonnegative integer solutions to

$$x_1 + x_2 + \ldots + x_q = q$$

with

$$x_1 \le x_2 \le \ldots \le x_q \quad .$$

If a solution is denoted by the ordered set of integers

$$(x_1, x_2, \ldots, x_q)$$

then the permutation set corresponding to this solution has

$$\frac{q!}{x_1!\, x_2! \ldots x_q!}$$

elements.

For q = 3, for example, there are three solutions to the above equation: (0, 0, 3), (0, 1, 2) and (1, 1, 1). The corresponding types of permutation sets have 1, 3 and 6 points respectively.

For q = 4 there are the five solutions: (0, 0, 0, 4), (0, 0, 1, 3), (0, 0, 2, 2), (0, 1, 1, 2) and (1, 1, 1, 1) with the corresponding permutation sets having 1, 4, 6, 12 and 24 points.

The concept of design factors can also be extended to the q-component case. Let D be a symmetric design for q components, then D is the adjunction of a number of permutation sets. Each such set can be represented by a number of design factors. The number of design factors required to define a given permutation set may be deduced as follows. Let $(x_1, x_2, \ldots, x_q)$ be the solution to the above mentioned equation which corresponds to the type permutation set in question. Let k be the number of nonzero integers in $(x_1, x_2, \ldots, x_q)$. Then the number of design factors required to define the permutation set is $k - 1$.

For example, with q = 3, the number of factors required to define a 6-point set with corresponding solution (1, 1, 1) is 3 - 1 = 2 and the number of factors for a 1-point set with solution (0, 0, 3) is 1 - 1 = 0.

With q = 4, the number of factors required to define a 12-point set with solution, (0, 1, 1, 2), is 3 - 1 = 2. And with q = 5, the number of factors required to define a 10-point set corresponding to the solution, (0, 0, 0, 1, 4), is 2 - 1 = 1.

To pursue the search for optimum designs for q-component mixtures it would be necessary to find the functional relationship between the criterion measure, e.g., average variance, and the design factors as was done for the case of three components. The developments in Chapters IV and V and the search programs would then have to be modified to incorporate these changes. Similarly such modifications would be required if the three-component problem were extended to the case of cubic or higher order models.

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APPENDIX A

LATTICE SEARCH PROGRAM FOR OPTIMUM GENERALIZED VARIANCE DESIGNS

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C          1/GENERALIZED VARIANCE OF SYMMETRIC DESIGNS
C                 FOR MIXTURES OF THREE COMPONENTS
C       INPUT
C             CARD 1  -    ENTERED FOR EACH COMPUTER RUN
C                    D3 = SIZE INCREMENTS IN F1
C                    D6 = SIZE INCREMENTS IN F312
C                    LOOK   =  NO. OF DESIGNS TO OUTPUT
C                    FORMAT(2F10.0,I2)
C             CARD 2  -    ONE FOR EACH PROBLEM
C                    NG = NO. CENTER POINTS
C                    NT = NO. 3-POINT SETS
C                    NZ = NO. 6-POINT SETS
C                    FORMAT(3I3)
      DIMENSION K(20),MAX(20),NC(20),C1(160),D1(160),F1(160)
      DIMENSION Z2(2000),Z3(2000),C2(2000),D2(2000),F2(2000)
      DIMENSION ADET(40),Z1(160)
      DIMENSION A(40,20)
C     SET UP C,D AND F ARRAYS
 1000 READ(5,900) D3,D6,LOOK
  900 FORMAT(2F10.0,I2)
      IF(D3.LT.0.01) D3=.01
      IF(D6.LT.0.02) D6=0.02
      WRITE(6,850) D3,D6
  850 FORMAT(4H1D3=,F6.3,1X,3HD6=,F6.3//)
      R2=SQRT(2.)
      R3=SQRT(3.)
      R6=SQRT(6.)
      NCNT1=2
      NCNT2=1
      LEAST=0
      MOST=0
      C1(1)=0.5
      D1(1)=R3/12.0
      F1(1)=0.04166667
      Z1(1)=1.0
      X=-0.5-D3
      U1X=1.0-.001
  800 X=X+D3
      IF(X.GE.U1X) GO TO 700
      NCNT2=NCNT2+1
      C1(NCNT2)=X**2/2.0
      D1(NCNT2)=R3*X**3/12.0
      F1(NCNT2)=X**4/24.0
      Z1(NCNT2)=X
      GO TO 800
  700 WRITE(6,801)NCNT2
  801 FORMAT(7H0NCNT2=,I10/9X,1HX,6X,7X,1HC,14X,1HD,14X,1HF)
      DO 802 J=1,NCNT2
  802 WRITE(6,803) Z1(J),C1(J),D1(J),F1(J)
```

```
  803 FORMAT(1X,F10.2,5X,3E15.8)
      X=-1.0/R2-D6
      B=-1.0/R2+.0001
  600 X=X+D6
      IF(X.GT.0.0) X=0.0
      Y=0.0-D6
      X2=X**2
      UY=-3.0*X
      BB=UY-.0001
  500 Y=Y+D6
      IF(Y.GT.UY) Y=UY
      MOST=MOST+1
      C2(MOST)=(Y**2+3.*X2)/6.0
      D2(MOST)=(X2-Y**2)*X/(4.*R6)
      F2(MOST)=(C2(MOST))**2/12.0
      Z2(MOST)=X
      Z3(MOST)=Y
      IF(X.LE.B) LEAST=LEAST+1
      IF(Y.LT.BB) GO TO 500
      IF(X.LT.0.0) GO TO 600
      WRITE(6,501)LEAST,MOST
  501 FORMAT(8H0LEAST =,I10,5X,6HMOST =,I10/9X,1HX,9X,1HY,
     16X,7X,1HC,14X,1HD,14X,1HF)
      DO 502 J=1,MOST
  502 WRITE(6,503)Z2(J),Z3(J),C2(J),D2(J),F2(J)
  503 FORMAT(1X,2F10.2,5X,3E15.8)
      WRITE(6,504)
  504 FORMAT(1H1)
C     SET UP PARAMETERS FOR THE GIVEN CLASS OF DESIGNS
   40 READ(5,50) NG,NT,NZ
   50 FORMAT(3I3)
      DO 51 II=1,LOOK
   51 ADET(II)=0.0
      NDCNT=0
      NVAR=NT+NZ
      NFAC=NT+2*NZ
      N=NG+3*NT+6*NZ
      XN=N
      DO 52 J=1,NVAR
   52 NC(J)=2
      IF(NT.EQ.0) GO TO 54
      DO 53 J=1,NT
   53 MAX(J)=NCNT2
   54 IF(NZ.EQ.0) GO TO 56
      J1=NT+1
      DO 55 J=J1,NVAR
   55 MAX(J)=MOST
   56 IF(NT.GT.0) GO TO 57
      MAX(1)=LEAST
      GO TO 60
   57 IF(NZ.GT.0) GO TO 58
      IF(NT.LT.2) GO TO 58
      MAX(1)=NCNT1
      NC(2)=1
```

```
      GO TO 60
   58 J1=NT+1
      NC(J1)=1
   60 WRITE(6,61) NG,NT,NZ,(J,J=1,NFAC)
   61 FORMAT(43H01/GENERALIZED VARIANCE OF DESIGNS FROM THE,
     19H CLASS S(,3I3,1H)/4X,9H1/GEN VAR,I9,9I11)
C     ITERATIONS
      I=1
    1 K(I)=0
    2 K(I+1)=K(I)
      K(I)=K(I)+1
      I=I+1
      IF(I.GT.NVAR) GO TO 100
      NN=NC(I)
      GO TO (1,2), NN
    5 I=I-1
      IF(I.EQ.0) GO TO 7
      IF(NC(I).EQ.2) GO TO 6
      IF(I.LE.NT) GO TO 6
      MAX(I)=LEAST
      IF(K(1).LE.2) MAX(I)=MOST
    6 IF(K(I).LT.MAX(I)) GO TO 2
      GO TO 5
C     OUTPUT
    7 DO 8 II=1,LOOK
    8 WRITE(6,9) ADET(II),(A(II,J),J=1,NFAC)
    9 FORMAT(1X,E15.8,10F11.8)
      WRITE(6,10)LOOK,NDCNT
   10 FORMAT(5H0BEST,I3,3H OF,I10,8H DESIGNS//)
      GO TO 40
C     CALCULATE 1/GENERALIZED VARIANCE
  100 C=0.0
      D=0.0
      F=0.0
      NDCNT=NDCNT+1
      IF(NT.EQ.0) GO TO 110
      DO 105 J=1,NT
      L=K(J)
      C=C+C1(L)
      D=D+D1(L)
  105 F=F+F1(L)
  110 IF(NZ.EQ.0) GO TO 120
      J1=NT+1
      DO 115 J=J1,NVAR
      L=K(J)
      C=C+C2(L)
      D=D+D2(L)
  115 F=F+F2(L)
  120 DET=4.0*(2.0*XN*F-C**2)*(C*F-D**2)**2
      LL=1
      DO 130 II=1,LOOK
      IF(ADET(II).LT.ADET(LL)) LL=II
  130 CONTINUE
      IF(DET.LE.ADET(LL)) GO TO 140
```

```
      ADET(LL)=DET
      IF(NT.EQ.0) GO TO 135
      DO 131 II=1,NT
      L=K(II)
  131 A(LL,II)=Z1(L)
  135 IF(NZ.FQ.0) GO TO 140
      J1=NT+1
      J2=NT-1
      DO 136 II=J1,NVAR
      J2=J2+2
      J3=J2+1
      L=K(II)
      A(LL,J2)=Z2(L)
  136 A(LL,J3)=Z3(L)
  140 GO TO 5
      END
```

APPENDIX B

LATTICE SEARCH PROGRAM FOR OPTIMUM AVERAGE VARIANCE DESIGNS

```
C             AVERAGE VARIANCE OF SYMETRIC DESIGNS
C               FOR MIXTURES OF THREE COMPONENTS
C       INPUT
C            CARD 1  -   ENTERED FOR EACH COMPUTER RUN
C                 D3 = SIZE INCREMENTS IN F1
C                 D6 = SIZE INCREMENTS IN F312
C                 THETA = RATIO OF Q TO R
C                 LOOK  =  NO. OF DESIGNS OF EACH TYPE
C                          (D AND D*) TO OUTPUT
C                 FORMAT(3F10.0,I2)
C            CARD 2  -   ONE FOR EACH PROBLEM
C                 NG = NO. CENTER POINTS
C                 NT = NO. 3-POINT SETS
C                 NZ = NO. 6-POINT SETS
C                 FORMAT(3I3)
      DIMENSION Z2(2000),Z3(2000),C2(2000),D2(2000),F2(2000)
      DIMENSION K(20),MAX(20),NC(20),C1(160),D1(160),F1(160)
      DIMENSION A(40,20),ZF(20),COSIN(20),AA(40,20),AVAR(40)
      DIMENSION ADET(40),Z1(160)
C     SET UP C,D AND F ARRAYS
 1000 READ(5,900) D3,D6,THETA,LOOK
  900 FORMAT(3F10.0,I2)
      IF(THETA.LE.0.) THETA=1.
      IF(D3.LT.0.01) D3=.01
      IF(D6.LT.0.02) D6=0.02
      D3=D3*THETA
      D6=D6*THETA
      WRITE(6,850) D3,D6,THETA
  850 FORMAT(4H1D3=,F6.3,1X,3HD6=,F6.3,1X,6HTHETA=,F6.3//)
      R2=SQRT(2.)
      R3=SQRT(3.)
      R6=SQRT(6.)
      IF(LOOK.GT.40) LOOK=40
      NCNT1=2
      NCNT2=1
      LEAST=0
      MOST=0
      C1(1)=THETA**2/2.
      D1(1)=R3*THETA**3/12.
      F1(1)=THETA**4/24.
      Z1(1)=THETA
      X=-0.5*THETA-D3
      U1X=THETA-.001
  800 X=X+D3
      IF(X.GE.U1X) GO TO 700
      NCNT2=NCNT2+1
      C1(NCNT2)=X**2/2.0
      D1(NCNT2)=R3*X**3/12.0
      F1(NCNT2)=X**4/24.0
```

```
      Z1(NCNT2)=X
      GO TO 800
  700 WRITE(6,801)NCNT2
  801 FORMAT(7HONCNT2=,I10/9X,1HX,6X,7X,1HC,14X,1HD,14X,1HF)
      DO 802 J=1,NCNT2
  802 WRITE(6,803) Z1(J),C1(J),D1(J),F1(J)
  803 FORMAT(1X,F10.2,5X,3E15.8)
      X=-THETA/R2-D6
      B=-THETA/R2+.001
  600 X=X+D6
      IF(X.GT.0.0) X=0.0
      Y=0.0-D6
      X2=X**2
      UY=-3.0*X
      BB=UY-.0001
  500 Y=Y+D6
      IF(Y.GT.UY) Y=UY
      MOST=MOST+1
      C2(MOST)=(Y**2+3.*X2)/6.0
      D2(MOST)=(X2-Y**2)*X/(4.*R6)
      F2(MOST)=(C2(MOST))**2/12.0
      Z2(MOST)=Y
      Z3(MOST)=X
      IF(X.LE.B) LEAST=LEAST+1
      IF(Y.LT.BB) GO TO 500
      IF(X.LT.0.0) GO TO 600
      WRITE(6,501)LEAST,MOST
  501 FORMAT(8HOLEAST =,I10,5X,6HMOST =,I10/9X,1HX,9X,1HY,
     16X,7X,1HC,14X,1HD,14X,1HF)
      DO 502 J=1,MOST
  502 WRITE(6,503)Z2(J),Z3(J),C2(J),D2(J),F2(J)
  503 FORMAT(1X,2F10.2,5X,3E15.8)
      WRITE(6,504)
  504 FORMAT(1H1)
C     SET UP PARAMETERS FOR THE GIVEN CLASS OF DESIGNS
   40 READ(5,50) NG,NT,NZ
   50 FORMAT(3I3)
      DO 51 II=1,LOOK
      AVAR(II)=99999999.
   51 ADET(II)=99999999.
      NDCNT=0
      MDCNT=0
      NVAR=NT+NZ
      NFAC=NT+2*NZ
      N=NG+3*NT+6*NZ
      XN=N
      DO 52 J=1,NVAR
   52 NC(J)=2
      IF(NT.EQ.0) GO TO 54
      DO 53 J=1,NT
   53 MAX(J)=NCNT2
   54 IF(NZ.EQ.0) GO TO 56
      J1=NT+1
      DO 55 J=J1,NVAR
```

```
   55 MAX(J)=MOST
   56 IF(NT.GT.0) GO TO 57
      MAX(1)=LEAST
      GO TO 60
   57 IF(NZ.GT.0) GO TO 58
      IF(NT.LT.2) GO TO 58
      MAX(1)=NCNT1
      NC(2)=1
      GO TO 60
   58 J1=NT+1
      NC(J1)=1
   60 WRITE(6,61) NG,NT,NZ,(J,J=1,NFAC)
   61 FORMAT(43H0          AVERAGE VARIANCE OF DESIGNS FROM THE,
     19H CLASS S(,3I3,1H)/4X,9H  AVG VAR,I9,9I11)
C     ITERATIONS
      I=1
    1 K(I)=0
    2 K(I+1)=K(I)
      K(I)=K(I)+1
      I=I+1
      IF(I.GT.NVAR) GO TO 100
      NN=NC(I)
      GO TO (1,2), NN
    5 I=I-1
      IF(I.EQ.0) GO TO 7
      IF(NC(I).EQ.2) GO TO 6
      IF(I.LE.NT) GO TO 6
      MAX(I)=LEAST
      IF(K(1).LE.2) MAX(I)=MOST
    6 IF(K(I).LT.MAX(I)) GO TO 2
      GO TO 5
C     OUTPUT
    7 DO 8 II=1,LOOK
    8 WRITE(6,9) ADET(II),(A(II,J),J=1,NFAC)
    9 FORMAT(1X,E15.8,10F11.8)
      WRITE(6,10)LOOK,NDCNT
   10 FORMAT(5H0BEST,I3,3H OF,I10,8H DESIGNS//)
      DO 11 II=1,LOOK
   11 WRITE(6,9) AVAR(II),(AA(II,J),J=1,NFAC)
      WRITE(6,10) LOOK,MDCNT
      GO TO 40
C     CALCULATE AVERAGE VARIANCE
  100 C=0.0
      D=0.0
      F=0.0
      NDCNT=NDCNT+1
      IF(NT.EQ.0) GO TO 110
      DO 105 J=1,NT
      L=K(J)
      C=C+C1(L)
      D=D+D1(L)
  105 F=F+F1(L)
  110 IF(NZ.EQ.0) GO TO 120
      J1=NT+1
```

```
      DO 115 J=J1,NVAR
      L=K(J)
      C=C+C2(L)
      D=D+D2(L)
  115 F=F+F2(L)
  120 FMCS=2.*XN*F-C**2
      CFMD=C*F-D**2
      FMCS=ABS(FMCS)
      CFMD=ABS(CFMD)
      IF(FMCS.LT.0.00001) GO TO 5
      IF(CFMD.LT.0.00001) GO TO 5
      DET=(720.*F-30.*C+XN)/(360.*FMCS)
      DET=DET+(30.*F-4.*R3*D+C)/(360.*CFMD)
      IF(NT.EQ.0) GO TO 135
      DO 131 II=1,NT
      L=K(II)
  131 ZF(II)=Z1(L)
  135 IF(NZ.EQ.0) GO TO 140
      J1=NT+1
      J2=NT-1
      DO 136 II=J1,NVAR
      J2=J2+2
      J3=J2+1
      L=K(II)
      ZF(J2)=Z2(L)
  136 ZF(J3)=Z3(L)
  140 SZF=0.
      DO 141 II=1,NFAC
  141 SZF=SZF+ZF(II)**2
      SZF=SQRT(SZF)
      DO 142 II=1,NFAC
  142 COSIN(II)=ZF(II)/SZF
      G4=XN/(360.*FMCS)+C/(360.*CFMD)
      G3=-R3*D/(120.*CFMD)
      G2=F/(12.*CFMD)-C/(12.*FMCS)
      LL=1
      DO 130 II=1,LOOK
      IF(ADET(II).GT.ADET(LL)) LL=II
  130 CONTINUE
      IF(DET.GE.ADET(LL)) GO TO 150
      ADET(LL)=DET
      DO 145 II=1,NFAC
  145 A(LL,II)=ZF(II)
  150 DSCMNT=9.*G3**2-32.*G2*G4
      IF(DSCMNT.LE.0.) GO TO 5
      DSCMNT=SQRT(DSCMNT)
      RHO=(-3.*G3+DSCMNT)/(8.*G4)
      IF(RHO.LE.1.) GO TO 5
      RSTAR=SZF/RHO
      DO 160 II=1,NFAC
  160 ZF(II)=RSTAR*COSIN(II)
      C=0.
      D=0.
      F=0.
```

```
      IF(NT.EQ.0) GO TO 170
      DO 165 II=1,NT
      C=C+ZF(II)**2
      D=D+ZF(II)**3
  165 F=F+ZF(II)**4
      C=C/2.
      D=D*R3/12.
      F=F/24.
  170 IF(NZ.EQ.0) GO TO 180
      J1=NT+1
      DO 166 II=J1,NFAC,2
      C=C+(ZF(II)**2+3.*ZF(II+1)**2)/6.
      D=D+(ZF(II+1)**2-ZF(II)**2)*ZF(II+1)/(4.*R6)
  166 F=F+(ZF(II)**2+3.*ZF(II+1)**2)**2/432.
  180 FMCS=2.*XN*F-C**2
      CFMD=C*F-D**2
      MDCNT=MDCNT+1
      VAR=(720.*F-30.*C+XN)/(360.*FMCS)
      VAR=VAR+(30.*F-4.*R3*D+C)/(360.*CFMD)
      LL=1
      DO 190 II=1,LOOK
      IF(AVAR(II).GT.AVAR(LL)) LL=II
  190 CONTINUE
      IF(VAR.GE.AVAR(LL)) GO TO 5
      AVAR(LL)=VAR
      DO 200 II=1,NFAC
  200 AA(LL,II)=ZF(II)
      GO TO 5
      END
```

APPENDIX C

PATTERN SEARCH PROGRAM FOR OPTIMUM AVERAGE
VARIANCE DESIGNS

```
C       INPUT
C            CARD 1
C                  NG = NO. CENTER POINTS
C                  NT = NO. 3-POINT SETS
C                  NZ = NO. 6-POINT SETS
C                  MCALC = MAX. NO. ITERATIONS
C                  TOL = SMALLEST CHANGE IN FACTORS
C                  THETA = RATIO OF Q TO R
C                  FORMAT(3I3,1X,I5,2F10.0)
C            CARD 2
C                  D(I) = THE T+2S  (NT+2NZ)  STEP SIZES
                   FORMAT(8F10.0)
C            CARD 3
C                  B(I) = THE T+2S  (NT+2NZ)  STARTING VALUES
C                  FORMAT(5F15.0)
      DIMENSION B(2,10),T(10,10),D(10),X(10)
      R2=SQRT(2.0)
      R3=SQRT(3.0)
      R6=SQRT(6.0)
    1 READ(5,2) NG,NT,NZ,MCALC,TOL,THETA
    2 FORMAT(3I3,1X,I5,2F10.0)
      K=NT+2*NZ
      NVAR=NT+NZ
      READ(5,3)(D(I),I=1,K)
    3 FORMAT(8F10.0)
      IF(D(1).EQ.0.0)STOP
      DO 4 I=2,K
      IF(D(I).EQ.0.0)D(I)=D(1)
    4 CONTINUE
      READ(5,5)(B(1,I),I=1,K)
    5 FORMAT(5F15.0)
      WRITE(6,6)NG,NT,NZ,MCALC,TOL,THETA,(I,I=1,K)
    6 FORMAT(43H1SEARCH FOR MIN AVG VAR DESIGN IN THE CLASS,
     13H S(,3I3,1H)/1X,14HMAX NO TRIALS=,I10/1X, 8HSMALLEST,
     210H INTERVAL=,F10.8/1X,6HTHETA=,F10.4/5X,7HAVG VAR,4X,
     310(I6,5X))
      ICALC=0
      XU=THETA
      XL=-0.5*THETA
      YL=THETA*(-1.0)/R2
      XN=NG+3*NT+6*NZ
C     ESTABLISH PATTERN
  100 DO 101 I=1,K
      T(1,I)=B(1,I)
  101 X(I)=B(1,I)
      CALL AVAR(NT,NZ,NVAR,ICALC,R2,R3,R6,XU,XL,YL,X,VAR,
     1MCALC,XN)
   37 VARM=VAR
   50 DO 110 I=1,K
```

```
      DO 109 J=1,2
      JJ=J+1
      DO 102 L=1,K
      IF(I.EQ.1)GO TO 33
      T(I,L)=T(I-1,L)
   33 X(L)=T(I,L)
      IF(L.EQ.I) X(L)=T(I,L)+(-1.0)**JJ*D(L)
  102 CONTINUE
      CALL AVAR(NT,NZ,NVAR,ICALC,R2,R3,R6,XU,XL,YL,X,VAR,
     1MCALC,XN)
      IF(ICALC.GT.MCALC) GO TO 1
   34 IF(VAR.GE.VARM)GO TO 109
      VARM=VAR
      DO 103 L=1,K
  103 T(I,L)=X(L)
      GO TO 110
  109 CONTINUE
  110 CONTINUE
      ICHK=0
      DO 111 I=1,K
      B(2,I)=T(K,I)
      DIF=ABS(B(1,I)-B(2,I))
      IF(DIF.LT.0.00000002)ICHK=ICHK+1
  111 CONTINUE
      IF(ICHK.LT.K)GO TO 500
      DO 112 I=1,K
      D(I)=D(I)/2.0
      IF(D(I).LT.TOL)GO TO 1
  112 CONTINUE
      GO TO 100
C     PATTERN MOVES
  500 DO 501 I=1,K
      T(1,I)=2.0*B(2,I)-B(1,I)
  501 X(I)=T(1,I)
      CALL AVAR(NT,NZ,NVAR,ICALC,R2,R3,R6,XU,XL,YL,X,VAR,
     1MCALC,XN)
      IF(ICALC.GT.MCALC) GO TO 1
   35 VAR1=VAR
      DO 510 I=1,K
      DO 509 J=1,2
      JJ=J+1
      DO 502 L=1,K
      IF(I.EQ.1) GO TO 53
      T(I,L)=T(I-1,L)
   53 X(L)=T(I,L)
      IF(L.EQ.I)X(L)=T(I,L)+(-1.0)**JJ*D(L)
  502 CONTINUE
      CALL AVAR(NT,NZ,NVAR,ICALC,R2,R3,R6,XU,XL,YL,X,VAR,
     1MCALC,XN)
      IF(ICALC.GT.MCALC) GO TO 1
   36 IF(VAR.GE.VAR1)GO TO 509
      VAR1=VAR
      DO 503 L=1,K
  503 T(I,L)=X(L)
```

```
      GO TO 510
  509 CONTINUE
  510 CONTINUE
      IF(VAR1.GT.VARM)GO TO 512
      VARM=VAR1
      DO 511 I=1,K
      B(1,I)=B(2,I)
  511 B(2,I)=T(K,I)
      GO TO 500
  512 DO 513 I=1,K
      B(1,I)=B(2,I)
      T(1,I)=B(1,I)
      D(I)=D(I)/2.0
      IF(D(I).LT.TOL)GO TO 1
  513 CONTINUE
      GO TO 50
      END


      SUBROUTINE AVAR(NT,NZ,NVAR,ICALC,R2,R3,R6,XU,XL,YL,X,
     1VAR,MCALC,XN)
      DIMENSION X(10)
  700 ICALC=ICALC+1
      K=NT+2*NZ
      IF(ICALC.GT.MCALC)GO TO 802
      IF(NT.EQ.0) GO TO 705
      DO 701 I=1,NT
      IF(X(I).GT.XU)GO TO 800
      IF(X(I).LT.XL) GO TO 800
  701 CONTINUE
  705 IF(NZ.EQ.0) GO TO 710
      J1=NT+1
      J2=NT-1
      DO 706 I=J1,NVAR
      J2=J2+2
      J3=J2+1
      IF(X(J3).LT.YL)GO TO 800
      IF(X(J3).GT.0.0) GO TO 800
      IF(X(J2).LT.0.0) GO TO 800
      YU=-3.0*X(J3)
      IF(X(J2).GT.YU)GO TO 800
  706 CONTINUE
  710 CC=0.0
      DD=0.0
      FF=0.0
      IF(NT.EQ.0) GO TO 720
      DO 715 I=1,NT
      CC=CC+X(I)**2/2.0
      DD=DD+R3*X(I)**3/12.0
  715 FF=FF+X(I)**4/24.0
  720 IF(NZ.EQ.0) GO TO 735
      J1=NT+1
      J2=NT-1
```

```
      DO 725 I=J1,NVAR
      J2=J2+2
      J3=J2+1
      CC=CC+(X(J2)**2+3.0*X(J3)**2)/6.0
      DD=DD+(X(J3)**2-X(J2)**2)*X(J3)/(4.0*R6)
  725 FF=FF+(X(J2)**2+3.0*X(J3)**2)**2/432.0
  735 FMCS=2.0*XN*FF-CC**2
      IF(FMCS.LT.0.0000001) GO TO 800
      CFMD=CC*FF-DD**2
      IF(CFMD.LT.0.0000001)GO TO 800
      VAR=(720.0*FF-30.0*CC+XN)/(360.0*FMCS)
      VAR=VAR+(30.0*FF-4.0*R3*DD+CC)/(360.0*CFMD)
      GO TO 801
  800 VAR=99999999.0
  801 WRITE(6,7)VAR,(X(I),I=1,K)
    7 FORMAT(1X,E15.8,10F11.8)
  802 RETURN
      END
```

APPENDIX D

SAMPLE OUTPUT FROM LATTICE SEARCH PROGRAM FOR OPTIMUM AVERAGE VARIANCE DESIGNS

The output below was obtained from a search in the design factor space, $F = F_1^2 F_{312}$, corresponding to 12-point designs in the subclass S[0, 2, 1]. The search was conducted on a grid of increments of 0.1 in the design factors.

Output for each design consists of the average variance, AV, and the corresponding point in F:

$$[y_1, y_2, (y_{31}, y_{32})].$$

The first five points below are from B(F), that is from the region of F corresponding to designs having some points on the boundary of R. These five were the best of 5546 such points investigated. The last five points correspond to designs with no points on the boundary of R. These were the best of 53 such points found in the 5546 cases considered.

AV	y_1	y_2	y_{31}	y_{32}
0.27663	1.000	-0.400	0.000	-0.707
0.27685	1.000	-0.400	0.100	-0.707
0.27755	1.000	-0.400	0.200	-0.707
0.27778	1.000	-0.500	0.000	-0.707
0.27793	1.000	-0.300	0.000	-0.707
0.85705	0.798	0.898	1.097	-0.705
0.95025	0.885	0.885	1.180	-0.695
1.04110	0.778	0.778	0.972	-0.687
1.09145	0.767	0.863	1.151	-0.678
1.13056	0.692	0.890	1.285	-0.699

APPENDIX E

TABLE X

SOME "NEAR OPTIMUM" AVERAGE VARIANCE DESIGNS IN R
SELECTED FROM LATTICE PROGRAM OUTPUT

N	AV	r	x_1	x_2	x_3
6	0.68995	1	0.500	0.500	0.000
		1	0.033	0.033	0.934
7	0.53116	1	0.333	0.333	0.333
		1	0.500	0.500	0.000
		1	0.033	0.033	0.934
8	0.46835	2	0.333	0.333	0.333
		1	0.500	0.500	0.000
		1	0.033	0.033	0.934
9	0.39679	1	0.000	0.000	1.000
		1	0.047	0.382	0.571
10	0.36273	1	0.333	0.333	0.333
		1	0.000	0.000	1.000
		1	0.047	0.382	0.571
11	0.34121	2	0.333	0.333	0.333
		1	0.000	0.000	1.000
		1	0.047	0.382	0.571
12	0.27997	1	0.000	0.000	1.000
		1	0.500	0.500	0.000
		1	0.047	0.429	0.524
13	0.26349	1	0.333	0.333	0.333
		1	0.000	0.000	1.000
		1	0.500	0.500	0.000
		1	0.047	0.429	0.524
14	0.24804	2	0.333	0.333	0.333
		1	0.000	0.000	1.000
		1	0.467	0.467	0.066
		1	0.000	0.406	0.594

VITA

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