

Rotatable designs: Constructions and considerations
in the robust design of experiments

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Thesis submitted for the Degree of
Doctor of Philosophy
in the University of London

Imperial College of Science and Technology
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January 1981

ABSTRACT

Results concerning response surface designs are presented. Well-known one-dimensional designs are compared with one another under various optimality criteria and new designs are obtained. Several new methods of construction of second-order and third-order rotatable designs are also provided. In particular, methods of construction of designs from designs of the same order in lower dimensions are obtained. In applying these methods the results of the experiments performed according to the lower-dimensional designs need not be discarded. Many new second-order and third-order rotatable designs, including some which require the minimum number of points among the designs known so far, are constructed by these methods. Cylindrically rotatable designs of type 3 are generalized and the conditions which have to be satisfied by such a design are derived. A method of construction of second-order cylindrically rotatable designs of type 3 with three or more groups of factors is provided. The effects of departure of the observations from second-order distributional assumptions on the rotatability of designs are studied by considering some specific families of variance-covariance structures. Some robust designs are obtained.

ACKNOWLEDGEMENTS

The work presented was carried out under the supervision of Dr. A.M. Herzberg and I am deeply indebted to her for her patient guidance and encouragement. I am also grateful to Professor D.R. Cox for his many helpful comments.

Thanks are also due to the Science Research Council for the financial support.

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CHAPTER 1

INTRODUCTION

To study the dependence of one or more response variables upon some explanatory variables, information is often collected by performing experiments. The statistical design of experiments is concerned with the selection of the values of the explanatory variables at which experiments are to be carried out when the observations are subject to error.

It is usually desirable to choose a design which is optimal in some sense. An appreciable number of interesting results are known about the various optimal designs for polynomial regression models in one variable. Some of these optimal designs are considered in Chapter 2. The 'uniform' design is compared with the optimal designs under various optimality criteria. The D-optimality criterion is considered in Section 2.2 and the efficiency of the uniform design under this criterion is derived. The G-optimality and related criteria are considered in Section 2.3. In Section 2.4, the uniform design is compared with the optimal design under the 'Integrated-variance' criterion. In Section 2.5 the optimal extrapolation design is compared with the uniform design. Results of Section 2.6 show that under certain restrictions, among all the design measures with density functions the 'continuous uniform design' is optimal for minimizing the maximum possible 'bias' in the expected mean squared error arising from inadequacy in the assumed model.

In response surface designs the main interest has usually been on the absolute response. However, as in Herzberg (1967c), Atkinson (1970) and Box and Draper (1980), there may be instances where the

differences in response are of greater interest than the absolute response. In Section 3.2 the problem of obtaining optimal designs in such situations is considered for the simple one-dimensional polynomial regression models.

In many problems the use of one particular optimality criterion may not lead to a unique optimal design. However, by applying various criteria in an hierarchical order, it may be possible to discriminate between competing designs. These applications are illustrated by some simple examples in Section 3.3.

Response surface designs for multi-dimensional factor spaces are considered in Chapter 4 and Chapter 5. Box and Hunter (1957) introduced the class of designs called rotatable designs for the exploration of response surfaces; these designs have the property that the variance of the estimated response at all points equidistant from the centre of the design is constant. Some situations where the optimal designs belong to the class of rotatable designs are given in Box and Draper (1959, 1963), Kiefer (1960) and Galil and Kiefer (1977a,b, 1979). Many second-order and third-order rotatable designs are now well-known. However, there still exist several interesting combinatorial problems associated with the construction of rotatable designs and some of these problems are investigated in Chapter 4. The main emphasis is on obtaining new methods of construction and on deriving new designs by these methods.

Methods for the construction of second-order rotatable designs in k dimensions from any given second-order rotatable design in $(k-1)$ dimensions ($2 \leq k-1$) are provided in Section 4.3. The methods are such that the results of the experiments performed according to the given design need not be discarded. In Section 4.4 several new third-order rotatable designs in 5, 6, 7 and 8 dimensions are derived by

combining symmetric point sets or suitably balanced subsets of these sets. Many of these derived designs are of a sequential nature and some require fewer experiments than the known designs. In Section 4.5 a method for the construction of third-order rotatable designs in k dimensions from third-order rotatable designs in $(k-1)$ dimensions is presented. The results of the experiments of the $(k-1)$ -dimensional design need not be discarded. The method cannot be applied to all given designs since it only works under some restrictive conditions. A new third-order rotatable design in 3 dimensions is derived by the application of the method. In Section 4.6 third-order rotatable designs in k dimensions are constructed by taking projections of third-order rotatable designs in $(k+1)$ dimensions onto k -dimensional orthogonal subspaces. Several new designs, including some with the minimum number of points among the designs available so far, are constructed by this method. A method for the construction of third-order rotatable designs in k dimensions from third-order rotatable designs in $(k-\ell)$ dimensions ($\ell \leq k-1$) is presented in Section 4.7 and some new designs are derived by the method. The results of the experiments from the $(k-\ell)$ -dimensional design need not be discarded when this method is used. In Section 4.8, pairwise balanced designs with unequal block sizes derived from well-known balanced incomplete block designs are used to construct some new second-order rotatable designs, including some which require the minimum number of points among the designs available so far. In Section 4.9, second-order rotatable designs are constructed by combining asymmetric point-sets.

Cylindrically rotatable designs of type 3, introduced independently by Herzberg (1967a) and Das and Dey (1967), split up the factors into two groups such that the designs are rotatable for each group of

factors when the sum of squares of the factors in the other group is held constant. In Section 4.10, cylindrically rotatable designs of type 3 are generalized to consider factors split up into any number of groups. The conditions which have to be satisfied by such a design are derived and a method of construction is provided for the designs with three or more groups of factors.

In many situations the assumption of independent and identically distributed observations may be unrealistic. A design which is rotatable when the observations are independent and identically distributed may not necessarily be rotatable when the observations are correlated or non-identically distributed. Hence it may be of interest to obtain rotatable designs whose rotatability is little or not affected by simple departures of the observations from the second-order distributional assumption, that is, the assumption of independent and identically distributed observations. The effects of the non-constancy of variance of the observations and correlation among the observations on the rotatability of designs are investigated in Chapter 5. In Section 5.2, uncorrelated observations with non-constant variances dependent on distance from the origin are considered and it is shown that the rotatability of designs consisting of equiradial rotatable sets of the same order is robust against such departures from the second-order distributional assumption. In Section 5.3, the observations are allowed to be correlated and the effects of the correlation upon the rotatability of designs are studied via some specific families of variance-covariance functions. Section 5.4 is concerned with the rotatability of designs in terms of the best linear unbiased estimates rather than the least squares estimates. In Section 5.5 the two-dimensional rotatable designs consisting of equally spaced points on concentric circles are considered. The rotatability of a

particular sub-family of these designs is shown to be robust against wide classes of departures from the second-order distributional assumption.

CHAPTER 2
UNIFORM DESIGNS FOR LARGE-DEGREE
POLYNOMIAL REGRESSION

2.1 Introduction

Let $\underline{f}' = (f_0, f_1, \dots, f_d)$ be a vector of linearly independent functions on a space X . Let $y(\underline{x})$ be the observation corresponding to the experiment performed at point $\underline{x} \in X$. It is assumed that the observations are independent with a common variance σ^2 and expected value $E\{y(\underline{x})\} = \underline{\beta}' \underline{f}(\underline{x})$, where $\underline{\beta}' = (\beta_0, \beta_1, \dots, \beta_d)$ is the vector of unknown parameters. Let ξ denote a design measure on X . If the experiments are performed in accordance with the design measure ξ the variance-covariance matrix of the least squares estimates of the parameters β_i is given by $\frac{\sigma^2}{N} \underline{M}^{-1}(\xi)$, where $\underline{M}(\xi) = \int_X \underline{f}(\underline{x}) \underline{f}'(\underline{x}) d\xi(\underline{x})$ is the information matrix of ξ and N is the total number of experiments performed.

It is usually desirable to choose a design measure ξ which minimizes a particular function of the matrix $\underline{M}(\xi)$. Among the many commonly used are:

(i) $|\underline{M}^{-1}(\xi)|;$

(ii) $\sup_{\underline{x} \in X} \underline{f}'(\underline{x}) \underline{M}^{-1}(\xi) \underline{f}(\underline{x}),$

where $\underline{f}'(\underline{x}) \underline{M}^{-1}(\xi) \underline{f}(\underline{x})$ is proportional to the variance of the estimated response at $\underline{x}$;

(iii) $\underline{f}'(\underline{x}_e) \underline{M}^{-1}(\xi) \underline{f}(\underline{x}_e);$

(iv) $\underline{c}' \underline{M}^{-1}(\xi) \underline{c} \quad \text{or} \quad \text{tr}\{\underline{M}^{-1}(\xi) \underline{A}\},$

where $\underline{c}$ is any $(d+1) \times 1$ vector and $\underline{A}$ is any $(d+1) \times (d+1)$ symmetric non-negative definite matrix;

(v) $\sup_i \text{var}(\hat{\beta}_i).$

Kiefer and Wolfowitz (1960) showed that (i) and (ii) are equivalent. A detailed account of these and other criteria are given in, for example, Fedorov (1972, page 51-58) and Kiefer (1974). The criteria (i), (iv) with $A = I$ and (v) are in fact special cases of the ' Φ -optimality criterion' discussed in Kiefer (1974, 1975a) and Galil and Kiefer (1977a,b,c).

Let $X = [-1, 1]$ and $f'(x) = (1, x, \dots, x^d)$. Then it is known that for each d there exists a unique design measure ξ_d optimal under (i) and a unique design measure ξ_d^e optimal under (iii) with a fixed x_e , $|x_e| > 1$. Kiefer and Studden (1976) compared ξ_d with ξ_∞ under criteria (i) and (ii) and ξ_d^e with ξ_∞^e under criterion (iii) where $\xi_\infty = \lim_{d \rightarrow \infty} \xi_d$ and $\xi_\infty^e = \lim_{d \rightarrow \infty} \xi_d^e$, respectively.

The uniform design is the continuous design measure ξ_u with a derivative $m_u(x) = \frac{d\xi_u(x)}{dx} = \frac{1}{2}$. Some new results are now obtained on the comparison of ξ_u with the optimal design measures and the limiting optimal design measures. The design measures are also compared under other criteria.

For any given d there exists a discrete design measure with a finite number of support points providing the same information matrix as ξ_u . The discrete design measure with $(d+1)$ support points x_i with weights

$$\frac{1}{(1-x_i^2)\{P'_{d+1}(x_i)\}^2}$$

has moments up to and including order $(2d+1)$ matching those of ξ_u , where x_i ($i = 1, 2, \dots, d+1$) are the zeros of the Legendre's polynomial $P_{d+1}(x)$ of degree $d+1$. For the results of Sections 2.2-2.5, no distinction needs to be made between ξ_u and these discrete design measures since under the criteria to be considered design measures are characterized by their information matrices only.

Let $f'_d(x) = (1, x, \dots, x^d)$ and $M_d(\xi) = \int_{-1}^1 f_d(x) f'_d(x) d\xi(x)$.
Denote $f'_d(x) M_d^{-1}(\xi) f_d(x)$ by $V_d(x, \xi)$ and $\sup_{x \in [-1, 1]} V_d(x, \xi)$ by $V_d(\xi)$. Further, let $A_d(\xi) = \text{tr}\{M_d^{-1}(\xi) M_d(\xi_u)\}$.

2.2. Efficiency under the D-optimality criterion

In order to compare ξ_u with the D-optimal design measure ξ_d under the D-optimality criterion and to derive the results on the efficiency of ξ_u the following lemmata are required.

Lemma 2.2.1: The sequence ξ_d ($d = 1, 2, \dots$) of D-optimal design measures converges weakly to ξ_∞ where ξ_∞ has density $\frac{1}{\pi\sqrt{(1-x^2)}}$ [Fedorov (1972, page 91)].

Lemma 2.2.2: For the limiting design measure ξ_∞ , $|M_d(\xi_\infty)| = 2^{-d^2}$ [Szego (1959, page 28)].

Lemma 2.2.3: For the D-optimal design measure ξ_d ,

$$|M_d(\xi_d)| = 2^{d(d+1)} \left(\prod_{v=1}^d v^v \right)^4 d^{-d} \left(\prod_{v=1}^{2d} v^{-v} \right)$$

[Karlin and Studden (1966)].

Lemma 2.2.4: If

$$\zeta_d(\ell) = \sum_{m=1}^d \frac{1}{m^\ell}, \quad \zeta(\ell) = \sum_{m=1}^{\infty} \frac{1}{m^\ell}$$

and

$$\delta_d = \frac{1}{4} \left\{ \sum_{\ell=1}^d \frac{1}{\ell} - \ln d \right\} - \sum_{\ell=2}^{\infty} (-1)^\ell \frac{\zeta_d(\ell)}{\ell(\ell+1)} \left(1 - \frac{1}{2^\ell} \right),$$

then $\lim_{d \rightarrow \infty} \delta_d = \frac{1}{2} - \frac{13}{12} \ln 2 - 3\zeta'(-1)$.

[Kiefer and Studden (1976)].

Lemma 2.2.5: For any real or complex z ,

$$\sin z = z \prod_{j=1}^{\infty} \left(1 - \frac{z^2}{\pi^2 j^2}\right).$$

Lemma 2.2.6: For $n \geq d+1$, let ξ_{en} be the discrete design measure with mass $\frac{1}{n}$ at each of the n equally spaced points

$$x_i = -1 + \frac{2(i-1)}{(n-1)} \quad (i = 1, \dots, n).$$

Then the sequence ξ_{en} ($n = d+1, d+2, \dots$) converges weakly to ξ_u .

Let $E_{\xi}^D(d) = \{ |M_d(\xi)| / |M_d(\xi_d)| \}^{1/(d+1)}$. Then $E_{\xi}^D(d)$ is a measure of efficiency of ξ under criterion (i).

Theorem 2.2.1: If $\alpha_{\ell} = \prod_{j=1}^{\ell+1} \left(1 - \frac{1}{4j^2}\right)$ and δ_d is defined as in Lemma 2.2.4, then

$$|M_{d+1}(\xi_{d+1})| / |M_{d+1}(\xi_u)| = 3d^{1/4} e^{\delta_d} 2^d \prod_{\ell=1}^d \alpha_{\ell}. \quad (2.2.1)$$

Lemma 2.2.7: For the uniform design measure ξ_u ,

$$|M_d(\xi_u)| = 2^{d(d+1)} \frac{(1!2!\dots d!)^4}{\{1!2!\dots (2d+1)!\}}. \quad (2.2.2)$$

Proof: Let ε_{en} be the design measure which puts equal mass at each of n equally spaced points $x_i = \frac{(i-1)}{(n-1)}$ ($i = 1, 2, \dots, n$; $n \geq d+1$), in the interval $[0, 1]$. Then, from Hoel (1958, 1961), it is known that

$$|nM_d(\varepsilon_{en})| = \left(\frac{1}{n-1}\right)^{d(d+1)} n^{d+1} (n^2-1^2)^d (n^2-2^2)^{d-1} \dots (n^2-d^2) \frac{(1!2!\dots d!)^4}{\{1!2!\dots (2d+1)!\}}.$$

On taking a suitable transformation of the interval $[0, 1]$ to $[-1, 1]$

it readily follows that

$$|M_d(\xi_{en})| = \left(\frac{2}{n-1}\right)^{d(d+1)} (n^2-1)^d (n^2-2)^{d-1} \dots (n^2-d)^2 \frac{(1!2!\dots d!)^4}{\{1!2!\dots(2d+1)!\}}.$$

Therefore, by taking $\lim_{n \rightarrow \infty} |M_d(\xi_{en})|$ and using Lemma 2.2.6 one obtains Lemma 2.2.7.

Proof of Theorem 2.2.1. Let $v_d = |M_d(\xi_d)| / |M_d(\xi_u)|$. Then by using Lemma 2.2.3 and Lemma 2.2.7, one obtains that

$$\begin{aligned} \frac{v_{d+1}}{v_d} &= \frac{\{2^{(d+1)(d+2)} (\prod_{v=1}^{d+1} v^v)^{4(d+1)} 2^{d+2} (\prod_{v=1}^{2d+2} v^{-v})\}}{\{2^{d(d+1)} (\prod_{v=1}^d v^v)^{4d} 2^d (\prod_{v=1}^{2d} v^{-v})\}} \\ &\times \frac{2^{d(d+1)} (1!2!\dots d!)^4}{\{1!2!\dots(2d+1)!\}} \frac{\{1!2!\dots(2d+3)!\}}{2^{(d+1)(d+2)} \{1!2!\dots(d+1)!\}^4}, \end{aligned}$$

and after some simplification it follows that

$$\frac{v_{d+1}}{v_d} = \frac{(1 + \frac{1}{d})^{d+1}}{(1 + \frac{1}{2d})^{2d+1}} \times 2 \cdot \prod_{j=1}^{d+1} (1 - \frac{1}{4j^2}).$$

Therefore,

$$\ln \frac{v_{\ell+1}}{v_\ell} = \frac{1}{4\ell} - \sum_{m=2}^{\infty} \frac{(-1)^m (1 - \frac{1}{2^m})}{\ell^m m(m+1)} + \ln 2 + \ln \prod_{j=1}^{\ell+1} (1 - \frac{1}{4j^2})$$

and

$$\ln \frac{v_{d+1}}{v_1} = \frac{1}{4} \sum_{\ell=1}^d \frac{1}{\ell} - \sum_{m=2}^{\infty} \frac{\zeta_d(m) (-1)^m (1 - \frac{1}{2^m})}{m(m+1)} + d \ln 2 + \sum_{\ell=1}^d \ln \prod_{j=1}^{\ell+1} (1 - \frac{1}{4j^2}).$$

Hence,

$$\begin{aligned} \ln \frac{V_{d+1}}{V_1 d^{1/4}} &= \frac{1}{4} \left\{ \sum_{\ell=1}^d \frac{1}{\ell} - \ln d \right\} - \sum_{m=2}^{\infty} \frac{\zeta_d(m) (-1)^m (1 - \frac{1}{2^m})}{m(m+1)} + d \ln 2 \\ &+ \sum_{\ell=1}^d \ln \prod_{j=1}^{\ell+1} \left(1 - \frac{1}{4j^2}\right) = \delta_d + d \ln 2 + \sum_{\ell=1}^d \ln \alpha_{\ell}, \end{aligned}$$

and the theorem follows because $V_1 = 3$.

From the results obtained it can be seen that the efficiency of the uniform design measure under the D-optimality criterion is given by

$$E_{\xi_u}^D(d+1) = \{3d^{1/4} e^{\delta_d} 2^d \prod_{\ell=1}^d \alpha_{\ell}\}^{-\frac{1}{(d+2)}}, \quad (2.2.3)$$

and the asymptotic efficiency is given by the following theorem.

Theorem 2.2.2: For the uniform design measure ξ_u ,

$$\lim_{d \rightarrow \infty} E_{\xi_u}^D(d) = \frac{1}{4} \pi. \quad (2.2.4)$$

Proof: From (2.2.3), it follows that

$$\ln\{E_{\xi_u}^D(d+1)\}^{-1} = \frac{1}{d+2} (\delta_d + d \ln 2 + \ln 3 + \frac{1}{4} \ln d + \sum_{\ell=1}^d \ln \alpha_{\ell}).$$

By Lemma 2.2.4,

$$\lim_{d \rightarrow \infty} \frac{\delta_d}{d+1} = 0$$

and by Lemma 2.2.5,

$$\lim_{d \rightarrow \infty} \frac{1}{d+2} \sum_{\ell=1}^d \ln \alpha_{\ell} = \ln \frac{2}{\pi}.$$

Therefore, the theorem follows.

Since $\xi_\infty = \lim_{d \rightarrow \infty} \xi_d$, the result of Theorem 2.2.2 may also be proved by comparing ξ_u with ξ_∞ directly as in the following lemma.

Lemma 2.2.8: For the limiting design measure ξ_∞ and the uniform design measure ξ_u ,

$$\lim_{d \rightarrow \infty} \{ |M_d(\xi_u)| / |M_d(\xi_\infty)| \}^{\frac{1}{(d+1)}} = \frac{1}{4} \pi . \tag{2.2.5}$$

Proof: Let $R_\ell = |M_\ell(\xi_u)| / |M_\ell(\xi_\infty)|$. Then

$$R_{\ell+1} / R_\ell = 2^{4\ell+3} \{(\ell+1)!\}^4 / \{(2\ell+2)!(2\ell+3)!\}$$

and by Lemma 2.2.5 it follows that $\lim_{\ell \rightarrow \infty} R_{\ell+1} / R_\ell = \frac{1}{4} \pi$. Therefore,

$$\begin{aligned} \lim_{d \rightarrow \infty} \ln \{ R_{\frac{d+1}{2}}^{\frac{1}{(d+2)}} \} &= \lim_{d \rightarrow \infty} \ln \{ R_1^{\frac{1}{(d+2)}} \} + \lim_{d \rightarrow \infty} \frac{1}{(d+2)} \sum_{\ell=1}^d \ln \frac{R_{\ell+1}}{R_\ell} \\ &= \ln \frac{\pi}{4} , \end{aligned}$$

and hence the desired result.

Table 2.2.1 displays $E_{\xi_u}^D(d)$ for some selected values of d .

TABLE 2.2.1
The D-efficiency of uniform design

d	1	2	3	4	5	6	7	8
$E_{\xi_u}^D(d)$	0.577	0.585	0.603	0.620	0.634	0.646	0.656	0.665
d	9	19	49	99	999	∞		
$E_{\xi_u}^D(d)$	0.672	0.714	0.749	0.764	0.782	$\frac{\pi}{4}$		

2.3 Efficiency under the G-optimality and related criteria

In order to compare ξ_u with ξ_d and ξ_∞ under the variance of the estimated response criteria one may look at $V_d(x, \xi_d)/V_d(x, \xi_u)$ and $V_d(x, \xi_\infty)/V_d(x, \xi_u)$, respectively, for various values of x . The G-efficiency of a design measure ξ considers $V_d(x, \xi)$ only at its maximum value and is defined (see Atwood, 1969) as $V_d(\xi_d)/V_d(\xi)$. Further, from Kiefer and Studden (1976) it is known that a limiting D-efficiency equal to one does not imply a limiting G-efficiency equal to one.

From Guest (1958) it is known that

$$V_d(x, \xi_d) = (d+1) - \frac{(1-x^2)}{d} (P'_d(x))^2,$$

$$V_d(\xi_d) = \sup_{x \in [-1, 1]} V_d(x, \xi_d) = (d+1),$$

the supremum being achieved at the points where ξ_d concentrates its equal mass. These points are zeros of $(1-x^2)P'_d(x)$ where $P_d(x)$ is the Legendre's polynomial of degree d . Further, in the region of extrapolation, that is, for $|x| > 1$, $V_d(x, \xi_d)$ is dominated by the term $d\{(2d)!/2^d(d!)^2\}x^{2d}$.

From Kiefer and Studden (1976) it is known that for the limiting design measure ξ_∞ , $V_d(x, \xi_\infty) = 1 + 2 \sum_{\ell=1}^d T_\ell^2(x) = d + \frac{1}{2} + \frac{1}{2} U_{2d}(x)$, where

$$T_\ell(\cos \theta) = \cos(\ell\theta) \quad \text{and} \quad U_\ell(\cos \theta) = \frac{\sin(\ell+1)\theta}{\sin \theta}$$

are the Chebyshev polynomials of the first and second kinds, respectively. Further,

$$V_d(\xi_\infty) = \sup_{x \in [-1, 1]} V_d(x, \xi_\infty) = (2d+1),$$

the supremum being achieved only at the end points $x = \pm 1$. From Szego (1959, page 28), it is known that the coefficient of x^{2d} in $V_d(x, \xi_\infty)$ is 2^{2d-1} so that in the extrapolation region, $|x| > 1$, $V_d(x, \xi_\infty)$ is dominated by $2^{2d-1} x^{2d}$.

From Guest (1958) it is known that

$$V_d(x, \xi_u) = \sum_{\ell=0}^d (2\ell+1) P_\ell^2(x) = \{(d+1)^2 P_d^2(x) - (x^2-1) P_d'^2(x)\}$$

and $V_d(x, \xi_u)$ attains its maximum values at the very points where ξ_d puts its masses. Hence it is known that

$$V_d(\xi_u) = \sup_{x \in [-1, 1]} V_d(x, \xi_u) = V_d(\pm 1, \xi_u) = (d+1)^2.$$

It was also shown in Guest (1958) that

$$V_d(0, \xi_u) = \left\{ \frac{(2q+1)(2q-1) \dots 1}{2^q q!} \right\}^2,$$

where $q = \frac{d}{2}$ when d is even and $q = \frac{d-1}{2}$ when d is odd. Therefore, from Guest (1958) it is known that

$$\lim_{d \rightarrow \infty} V_d(0, \xi_d) / V_d(0, \xi_u) = \frac{\pi}{2},$$

$$V_d(\xi_d) / (V_d(\xi_u)) = \frac{1}{d+1},$$

and for $|x| > 1$,

$$\lim_{d \rightarrow \infty} \frac{V_d(x, \xi_d)}{V_d(x, \xi_u)} = \frac{1}{2}.$$

Theorem 2.3.1: For the design measures ξ_∞ and ξ_u ,

$$V_d(\xi_\infty)/V_d(\xi_u) = \frac{2}{(d+1)}, \quad (2.3.1)$$

$$\lim_{d \rightarrow \infty} V_d(0, \xi_\infty)/V_d(0, \xi_u) = \frac{\pi}{2}, \quad (2.3.2)$$

and for $|x| > 1$,

$$\lim_{d \rightarrow \infty} V_d(x, \xi_\infty)/V_d(x, \xi_u) = \frac{\pi}{4}. \quad (2.3.3)$$

The equation (2.3.1) is obvious. To prove (2.3.2) the following lemma is needed.

Lemma 2.3.1: For any real or complex z ,

$$\{\Gamma(z)\}^{-1} = ze^{\gamma z} \prod_{q=1}^{\infty} \left[\left(1 + \frac{z}{q}\right) e^{-\frac{z}{q}} \right],$$

where $\gamma = \lim_{n \rightarrow \infty} \left(\sum_{q=1}^n \frac{1}{q} - \ln n \right)$ is the Euler's constant.

Proof of Theorem 2.3.1: From the known results it follows that

$$\frac{V_d(0, \xi_\infty)}{V_d(0, \xi_u)} = \left\{ d + \frac{1}{2} + \frac{1}{2}(-1)^d \right\} / \left\{ \frac{(2q+1)(2q-1) \dots 1}{2^q q!} \right\}^2,$$

where $q = \frac{d}{2}$ when d is even and $q = \frac{d-1}{2}$ when d is odd. Therefore,

$$\begin{aligned} \frac{V_d(0, \xi_\infty)}{V_d(0, \xi_u)} &= (2q+1) / \left\{ \frac{(2q+1)(2q-1) \dots 1}{2^q q!} \right\}^2 \\ &= \left\{ (2q+1) \frac{\pi}{4q} \right\} \left[\frac{4q}{\pi} / \left\{ \prod_{i=1}^q \left(1 + \frac{1}{2i}\right) \right\}^2 \right]. \end{aligned} \quad (2.3.4)$$

Putting $z = \frac{1}{2}$ in Lemma 2.3.1 it can be seen that the second term on the right hand side of (2.3.4) tends to the limiting value 1 as q tends to infinity, and hence (2.3.2) follows. Also, for $|x| > 1$,

$$\begin{aligned} \lim_{d \rightarrow \infty} \frac{V_d(x, \xi_\infty)}{V_d(x, \xi_u)} &= \lim_{d \rightarrow \infty} \frac{2^{2d-1}}{(2d+1)\{(2d)!/2^d(d!)^2\}^2} \\ &= \lim_{d \rightarrow \infty} \left\{ 2 \prod_{i=1}^d \left(1 - \frac{1}{4i^2}\right) \right\}^{-1}. \end{aligned}$$

Therefore, by lemma (2.2.5), the last part of the theorem is obtained.

It is interesting to note that for $|x| > 1$,

$$\lim_{d \rightarrow \infty} \frac{V_d(x, \xi_d)}{V_d(x, \xi_u)} = \frac{1}{2} \quad \text{and} \quad \lim_{d \rightarrow \infty} \frac{V_d(x, \xi_\infty)}{V_d(x, \xi_u)} = \frac{\pi}{4}$$

implying that $\lim_{d \rightarrow \infty} \frac{V_d(x, \xi_d)}{V_d(x, \xi_\infty)} = \frac{2}{\pi}$. The limiting design measure ξ_∞ , therefore, never achieves the efficiency of ξ_d in predicting the response in the extrapolation region. This is to be expected from the results of Kiefer and Studden (1976) on the G-efficiency of ξ_∞ which showed that ξ_∞ has a limiting G-efficiency equal to $\frac{1}{2}$ although it has a limiting D-efficiency equal to 1.

2.4 Efficiency under the integrated variance criterion

It may be of interest to know how well a design behaves over a whole region rather than at individual points in the region. Then it may be more useful to compare designs under the criterion of integrated variance. Let

$$A_d(\xi) = \int_{-1}^1 V_d(x, \xi) \frac{dx}{2} = \text{Tr } M_d^{-1}(\xi) M_d(\xi_u).$$

Then the following results are obtained.

Theorem 2.4.1: For design measures ξ_u , ξ_d and ξ_∞ ,

$$\begin{aligned} A_d(\xi_u) - A_d(\xi_d) &= \frac{(d+1)}{(2d+1)} , \\ A_d(\xi_u) - A_d(\xi_\infty) &= \frac{d}{(2d+1)} . \end{aligned} \tag{2.4.1}$$

Proof: From Guest (1958),

$$V_d(x, \xi_u) = (d+1)^2 (P_d(x))^2 + (1-x^2) P_d'^2(x).$$

Therefore, it follows that

$$\int_{-1}^1 (1-x^2) P_d'^2(x) \frac{dx}{2} = \frac{d(d+1)}{(2d+1)} .$$

Now, from Guest (1958),

$$V_d(x, \xi_d) = (d+1) - \frac{(1-x^2)}{d} P_d'^2(x) .$$

Therefore,

$$A_d(\xi_d) = (d+1) - \frac{(d+1)}{(2d+1)} .$$

From Kiefer and Studden (1976),

$$V_d(x, \xi_\infty) = d + \frac{1}{2} + \frac{1}{2} U_{2d}(x) ,$$

where $U_n(\cos \theta) = \sin(n+1)\theta / \sin \theta$. Therefore,

$$A_d(\xi_\infty) = (d+1) - \frac{d}{(2d+1)}$$

and the theorem follows.

Note that

$$\lim_{d \rightarrow \infty} \{A_d(\xi_u) - A_d(\xi_d)\} = \frac{1}{2} \text{ and } \lim_{d \rightarrow \infty} \{A_d(\xi_u) - A_d(\xi_\infty)\} = \frac{1}{2}.$$

Therefore, for large-degree polynomials, under the integrated variance criterion, there is hardly any difference in efficiency of the design measures ξ_u , ξ_d and ξ_∞ . Figure 2.4.1 displays the behaviour of $A_d(\xi_u) - A_d(\xi_d)$ and $A_d(\xi_u) - A_d(\xi_\infty)$ for some selected values of d .

If the central region of $[-1,1]$ is of greater interest than the boundary regions, it would be more appropriate to integrate $V_d(x, \xi)$ with respect to a measure that puts greater weight in the central region than the uniform measure. Since Guest (1958) showed that $V_d(x, \xi_u)$ is smaller than $V_d(x, \xi_d)$ in the central region, in this case the performance of ξ_u would be even better under the integrated variance criterion.

Studden (1977) considered the problem of finding optimal designs under uniformly integrated variance criterion. Let ξ_d^I be the optimal design measure under the criterion and let ξ_d^{IA} be the design measure that concentrates on the zeros $x_0, x_1, \dots, x_d$ of $(1-x^2)P'_d(x)$ with weights proportional to $|P_d(x_i)|^{-1}$. Studden (1977) proved that

$$A_d(\xi_d^{IA}) = \frac{2d}{d(d+1)(2d+1)} \left(\sum_{i=0}^d |P_d(x_i)|^{-1} \right)^2, \quad (2.4.2)$$

$$A_d(\xi_d^{IA}) - A_d(\xi_d^I) \leq \frac{1}{d(d+1)(2d+1)} \left(\sum_{i=0}^d |P_d(x_i)|^{-1} \right)^2.$$

Using a few known results on orthogonal polynomials, stated in the following lemma, some asymptotic results about the design measures ξ_d^I and ξ_d^{IA} may be derived.

Lemma 2.4.1: (a): For $d \geq 2$, the successive relative maxima of $|P_d(x)|$ when x decreases from 1 to 0, form a decreasing sequence. If $\mu_{1d}, \mu_{2d}, \dots, \mu_{[d/2],d}$ denote these maxima corresponding to decreasing values of x , then

$$1 > \mu_{1,d} > \mu_{2d} > \dots > \mu_{[d/2],d}$$

and for d even,

$$\mu_{\frac{d}{2},d} = |P_d(0)| = \frac{1.3 \dots (d-1)}{2.4 \dots d};$$

(b) for a fixed r ,

$$\mu_{r,d} > \mu_{r,d+1}$$

so that when d is odd,

$$1 > \mu_{1,d} > \dots > \mu_{\frac{d-1}{2},d} > \mu_{\frac{d-1}{2},d+1} > \mu_{\frac{d+1}{2},d+1} = |P_{d+1}(0)|.$$

Proof of the lemma is given in Szego (1959) ((a) corresponds to theorem 7.3.1, pp.164, 165 and (b) corresponds to the result 7.8.1, p.190).

Lemma 2.4.2. For the design measures ξ_d^{IA} and ξ_d^I ,

$$\lim_{d \rightarrow \infty} \{A_d(\xi_d^{IA}) - A_d(\xi_d^I)\} \leq \frac{1}{4} \pi. \quad (2.4.3)$$

Proof: Let d be even. Then by lemma 2.4.1,

$$|P_d(x_1)|^{-1} \leq \frac{2.4 \dots d}{1.3 \dots (d-1)}.$$

Therefore,

$$\begin{aligned} A_d(\xi_d^{IA}) - A_d(\xi_d^I) &\leq \frac{(d+1)}{d(2d+1)} \prod_{i=1}^{d/2} \left(\frac{2i}{2i-1}\right)^2 \\ &= \left\{ \frac{2(d+1)^3}{d^2(2d+1)} \right\} \left\{ \frac{d}{2} \prod_{i=1}^{d/2} \left(\frac{2i}{2i+1}\right)^2 \right\}, \end{aligned}$$

and hence by taking limits and by applying Lemma 2.3.1 the desired result is obtained.

Let d be odd. Then by Lemma 2.4.1

$$|P_d(x_i)|^{-1} \leq |P_{d+1}(0)|^{-1} = \frac{2.4 \dots (d+1)}{1.3 \dots d}.$$

Therefore,

$$\begin{aligned} A_d(\xi_d^{IA}) - A_d(\xi_d^I) &< \frac{(d+1)}{d(2d+1)} \prod_{i=1}^{(d+1)/2} \left(\frac{2i}{2i-1}\right)^2 \\ &= \frac{(d+1)(d+2)^2}{d(2d+1)} \prod_{i=1}^{(d+1)/2} \left(\frac{2i}{2i+1}\right)^2 \\ &= \left\{ \frac{2}{d} \frac{(d+2)^2}{(2d+1)} \right\} \left\{ \frac{(d+1)}{2} \prod_{i=1}^{(d+1)/2} \left(\frac{2i}{2i+1}\right)^2 \right\} \end{aligned}$$

and hence by taking limits the desired result is obtained.

The result (2.4.3) shows that the design measure ξ_d^{IA} proposed by Studden (1977) is extremely efficient for large-degree polynomials under the integrated variance criterion. In fact the limiting bound in (2.4.3) can be decreased as shown by the following lemma.

Lemma 2.4.3: For the design measures ξ_d^{IA} and ξ_d^I ,

$$\lim_{d \rightarrow \infty} \{A_d(\xi_d^{IA}) - A_d(\xi_d^I)\} \leq \frac{1}{2} \quad (2.4.4)$$

Proof: From (2.4.2) it can be seen that,

$$(1 - \frac{1}{2d}) A_d(\xi_d^{IA}) \leq A_d(\xi_d^I) .$$

Therefore,

$$A_d(\xi_d^{IA}) - A_d(\xi_d^I) \leq \frac{1}{(2d-1)} A_d(\xi_d^I) \leq \frac{A_d(\xi_u)}{(2d-1)}$$

and hence the Lemma follows.

In terms of G-efficiency the design measure ξ_d^{IA} is better than the uniform design measure ξ_u . This can readily be seen since, for ξ_d^{IA} ,

$$\begin{aligned} V_d(\xi_d^{IA}) &= \sup_{x \in [-1, 1]} V_d(x, \xi_d^{IA}) \\ &= \sup_{x \in [-1, 1]} \left(\sum_{i=0}^d |P_d(x_i)|^{-1} \right) \left\{ \sum_{i=0}^d |P_d(x_i)| \ell_i^2(x) \right\} \\ &\leq \sup_{x \in [-1, 1]} \left(\sum_{i=0}^d |P_d(x_i)|^{-1} \right) \left(\sum_{i=0}^d \ell_i^2(x) \right) \\ &= \left(\sum_{i=0}^d |P_d(x_i)|^{-1} \right) , \end{aligned}$$

where x_i are the zeroes of $(1-x^2)P_d'(x)$ and $\ell_i(x)$ are the corresponding Lagrange's interpolation polynomials given by

$$\ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^d \frac{(x - x_j)}{(x_i - x_j)} .$$

Thus, $V_d(\xi_d^{IA}) < (d+1)^2 (\frac{\pi}{2d})^{1/2}$ for even d and $V_d(\xi_d^{IA}) < (d+1)(d+2) \{\frac{\pi}{2(d+1)}\}^{1/2}$ for odd d . Therefore $V_d(\xi_d^{IA})$ is at most of $O(d^{3/2})$ whereas $V_d(\xi_u)$ is of $O(d^2)$. Due to the well-known inequality

$$|M_d(\xi)| / |M_d(\xi_d)| \geq e^{\{d+1-V_d(\xi)\}},$$

this suggests that in terms of D-efficiency also ξ_d^{IA} is better than ξ_u .

Let $\phi(x, \xi) = f_d'(x) M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) f_d(x)$. It is known from Kiefer (1974, p. 877) or Studden (1977) that

$$A_d(\xi) - A_d(\xi_d^I) \leq \sup_{x \in [-1, 1]} \phi(x, \xi) - A_d(\xi).$$

Hence

$$A_d(\xi_d) - A_d(\xi_d^I) \leq \frac{(d+1)}{2d+1} + (d+1) \left\{ \frac{1}{d|P_d(0)|^2} - 1 \right\}.$$

Therefore,

$$A_d(\xi_u) - A_d(\xi_d^I) \leq \frac{2(d+1)}{(2d+1)} + (d+1) \left\{ \frac{1}{d|P_d(0)|^2} - 1 \right\}$$

and

$$\lim_{d \rightarrow \infty} \frac{A_d(\xi_u) - A_d(\xi_d^I)}{(d+1)} \leq \frac{\pi}{2} - 1.$$

It follows that

$$\lim_{d \rightarrow \infty} \frac{A_d(\xi_d^I)}{(d+1)} \geq 2 - \frac{\pi}{2}.$$

Hence, if $A_d(\xi_d^I)/A_d(\xi)$ is taken as a measure of efficiency of the design measure ξ in terms of the integrated variance criterion, it is seen that the design measure ξ_u has an asymptotic efficiency of at least 0.43, approximately.

It is interesting to note that under the integrated variance criterion there may be distinct designs with the same efficiency. For example, consider the measure $\xi_d^{(N)}$ which puts weights $|P_d(x_i)|^{-2}/\{d(d+1)\}$ at the zeros x_i of $(1-x^2)P'_d(x)$. Then $\xi_d^{(N)}$ is clearly a nonsingular design measure for polynomial regression model of degree d since from the Lobatto formula of quadrature (see Ghizzetti and Ossicini, 1970)

$$\sum_{i=0}^d |P_d(x_i)|^{-2}/d(d+1) = 1.$$

Then, for the design measure $\xi_d^{(N)}$,

$$V_d(x, \xi_d^{(N)}) = d(d+1) \sum_{i=0}^d |P_d(x_i)|^2 \ell_i^2(x)$$

and

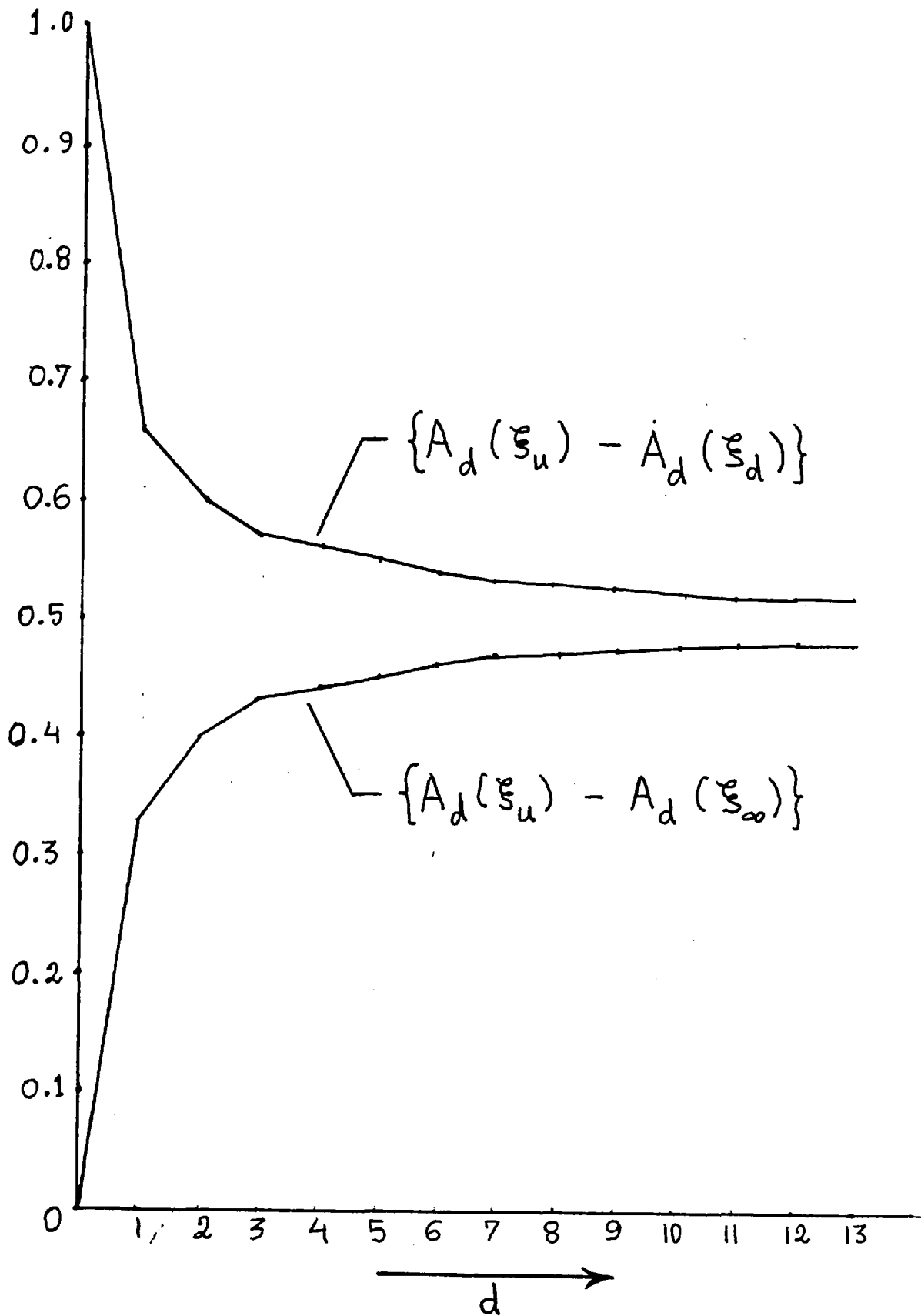
$$\begin{aligned} A_d(\xi_d^{(N)}) &= d(d+1) \sum_{i=0}^d |P_d(x_i)|^2 \int_{-1}^1 \ell_i^2(x) \frac{dx}{2} \\ &= d(d+1) \sum_{i=0}^d \frac{2d}{d(d+1)(2d+1)} \\ &= \frac{2d(d+1)}{(2d+1)}. \end{aligned}$$

Therefore, in terms of the integrated variance criterion, the design measure $\xi_d^{(N)}$ has the same efficiency as the D-optimum design measure ξ_d since $A_d(\xi_d) = \frac{2d(d+1)}{(2d+1)}$. Another interesting feature of $\xi_d^{(N)}$ is that $\int_{-1}^1 x^i d\xi_d^{(N)}(x) = \int_{-1}^1 x^i d\xi_u(x)$ ($i = 0, 1, \dots, 2d-1$), that is, for $\xi_d^{(N)}$ and for the uniform design measure ξ_u the moments up to order $2d-1$ match. However, the $2d$ -th moments are different. In fact,

$$\int_{-1}^1 x^{2d} d\xi_d^{(N)}(x) = \int_{-1}^1 x^{2d} d\xi_u(x) + \frac{2^{2d}(d-1)!(d!)^2(d+1)!}{(2d+1)!(2d)!}.$$

FIGURE 2.4.1

THE BEHAVIOUR OF $A_d(\xi_u) - A_d(\xi_d)$ AND $A_d(\xi_u) - A_d(\xi_\infty)$



2.5 Comparison with the extrapolation designs

From Hoel and Levine (1964) or Studden (1968) it is known that ξ_d^e , the optimal design measure for extrapolation at x_e , concentrates mass w_i at points $x_i = \cos \frac{i\pi}{d}$ ($i = 0, 1, 2, \dots, d$), where

$$w_i = |l_i(x_e)| / \sum_{i=0}^d |l_i(x_e)|$$

and $l_i(x)$ are the Lagrange's polynomials of degree d specified by $l_i(x_j) = \delta_{ij}$. Further, $V_d(x_e, \xi_d^e) = T_d^2(x_e)$ which has 2^{2d-2} as the coefficient of x_e^{2d} .

From Kiefer and Studden (1976) it is also known that

$\lim_{d \rightarrow \infty} \xi_d^e = \xi_\infty^e$, where ξ_∞^e has the density

$$\frac{(x_e^2 - 1)^{1/2}}{\pi |x_e - 1| (1 - x^2)^{1/2}}.$$

Further, if $r_d(x_e) = V_d(x_e, \xi_d^e) / V_d(x_e, \xi_\infty^e)$ then $r_d(x_e)$ decreases to $\frac{1}{2}$ as d increases.

By comparing ξ_d^e and ξ_∞^e with ξ_u the following theorem is obtained.

Theorem 2.5.1: For the design measures ξ_u , ξ_d^e and ξ_∞^e ,

$$\lim_{d \rightarrow \infty} \{V_d(x_e, \xi_d^e) / V_d(x_e, \xi_u)\} = \frac{1}{8} \pi, \quad (2.5.1)$$

$$\lim_{d \rightarrow \infty} \{V_d(x_e, \xi_\infty^e) / V_d(x_e, \xi_u)\} = \frac{1}{4} \pi.$$

Proof: For any fixed $|x_e| > 1$,

$$\begin{aligned} \lim_{d \rightarrow \infty} \frac{V_d(x_e, \xi_\infty^e)}{V_d(x_e, \xi_u)} &= \lim_{d \rightarrow \infty} 2^{2d-2} / [(2d+1) \left\{ \frac{(2d)!}{2^d (d!)^2} \right\}^2] \\ &= \lim_{d \rightarrow \infty} 2^{-2} / \prod_{i=1}^d \left(1 - \frac{1}{4i^2}\right). \end{aligned}$$

But by Lemma 2.2.5,

$$\frac{2}{\pi} = \lim_{d \rightarrow \infty} \prod_{i=1}^d \left(1 - \frac{1}{4i^2}\right),$$

and hence the first part of the theorem. The second part of the theorem follows immediately from the first part and the results of Kiefer and Studden (1976).

By comparing the D-optimal design measures with the optimal extrapolation design measures the following theorem is obtained.

Theorem 2.5.2: For any fixed $|x_e| > 1$ and the design measures ξ_d , ξ_∞ , ξ_d^e , ξ_∞^e as defined,

$$\begin{aligned} \lim_{d \rightarrow \infty} \{V_d(x_e, \xi_d^e) / V_d(x_e, \xi_d)\} &= \frac{\pi}{4}, \\ \lim_{d \rightarrow \infty} \{V_d(x_e, \xi_\infty^e) / V_d(x_e, \xi_d)\} &= \frac{\pi}{2}, \\ \lim_{d \rightarrow \infty} \{V_d(x_e, \xi_d^e) / V_d(x_e, \xi_\infty)\} &= \frac{1}{2}, \\ \lim_{d \rightarrow \infty} \{V_d(x_e, \xi_\infty^e) / V_d(x_e, \xi_\infty)\} &= 1. \end{aligned} \tag{2.5.2}$$

The proof of Theorem 2.5.2 follows from the previous theorem and earlier results.

2.6 The uniform design as a 'Mini-Max. bias' design

Box and Draper (1959) showed that deviations from the assumed model can introduce so much bias that "the optimal design in typical situations in which both variance and bias occur is very nearly the same as would be obtained if variance were ignored completely and the experiment designed so as to minimize bias alone". Karson, Manson and Hader (1969), Atwood (1971) and Stigler (1971) also considered the problem of bias arising from inadequacy in the assumed model. Huber

(1975) appears to be the first to show that the only way to make reasonably sure that no small deviation from the model has been overlooked "seems to consist in solving some minimax problems with unrestricted (i.e. not necessarily polynomials) alternatives". Huber (1975) considered the problem in which the assumed model is a straight line in a single variable and the designs are continuous with density functions. Marcas and Sacks (1977) obtained combinations of the best discrete designs and estimators for the straight line model with similar bias.

Some of the results obtained by Huber (1975) may be extended to polynomials of higher order. Let the assumed model be a polynomial of degree d as considered in Sections 2.1-2.5, that is, it is assumed that $E\{y(x)\} = \beta' f_d(x)$. Let the observations be independent and identically distributed with variance σ^2 . If ξ is the design measure on $[-1,1]$ according to which the observations are taken and if $\hat{\beta}$ is the least squares estimate of β , then

$$\hat{\beta} = M_d^{-1}(\xi) \int_{-1}^1 f_d(x) y(x) d\xi(x). \quad (2.6.1)$$

Now suppose the true model is given by

$$E\{y(x)\} = g(x), \quad (2.6.2)$$

where it is known that $g \in G$ which is the family of all functions g satisfying

$$Q_g = \inf_{\beta} \int_{-1}^1 \{g(x) - \beta' f_d(x)\}^2 \frac{dx}{2} = \int_{-1}^1 \{g(x) - \beta_0' f_d(x)\}^2 \frac{dx}{2} \leq Q_0 \quad (2.6.3)$$

for a value Q_0 fixed in advance.

It is evident that

$$\beta_0 = M_d^{-1}(\xi_u) \int_{-1}^{+1} f_d(x) g(x) \frac{dx}{2} . \quad (2.6.4)$$

Without loss of generality, it may be assumed that $\beta_0 = 0$, that is,

$$\int_{-1}^{+1} f_d(x) g(x) \frac{dx}{2} = 0 \quad (2.6.5)$$

and hence

$$Q_g = \int_{-1}^{+1} g^2(x) \frac{dx}{2} \leq Q_0 . \quad (2.6.6)$$

Consider the supremum of the average mean square error

$$\sup_{g \in G} E \left[\int_{-1}^{+1} \{g(x) - \hat{\beta}' f_d(x)\}^2 \frac{dx}{2} \right] . \quad (2.6.7)$$

For a fixed g let

$$\begin{aligned} Q(g, \xi) &= E \left[\int_{-1}^{+1} \{g(x) - \hat{\beta}' f_d(x)\}^2 \frac{dx}{2} \right] \\ &= \int_{-1}^{+1} g^2(x) \frac{dx}{2} + \beta_1' M_d(\xi_u) \beta_1 + \frac{\sigma^2}{n} \text{tr } M_d^{-1}(\xi) M_d(\xi_u), \end{aligned} \quad (2.6.8)$$

where

$$\beta_1 = E(\hat{\beta}) = M_d^{-1}(\xi) \int_{-1}^{+1} f_d(x) g(x) d\xi(x) . \quad (2.6.9)$$

Alternatively,

$$Q(g, \xi) = B(g, \xi) + \frac{\sigma^2}{n} A_d(\xi), \quad (2.6.10)$$

where

$$B(g, \xi) = Q_g + \beta_1' M_d(\xi_u) \beta_1 . \quad (2.6.11)$$

Studden (1977) considered the problem of minimizing $A_d(\xi)$ with respect to the design measure ξ . However, in view of the results of Box and Draper (1959), $B(g, \xi)$ is the more important component of the average mean square error and hence consider the problem of minimizing

$$\sup_g B(g, \xi) \quad (2.6.12)$$

with respect to the design measure ξ .

Let ξ be a design measure with density $m(x)$. Then for a fixed ξ , the bias term $B(g, \xi)$ is clearly maximized by maximizing the quadratic form

$$\begin{aligned} \beta'_{1-d} M_d(\xi_u) \beta_{1-d} &= \left(\int_{-1}^1 f_d(x) g(x) m(x) dx \right)' M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \\ &\quad \times \left(\int_{-1}^1 f_d(x) g(x) m(x) dx \right), \end{aligned} \quad (2.6.13)$$

with respect to $g(x)$ subject to the constraints (2.6.5) and (2.6.6).

Let $g_0(x)$ be the maximizing $g(x)$.

Lemma 2.6.1: The maximizing $g(x)$ is given by $g_0(x)$, where

$$g_0(x) = b' \{ f_d(x) - 2 M_d(\xi_u) M_d^{-1}(\xi) f_d(x) m(x) \}, \quad (2.6.14)$$

with b a vector of constants.

Proof: The proof relies on variational arguments. Let $\eta(x)$ be such that $\eta(1) = \eta(-1) = 0$ and let

$$\begin{aligned} \psi(\alpha) &= \left[\int_{-1}^1 f_d(x) \{ g_0(x) + \alpha \eta(x) \} m(x) dx \right]' M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \\ &\quad \left[\int_{-1}^1 f_d(x) \{ g_0(x) + \alpha \eta(x) \} m(x) dx \right] \\ &\quad + b' \int_{-1}^1 f_d(x) \{ g_0(x) + \alpha \eta(x) \} \frac{dx}{2} - \lambda \left[\int_{-1}^1 \{ g_0(x) + \alpha \eta(x) \}^2 \frac{dx}{2} - Q_0 \right], \end{aligned}$$

where λ and $\underline{b}$ are Lagrange's multipliers. Then by definition $\psi(\alpha)$ has a maximum at $\alpha = 0$, that is, $\psi'(0) = 0$ and $\psi''(0) \leq 0$. Therefore,

$$2\left\{ \int_{-1}^1 \underline{f}'_d(x) \eta(x) m(x) dx \right\} M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \left\{ \int_{-1}^1 \underline{f}_d(x) g_0(x) m(x) dx \right\} \\ + \underline{b}' \int_{-1}^1 \underline{f}_d(x) \eta(x) \frac{dx}{2} - 2\lambda \int_{-1}^1 g_0(x) \eta(x) \frac{dx}{2} = 0$$

that is,

$$\int_{-1}^1 [4\underline{f}'_d(x) m(x) M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \left\{ \int_{-1}^1 \underline{f}_d(x) g_0(x) m(x) dx \right\} + \underline{f}'_d(x) \underline{b} - 2\lambda g_0(x)] \\ \eta(x) \frac{dx}{2} = 0.$$

But $\eta(x)$ is arbitrary. Therefore,

$$4m(x) \underline{f}'_d(x) M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \int_{-1}^1 \underline{f}_d(x) g_0(x) m(x) dx + \underline{f}'_d(x) \underline{b} - 2\lambda g_0(x) = 0$$

and it follows that

$$g_0(x) = \frac{1}{2\lambda} [\underline{f}'_d(x) \underline{b} + 4m(x) \underline{f}'_d(x) M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \int_{-1}^1 \underline{f}_d(x) g_0(x) m(x) dx].$$

But by constraint (2.6.5),

$$\int_{-1}^1 \underline{f}_d(x) g_0(x) \frac{dx}{2} = 0.$$

Therefore,

$$4M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \int_{-1}^1 \underline{f}_d(x) g_0(x) m(x) dx = -2M_d^{-1}(\xi) M_d(\xi_u) \underline{b}.$$

Hence

$$g_0(x) = \frac{1}{2\lambda} \underline{b}' [\underline{f}_d(x) - 2M_d(\xi_u) M_d^{-1}(\xi) \underline{f}_d(x) m(x)]$$

and writing $\underline{b}$ for $\frac{1}{2\lambda} \underline{b}$ gives the desired result.

Because of the particular dependence of $g_0(x)$ on $m(x)$ an important feature of the uniform design measure ξ_u follows from Lemma 2.6.1.

Theorem 2.6.1: Among all design measures with density functions, ξ_u is optimal for minimizing the maximum bias arising from inadequacy in the polynomial model when the alternative model is not necessarily a polynomial and may be any member of the family given by (2.6.3).

Proof: Theorem 2.6.1 is a consequence of Lemma 2.6.1. For the uniform design measure ξ_u , the density $m(x) = \frac{1}{2}$ and hence $g_0(x) = 0$. Therefore, $B(g_0, \xi_u) = 0$ and the theorem follows.

Note that for a fixed ξ , the bias term $B(g, \xi)$ has the maximum value

$$B(g_0, \xi) = a' \left[4 \int_{-1}^1 f_d(x) f_d'(x) m^2(x) dx M_d^{-1}(\xi) M_d(\xi_u) M_d^{-1}(\xi) \int_{-1}^1 f_d(x) f_d'(x) m^2(x) dx \right. \\ \left. - 2 \int_{-1}^1 f_d(x) f_d'(x) m^2(x) dx \right] a,$$

where $a = M_d^{-1}(\xi) M_d(\xi_u) b$.

It can also be shown that Lemma 2.6.1 and Theorem 2.6.1 have higher-dimensional analogues. However, these are not pursued here.

CHAPTER 3

THE VARIANCE OF THE DIFFERENCE OF ESTIMATED RESPONSES AND

OTHER CRITERIA

3.1 Introduction

It may be seen from Herzberg (1967c), Atkinson (1970) and Box and Draper (1980) that even in response surface experiments differences in response may sometimes be of greater interest than the absolute response. Hence in Section 3.2, an attempt is made to obtain some one-dimensional designs for polynomial regression that try to minimize the variance of the difference of estimated responses.

In many design problems, the use of a particular optimality criterion may not lead to a unique design. Often one would be left with a very large number of designs all of which are optimal under the particular criterion. In such situations other criteria may be applied to the designs selected so as to have a reduction in the number of designs one would have to choose from. The introduction of fresh criteria may be continued until one is left with a unique optimal design. The hierarchical ordering of the various criteria in any such selection programme would of course depend on the goal of the experiments and hence on the available information about the mechanism to be studied. Some simple examples of the application of such hierarchical ordering of criteria are provided in Section 3.3.

3.2 Variance of the difference of estimated responses

Consider first the simple example of one-dimensional quadratic regression model with the design space $X = [-1, 1]$. Let the observations be independent and identically distributed with a common variance σ^2 . Then the design that minimizes the maximum variance of the difference in two estimated responses in the design region for a quadratic model is obtained in Theorem 3.2.1.

Theorem 3.2.1: The design measure $\xi^{(0)}$ which minimizes

$$\sup_{x, z \in [-1, 1]} \{f_2'(x) - f_2'(z)\} \left[\int_{-1}^1 f_2(x) f_2'(x) d\xi(x) \right]^{-1} \{f_2(x) - f_2(z)\}, \quad (3.2.1)$$

over all non-singular design measures ξ puts weights $\frac{1}{2}(23-10\sqrt{5})$ at each of ± 1 and $(10\sqrt{5}-22)$ at 0.

consideration

Proof: Without loss of generality one may restrict to the class of symmetric design measures so that

$$\begin{aligned} M_2(\xi) &= \int_{-1}^1 f_2(x) f_2'(x) d\xi(x) \\ &= \begin{bmatrix} 1 & 0 & \alpha \\ 0 & \alpha & 0 \\ \alpha & 0 & \beta \end{bmatrix}, \end{aligned}$$

where $\alpha = \int_{-1}^1 x^2 d\xi(x)$ and $\beta = \int_{-1}^1 x^4 d\xi(x)$. Then,

$$\begin{aligned} \text{var}\{\hat{y}(x) - \hat{y}(z)\} &= \{f_2'(x) - f_2'(z)\} M_2^{-1}(\xi) \{f_2(x) - f_2(z)\} \\ &= \frac{(x-z)^2}{\alpha} + \frac{(x^2 - z^2)^2}{(\beta - \alpha^2)}, \end{aligned} \quad (3.2.2)$$

where $\hat{y}(x)$ is the response at point x fitted by the method of least squares having taken observations according to the design measure ξ .

Since for any fixed x , z and α , (3.2.2) may be minimized by making $(\beta - \alpha^2)$ as large as possible, that is, by making β as large as possible, and since always $\beta \leq \alpha$, only the design measures with $\beta = \alpha$, i.e. the design measures supported at 0 and ± 1 need to be considered. With $\beta = \alpha$, (3.2.2) reduces to

$$\text{var}\{\hat{y}(x) - \hat{y}(z)\} = \frac{(x-z)^2}{\alpha} + \frac{(x^2-z^2)^2}{(\alpha-\alpha^2)} \quad (3.2.3)$$

Let $z = tx$ so that (3.2.3) reduces to

$$\text{var}\{\hat{y}(x) - \hat{y}(z)\} = x^2 \left\{ \frac{(1-t)^2}{\alpha} + \frac{x^2(1-t^2)^2}{(\alpha-\alpha^2)} \right\} \quad (3.2.4)$$

which for any fixed t achieves a maximum if $x = \pm 1$, the same maximum value being achieved at both points. Hence, let x be one of those points, say, $x = 1$. Therefore, the problem reduces to

$$\text{Minimize } \sup_{\alpha \in (0,1) \ t \in [-1,1]} h(\alpha, t), \quad (3.2.5)$$

$$\text{where } h(\alpha, t) = \frac{(1-t)^2}{\alpha} + \frac{(1-t^2)^2}{\alpha(1-\alpha)}.$$

For a fixed α , differentiating $h(\alpha, t)$ with respect to t it can be seen that the turning points of $h(\alpha, t)$ are $t = -\frac{1}{2} \pm \frac{1}{2} \sqrt{2\alpha-1}$. Thus for $\alpha < \frac{1}{2}$ there is no turning point and therefore only the design measures with $\alpha \geq \frac{1}{2}$ need to be considered.

For any fixed $\alpha > \frac{1}{2}$, differentiating $h(\alpha, t)$ twice with respect to t it can be seen that $t_1 = -\frac{1}{2} + \frac{1}{2} \sqrt{2\alpha-1}$ is a maximum and $t_2 = -\frac{1}{2} - \frac{1}{2} \sqrt{2\alpha-1}$ is a minimum. Now

$$h(\alpha, t_1) = \frac{11 - 8\alpha - \alpha^2 + 2(2\alpha-1)^{3/2}}{4\alpha(1-\alpha)} \quad (3.2.6)$$

Therefore, for $\alpha \leq 23-10\sqrt{5}$, it follows that $h(\alpha, t_1) \leq \frac{4}{\alpha} = h(\alpha, -1)$ and for $\alpha = 23-10\sqrt{5}$, $h(\alpha, t_1) = \frac{4}{\alpha} = h(\alpha, -1)$. Hence the design measure $\xi^{(0)}$ with $\alpha = 23-10\sqrt{5}$ is better than the design measures with $\alpha < 23-10\sqrt{5}$ and thus only the design measures with $\alpha \geq 23-10\sqrt{5}$ need to be considered.

Now, $\frac{\partial}{\partial \alpha} h(\alpha, t_1)$ is a positive multiple of $2(\alpha^2 - \alpha + 1)(2\alpha - 1)^{1/2} - 11 - 9\alpha^2 + 22\alpha$. Therefore $\frac{\partial}{\partial \alpha} h(\alpha, t_1) > 0$ if and only if

$$2(\alpha^2 - \alpha + 1)(2\alpha - 1)^{1/2} > 11 + 9\alpha^2 - 22\alpha$$

Since $2(2\alpha - 1)^{1/2} > 1$ for $\alpha \geq 23-10\sqrt{5}$, it is sufficient to show that $8\alpha^2 - 21\alpha + 10 < 0$ in order that $\frac{\partial h}{\partial \alpha}(\alpha, t_1) > 0$. But $8\alpha^2 - 21\alpha + 10 \leq 0$ for all $\alpha \in [\frac{10}{16}, 2]$. Since $23-10\sqrt{5} > \frac{10}{16}$ it follows that $\frac{\partial h}{\partial \alpha}(\alpha, t_1) > 0$ and hence $h(\alpha, t_1)$ is strictly increasing for α increasing in the range $\alpha \in [23-10\sqrt{5}, 1]$. Hence it follows that $\xi^{(0)}$ is the optimal design measure for minimizing the maximum variance of the difference in two estimated responses and the theorem follows. The behaviour of $h(\alpha, t)$ for some selected values of α is sketched in Figure 3.2.1.

The optimal design measure $\xi^{(0)}$ has the same support points as the D-optimal design measure. Only the weights are different. $\xi^{(0)}$ puts greater weight at 0 than the D-optimal design measure.

For higher-order models the optimal design measures for minimizing the maximum variance of the difference of two estimated responses are likely to be extremely difficult to obtain. Also, the 'mini-max' optimality criterion may be criticized for being too pessimistic. Hence, it may be more desirable to obtain design measures which minimize the variance of the difference in two estimated responses integrated with respect to some measure α on $[-1, 1]^2$. For simplicity, it is assumed that $d\alpha(x, z) = d\mu(x)d\mu(z)$ for some measure μ on $[-1, 1]$. Using the notation of Chapter 2, the problem then may be formulated as that of obtaining a design measure $\bar{\xi}$ which minimizes

$$\int_{-1}^1 \int_{-1}^1 (f'_d(x) - f'_d(z)) M_d^{-1}(\xi) (f_d(x) - f_d(z)) d\mu(x) d\mu(z) \quad (3.2.7)$$

over all non-singular design measures ξ for the polynomial regression model $E\{y(x)\} = f'_d(x)\beta$. Equivalently, $\bar{\xi}$ has to minimize

$$V_d(\xi, \mu) = \text{tr } M_d^{-1}(\xi) [M_d(\mu) - \int_{-1}^1 f_d(x) d\mu(x) \int_{-1}^1 f'_d(x) d\mu(x)]. \quad (3.2.8)$$

It is assumed that μ has at least $(d+1)$ points of support.

Since $V_d(\xi, \mu)$ involves $M_d^{-1}(\xi)$ in an appropriate positive definite manner, from De La Graza (1954), Hoel and Levine (1964) or Levine (1966) it can be seen that only the design measures supported at ± 1 and at $(d-1)$ interior points need to be considered.

Suppose the design measure has support at the points

$-1 = x_0 < x_1 < \dots < x_{d-1} < x_d = 1$ with corresponding weights P_i

($i = 0, 1, \dots, d$). Let $\ell_i(x)$ ($i = 0, 1, \dots, d$) be the Lagrange's

interpolation polynomial of degree d corresponding to the points x_i ,

that is, $\ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^d \frac{(x - x_j)}{(x_i - x_j)}$. It is known that (3.2.8) is invariant

under linear transformations of $f_d(x)$. Hence (3.2.8) may be written as

$$V_d(\xi, \mu) = \sum_{i=0}^d \frac{1}{P_i} \left[\int_{-1}^1 \ell_i^2(x) d\mu(x) - \left\{ \int_{-1}^1 \ell_i(x) d\mu(x) \right\}^2 \right]. \quad (3.2.9)$$

It follows by Schwarz's inequality that the minimizing weights are given by

$$P_i = \sqrt{h_i} / \sum_{i=0}^d \sqrt{h_i}, \quad (3.2.10)$$

where $h_i = \left[\int_{-1}^1 \ell_i^2(x) d\mu(x) - \left\{ \int_{-1}^1 \ell_i(x) d\mu(x) \right\}^2 \right]$ ($i = 0, 1, \dots, d$).

With this optimal choice of weights for the support points

$x_0, x_1, \dots, x_d$ it follows that

$$V_d(\xi, \mu) = \left(\sum_{i=0}^d \sqrt{h_i} \right)^2. \quad (3.2.11)$$

Hence the problem is to choose the interior points $x_1, \dots, x_{d-1}$ such that the expression in (3.2.11) is minimized.

For any given non-singular design measure ξ the following result is true.

Lemma 3.2.1. Let $\bar{\xi}$ be the design measure minimizing $V_d(\xi, \mu)$. Then

$$V_d(\xi, \mu) - V_d(\bar{\xi}, \mu) \leq \sup_{x \in [-1, 1]} \phi(x, \xi, \mu) - V_d(\xi, \mu), \quad (3.2.12)$$

where

$$\phi(x, \xi, \mu) = f_d'(x) M_d^{-1}(\xi) [M_d(\mu) - \int_{-1}^1 f_d(x) d\mu(x) \int_{-1}^1 f_d'(x) d\mu(x)] M_d^{-1}(\xi) f_d(x). \quad (3.2.13)$$

Proof: The inequality (3.2.12) involves convexity of $V_d(\xi, \mu)$ in the design measure ξ and can be proved in the same way as for similar result in Kiefer (1960, p.388) for the D-optimal design measure.

The exact optimal design measures for large values of d may be rather difficult to obtain. However, the following lemmata show that there are design measures which are nearly as efficient as the optimal design measures. Let μ' be the measure for which the moments up to order $(2d-1)$ are the same as those for μ and which maximizes the $2d$ -th moment. If μ' is supported at $-1 = x_0 < x_1 < \dots < x_{d-1} < x_d = 1$, then let $\bar{\xi}^A$ be the design measure supported at the same points but with the optimal weights given by (3.2.10). The design measure $\bar{\xi}^A$ is a nearly optimal design measure under the criterion considered.

Lemma 3.2.2: If the measure μ concentrates mass $q_0, \dots, q_d$ on the points $x_0, \dots, x_d$ then the design measure $\bar{\xi}^A$ concentrates mass $\sqrt{h_i} / \sum_{i=0}^d \sqrt{h_i}$ with $h_i = q_i - q_i^2$ on x_i ($i = 0, 1, \dots, d$) and

$$V_d(\bar{\xi}^A, \mu) - V_d(\bar{\xi}, \mu) \leq (\sum \sqrt{h_i})^2 \left\{ \sup_x \sum_{i=0}^d \ell_i^2(x) - 1 \right\}. \quad (3.2.14)$$

Proof: From (3.2.11) it follows that $V_d(\bar{\xi}^A, \mu) = (\sum \sqrt{h_i})^2$. From (3.2.13) it can be seen that $\phi(x, \bar{\xi}^A, \mu) = (\sum \sqrt{h_i})^2$

$$\begin{aligned} & \times \left[\frac{\ell_0(x)}{\sqrt{h_0}}, \dots, \frac{\ell_d(x)}{\sqrt{h_d}} \right] \left[\begin{bmatrix} q_0 & & 0 \\ & \ddots & \\ 0 & & q_d \end{bmatrix} - \begin{bmatrix} q_0 \\ \vdots \\ q_d \end{bmatrix} [q_0, \dots, q_d] \right] \begin{bmatrix} \ell_0(x)/\sqrt{h_0} \\ \vdots \\ \ell_d(x)/\sqrt{h_d} \end{bmatrix} \\ & = (\sum \sqrt{h_i})^2 [\sum \ell_i^2(x)] \\ & + (\sum \sqrt{h_i})^2 \left[\frac{\ell_0(x)}{\sqrt{h_0}}, \dots, \frac{\ell_d(x)}{\sqrt{h_d}} \right] \left[\begin{bmatrix} q_0^2 & & 0 \\ & \ddots & \\ 0 & & q_d^2 \end{bmatrix} - \begin{bmatrix} q_0 \\ \vdots \\ q_d \end{bmatrix} [q_0, \dots, q_d] \right] \begin{bmatrix} \ell_0(x)/\sqrt{h_0} \\ \vdots \\ \ell_d(x)/\sqrt{h_d} \end{bmatrix}. \end{aligned}$$

Now the matrix

$$\begin{bmatrix} q_0^2 & & 0 \\ & \ddots & \\ 0 & & q_d^2 \end{bmatrix} - \begin{bmatrix} q_0 \\ \vdots \\ q_d \end{bmatrix} [q_0, \dots, q_d]$$

is clearly negative definite since the matrix may be written as

$$\begin{bmatrix} q_0 & & 0 \\ & \ddots & \\ 0 & & q_d \end{bmatrix} \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix} - \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} [1 \dots 1] \begin{bmatrix} q_0 & & 0 \\ & \ddots & \\ 0 & & q_d \end{bmatrix}$$

and its determinant is given (see Rao, 1973) by

$$\left\{ \prod_{i=0}^d q_i^2 \right\} \{0 - (-1)\}^d \{0 + d(-1)\} = -d \prod_{i=0}^d q_i^2.$$

Therefore

$$\phi(x, \bar{\xi}^A, \mu) \leq (\sum \sqrt{h_i})^2 \left\{ \sum_{i=0}^d \ell_i^2(x) \right\}$$

and hence by (3.2.12) the lemma follows.

Lemma 3.2.3: If the measure μ concentrates all its mass on the zeros of $(1-x^2)P'_d(x)$, whose $P_d(x)$ is the Legendre's polynomial of degree d then the nearly optimal design measure $\bar{\xi}^A$ is the exact optimal design measure $\bar{\xi}$.

Proof: In this case $\sup_x \sum_{i=0}^d \ell_i^2(x) = 1$ and hence the result.

Lemma 3.2.4: If $\mu = \xi_u$ then $\bar{\xi}^A$ puts mass proportional to

$$|P_d(x_i)|^{-1} \sqrt{\frac{2}{(d+1)(2d+1)} - \frac{|P_d(x_i)|^{-2}}{d^2(d+1)^2}}$$

at the zeros x_i ($i = 0, 1, \dots, d$) of $(1-x^2)P'_d(x)$, where $P_d(x)$ is Legendre's polynomial of degree d and

$$v_d(\bar{\xi}^A, \mu) = \left(\sum_{i=0}^d \sqrt{h_i} \right)^2,$$

where

$$h_i = \frac{2|P_d(x_i)|^{-2}}{(d+1)(2d+1)} - \frac{|P_d(x_i)|^{-4}}{d^2(d+1)^2} \quad (i = 0, 1, \dots, d).$$

Further,

$$v_d(\bar{\xi}^A, \mu) - v_d(\bar{\xi}, \mu) \leq (\sum \sqrt{h_i})^2 g(d), \quad (3.2.15)$$

where for even d , $g(d) \leq \frac{5d^2+6d+2}{2(d^3-3d^2-3d-1)}$

and for odd d , $g(d) \leq \frac{5d^3-4d^2+25d-8}{2(d^4+8d^2-12d+4)}$.

Proof: Since x_i 's are the zeros of $(1-x^2)P_d'(x)$ it follows from Lobatto quadrature formula that

$$\int_{-1}^1 \ell_i^2(x) \frac{dx}{2} = \frac{2|P_d(x_i)|^{-2}}{(d+1)(2d+1)} \quad \text{and}$$

$$\left\{ \int_{-1}^1 \ell_i(x) \frac{dx}{2} \right\}^2 = \left\{ \frac{|P_d(x_i)|^{-2}}{d(d+1)} \right\}^2.$$

Therefore,

$$h_i = \frac{2|P_d(x_i)|^{-2}}{(d+1)(2d+1)} - \left\{ \frac{|P_d(x_i)|^{-2}}{d(d+1)} \right\}^2$$

and the mass distribution of $\bar{\xi}^A$ as stated in the theorem follows.

Also, from (3.2.13)

$$\begin{aligned} \phi(x, \bar{\xi}^A, \mu) &= (\Sigma \sqrt{h_i})^2 \left[\sum_{i=0}^d \sum_{j=0}^d \frac{\ell_i(x)}{\sqrt{h_i}} \frac{\ell_j(x)}{\sqrt{h_j}} \int_{-1}^1 \ell_i(x) \ell_j(x) \frac{dx}{2} \right. \\ &\quad \left. - \left\{ \sum_{i=0}^d \frac{\ell_i(x)}{\sqrt{h_i}} \int_{-1}^1 \ell_i(x) \frac{dx}{2} \right\}^2 \right] \\ &\leq (\Sigma \sqrt{h_i})^2 \left[\sum_{i=0}^d \sum_{j=0}^d \frac{\ell_i(x)}{\sqrt{h_i}} \frac{\ell_j(x)}{\sqrt{h_j}} \int_{-1}^1 \ell_i(x) \ell_j(x) \frac{dx}{2} \right] \\ &= \frac{(\Sigma \sqrt{h_i})^2}{d(d+1)} \left[\sum_{i=0}^d \frac{\ell_i^2(x)}{h_i |P_d(x_i)|^2} - \frac{1}{(2d+1)} \left\{ \sum_{i=0}^d \frac{\ell_i(x)}{\sqrt{h_i} P_d(x_i)} \right\}^2 \right] \\ &\leq \frac{(\Sigma \sqrt{h_i})^2}{d(d+1)} \sum_{i=0}^d \frac{\ell_i^2(x)}{h_i |P_d(x_i)|^2}. \end{aligned}$$

Now,

$$h_i |p_d(x_i)|^2 = \frac{2}{(d+1)(2d+1)} - \frac{1}{d^2(d+1)^2 |p_d(x_i)|^2}.$$

Suppose d is even. Then

$$|p_d(x_i)|^2 \geq |p_d(0)|^2 = \left\{ \frac{1.3 \dots (d-1)}{2.4 \dots d} \right\}^2$$

and

$$\begin{aligned} \{d^2(d+1)^2 |p_d(x_i)|^2\}^{-1} &\leq \frac{1}{d^2(d+1)^2} \left\{ \frac{2.4 \dots d}{1.3 \dots (d-1)} \right\}^2 \\ &= \frac{1}{d^3} \left[\frac{d}{(d+1)^2} \left\{ \frac{2.4 \dots d}{1.3 \dots (d-1)} \right\}^2 \right] \leq \frac{\pi}{2d^3} \leq \frac{2}{d^3}. \end{aligned}$$

Therefore,

$$h_i |p_d(x_i)|^2 \geq \frac{2(d^3 - 2d^2 - 3d - 1)}{d^3(d+1)(2d+1)}$$

and

$$\sup_x \phi(x, \bar{\xi}^A, \mu) \leq \left(\sum_{i=0}^d \sqrt{h_i} \right)^2 \frac{(2d^3 + d^2)}{2(d^3 - 2d^2 - 3d - 1)}$$

$$\text{since } \sup_x \sum_{i=0}^d \ell_i^2(x) = 1.$$

Similarly when d is odd,

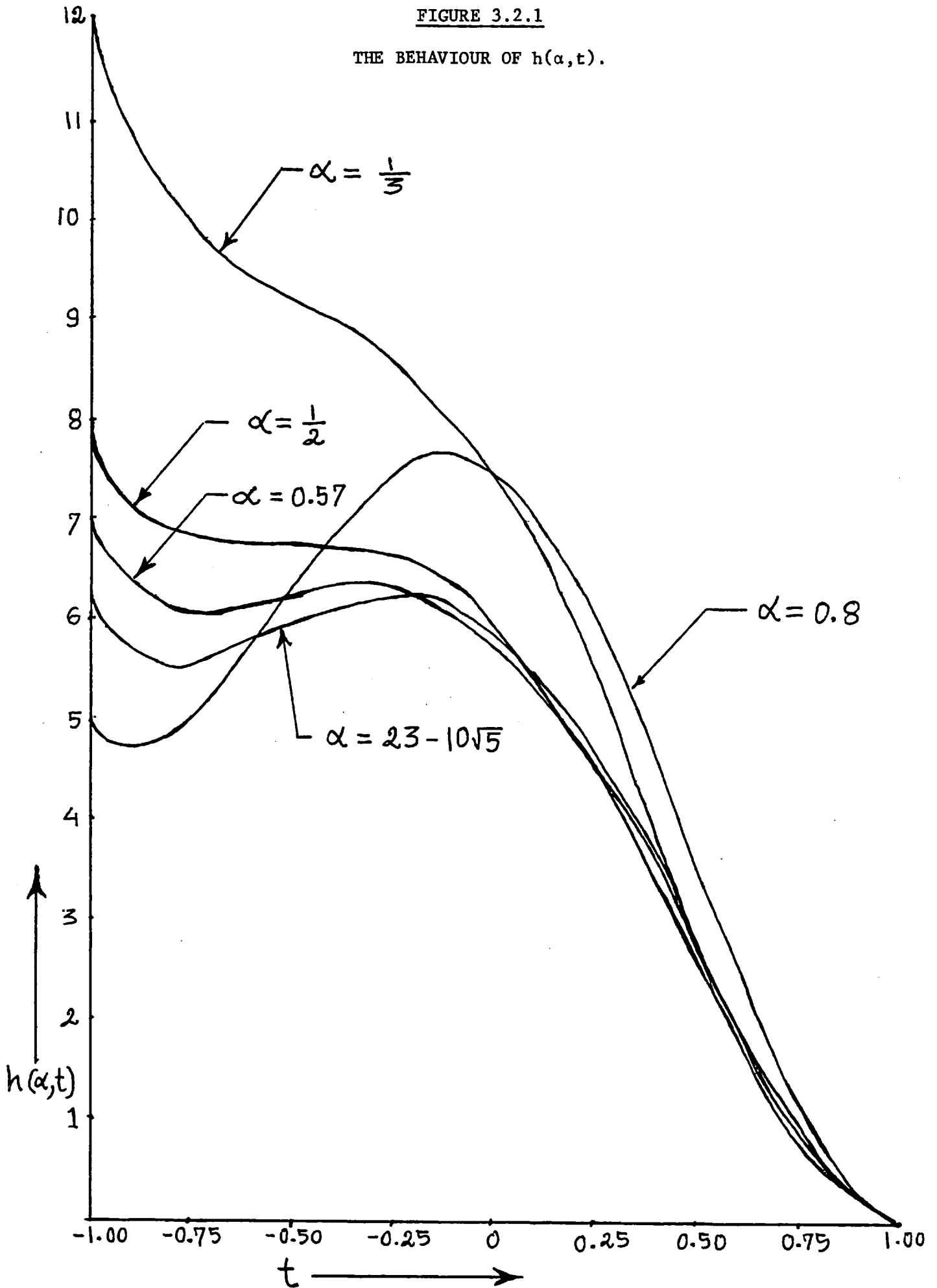
$$h_i |p_d(x_i)|^2 \geq \frac{2[d^4 + 8d^2 - 12d + 4]}{d^2(d+1)^3(2d+1)}$$

and

$$\sup_x \phi(x, \bar{\xi}^A, \mu) \leq \left(\sum_{i=0}^d \sqrt{h_i} \right)^2 \frac{d(d+1)^2(2d+1)}{2(d^4 + 8d^2 - 12d + 4)}.$$

Therefore, (3.2.15) follows.

FIGURE 3.2.1
THE BEHAVIOUR OF $h(\alpha, t)$.



3.3 Application of hierarchical ordering of criteria

The hierarchical ordering of various optimality criteria may be useful in discriminating between designs that are equally good under a particular criterion. Some simple examples are provided to illustrate the idea. The first two examples are chosen from the weighing design problems but have equivalent formulation in terms of first-order polynomial models in response surface designs [see Galil, Z. and Kiefer, J. (1980)].

Example 3.3.1: Consider the problem of determining the weights of four objects by a spring balance in four observations or weighing operations. Observations are independent with variance σ^2 . Let the designs D_1 and D_2 have design matrices $\underline{X}_1$ and $\underline{X}_2$, respectively, with

$$\underline{X}_1 = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}, \quad \underline{X}_2 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix},$$

where

$$(\underline{X}_i)_{j,l} = \begin{cases} 1 & \text{if } l\text{-th object is weighed in } j\text{-th operation,} \\ 0 & \text{otherwise.} \end{cases} \quad (i = 1, 2,)$$

It is known that both the designs are D-optimum with $|\underline{X}_i' \underline{X}_i| = 9$ ($i = 1, 2$). However,

$$(\underline{X}'_1 \underline{X}_1)^{-1} = \frac{1}{9} \begin{bmatrix} 7 & -2 & -2 & -2 \\ -2 & 7 & -2 & -2 \\ -2 & -2 & 7 & -2 \\ -2 & -2 & -2 & 7 \end{bmatrix}, \quad (\underline{X}'_2 \underline{X}_2)^{-1} = \frac{1}{9} \begin{bmatrix} 7 & -2 & -2 & -1 \\ -2 & 7 & -2 & -1 \\ -2 & -2 & 7 & -1 \\ -1 & -1 & -1 & 4 \end{bmatrix}$$

Therefore, $\text{tr}(\underline{X}'_1 \underline{X}_1)^{-1} = \frac{28}{9}$ and $\text{tr}(\underline{X}'_2 \underline{X}_2)^{-1} = \frac{25}{9}$.

Hence if the A-optimality criterion is applied to the set of D-optimal designs, the design D_2 is obtained as the unique optimal design.

Example 3.3.2: Consider the problem of determining the weights of three objects by a chemical balance in three independent and identically distributed observations or weighing operations. It is known from Mood (1946) that for this problem there are three D-optimal designs D_1 , D_2 and D_3 having design matrices $\underline{X}_1$, $\underline{X}_2$ and $\underline{X}_3$, respectively, with

$$\underline{X}_1 = \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{bmatrix}, \quad \underline{X}_2 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{bmatrix}, \quad \underline{X}_3 = \begin{bmatrix} 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{bmatrix},$$

where $(\underline{X}_i)_{j\ell} = \begin{cases} 1 & \text{if } \ell\text{-th object is in left pan in } j\text{-th operation,} \\ -1 & \text{" " " " " " " right " " " "} \\ 0 & \text{" " " " is not included " " " "} \end{cases}$

and $|\underline{X}'_i \underline{X}_i| = 16$ ($i = 1, 2, 3$). However,

$$(\underline{X}'_1 \underline{X}_1)^{-1} = \frac{1}{8} \begin{bmatrix} 3 & 1 & 0 \\ 1 & 3 & 0 \\ 0 & 0 & 4 \end{bmatrix}, \quad (\underline{X}'_2 \underline{X}_2)^{-1} = \frac{1}{4} \begin{bmatrix} 2 & 1 & -1 \\ 1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}, \quad (\underline{X}'_3 \underline{X}_3)^{-1} = \frac{1}{4} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

and hence if the A-optimality criterion is applied to the set of

D-optimal designs the design D_1 is obtained as the unique optimal

design since $\text{tr}(\underline{X}'_1 \underline{X}_1)^{-1} = \frac{5}{4}$ and $\text{tr}(\underline{X}'_2 \underline{X}_2)^{-1} = \text{tr}(\underline{X}'_3 \underline{X}_3)^{-1} = \frac{6}{4}$. Let the

weights of the objects be w_1 , w_2 and w_3 . Consider the linear combination

3
 $\sum_{i=1}^3 a_i w_i$ where each a_i can take the values 0, 1 or -1. Then
 $\max_a \text{var}(\sum_{i=1}^3 a_i \hat{w}_i)$ for D_1 is smaller than that for D_2 and D_3 , that is,
 under the G-optimality criterion also D_1 is superior to D_2 and D_3 .

Example 3.3.3: Consider the simple linear regression model

$$E\{y(x)\} = \beta_0 + \beta_1 x_1 + \beta_2 x_2,$$

where $\underline{x} = (x_1, x_2) \in [-1, 1]^2$.

Suppose the parameters are to be estimated by the least squares method using a three point discrete design. Then under the assumption of independent and identically distributed observations, any design with equal weights on any two of vertices of $[-1, 1]^2$ and a point on the opposite edge is D-optimal. Thus there is an infinite family of D-optimal designs. Now consider the behaviour of these designs when the observations are correlated. As a typical situation consider the variance-covariance function given by

$$\text{cov}(y(\underline{x}), y(\underline{z})) = \sigma^2 e^{-\lambda \sum_{i=1}^2 |x_i - z_i|} \quad (\lambda > 0).$$

Without loss of generality let $\sigma^2 = 1$. For a design with support points (x_{1i}, x_{2i}) ($i = 1, 2, 3$) the corresponding matrix of 'independent variables' is given by the 3×3 matrix

$$\underline{X} = \begin{bmatrix} 1 & x_{11} & x_{21} \\ 1 & x_{12} & x_{22} \\ 1 & x_{13} & x_{23} \end{bmatrix}.$$

The generalized variance of the least squares estimates of the parameters is then given by

$$\text{G.V.}(\underline{\ell}) = |\underline{X}' \underline{S} \underline{X}| / |\underline{X}' \underline{X}|^2 = |\underline{S}| / |\underline{X}|^2,$$

where $\underline{S}$ is the corresponding variance-covariance matrix. The generalized variance of the best linear unbiased estimates of the parameters is

given by

$$G.V. (b) = |(\underline{X}'\underline{S}^{-1}\underline{X})^{-1}| = |\underline{S}|/|\underline{X}|^2.$$

Consider the designs ξ_1 and ξ_x supported on $(-1,1)$, $(1,-1)$, $(1,1)$ and $(-1,-1)$, $(1,-1)$, $(x,1)$ respectively. Let $\underline{S}_1$ and $\underline{S}_x$ be the corresponding variance-covariance matrices. Then,

$$|\underline{S}_1| = \begin{vmatrix} 1 & w & w^2 \\ w & 1 & w \\ w^2 & w & 1 \end{vmatrix} = 1 - 2w^2 + w^4,$$

where $w = e^{-2\lambda}$,

$$|\underline{S}_x| = \begin{vmatrix} 1 & (e^{-\lambda})^2 & (e^{-\lambda})^{3+x} \\ (e^{-\lambda})^2 & 1 & (e^{-\lambda})^{3-x} \\ (e^{-\lambda})^{3+x} & (e^{-\lambda})^{3-x} & 1 \end{vmatrix} = 1 - w^2 + 2w^4 - w^{3-x} - w^{3+x}.$$

Thus $|\underline{S}_x|$ is symmetric in x . Now since $0 \leq w \leq 1$ and $0 \leq x \leq 1$ it follows that

$$w \leq w^x \leq 1$$

and

$$\frac{(1-w)^2}{w} \geq \frac{(1-w^x)^2}{w^x},$$

which implies that

$$|\underline{S}_x| \geq |\underline{S}_1|.$$

Therefore, regardless of the value of λ , under the type of variance-covariance function assumed, within the class of D-optimal designs, those supported on three vertices of $[-1,1]^2$ minimize the generalized variance of the least squares estimates and the best linear unbiased estimates. Let ξ_2 , ξ_3 and ξ_4 be the designs with support points

$\{(-1,-1), (1,-1), (-1,1)\}$, $\{(-1,-1), (1,1), (-1,1)\}$ and $\{(1,-1), (1,1), (-1,1)\}$, respectively. It is interesting to note that if the variance-covariance function is given by

$$\text{cov}(y(\underline{x}), y(\underline{z})) = \sigma^2 e^{-\lambda \{(x_1 - z_1)^2 + (x_2 - z_2)^2\}^{1/2}}$$

then for all $\lambda \geq 1.032$ the designs ξ_i ($i = 1, 2, 3, 4$) have smaller generalized variances than the other D-optimal designs. Let us assume that the variance-covariance function may only be of the first type considered. Then on applying the criterion of minimizing generalized variance or equivalently robustness against correlation, to the set of D-optimal designs a subset consisting of ξ_i ($i = 1, \dots, 4$) is obtained. From symmetry considerations or otherwise it can be seen that these four designs are equally good under A-optimality, E-optimality or the integrated variance criteria. However, it is possible to discriminate between these designs if robustness against possible quadratic bias in the model is considered. Suppose the true model is given by

$$E\{y(\underline{x})\} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{22} x_2^2.$$

Then from the results of Box and Draper (1959) it can be shown that the designs ξ_1 and ξ_3 have larger expected integrated square error than ξ_2 and ξ_4 if β_{11} , β_{12} and β_{22} are of the same magnitude and sign. ξ_1 and ξ_3 are preferable to ξ_2 and ξ_4 if β_{11} , β_{12} and β_{22} are of the same magnitude but β_{12} is of a different sign.

The examples show how it is possible to reduce the class of designs to be considered in any given experimental situation by applying an hierarchy of optimal criteria. An application of this idea is to be found in Kiefer and Wynn (1980) where a criterion is used to select a subset of designs optimal under correlated error structure from the set of designs that are optimal under the criterion when the observations are independent and identically distributed.

CHAPTER 4

SECOND-ORDER AND THIRD-ORDER ROTATABLE DESIGNS

4.1 Introduction

A response surface design involving k quantitative factors may be considered as a set of N points in k -dimensional space, each point representing a particular combination of the levels of the factors. Let $x_1, \dots, x_k$ denote the standardized levels of the factors and let $y(\underline{x})$ denote the response at $\underline{x}$, where $\underline{x} = (x_1, \dots, x_k)$. It is assumed that the response is a random variable with expected value $\eta(\underline{x})$, where

$$\eta(\underline{x}) = b_0 + b_1 x_1 + \dots + b_k x_k + b_{11} x_1^2 + \dots + b_{kk} x_k^2 \quad (4.1.1)$$

$$+ b_{12} x_1 x_2 + \dots + b_{k-1,k} x_{k-1} x_k + \dots$$

includes all terms up to and including order d . In matrix notation

$$\eta(\underline{x}) = \underline{x}'^{[d]} \underline{b}, \quad (4.1.2)$$

where $\underline{x}' = (1, x_1, \dots, x_k)$, $\underline{x}'^{[d]}$ is the derived power vector of degree d , that is, $\underline{x}'^{[d]} \underline{x}^{[d]} = (\underline{x}' \underline{x})^d$ and $\underline{b}$ contains all the $b_{1\alpha_1 \dots k\alpha_k}$'s along with suitable multipliers, in order that (4.1.1) equals (4.1.2). Let $\underline{x}_u = (x_{1u}, \dots, x_{ku})$ ($u = 1, \dots, N$) be the design points with y_u 's the corresponding responses. The design is said to be of order d if it allows the estimation of all the coefficients in (4.1.1). If the coefficients are estimated by the method of least squares and if the y_u 's are uncorrelated with a common variance σ^2 , then from the least squares theory the variance of the estimated response $\hat{y}(\underline{x})$ at $\underline{x}$ is given by

$$\text{var}\{\hat{y}(\underline{x})\} = \sigma^2 \underline{x}'^{[d]} (\underline{X}' \underline{X})^{-1} \underline{x}^{[d]}, \quad (4.1.3)$$

where $\underline{X}$ is the $N \times \binom{k+d}{k}$ matrix of 'independent variables', that is,

$$\underline{X}' = (\underline{x}_1^{[d]}, \dots, \underline{x}_N^{[d]}). \quad (4.1.4)$$

4.2 Rotatable designs

Rotatable designs, introduced by Box and Hunter (1957), have the property that the variance of the estimated response at any point is a function of the distance of the point from the origin of the design.

For rotatable designs (4.1.3) is constant on spheres centred at the origin of the design. Suppose $\underline{z} = \underline{M}\underline{x}$, where $\underline{z}' = (1, z_1, \dots, z_k)$, $\underline{x}' = (1, x_1, \dots, x_k)$ and $\underline{M}$ is an orthonormal $(k+1) \times (k+1)$ matrix consisting of an arbitrary orthonormal matrix H bordered by a first row $\underline{u}' = (1, 0, \dots, 0)$ and a first column $\underline{u}$. Then from (4.1.3)

$$\begin{aligned} \text{var}\{\hat{y}(\underline{z})\} &= \sigma^2 \underline{z}'^{[d]} (\underline{X}'\underline{X})^{-1} \underline{z}^{[d]} \\ &= \sigma^2 \underline{x}'^{[d]} \underline{M}'^{[d]} (\underline{X}'\underline{X})^{-1} \underline{M}^{[d]} \underline{x}^{[d]} \\ &= \sigma^2 \underline{x}'^{[d]} (\underline{M}'^{[d]} \underline{X}'\underline{X}\underline{M}^{[d]})^{-1} \underline{x}^{[d]}, \end{aligned} \quad (4.2.1)$$

where $\underline{M}^{[d]}$ is the d -th Schläflian matrix such that $\underline{z}^{[d]} = \underline{M}^{[d]} \underline{x}^{[d]}$.

Therefore, for a rotatable design it is required that (4.2.1) and (4.1.3) be identically equal for every $\underline{x}$ and every $\underline{M}$ or equivalently

$$\underline{M}'^{[d]} \underline{X}'\underline{X}\underline{M}^{[d]} = \underline{X}'\underline{X}, \quad (4.2.2)$$

for every orthonormal matrix $\underline{M}$ of the form described. Let

$$[1^{\alpha_1}, \dots, k^{\alpha_k}] = N^{-1} \sum_{u=1}^N \begin{matrix} \alpha_1 & & \alpha_k \\ x_{1u} & \dots & x_{ku} \end{matrix}$$

and let $\underline{t}' = (1, t_1, \dots, t_k)$. Box and Hunter (1957) showed that

$$\begin{aligned}
Q &= N^{-1} \underline{t}'^{[d]} \underline{X}' \underline{X} \underline{t}^{[d]} \\
&= N^{-1} \sum_{u=1}^N (1 + t_{11} x_{1u} + \dots + t_{k1} x_{ku})^{2d}
\end{aligned} \tag{4.2.3}$$

is the generating function of moments of order $2d$ or less of a design and a design is rotatable if and only if

$$\lambda_{\alpha}^{[\alpha_1, \dots, \alpha_k]} = \begin{cases} 0 & \text{if one or more of the } \alpha_i \text{ are odd,} \\ \lambda_{\alpha} \prod_{i=1}^k \alpha_i! / \{2^{\alpha/2} \prod_{i=1}^k (\frac{1}{2}\alpha_i)!\} & \text{if all the } \alpha_i \text{ are even,} \end{cases} \tag{4.2.4}$$

where $\alpha = \sum_{i=1}^k \alpha_i$ and $0 \leq \alpha \leq 2d$.

A set of points is said to be a rotatable arrangement of order d if (4.2.4) is satisfied. A rotatable arrangement is a rotatable design only if the arrangement forms a nonsingular design.

4.3 Construction of second-order rotatable designs in k dimensions from those in $(k-2)$ dimensions

For a second-order rotatable arrangement in k dimensions (4.2.4) reduces to

$$\sum_{u=1}^N x_{iu}^2 = A \quad (i = 1, \dots, k), \tag{4.3.1}$$

$$\sum_{u=1}^N x_{iu}^4 = 3 \sum_{u=1}^N x_{iu}^2 x_{ju}^2 = 3B \quad (i \neq j; i, j = 1, \dots, k),$$

all other sums of powers and products up to order four being zero. From Box and Hunter (1957), the arrangement forms a second-order rotatable design if in addition

$$\frac{NB}{A} > \frac{k}{(k+2)}, \tag{4.3.2}$$

which can always be satisfied by a rotatable arrangement merely by the addition of centre points.

A large number of methods for constructing second-order rotatable designs are now available. Some of these were given by Box and Hunter (1957), Bose and Draper (1959), Debaum (1959), Box and Behnken (1960a,b), Draper (1960a), Das (1961), Das and Narasimham (1962), Thaker (1962), Tyagi (1964), Herzberg (1967b), Draper and Herzberg (1968). In particular, Draper (1960a) presented a method of constructing a second-order rotatable design in k dimensions from a second-order rotatable design in $(k-1)$ dimensions. Draper's method may be used only for some restrictive classes of given designs. Herzberg (1967b) presented an alternative method which works in all cases and which does not need to discard the results of the experiments that may have already been performed according to the $(k-1)$ -dimensional design.

Two simple methods of constructing second-order rotatable designs in k dimensions from second-order rotatable designs in $(k-1)$ dimensions are presented here. The methods work in all cases and, as with Herzberg's method, the results of the experiments performed according to the $(k-1)$ -dimensional design need not be discarded.

Let $S(z_1, \dots, z_k)$ denote all permutations of $(\pm z_1, \dots, \pm z_k)$ and let $2^{-P}S(a, \dots, a)$ be any one of the smallest 2^{-P} 'Resolution V' fractions of the two-level factorial design $S(a, \dots, a)$. Further let T be the transformation defined by $T(z_1, z_2, \dots, z_k) = (z_2, \dots, z_k, z_1)$.

Suppose for the set of N' points $\underline{x}_u = (x_{1u}, \dots, x_{k-1,u})$ ($u = 1, \dots, N'$) in $(k-1)$ -dimensions, (4.3.1) is satisfied. Now consider the set of k -dimensional points given by $2^{-P}S(b, \dots, b)$ and for $u = 1, \dots, N'$:

$$\begin{aligned}
& (x_{1u}, x_{2u}, x_{3u}, \dots, x_{k-2,u}, x_{k-1,u}, 0), \\
& (x_{1u}, x_{2u}, x_{3u}, \dots, x_{k-2,u}, 0, x_{k-1,u}), \\
& \quad \vdots \\
& (x_{1u}, 0, x_{3u}, \dots, x_{k-2,u}, x_{k-1,u}, x_{2u}), \\
& (0, x_{2u}, x_{3u}, \dots, x_{k-2,u}, x_{k-1,u}, x_{1u}).
\end{aligned}$$

The number of points in this set is $N = N'k + 2^{k-p}$. For this derived set of points

$$\sum_{u=1}^N x_{iu}^2 = (k-1)A + 2^{k-p}b^2 \quad (i = 1, \dots, k), \quad (4.3.3)$$

$$\sum_{u=1}^N x_{iu}^4 = (k-1)3B + 2^{k-p}b^4 \quad (i = 1, \dots, k),$$

$$\sum_{u=1}^N x_{iu}^2 x_{ju}^2 = (k-2)B + 2^{k-p}b^4 \quad (i \neq j; i, j = 1, \dots, k),$$

where all other sums of powers and products up to order four are zero.

Therefore, the derived set forms a second-order rotatable arrangement if

$$b = (3B/2^{k-p+1})^{1/4}. \quad (4.3.4)$$

Also consider the set of k -dimensional points given by

$$\{T^\ell(x_{1u}, \dots, x_{k-1,u}, 0); \quad \ell = 1, \dots, k; \quad u = 1, \dots, N'\}$$

and $2^{-p}S(b, \dots, b)$. This set also has $N = kN' + 2^{k-p}$ points and satisfies (4.3.3). Therefore, this set forms a second-order rotatable arrangement if b is chosen according to (4.3.4).

Both the k -dimensional arrangements described would almost always form nonsingular designs. If not, some centre points may be added to obtain the designs. If the $(k-1)$ -dimensional arrangement is nonsingular then the derived k -dimensional arrangements are necessarily non-singular. If the given arrangement consists of combinations of symmetric point

sets then both the methods described would lead to the same k -dimensional designs. Otherwise, distinct designs would be obtained by the two methods. As an example consider the case $k = 3$. Suppose the given 2-dimensional arrangement consists of 8 equally spaced points on a circle of radius ρ centred at the origin given by $S(\rho, 0)$ and $S(\frac{\rho}{\sqrt{2}}, \frac{\rho}{\sqrt{2}})$. Then the 3-dimensional arrangements derived by the two methods are identical and is given by

$$S(\frac{\rho}{\sqrt{2}}, \frac{\rho}{\sqrt{2}}, 0), S(\frac{3^{1/4}}{2} \rho, \frac{3^{1/4}}{2} \rho, \frac{3^{1/4}}{2} \rho)$$

and 2 sets of $S(\rho, 0, 0)$. On the other hand if the given arrangement consists of the vertices of a hexagon, the derived designs would be different.

For small values of k the methods described are nearly as efficient as Herzberg's method in terms of the number of experiments required. However, for large values of k , these methods are likely to be of theoretical interest only since the derived designs would require too many experiments. It is interesting to note that some new classes of 3-dimensional second-order rotatable designs with 23 points may be obtained by applying these methods to a second-order rotatable arrangement in 2 dimensions with 5 equally spaced points on a circle.

It may be desirable to extend a $(k-\ell)$ -dimensional second-order rotatable design into a k -dimensional second-order rotatable design, for some $\ell \in \{1, \dots, k-1\}$. In such a situation, the k -dimensional design may be derived by ℓ iterative application of any of the methods considered earlier. Since Draper's method cannot always be used and since it may be desirable not to discard the results of the experiments that may have been performed according to the $(k-\ell)$ -dimensional design, Herzberg's method appears to be the only one which on successive application may provide a k -dimensional design with a practicable number of experiments.

However, there exists a method for extending any given $(k-l)$ -dimensional second-order rotatable design directly into a k -dimensional second-order rotatable design without discarding the results of the experiments already performed. The method uses balanced incomplete block designs to derive the k -dimensional points. When an appropriate block design with a small number of blocks exists, the method can provide a design with fewer points than the design derived by successive application of Herzberg's method or by Draper's method when it works. Construction of second-order rotatable designs through balanced incomplete block designs has also been considered by Box and Behnken (1960b), Das and Narasimham (1962), Das (1963), Raghavarao (1963), Nigam and Das (1966). However, the problem of obtaining methods for extending the dimensionality of a rotatable design was not considered by them.

Let $(x_{1u}, \dots, x_{k-l,u})$ ($u = 1, \dots, N'$) be a second-order rotatable arrangement in $(k-l)$ dimensions. The problem is to obtain a k -dimensional second-order rotatable arrangement such that the points $(x_{1u}, \dots, x_{k-l,u}, 0, \dots, 0)$ ($u = 1, \dots, N'$) are included in the arrangement.

Let BIB (t, b, r, s, λ) denote a balanced incomplete block design with t treatments in b blocks of size s , with r and λ representing the number of occurrences of each treatment and each pair of treatments. To each block associate the points $(\pm h_1, \dots, \pm h_t)$, where each h_i ($i = 1, \dots, t$) has the value a or 0 corresponding to the presence or absence of the i -th treatment in the block. Let $\text{BIB} - a(t, b, r, s, \lambda)$ denote the set of all such points associated with the corresponding block design and let $2^{-q} \text{BIB} - a(t, b, r, s, \lambda)$ be any one of the smallest 2^{-q} fractions of 'Resolution V' of this set.

Now consider the balanced incomplete block designs with $t = k$ and $s = k-l$. Without loss of generality it is assumed that for the first block $h_i = a$ ($i = 1, \dots, k-l$) and $h_i = 0$ ($i = k-l+1, \dots, k$). For each block of BIB $(k, b, r, k-l, \lambda)$ and each u ($u = 1, \dots, N'$) there is an associated point generated by replacing the $(k-l)$ nonzero entries of $(h_1, \dots, h_k)$ by $x_{1u}, \dots, x_{k-l,u}$ in any order without repeating the x_{iu} 's ($i = 1, \dots, k-l$). Without loss of generality, let the x_{iu} 's be placed in the ascending order of the i 's in the first block. Let ABIB $(k, b, r, k-l, \lambda)$ denote the set of all such points generated from the corresponding block design using the given $(k-l)$ dimensional arrangement. The set ABIB $(k, b, r, k-l, \lambda)$ thus contains $(x_{1u}, \dots, x_{k-l,u}, 0, \dots, 0)$ ($u = 1, \dots, N'$).

Consider the set of $N = bN' + 2^{k-p}$ points in k dimensions given by ABIB $(k, b, r, k-l, \lambda)$ and $2^{-p}S(a, \dots, a)$. For this set the following conditions are satisfied:

$$\begin{aligned} \sum_{u=1}^N x_{iu}^2 &= rA + 2^{k-p} a^2 \quad (i = 1, \dots, k), \\ \sum_{u=1}^N x_{iu}^4 &= r3B + 2^{k-p} a^4 \quad (i = 1, \dots, k), \\ \sum_{u=1}^N x_{iu}^2 x_{ju}^2 &= \lambda B + 2^{k-p} a^4 \quad (i \neq j; \quad i, j = 1, \dots, k), \end{aligned} \tag{4.3.5}$$

where all other sums of powers and products up to order four are zero.

Therefore, the arrangement satisfies (4.3.1) if

$$a = \{(r-\lambda)3B/2^{k-p+1}\}^{1/4}. \tag{4.3.6}$$

The k -dimensional arrangement, with centre points if necessary, therefore forms a second-order rotatable design if a is chosen according to (4.3.6).

The method described can be quite useful in practice. For example consider the case $k = 7$ and $k-l = 3$. If the 3-dimensional design is of the 'cube + cross-polytope' type, then $N' = 14$. The design derived by the method described consists of the $7N' + 64$ points of ABIB $(7,7,3,3,1)$ and $2^{-1}S(a, \dots, a)$. The design in 7 dimensions obtained by successive application of Herzberg's method requires $N' + 180$ points which is considerably larger than $7N' + 64$ when $N' = 14$. As another example consider the case $k = 11$, $k-l = 5$. The design derived by the method described consists of the $11N' + 128$ points of ABIB $(11,11,5,5,2)$ and $2^{-4}S(a, \dots, a)$. The design derived by successive application of Herzberg's method requires $N' + 658$ points, which is considerably larger than $11N' + 128$ when $N' = 26$, the minimal value for N' .

As an alternative, consider the k -dimensional arrangement given by ABIB $(k, b, r, k-l, \lambda)$ and $2^{-q}BIB - a(k, b_1, r_1, s_1, \lambda_1)$ with $r_1 < 3\lambda_1$. This set has $N = bN' + b_1 2^{s_1-1-q}$ points and satisfies the following relations:

$$\begin{aligned} \sum_{u=1}^N x_{iu}^2 &= rA + r_1 2^{s_1-1-q} a^2 \quad (i = 1, \dots, k), \\ \sum_{u=1}^N x_{iu}^4 &= r3B + r_1 2^{s_1-1-q} a^4 \quad (i = 1, \dots, k), \\ \sum_{u=1}^N x_{iu}^2 x_{ju}^2 &= \lambda B + \lambda_1 2^{s_1-1-q} a^4 \quad (i \neq j; i, j = 1, \dots, k), \end{aligned} \quad (4.3.7)$$

where all other sums of powers and products up to order four are zero. Therefore, this arrangement forms a second-order rotatable design if

$$a = \left\{ \frac{3B(r-\lambda)}{(3\lambda_1 - r_1) 2^{s_1-1-q}} \right\}^{1/4}. \quad (4.3.8)$$

For example, when $k = 11$, $k-l = 5$, the $11N' + 176$ points of ABIB $(11,11,5,5,2)$ and 2^{-1} BIB - $a(11,11,5,5,2)$ form a second-order rotatable design in 11 dimensions if a is chosen to satisfy (4.3.8).

If N' is the number of points in a $(k-l)$ -dimensional design, then $N' + 2^{k-p} + 2k+2$ points are needed in the k -dimensional design derived by Herzberg's method. Therefore, when k and l are both large the design in k dimensions derived from a $(k-l)$ -dimensional design by successive application of Herzberg's method is likely to require more experiments than the designs derived by the methods described if a suitable balanced incomplete block design with a small number of blocks exists. If such a suitable block design does not exist, Herzberg's method could be applied iteratively until the dimensions are such that the existence of a balanced incomplete block design with small number of blocks is ensured. These methods are useful also in the actual performance of experiments. If, after performing the experiments according to a second-order rotatable design in $(k-l)$ factors, the experimenter feels that l more factors should have been included, he can then proceed by the methods described without discarding the original results.

The designs derived by the method may also be of use when certain $(k-l)$ -subsets of the k factors are of greater interest than others. When possible, these subsets may be identified with some of the $(k-l)$ -dimensional rotatable designs contained in the derived k -dimensional design.

Some of the designs derived by the methods described are displayed in Table 4.3.1. Only the nature of the derived point sets are indicated rather than the actual point sets since these depend on the given $(k-l)$ -dimensional arrangements. The number of experiments required by these designs may be compared with the number of experiments in the

TABLE 4.3.1

Second-order rotatable designs in k dimensions from
second-order rotatable designs in (k-2) dimensions

k-2	k	Design	Number of points	Type of point sets	Number of points needed by Herzberg's method	Number of points needed by Draper's method
2	4	1	$6N' + 16$	ABIB (4,6,3,2,1) $S(a,a,a,a)$	$N' + 42$	$4N' + 12$
	5	1	$10N' + 16$	ABIB (5,10,4,2,1) $2^{-1}S(a,\dots,a)$	$N' + 70$	$8N' + 28$
	6	1	$15N' + 32$	ABIB (6,15,5,2,1) $2^{-1}S(a,\dots,a)$	$N' + 116$	$16N' + 60$
3	7	1	$7N' + 64$	ABIB(7,7,3,3,1) $2^{-1}S(a,\dots,a)$	$N' + 180$	$16N' + 60$
4	7	1	$7N' + 64$	ABIB(7,7,4,4,2) $2^{-1}S(a,\dots,a)$	$N' + 154$	$8N' + 28$
5	11	1	$11N' + 128$	ABIB (11,11,5,5,2) $2^{-4}S(a,\dots,a)$	$N' + 658$	$64N' + 252$
		2	$11N' + 176$	ABIB(11,11,5,5,2) $2^{-1}BIB-a(11,11,5,5,2)$		
6	11	1	$11N' + 128$	ABIB(11,11,6,6,3)	$N' + 612$	$32N' + 124$
		2	$11N' + 176$	ABIB(11,11,6,6,3) $2^{-1}BIB-a(11,11,5,5,2)$		
	16	1	$16N' + 256$	ABIB(16,16,6,6,2) $2^{-8}S(a,\dots,a)$	$N' + 2042$	$2^{10}N' + 2^{12}-4$
7	15	1	$15N' + 256$	ABIB(15,15,7,7,3) $2^{-7}S(a,\dots,a)$	$N' + 1672$	$2^8N' + 2^{10}-4$
8	15	1	$15N' + 256$	ABIB(15,15,8,8,4) $2^{-7}S(a,\dots,a)$	$N' + 1590$	$2^7N' + 2^9-4$
9	13	1	$13N' + 256$	ABIB(13,13,9,9,6) $2^{-5}S(a,\dots,a)$	$N' + 868$	$16N' + 60$

designs derived by Herzberg's method and by Draper's method, assuming that his method also works.

4.4 Some new third-order rotatable designs

For a third-order rotatable arrangement, that is, when $d = 3$, condition (4.2.4) reduces to

$$\begin{aligned} \sum_{u=1}^N x_{iu}^2 &= A \quad (i = 1, \dots, k), \\ \sum_{u=1}^N x_{iu}^4 &= 3 \sum_{u=1}^N x_{iu}^2 x_{ju}^2 = 3B \quad (i \neq j; i, j = 1, \dots, k), \\ \sum_{u=1}^N x_{iu}^6 &= 5 \sum_{u=1}^N x_{iu}^4 x_{ju}^2 = 15 \sum_{u=1}^N x_{iu}^2 x_{ju}^2 x_{lu}^2 = 15C \quad (i \neq j \neq l; \\ &\quad i, j, l = 1, 2, \dots, k), \end{aligned} \quad (4.4.1)$$

where all other sums of powers and products up to order six are zero. From Gardiner, Grandage and Hader (1959), the arrangement forms a nonsingular design if in addition

$$\begin{aligned} \frac{NB}{A} &> \frac{k}{(k+2)}, \\ \frac{AC}{B} &> \frac{(k+2)}{(k+4)}. \end{aligned} \quad (4.4.2)$$

Draper (1960b) showed that (4.4.2) is satisfied by the arrangement if the points lie on two or more concentric circles centred at the origin.

Gardiner, Grandage and Hader (1959) used vertices of symmetric figures to construct third-order rotatable designs in three and four dimensions. Subsequently, Draper (1960b,c), Das and Narasimham (1962) and Herzberg (1964) constructed many new third-order rotatable designs. Designs in five and higher dimensions are provided by Das and

Narasimham (1962) who used a method involving balanced incomplete block designs and their complements and doubly balanced incomplete block designs. A similar method was used by Box and Behnken (1960b) to construct second-order rotatable designs.

Using these methods several new third-order rotatable designs are constructed in five, six, seven and eight dimensions. Many of these designs are of a sequential type and some require fewer observations than the known designs with minimal number of observations. A design is said to be of a sequential type if the experiments can be performed in blocks with the first block forming a lower-order rotatable design.

Let DBIB $(t, b, r, s, \lambda, \mu)$ denote a doubly balanced incomplete block design with μ representing the number of times any three treatments occur together and the other parameters as defined in Section 4.3. Let BIB-a (t, b, r, s, λ) and DBIB-a $(t, b, r, s, \lambda, \mu)$ denote the sets of point generated from the corresponding block designs in the manner illustrated in Section 4.3. If the block designs are irreducible, alternative notations are used to denote these point sets. For example, $S(a, a, a, 0)$ denotes DBIB-a $(4, 4, 3, 3, 2, 1)$. Let $2^{-P}S(a, \dots, a)$ be any one of the smallest 2^{-P} Resolution VII fractions of the factorial experiment $S(a, \dots, a)$.

The methods of construction require a suitable combination of 'symmetric' point sets such that conditions (4.4.1) and (4.4.2) are satisfied. For example, in five dimensions, consider the points given by $S(a, a, a, a, a)$, $S(d, d, d, d, d)$, $S(2d, 2d, 0, 0, 0)$ and 2 sets of $S(2a, 0, 0, 0, 0)$. Then

$$\begin{aligned}
\sum_{u=1}^N x_{iu}^2 &= 48a^2 + 96d^2 \quad (i = 1, \dots, 5), \\
\sum_{u=1}^N x_{iu}^4 &= 96a^4 + 288d^4 \quad (i = 1, \dots, 5), \\
\sum_{u=1}^N x_{iu}^2 x_{ju}^2 &= 32a^4 + 96d^4 \quad (i \neq j; i, j = 1, \dots, 5), \\
\sum_{u=1}^N x_{iu}^6 &= 288a^6 + 1056d^6 \quad (i = 1, \dots, 5), \\
\sum_{u=1}^N x_{iu}^4 x_{ju}^2 &= 32a^6 + 288d^6 \quad (i \neq j; i, j = 1, \dots, 5), \\
\sum_{u=1}^N x_{iu}^2 x_{ju}^2 x_{lu}^2 &= 32a^6 + 32d^6 \quad (i \neq j \neq l; i, j, l = 1, \dots, 5),
\end{aligned} \tag{4.4.3}$$

where all other sums of powers and products up to order six are zero.

Therefore, the points form a third-order rotatable arrangement if

$$\begin{aligned}
32a^6 + 288d^6 &= 3(32a^6 + 32d^6), \\
288a^6 + 1056d^6 &= 15(32a^6 + 32d^6).
\end{aligned} \tag{4.4.4}$$

Equation (4.4.4) is satisfied when $a^6 = 3d^6$. From Draper (1960b), the arrangement is also a non-singular design.

As another example consider the set of points given by $S(a, 0, 0, 0, 0)$, $S(b, b, 0, 0, 0)$ and two sets of $S(c, \dots, c)$ and $S(d, 0, 0, 0, 0)$, each. The set of points satisfy (4.4.1) if $b^2 = 2^{5/3}c^2$ and

$$a^4 + 2d^4 = (64 - 2^{13/3})c^4, \tag{4.4.5a}$$

$$a^6 + 2d^6 = 192c^6. \tag{4.4.5b}$$

Let $d^2 = ta^2$, $t \geq 0$. Then (4.4.5a) and (4.4.5b) are simultaneously satisfied if there is a non-negative t such that

$$f(t) = \frac{(1+2t^2)^3}{(1+2t^3)^2} = \frac{(64-2^{13/3})^3}{(192)^2}. \quad (4.4.6)$$

Clearly there exists a solution to (4.4.6) in the range $t \in (0,1)$ and it is in fact given by $t = 0.5372$. Thus for $b^2 = 2^{5/3}c^2$, $a^2 = 1.2039 c^2$ and $d^2 = 0.6467 c^2$ the arrangement obtained is a third-order rotatable design in five dimensions.

All the new designs obtained are displayed in Tables 4.4.1, 4.4.2, 4.4.3 and 4.4.4. For designs of the sequential type, possible blocking arrangements are illustrated with the first block forming a second-order rotatable design in each case.

In five dimensions, Das and Narasimham (1962) provided two non-sequential designs and one sequential design requiring 100, 150 and 192 experiments, respectively. Of all the designs in Table 4.4.1, Design 1 is the most efficient one in terms of the number of experiments required. This sequential design needs only 124 experiments instead of the 192 experiments needed for the sequential design of Das and Narasimham (1962). Further, Design 1 requires only 24 more points than the known design with minimal number of points among all third order rotatable designs in five dimensions.

In six dimensions, Das and Narasimham (1962) obtained three nonsequential and one sequential design with 260, 348, 360 and 260 points, respectively. Among the six-dimensional designs listed in Table 4.4.2, Design 1 is the most useful one. This sequential design requires only 236 points which is fewer than the number of points required by all the other six-dimensional third-order rotatable designs listed in the table and in Das and Narasimham (1962).

Das and Narasimham (1962) provided two nonsequential and one sequential designs in 7 dimensions with 238, 372 and 238 points, respectively. Note that the Design 1 of Table 4.4.3 is also listed by

TABLE 4.4.1

THIRD-ORDER ROTATABLE DESIGNS IN FIVE DIMENSIONS

Design number	Number of points	Block	Point sets	Replicates	Solutions in terms of a^2
1	124	1	$S(a, \dots, a)$ $S(2a, 0, 0, 0, 0)$	1 2	$d^2 = 3^{-1/3} a^2$
		2	$S(d, \dots, d)$ $S(2d, 2d, 0, 0, 0)$	1 1	
2	182	1	$S(a, \dots, a)$ $S(b, 0, 0, 0, 0)$ $S(c, 0, 0, 0, 0)$	1 1 2	$b^2 = 4.4832a^2$ $c^2 = 2.4393a^2$
		2	$S(d, d, d, d, 0)$ $S(f, f, 0, 0, 0)$	1 1	$d^2 = 0.5911a^2$ $f^2 = 2.6438a^2$
3	228	1	$S(a, \dots, a)$ $S(2a, 0, 0, 0, 0)$	1 2	
		2	$S(a, \dots, a)$ $S(2a, 0, 0, 0, 0)$ $S(2a, 2a, 0, 0, 0)$	3 4 1	
4	144		$S(a, \dots, a)$ $S(b, 0, 0, 0, 0)$ $S(c, 0, 0, 0, 0)$ $S(d, d, 0, 0, 0)$	2 2 2 1	$b^2 = 4.5597a^2$ $c^2 = 1.0630a^2$ $d^2 = 2^{5/3}a^2$
5	134		$S(a, \dots, a)$ $S(b, b, 0, 0, 0)$ $S(c, 0, 0, 0, 0)$ $S(d, 0, 0, 0, 0)$	2 1 1 2	$b^2 = 2^{5/3}a^2$ $c^2 = 1.2039a^2$ $d^2 = 0.6467a^2$

TABLE 4.4.2

THIRD-ORDER ROTATABLE DESIGNS IN SIX DIMENSIONS

Design number	Number of points	Block	Point sets	Replicates	Solutions in terms of a^2
1	236	1	$S(a, \dots, a)$ $S(2a, 2a, 0, 0, 0, 0)$	1 1	
		2	$S(a, \dots, a)$ $S(2a, 0, \dots, 0)$	1 4	
2	368	1	$S(a, \dots, a)$ $S(b, 0, \dots, 0)$ $S(c, 0, \dots, 0)$	1 1 1	$b^2 = 7.5421a^2$ $c^2 = 2.6684a^2$ $d^2 = 2a^2$
		2	$S(d, d, d, 0, 0, 0)$ $S(d, d, 0, 0, 0, 0)$	1 2	
3	272		$S(a, \dots, a)$ $S(b, b, b, 0, 0, 0)$ $S(c, 0, \dots, 0)$ $S(d, 0, \dots, 0)$	1 1 2 2	$b^2 = 2^{4/3}a^2$ $c^2 = 7.1773a^2$ $d^2 = 2.4260a^2$
4	348		$S(0, a, \dots, a)$ $S(b, b, 0, 0, 0, 0)$ $S(c, 0, \dots, 0)$ $S(d, 0, \dots, 0)$	1 1 4 4	$b^2 = 2(5)^{1/3}a^2$ $c^2 = 3.8859a^2$ $d^2 = 1.0970a^2$
5	324		$S(0, a, \dots, a)$ $S(b, b, 0, 0, 0, 0)$ $S(c, 0, \dots, 0)$ $S(d, 0, \dots, 0)$	1 1 2 4	$b^2 = 2(5)^{1/3}a^2$ $c^2 = 4.4293a^2$ $d^2 = 2.5484a^2$
6	312		$S(0, a, \dots, a)$ $S(b, b, 0, 0, 0, 0)$ $S(c, 0, \dots, 0)$ $S(d, 0, \dots, 0)$	1 1 1 4	$b^2 = 2(5)^{1/3}a^2$ $c^2 = 4.3659a^2$ $d^2 = 3.3968a^2$

TABLE 4.4.3

THIRD-ORDER ROTATABLE DESIGNS IN SEVEN DIMENSIONS

Design number	Number of points	Block	Point sets	Repli-cates	Solutions in terms of a^2
1	372	1	$2^{-1}S(a, \dots, a)$ $S(b, 0, \dots, 0)$ $S(c, 0, \dots, 0)$	1 1 1	$b^2 = 7.5421a^2$ $c^2 = 2.6678a^2$ $d^2 = 2a^2$
		2	$S(d, d, d, 0, 0, 0, 0)$	1	
2	240		$S(a, \dots, a)$ $S(2a, 2a, 0, \dots, 0)$ $S(2a, 0, \dots, 0)$	1 1 2	

TABLE 4.4.4

THIRD-ORDER ROTATABLE DESIGNS IN EIGHT DIMENSIONS

Design number	Number of points	Block	Point sets	Repli-cates	Solutions in terms of a^2
1	480 + n_0	1	$2^{-1}S(a, \dots, a)$ $S(2a, 2a, 0, \dots, 0)$	1 1	$b^2 \neq a^2$
		2	$2^{-1}S(b, \dots, b)$ $S(2b, 2b, 0, \dots, 0)$	1 1	
2	480 + n_0	1	DBIB-a(8, 14, 7, 4, 3, 1) $S(2a, 0, \dots, 0)$	1 1	$b^2 \neq a^2$
		2	DBIB-b(8, 14, 7, 4, 3, 1) $S(2b, 0, \dots, 0)$	1 1	
3	480 + n_0	1	$2^{-1}S(a, \dots, a)$ $S(2a, 2a, 0, \dots, 0)$	1 1	$b^2 \neq 2a^2$
		2	DBIB-b(8, 14, 7, 4, 3, 1) $S(2b, 0, \dots, 0)$	1 1	

them but only as a nonsequential design and the values of b^2 and c^2 seem to be in slight error.

In the designs of Table 4.4.4, n_0 is the number of centre-points. If the designs are performed non-sequentially then the centre points are not necessary. The designs of Das and Narasimham (1962) in 8 dimensions also require 480 points. Note that each block of the designs in Table 4.4.4 is a third-order rotatable arrangement.

4.5 A method for the construction of third-order rotatable designs in k dimensions

A simple method for the construction of third-order rotatable designs in k dimensions from third-order rotatable designs in (k-1) dimensions is presented. This method works only when the given designs satisfy some restrictive conditions. However, even if these conditions are not satisfied, the method may almost always be slightly modified to construct a k-dimensional design from the given design. Further, the results of the experiments performed according to the given design need not be discarded.

Suppose the set of N' points $\mathbf{x}_u = (x_{1u}, \dots, x_{k-1,u})$ ($u = 1, \dots, N'$) in (k-1)-dimensional space satisfy the condition (4.4.1). Now consider the $N = (2k-1)N' + 6$ points in k dimensions given by

$$(x_{1u}, \dots, x_{k-1,u}, 0) \quad (u = 1, \dots, N'),$$

$$\alpha(x_{1u}, \dots, x_{k-1,u}, \pm x_{iu}) \quad (i = 1, \dots, k-1; u=1, \dots, N'),$$

$$(0, \dots, 0, \pm\beta), \quad (0, \dots, 0, \pm\gamma) \text{ and } (0, \dots, 0, \pm\delta),$$

where $\alpha(a_1, \dots, a_k) = (\alpha a_1, \dots, \alpha a_k)$.

Then for this set of points

$$\sum_{u=1}^N x_{iu}^2 = \{1+2(k-1)\alpha^2\}A \quad (i = 1, \dots, k-1),$$

$$\sum_{u=1}^N x_{iu}^4 = 3\{1+2(k-1)\alpha^4\}B \quad (i = 1, \dots, k-1),$$

$$\sum_{u=1}^N x_{iu}^2 x_{ju}^2 = \{1+2(k-1)\alpha^4\}B \quad (i \neq j; i, j = 1, \dots, k-1),$$

$$\sum_{u=1}^N x_{iu}^6 = 15\{1+2(k-1)\alpha^6\}C \quad (i = 1, \dots, k-1),$$

$$\sum_{u=1}^N x_{iu}^4 x_{ju}^2 = 3\{1+2(k-1)\alpha^6\}C \quad (i \neq j; i, j = 1, \dots, k-1),$$

$$\sum_{u=1}^N x_{iu}^2 x_{ju}^2 x_{lu}^2 = \{1+2(k-1)\alpha^6\}C \quad (i \neq j \neq l; i, j, l = 1, \dots, k-1),$$

$$\sum_{u=1}^N x_{ku}^2 = 2(k-1)\alpha^2 A + 2(\beta^2 + \gamma^2 + \delta^2), \quad (4.5.1)$$

$$\sum_{u=1}^N x_{ku}^4 = 6(k-1)\alpha^4 B + 2(\beta^4 + \gamma^4 + \delta^4),$$

$$\sum_{u=1}^N x_{ku}^2 x_{iu}^2 = 6(k+3)\alpha^4 B \quad (i \leq k-1),$$

$$\sum_{u=1}^N x_{ku}^6 = 30(k-1)\alpha^6 C + 2(\beta^6 + \gamma^6 + \delta^6),$$

$$\sum_{u=1}^N x_{ku}^4 x_{iu}^2 = 6(k+3)\alpha^6 C \quad (i \leq k-1),$$

$$\sum_{u=1}^N x_{ku}^2 x_{iu}^4 = 6(k+3)\alpha^6 C \quad (i \leq k-1),$$

$$\sum_{u=1}^N x_{ku}^2 x_{iu}^2 x_{ju}^2 = 2(k+3)\alpha^6 C \quad (i \neq j; i, j \leq k-1),$$

where all the other sums of powers and products up to order six are zero.

It follows that the set of points forms a third order rotatable arrangement in k dimensions if

$$\begin{aligned}\beta^2 + \gamma^2 + \delta^2 &= \frac{1}{2} A, \\ \beta^4 + \gamma^4 + \delta^4 &= \frac{3}{2} B, \\ \beta^6 + \gamma^6 + \delta^6 &= \frac{15}{2} C,\end{aligned}\tag{4.5.2}$$

and

$$\alpha^2 = \frac{1}{2} .\tag{4.5.3}$$

Further, if conditions (4.5.2) and (4.5.3) are satisfied then from Draper (1960b), the arrangement forms a nonsingular design since the points lie on at least two distinct spheres centred at the origin.

From (4.5.2), it follows that β^2 , γ^2 and δ^2 have to be real nonnegative roots of the cubic equation

$$t^3 - \frac{A}{2} t^2 + \frac{(A^2 - 6B)t}{8} - \frac{(120C + A^3 - 18AB)}{48} = 0 .\tag{4.5.4}$$

From the theory of cubic equations, (Turnbull, 1947), the roots of equation (4.5.4) are all real if and only if

$$(10C - AB + \frac{A^3}{27})^2 + (\frac{A^2 - 18B}{18})^3 \leq 0,\tag{4.5.5}$$

and the roots are then given by

$$t_i = \frac{1}{2} \left\{ \frac{A}{3} + 2 \left(\frac{18B - A^2}{18} \right)^{1/2} \cos \left(\frac{\theta + 2\pi i}{3} \right) \right\} \quad (i = 0, 1, 2),\tag{4.5.6}$$

where

$$\theta = \text{Arc cos} \left\{ (10C - AB + \frac{A^3}{27}) / \left(\frac{18B - A^2}{18} \right)^{3/2} \right\} .$$

Therefore, a sufficient condition for the roots of equation (4.5.4) to be real and nonnegative is inequality (4.5.5) with

$$A^2 \geq 12B. \quad (4.5.7)$$

It can also be seen that if

$$120C + A^3 - 18AB \geq 0, \quad (4.5.8)$$

then the inequality (4.5.7) may become

$$A^2 \geq 6B. \quad (4.5.9)$$

Therefore, given any $(k-1)$ -dimensional third-order rotatable design or arrangement for which the conditions (4.5.5) and (4.5.7) or (4.5.5), (4.5.8) and (4.5.9) are satisfied, the corresponding set of points derived by the method described provides a third-order rotatable design in k dimensions.

It is interesting to note that even if condition (4.5.5) is not satisfied, designs may often be obtained by modifying the method slightly. To see this suppose the points $(0, \dots, 0, \pm\beta)$, $(0, \dots, 0, \pm\gamma)$ and $(0, \dots, 0, \pm\delta)$ are replicated, say, r times. Then condition (4.5.2) reduces to

$$\begin{aligned} \beta^2 + \gamma^2 + \delta^2 &= \frac{1}{2} \frac{A}{r}, \\ \beta^4 + \gamma^4 + \delta^4 &= \frac{3}{2} \frac{B}{r}, \\ \beta^6 + \gamma^6 + \delta^6 &= \frac{15}{2} \frac{C}{r}, \end{aligned} \quad (4.5.10)$$

and condition (4.5.5) reduces to

$$\left(10 \frac{C}{r} - \frac{AB}{r^2} + \frac{A^3}{27r^3}\right)^2 + \left(\frac{A^2 - 18Br}{18r^2}\right)^3 \leq 0. \quad (4.5.11)$$

By taking r sufficiently large one can always satisfy $A^2 \leq 18Br$ and for most given $(k-1)$ -dimensional designs, this would lead to fulfilment of condition (4.5.11). Condition (4.5.7) would in this case be replaced by

$$A^2 \geq 12Br, \quad (4.5.12)$$

and for most given designs (4.5.11) and (4.5.12) would be simultaneously satisfied for some suitable value of r . Conditions (4.5.8) and (4.5.9) are now to be replaced by

$$\frac{120C}{r} + \frac{A^3}{3} - \frac{18AB}{r^2} \geq 0 \quad (4.5.13)$$

and

$$A^2 \geq 6Br, \quad (4.5.14)$$

respectively. Even if (4.5.12) cannot be satisfied, it would usually be possible to find a suitable value of r for which (4.5.11), (4.5.13) and (4.5.14) may be satisfied simultaneously and hence obtain a k -dimensional design.

The method described may be applied to almost any given $(k-1)$ -dimensional design. However, only simple examples are looked into for $k = 2, 3$ and 4 .

Example 4.5.1: Consider the construction of a third-order rotatable design in 2 dimensions from a symmetric design in 1 dimension with support at $\pm a$ and $\pm b$, $b > a$. Then for the given design

$$A = 2(a^2 + b^2),$$

$$B = \frac{2}{3}(a^4 + b^4),$$

$$C = \frac{2}{15}(a^6 + b^6),$$

and hence

$$18B-A^2 = 8[a^4+b^4-a^2b^2],$$

$$A^2-6B = 8a^2b^2,$$

$$120C+A^3-18AB = 0,$$

$$(10C-AB + \frac{A^3}{27})^2 + (\frac{A^2-18AB}{18})^3 = -27(a^4b^2-a^2b^4)^2.$$

Therefore, for the given design, conditions (4.5.5), (4.5.8) and (4.5.9) are satisfied and the roots of the cubic equation (4.5.4) are $t = a^2, b^2, 0$. Thus the 2-dimensional third-order rotatable design derived by the method consists of two centrepoints and eight equally spaced points on each of the two circles of radii a and b , respectively. The centrepoints may be omitted. If the method were applied to a five-point symmetric design in 1 dimension the same 2-dimensional design with additional centrepoints would be obtained.

In the same way it can be seen that if the method is applied to a 1-dimensional symmetric design with six or seven support points, a 2-dimensional rotatable design based on eight equally spaced points on each of three distinct circles and some centrepoints which may be omitted is obtained.

If the given 1-dimensional design contains more than 7 symmetrically spaced points, then the design may be split up into component designs, none with more than 7 points, and the method may be applied to each component.

Example 4.5.2: Consider a 2-dimensional third-order rotatable arrangement based on n equally spaced points on a circle of radius ρ . From Box and Hunter (1957) or Bose and Carter (1959) it is required that $n \geq 7$.

Then for this arrangement

$$A = \frac{n}{2} \rho^2,$$

$$B = \frac{n}{8} \rho^4,$$

$$C = \frac{n}{48} \rho^6,$$

and hence the cubic equation (4.5.4) reduces to

$$t^3 - \frac{n}{4} \rho^2 t^2 + \frac{(n^2 - 3n)}{32} \rho^4 t - \frac{1}{48} \frac{(n^3 - 9n^2 + 20n)}{8} \rho^6 = 0. \quad (4.5.15)$$

It can readily be seen that for $n \geq 9$ the equation (4.5.15) cannot have three nonnegative real roots. Since, for $n \geq 9$, A^2 is always greater than or equal to $18B$, the condition (4.5.5) cannot be satisfied.

Suppose $n = 8$. Then

$$(10C - AB + \frac{A^3}{27})^2 + (\frac{A^2 - 18B}{18})^3 = 0$$

and therefore condition (4.5.5) is satisfied. Similarly it can be seen that the condition (4.5.7) is also satisfied. In fact for $n = 8$ the equation (4.5.15) reduces to

$$t^3 - 2\rho^2 t^2 + \frac{5}{4} \rho^4 - \frac{\rho^6}{4} = 0, \quad (4.5.16)$$

which has roots $t = \rho^2$, $\frac{\rho^2}{2}$ and $\frac{\rho^2}{2}$. Therefore, the method leads to a non-singular 3-dimensional third-order rotatable design with 46 points when applied to a 2-dimensional third order rotatable arrangement consisting of 8 equally spaced points on a circle. This 3-dimensional design in its standard orientation is in fact the design of Draper (1960b) with points given by

$$S(\frac{1}{2} \rho, \frac{1}{2} \rho, \frac{1}{2} \rho) \text{ twice,}$$

$$S(\rho, 0, 0),$$

$$S(\frac{1}{\sqrt{2}} \rho, 0, 0) \text{ twice,}$$

$$S(\frac{1}{\sqrt{2}} \rho, \frac{1}{\sqrt{2}} \rho, 0).$$

When $n = 7$,

$$A^2 - 12B = \frac{7\rho^4}{4},$$

$$(10C - AB + \frac{A^3}{27})^2 + (\frac{A^2 - 18B}{18})^3 = -\frac{49\rho^{12}}{27 \times 256}.$$

Therefore, conditions (4.5.5) and (4.5.7) are both satisfied. The equation (4.5.15), therefore, has three real nonnegative roots and the method thus leads to a non-singular three dimensional third-order rotatable design with 41 points. The application of the method provides a new class of 3-dimensional third-order rotatable designs distinct from the known classes of designs.

Consider a third order rotatable design with n equally spaced points on each of two circles of radii ρ_1 and ρ_2 , respectively. Then for this set of points

$$18B - A^2 = \frac{n}{4} \{9(\rho_1^4 + \rho_2^4) - n(\rho_1^2 + \rho_2^2)^2\},$$

and hence condition (4.5.5) cannot be satisfied if $n \geq 9$. Suppose $n = 8$. Let $R = \rho_1^2 / \rho_2^2$. It can be seen that in order to have $18B \geq A^2$, $R \notin (8 - \sqrt{63}, 8 + \sqrt{63})$. However, it can be seen that

$$\begin{aligned} (27)^2 \rho_2^{-12} \{ (10C - AB + \frac{A^3}{27})^2 + (\frac{A^2 - 18B}{18})^3 \} \\ = 216R^5 + 6453R^4 + 18306R^3 + 6453R^2 + 216R, \end{aligned}$$

which can never be non positive and hence condition (4.5.5) cannot be satisfied. The method, therefore, cannot be applied to a design based on eight points equally spaced on each of two concentric circles. However, the method may be applied to the points on each circle separately, providing a 3-dimensional design with 92 points against the 86 points that would have been required if the method could be applied to the circles together. If $n = 7$,

$$\begin{aligned}
 & (10C - AB + \frac{A^3}{27})^2 + (\frac{A^2 - 18B}{18})^3 \\
 & = (\frac{7}{16 \times 27})^2 \rho_2^{12} \{-27R^6 + 378R^5 + 6615R^4 + 32832R^3 + 6615R^2 + 378R - 27\}
 \end{aligned}$$

and hence to satisfy condition (4.5.5) it is required that $R > 25.5$ approximately, that is, the radius of one circle must be about five times that of the other. However, even if the circles do not have such radii, the method may be applied separately to each circle, providing a 3-dimensional design with 82 points.

Example 4.5.3: Consider the three-dimensional design with points $S(\frac{1}{2}a, \frac{1}{2}a, \frac{1}{2}a)$ twice, $S(\frac{1}{\sqrt{2}}a, 0, 0)$ twice, $S(a, 0, 0)$ and $S(\frac{1}{\sqrt{2}}a, \frac{1}{\sqrt{2}}a, 0)$. For this design,

$$\begin{aligned}
 A &= 12a^2, \\
 B &= 2a^4, \\
 C &= \frac{1}{4}a^6.
 \end{aligned}$$

Clearly, the method cannot be applied to this design to generate a third-order rotatable design in 4 dimensions. However, consider the method modified to take r replicates of the points $(0, 0, 0, \pm\beta)$, $(0, 0, 0, \pm\gamma)$ and $(0, 0, 0, \pm\delta)$. Then for $6 \geq p \geq 4$, the condition (4.5.12) is satisfied. Also, for $r = 5$ and 6 the condition (4.5.11) is satisfied. Therefore, when the modified method is applied to the given 3-dimensional design a third-order rotatable design in 4-dimensions is obtained.

The method of construction, as described, can always be utilized to extend third-order rotatable designs in 2 dimensions based on concentric circles with 7 or 8 equally spaced points on each circle, into a third-order rotatable design in 3 dimensions. It is not necessary to restrict to designs based on circles. The method may be applied to any design as long as the design moments are such that (4.5.4) has real nonnegative roots.

In the same manner, for $k \geq 4$, the method, with suitable modification if necessary, may almost always be applied to a $(k-1)$ -dimensional design to provide a k -dimensional design. For $k \geq 5$, the method may not be of much practical use since the resultant designs may require too many experiments.

The method may be applied to singular designs in $(k-1)$ dimensions. This has an added advantage in the performance of experiments. For example, if the 2-dimensional design is arranged in blocks with points on the same circle belonging to the same block, the experimenter can proceed in stages. If after performing some blocks of experiments in two dimensions, the experimenter feels that another factor should have been included in the analysis, he can then proceed by the method described without discarding the original results. In higher dimensions also the method has similar application.

4.6 The construction of third-order rotatable designs by projections

It is often possible to construct useful third-order rotatable designs in k dimensions from the available third-order rotatable designs or arrangements in $(k+l)$ dimensions. The method of construction relies on partitioning the $(k+l)$ -dimensional spaces into orthogonal subspaces and taking projections of the $(k+l)$ -dimensional designs onto these subspaces.

If $(x_1, \dots, x_{k+l})$ is a point in the $(k+l)$ -dimensional space, let its projection onto the k -dimensional subspace $x_{k+i} \equiv 0$ ($i = 1, \dots, l$) be denoted by $(x_1, \dots, x_k)$. It follows that if the set of points $(x_{1u}, \dots, x_{k+l,u})$ ($u = 1, \dots, N''$) satisfy (4.2.4) in the $(k+l)$ -dimensional

space then the set $(x_{1u}, \dots, x_{ku})$ ($u = 1, \dots, N''$) also automatically satisfy (4.2.4) in the k -dimensional space. From Gardiner, Grandage and Hader (1959) it is known that for a third-order rotatable arrangement in k dimensions, $\frac{AC}{B^2} > \frac{(k+2)}{(k+4)}$ is replaced by $\frac{AC}{B^2} \geq \frac{(k+2)}{(k+4)}$ in (4.4.2), where A , B and C are as defined in (4.4.1). In fact the inequality $\frac{AC}{B^2} \geq \frac{(k+2)}{(k+4)}$ cannot be reversed for any set of points satisfying (4.4.1). Therefore, it follows that the set of k -dimensional points derived by projecting the set of $(k+1)$ -dimensional points necessarily forms a non-singular third-order rotatable design in k dimensions even if the $(k+1)$ -dimensional design is singular. Hence, given any third-order rotatable design or arrangement in the $(k+1)$ -dimensional space, a third-order rotatable design in k dimensions may be derived by taking a projection of the given design or arrangement. Only the non-central k -dimensional points need to be kept in the derived design.

The usual methods of construction of third-order rotatable designs involve the use of balanced and doubly balanced incomplete block designs. As a consequence, it is easier in some dimensions than in others to construct designs or arrangements with small number of points. The method of construction described can be particularly useful whenever a $(k+1)$ -dimensional third-order rotatable arrangement with small number of points is available. Application of the method is best illustrated by considering some concrete examples.

Example 4.6.1: Draper (1960c) constructed a third-order rotatable arrangement in four dimensions consisting of $S(a, a, a, a)$, $S(2a, 0, 0, 0)$ and $S(2^{\frac{1}{2}}a, 2^{\frac{1}{2}}a, 0, 0)$. Consider the projection of this arrangement onto the three-dimensional subspace $x_4 \equiv 0$. Then ignoring the centre points, the 46 points of $S(2a, 0, 0, 0)$, $S(2^{\frac{1}{2}}a, 2^{\frac{1}{2}}a, 0, 0)$ and two sets of $S(a, a, a)$ and $S(2^{\frac{1}{2}}a, 0, 0)$, each, are obtained. Thus a three-dimensional third-order rotatable design with 46 points is derived. This derived design is listed in Draper (1960b).

Example 4.6.2: Consider the 5-dimensional design of Das and Narasimham (1962) given by the 100 points of $S(a,a,a,0,0)$, $S(b,0,0,0,0)$ and $S(d,0,0,0,0)$ where $b^2 = 3.24741a^2$, $d^2 = 1.20596a^2$. By projecting this design onto a 4-dimensional space, say, $x_5 \equiv 0$ and ignoring the centre points, a 4-dimensional third-order rotatable design is derived. The derived design consists of the 96 points given by $S(a,a,a,0)$, $S(b,0,0,0)$, $S(d,0,0,0)$ and 2 sets of $S(a,a,0,0)$. Note that this design is distinct from the other known 4-dimensional third-order rotatable design with 96 points described in Draper (1960c).

Example 4.6.3: Consider Design 2 of Table 4.4.3 with the 240 7-dimensional points given by $S(a,\dots,a)$, $S(2a,2a,0,\dots,0)$ and 2 sets of $S(2a,0,\dots,0)$. The 236 noncentral points derived in the 6-dimensional space are then given by $S(2a,2a,0,0,0,0)$, 2 sets of $S(a,\dots,a)$ and 4 sets of $S(2a,0,\dots,0)$. Thus, the six-dimensional Design 1 of Table 4.4.2 is obtained.

Example 4.6.4: Consider the 7-dimensional design of Das and Narasimham (1962) given by the 238 points of $S(2a,0,\dots,0)$, BIB-a(7,7,4,4,2) and 2 sets of Complementary BIB-a(7,7,3,3,1). On projecting these points onto the 6-dimensional subspace $x_7 \equiv 0$ and ignoring the centre points, a third-order rotatable design with 236 points is obtained. Note that this design is distinct from the other 236-point design - Design 1 of Table 4.4.2. In fact this design consists of the six-dimensional point-set given by

$$\begin{aligned} &S(2a,0,\dots,0), \\ &(0, \pm a, \pm a, \pm a, \pm a, 0), \\ &(\pm a, 0, \pm a, \pm a, 0, \pm a), \\ &(\pm a, \pm a, 0, 0, \pm a, \pm a), \end{aligned}$$

2 replicates of

$(\pm a, \pm a, \pm a, 0, 0, 0),$
 $(\pm a, 0, 0, \pm a, \pm a, 0),$
 $(0, \pm a, 0, \pm a, 0, \pm a),$
 $(0, 0, \pm a, 0, \pm a, \pm a),$
 $(0, 0, 0, \pm a, \pm a, \pm a),$
 $(0, \pm a, \pm a, 0, 0, \pm a),$
 $(\pm a, 0, \pm a, 0, \pm a, 0),$
 $(\pm a, \pm a, 0, \pm a, 0, 0),$

and 4 replicates of

$(\pm a, 0, 0, 0, 0, \pm a),$
 $(0, \pm a, 0, 0, \pm a, 0),$
 $(0, 0, \pm a, \pm a, 0, 0).$

Example 4.6.5: Consider the 8-dimensional third-order rotatable arrangement consisting of the 240 points of $2^{-1}S(a, \dots, a)$ and $S(2a, 2a, 0, \dots, 0)$. Its projection onto a 7-dimensional space provides the Design 2 of Table 4.4.3 consisting of the 240 points given by $S(a, \dots, a)$, $S(2a, 2a, 0, \dots, 0)$ and 2 sets of $S(2a, 0, \dots, 0)$.

Example 4.6.6: The 7-dimensional design of Das and Narasimham (1962) given by the 238 points of $S(2a, 0, \dots, 0)$, $\text{BIB-}a(7, 7, 4, 4, 2)$ and two sets of the Complementary $\text{BIB-}a(7, 7, 3, 3, 1)$ may be obtained from the projections of the 8-dimensional third-order rotatable arrangement with 240 points of $\text{DBIB-}a(8, 14, 7, 4, 3, \dots)$ and $S(2a, 0, \dots, 0)$.

Example 4.6.7: Consider the 11-dimensional design of Das and Narasimham (1962) given by $\text{DBIB-}a(11, 33, 15, 5, 6, 2)$, $S(b, 0, \dots, 0)$ and $S(d, 0, \dots, 0)$ with $b^2 = 5.44372a^2$ and $d^2 = 4.285562a^2$. This design with 1100 points is the minimal-point design among all available third-order

rotatable designs in 11 dimensions. As noted in Herzberg and Cox (1969), the minimal-point designs among the available third-order rotatable designs in 9 and 10 dimensions require 1202 and 1372 points, respectively and are listed in Das and Narasimham (1962). However, if orthogonal projections of the minimal-point 11-dimensional design onto a 10-dimensional subspace is taken then a new third-order rotatable design in 10 dimensions with only 1096 points is obtained. In the same way by projecting the 11-dimensional design onto a 9-dimensional subspace, a minimal-point design in 9 dimensions with only 1092 points is derived.

4.7 The construction of third-order rotatable designs in k dimensions from designs in (k-1) dimensions

A method for constructing second-order rotatable designs in k dimensions from second-order rotatable designs in (k-1) dimensions has been presented in Section 4.3. A similar method can often be used to construct new classes of k-dimensional third-order rotatable designs from given (k-1)-dimensional third-order rotatable arrangements or designs. Let $ADBIB-(k,b,r,k-1,\lambda,\mu)$ be the set of k-dimensional points generated from the given (k-1)-dimensional point-set through the doubly balanced incomplete block design $DBIB-(k,b,r,k-1,\lambda,\mu)$ in the manner illustrated in Section 4.3. Then by combining $ADBIB-(k,b,r,k-1,\lambda,\mu)$ with point sets of the form $S(a_1, \dots, a_1), \dots, S(a_k, 0, \dots, 0)$ or their suitably 'balanced fractions' it is often possible to satisfy (4.4.1) and (4.4.2). The following examples illustrate the method.

Example 4.7.1: Consider a third-order rotatable arrangement in 2-dimensions consisting of N' (≥ 7) equally spaced points on a circle of radius ρ . Then for this arrangement $B = \frac{N'}{8} \rho^4$, $C = \frac{N'}{48} \rho^6$, $A = \frac{N'}{2} \rho^2$ where A, B, C are as defined in (4.4.1). Consider the 3-dimensional

point set ADBIB-(3,3,2,2,1,0) generated from this arrangement. Combine the $3N'$ points of this set with the 28 points of $S(a,a,0)$, $S(b,b,b)$ and $S(d,d,d)$ where $d^2 = b^2 t$, $t \geq 0$. It can readily be verified that the $3N'+28$ points form a third-order rotatable arrangement in 3 dimensions if $a^2 = \left(\frac{9C}{20}\right)^{1/3}$ and if t is such that

$$f(t) = \frac{(1+t^2)^3}{(1+t^3)^2} = \frac{\{3B-4 \times \left(\frac{9C}{20}\right)^{2/3}\}^3}{16 \times 64} \times \frac{25}{9C^2}.$$

Consider $N' = 7$. Then a t is needed such that $\frac{(1+t^2)^3}{(1+t^3)^2} = 0.98144$.

Clearly no such non-negative t exists and hence one cannot obtain a third-order rotatable arrangement in 3 dimensions. Consider $N' = 8$. Then a nonnegative t is needed such that $\frac{(1+t^2)^3}{(1+t^3)^2} = 1.170636$. Clearly a solution exists and is given by $t = 0.25635$. Hence a third-order rotatable design in 3 dimensions with 52 points is obtained and is given by

$S\left(\frac{\rho}{\sqrt{2}}, \frac{\rho}{\sqrt{2}}, 0\right)$, 2 sets of $S(\rho, 0, 0)$, $S(a, a, 0)$, $S(b, b, b)$ and $S(d, d, d)$ with $a^2 = \left(\frac{3}{40}\right)^{1/3} \rho^2$, $b^2 = 0.5569\rho^2$, $d^2 = 0.1428\rho^2$.

Example 4.7.2: Consider the set of points given by $S(a, a, a, a)$, $S(b, b, 0, 0)$, 2 sets of $S(d, d, d, d)$ and the 42 points of ADBIB(4,6,3,2,1,0) generated from a third-order rotatable arrangement in 2 dimensions consisting of 7 equally spaced points on a circle of radius ρ . There are 114 points in this set. Let $d^2 = ta^2$, $t \geq 0$. It can be shown that the set forms a third-order rotatable design in 4 dimensions if $b^2 = \left(\frac{7}{32}\right)^{1/3} \rho^2$ and t is such that $\frac{(1+2t^2)^3}{(1+2t^3)^2} = \frac{21}{8}$. Therefore, for $t = 0.653356$, that is, for $a^2 = 0.29749\rho^2$ and $d^2 = 0.19437\rho^2$ the set of points described forms a 4-dimensional third-order rotatable design with 114 points derived from a 2-dimensional third-order rotatable arrangement. Note that this is a new design in 4 dimensions. Another new 4-dimensional third-order rotatable design is obtained by starting with a 2-dimensional third-order rotatable arrangement consisting of eight equally spaced points

on a circle of radius ρ . This design consists of 120 points and is given by $S(b,b,0,0)$, $S(a,a,a,a)$, 2 sets of $S(d,d,d,d)$ and the 48 points of ADBIB-(4,6,3,2,1,0). It can readily be verified that these 120 points satisfy (4.4.1) if $b^2 = \frac{\rho^2}{2^{2/3}}$, $d^2 = ta^2$ where t is such that $\frac{(1+2t^2)^3}{(1+2t^3)^2} = 3$. Therefore, the design is in fact given by $S(b,b,0,0)$, 3 sets of $S(a,a,a,a)$, $S(\frac{\rho}{\sqrt{2}}, \frac{\rho}{\sqrt{2}}, 0, 0)$ and 3 sets of $S(\rho,0,0,0)$, where $b^2 = \frac{\rho^2}{2^{2/3}}$, $a^2 = \frac{\rho^2}{4}$.

The method of construction illustrated through the simple examples is likely to be of practical use only when the suitable block designs with small number of blocks exist. Otherwise, the derived designs would require too many experiments. Nonetheless, the method has led to some new third-order rotatable designs.

4.8 Second-order rotatable designs constructed from pairwise balanced designs

The available second-order rotatable designs often require too many experiments. Here, a method of construction of second-order rotatable designs through pairwise balanced designs is provided and applied to construct some new designs with a small number of points.

A pairwise balanced design is an arrangement of t treatments in b blocks such that each block contains $s_1, s_2, \dots, s_m$ treatments that are all distinct ($s_i \leq t$, $s_i \neq s_j$) and every pair of treatments occurs exactly λ times. Corresponding to each block of size s_i there is a set of t -dimensional points $(\pm h_1, \dots, \pm h_t)$ where each h_j ($j = 1, \dots, t$) has the value ± 1 or 0 depending on the presence or absence of the j -th treatment in the block, respectively. As in Box and Behnken (1960b) and Das and Narasimham (1962) the actual design points of the second-order rotatable design which would correspond to the block may be any

one of the smallest 2^{-q} 'Resolution V' fractions of the set $(\pm h_1, \dots, \pm h_t)$ regarding the set as a 2^{s_i} factorial design in the factors at non-zero level.

Of particular interest are those pairwise balanced designs for which the number of times a treatment occurs in blocks of a particular size is the same for all treatments. If BIB (t, b, r, s, λ) is a balanced incomplete block design with parameters as defined earlier then many pairwise balanced designs of interest, with $m \geq 2$, may be obtained by deleting one or more treatments from the BIB (t, b, r, s, λ) . For convenience, let BIB- $a_1, \dots, a_m$ (t, b, r, s, λ) denote the k -dimensional design points corresponding to a pairwise balanced design of the desired type obtained by deleting treatments from the BIB (t, b, r, s, λ) ($t > k$). Also, as before, let $S(z_1, \dots, z_k)$ denote all permutations of $(\pm z_1, \dots, \pm z_k)$ and let $2^{-q}S(z_1, \dots, z_k)$ denote any one of the smallest 'Resolution V' fractions of $S(z_1, \dots, z_k)$.

If $r = 3\lambda$ then BIB- $a_1, \dots, a_m$ (t, b, r, s, λ) often forms a second-order rotatable design if the a_i ($i = 1, \dots, m$) are suitably chosen. If $r < 3\lambda$, a design may be obtained by adding $S(d, 0, \dots, 0)$ to the set with d appropriately chosen. If $r > 3\lambda$, the design may be formed by adding $2^{-q}S(p, \dots, p)$ to the set with p suitably chosen. This method of construction is best seen by considering some specific examples.

Example 4.8.1: Consider a BIB $(7, 7, 3, 3, 1)$. Then the corresponding 6-dimensional point set B.I.B- a_1, a_2 $(7, 7, 3, 3, 1)$ derived by deleting one treatment of B.I.B. $(7, 7, 3, 3, 1)$ is given by the 44 points

$$\begin{aligned}
& (\pm a_1, \pm a_1, \pm a_1, 0, 0, 0), \\
& (\pm a_1, 0, 0, \pm a_1, \pm a_1, 0), \\
& (\pm a_2, 0, 0, 0, 0, \pm a_2), \\
& (0, \pm a_1, 0, \pm a_1, 0, \pm a_1), \\
& (0, \pm a_2, 0, 0, \pm a_2, 0), \\
& (0, 0, \pm a_2, \pm a_2, 0, 0), \\
& (0, 0, \pm a_1, 0, \pm a_1, \pm a_1) .
\end{aligned} \tag{4.8.1}$$

For this set of points the following conditions are satisfied:

$$\begin{aligned}
\sum_u x_{iu}^2 &= 16a_1^2 + 4a_2^2 \quad (i = 1, \dots, 6), \\
\sum_u x_{iu}^4 &= 16a_1^4 + 4a_2^4 \quad (i = 1, \dots, 6), \\
\sum_u x_{iu}^2 x_{ju}^2 &= \begin{cases} 4a_2^4 & (i, j) = (1, 6), (2, 5), (3, 4), \\ 8a_1^4 & \text{otherwise } (i \neq j; i, j = 1, \dots, 6), \end{cases}
\end{aligned} \tag{4.8.2}$$

and all other sums of powers and products up to order four are zero.

Therefore BIB- $a_1, a_2(7, 7, 3, 3, 1)$ is a second-order rotatable design if

$a_2^4 = 2a_1^4$. Note that the design with smallest number of points among all the available second-order rotatable designs in six dimensions also requires 44 points and consists of $2^{-1}S(a, \dots, a)$ and $S(2^{5/4}a, 0, \dots, 0)$.

Example 4.8.2: Consider the BIB- $a_1, a_2(6, 10, 5, 3, 2)$ obtained by deleting one treatment of BIB $(6, 10, 5, 3, 2)$ and $S(d, 0, \dots, 0)$ in five dimensions.

For these points

$$\begin{aligned}
\sum_u x_{iu}^2 &= 24a_1^2 + 8a_2^2 + 2d^2 \quad (i = 1, \dots, 5), \\
\sum_u x_{iu}^4 &= 24a_1^4 + 8a_2^4 + 2d^4 \quad (i = 1, \dots, 5), \\
\sum_u x_{iu}^2 x_{ju}^2 &= 16a_1^4 \text{ or } 8a_1^4 + 4a_2^4 \quad (i \neq j; i, j = 1, \dots, 5),
\end{aligned} \tag{4.8.3}$$

and all other sums of powers and products up to order four are zero.

Therefore, these 70 points form a second-order rotatable design if $d^4 = 2a_2^4 = 4a_1^4$.

Example 4.8.3: Consider the 192 points of BIB- $a_1, a_2(10, 15, 6, 4, 2)$ which satisfy the conditions:

$$\begin{aligned} \sum x_{iu}^4 &= 64a_1^4 + 16a_2^2 \quad (i = 1, \dots, 9), \\ \sum x_{iu}^4 &= 64a_1^4 + 16a_2^4 \quad (i = 1, \dots, 9), \\ \sum x_{iu}^2 x_{ju}^2 &= 32a_1^4 \text{ or } 16a_1^4 + 8a_2^4 \text{ or } 16a_2^4 \quad (i \neq j; i, j = 1, \dots, 9), \end{aligned} \quad (4.8.4)$$

and all other sums of powers and products up to order four are zero. Therefore, BIB- $a_1, a_2(10, 15, 6, 4, 2)$ is a second-order rotatable design in 9 dimensions if $a_2^4 = 2a_1^4$.

Example 4.8.4: Consider a BIB (16, 16, 6, 6, 2). From the method of construction of BIB (16, 16, 6, 6, 2) it can readily be seen that the 16×16 incidence matrix $\underline{N}$ is $(\underline{N}_1 \otimes \underline{N}_1) + (\overline{\underline{N}}_1 \otimes \overline{\underline{N}}_1)$, where $\overline{\underline{A}}$ denotes the complement of $\underline{A}$, $\otimes$ denotes the Kronecker product and $\underline{N}_1$ is the 4×4 matrix given by

$$\underline{N}_1 = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}.$$

Let the treatments be partitioned into 4 sets of 4 treatments each so that the $\{(i-1)4+j\}$ -th treatment for $j = 1, 2, 3, 4$ belongs to the i -th set ($i = 1, 2, 3, 4$). By deleting any 4 treatments in the same set a BIB- $a_1, a_2(16, 16, 6, 6, 2)$ is obtained which is given by

$$\begin{aligned}
& (0, 0, 0, \pm b, 0, 0, 0, \pm b, 0, 0, 0, \pm b), \\
& (0, 0, \pm b, 0, 0, 0, \pm b, 0, 0, 0, \pm b, 0), \\
& (0, \pm b, 0, 0, 0, \pm b, 0, 0, 0, \pm b, 0, 0), \\
& (\pm b, 0, 0, 0, \pm b, 0, 0, 0, \pm b, 0, 0, 0), \\
& 2^{-1}(0, 0, 0, \pm a, 0, 0, 0, \pm a, \pm a, \pm a, \pm a, 0), \\
& 2^{-1}(0, 0, \pm a, 0, 0, 0, \pm a, 0, \pm a, \pm a, 0, \pm a), \\
& 2^{-1}(0, \pm a, 0, 0, 0, \pm a, 0, 0, \pm a, 0, \pm a, \pm a), \\
& 2^{-1}(\pm a, 0, 0, 0, \pm a, 0, 0, 0, 0, \pm a, \pm a, \pm a) \\
& 2^{-1}(0, 0, 0, \pm a, \pm a, \pm a, \pm a, 0, 0, 0, 0, \pm a), \\
& 2^{-1}(0, 0, \pm a, 0, \pm a, \pm a, 0, \pm a, 0, 0, \pm a, 0), \\
& 2^{-1}(0, \pm a, 0, 0, \pm a, 0, \pm a, \pm a, 0, \pm a, 0, 0), \\
& 2^{-1}(\pm a, 0, 0, 0, 0, \pm a, \pm a, \pm a, \pm a, 0, 0, 0), \\
& 2^{-1}(\pm a, \pm a, \pm a, 0, 0, 0, 0, \pm a, 0, 0, 0, \pm a), \\
& 2^{-1}(\pm a, \pm a, 0, \pm a, 0, 0, \pm a, 0, 0, 0, \pm a, 0), \\
& 2^{-1}(\pm a, 0, \pm a, \pm a, 0, \pm a, 0, 0, 0, \pm a, 0, 0), \\
& 2^{-1}(0, \pm a, \pm a, \pm a, \pm a, 0, 0, 0, \pm a, 0, 0, 0),
\end{aligned} \tag{4.8.5}$$

with $b = a_1$ and $a = a_2$. Clearly, BIB- $a_1, a_2(16, 16, 6, 6, 2)$ satisfy the following conditions:

$$\begin{aligned}
\sum x_{iu}^2 &= 8a_1^2 + 80a_2^2 \quad (i = 1, \dots, 12), \\
\sum_{u=1}^N x_{iu}^4 &= 8a_1^4 + 80a_2^4 \quad (i = 1, \dots, 12), \\
\sum x_{iu}^2 x_{ju}^2 &= \begin{cases} 8a_1^4 + 16a_2^4 & (|i-j| = 4, 8; i, j = 1, \dots, 12), \\ 32a_2^4 & (i \neq j; |i-j| \neq 4, 8; i, j = 1, \dots, 12), \end{cases}
\end{aligned} \tag{4.8.6}$$

where all other sums of powers and products up to order four are zero. Therefore, the 224 points of BIB- $a_1, a_2(16, 16, 6, 6, 2)$ obtained in (4.8.5) form a minimal-point second-order rotatable design in 12 dimensions if $a_1^4 = 2a_2^4$. This design may be used as an alternative to the other known minimal-point 12-dimensional second-order rotatable design

requiring 224 points which is provided by Adhikary and Panda (1977).

Many other second-order rotatable designs may be derived by the method described. Examples 4.8.1 and 4.8.4 are of special interest, since these provide alternatives to the available minimal-point designs in 6 and 12 dimensions, respectively.

4.9 Construction of second-order rotatable designs through asymmetric point-sets

In the methods of construction described, symmetric point-sets are combined to derive second-order rotatable designs. However, it is not necessary to restrict to symmetric point-sets. Often it may be possible to construct useful designs with small number of points by combining together point-sets which are asymmetric. Some examples of such designs with small number of points are provided. The first three designs require the minimum number of points among the available designs.

Example 4.9.1: Consider the four-dimensional points

$$(\pm b, \pm a, \pm a, 0),$$

$$(0, \pm a, \pm a, \pm b),$$

$$(0, \pm c, 0, 0),$$

$$(0, 0, \pm c, 0),$$

$$(\pm d, 0, 0, \pm d).$$

It can easily be verified that these 24 points form a second-order rotatable design if $b^2 = 2a^2$, $c^2 = 4a^2$ and $d^2 = 2a^2$.

Example 4.9.2: Consider the 44 six-dimensional points

$$2^{-1}(\pm 2^{\frac{1}{2}}a, \pm a, \pm a, \pm a, \pm a, 0),$$

$$2^{-1}(0, \pm a, \pm a, \pm a, \pm a, \pm 2^{\frac{1}{2}}a),$$

$$(0, s(2^{5/4}a, 0, 0, 0), 0),$$

$$(\pm 2^{3/4}a, 0, 0, 0, 0, \pm 2^{3/4}a).$$

These points clearly form a second-order rotatable design.

Example 4.9.3: Consider the 144 nine-dimensional points

$$\begin{aligned} &2^{-2} (\pm b, \pm a, \pm a, \pm a, \pm a, \pm a, \pm a, \pm a, 0), \\ &2^{-2} (0, \pm a, \pm a, \pm a, \pm a, \pm a, \pm a, \pm a, \pm b), \\ &(0, S(d, 0, 0, 0, 0, 0, 0, 0), 0), \\ &(\pm c, 0, 0, 0, 0, 0, 0, 0, \pm c). \end{aligned}$$

This set forms a second-order rotatable design if $b^2 = 2a^2$, $c^2 = 2^{5/2}a^2$, $d^2 = 2^{7/2}a^2$.

Example 4.9.4: Consider the 280 twelve-dimensional points

$$\begin{aligned} &2^{-4}(0, \pm a, \dots, \pm a, \pm\sqrt{2}a), \\ &2^{-4}(\pm\sqrt{2}a, \pm a, \dots, \pm a, 0), \\ &(0, S(4a, 0, \dots, 0), 0), \\ &(\pm 2\sqrt{2}a, 0, \dots, 0, \pm 2\sqrt{2}a). \end{aligned}$$

This set of points clearly satisfies all the requirements of a non-singular second-order rotatable design in 12 dimensions.

4.10 Cylindrically rotatable designs

Herzberg (1966, 1967a) introduced and classified the cylindrically rotatable designs. Of particular interest are the cylindrically rotatable designs of type 3 which are also known as the group-divisible rotatable designs. These designs were independently introduced by Das and Dey (1967). Cylindrically rotatable designs of type 3 split up the factors into two groups such that the designs are rotatable for each group of factors when the sum of squares of the factors in the other group is held constant. Das and Dey (1967) derived empirically the conditions under which second-order designs are cylindrically rotatable of type 3

and also provided some methods of construction. However, their analysis and the methods of construction of these designs appear to be incorrect. The correct analysis and some methods of construction of second-order cylindrically rotatable designs of type 3 are given in Adhikary and Sinha (1976). The methods provided in Dey and Nigam (1968) are only valid for those second-order models in which there is no product term involving factors from different groups.

Singh (1979) obtained the conditions under which the second-order designs are such that the factors may be split up into three groups for each of which the designs are rotatable when the sums of squares of the factors in the other groups are held constant.

More generally consider the k factors split up into m mutually exclusive groups with $k_i - k_{i-1}$ factors $x_{k_{i-1}+1}, \dots, x_{k_i}$ in the i -th group, ($i = 1, \dots, m$), where $k_0 = 0$, $k_m = k$. A design is to be called a m -grouped cylindrically rotatable design of type 3 if it is rotatable for each group of factors when the sums of squares of the factors in the other groups are held constant. The moment requirements of a m -grouped cylindrically rotatable design of type 3 of order d may be derived by a method very similar to the method used by Box and Hunter (1957) and Herzberg (1966, 1967a) to derive the moment requirements of a rotatable design and a cylindrically rotatable design of order d , respectively.

Consider $\hat{y}(\underline{x})$ and $\hat{y}(\underline{z})$ where

$$\sum_{j=k_{i-1}+1}^{k_i} x_j^2 = \sum_{j=k_{i-1}+1}^{k_i} z_j^2 \quad (i = 1, \dots, m). \quad (4.10.1)$$

Suppose $\underline{z} = \underline{R}\underline{x}$, where $\underline{x}' = (1, x_1, \dots, x_k)$, $\underline{z}' = (1, z_1, \dots, z_k)$ and $\underline{R}$ is a $(k+1) \times (k+1)$ orthonormal matrix of the form

$$\underline{R} = \text{Diag} \{1, \underline{R}_1, \dots, \underline{R}_m\}, \quad (4.10.2)$$

with each R_i an orthonormal matrix of order $(k_i - k_{i-1}) \times (k_i - k_{i-1})$, $(i = 1, \dots, m)$. Therefore, for a m -grouped cylindrically rotatable design of type 3 it is required that

$$\tilde{R}'^{[d]} \tilde{X}' \tilde{X} \tilde{R}^{[d]} = \tilde{X}' \tilde{X}, \quad (4.10.3)$$

for every orthonormal matrix $\tilde{R}$ of the form described. It follows that, Q , the moment generating function of a m -grouped cylindrically rotatable design type 3 must be a function of

$$\sum_{j=k_{i-1}+1}^{k_i} t_j^2 \quad (i = 1, \dots, m)$$

and since Q is a polynomial in the t_j 's, it must be of the form

$$Q = \sum_{p_1=0}^d \dots \sum_{p_m=0}^d a_{2p_1, \dots, 2p_m} \left\{ \prod_{i=1}^m \left(\sum_{j=k_{i-1}+1}^{k_i} t_j^2 \right)^{p_i} \right\}, \quad (4.10.4)$$

where $\sum_{i=1}^m p_i \leq d$. The coefficient of $t_1^{\alpha_1} \dots t_k^{\alpha_k}$ in Q is zero if any of the α_j , $j = 1, \dots, k$ is odd and is

$$a_{\sum_{i=1}^m \alpha_i} \left\{ \prod_{i=1}^m \left(\frac{1}{2} \sum_{j=k_{i-1}+1}^{k_i} \alpha_j \right)! \right\} / \left\{ \prod_{j=1}^k \left(\frac{1}{2} \alpha_j \right)! \right\} \quad (4.10.5)$$

by
if all the α_j ($j = 1, \dots, k$) are even integers. Therefore, equating (4.10.5) with the coefficient of $t_1^{\alpha_1} \dots t_k^{\alpha_k}$ in (4.2.3) it can be seen that for a m -grouped cylindrically rotatable design of type 3 of order d

$$[1^{\alpha_1}, \dots, k^{\alpha_k}] = \begin{cases} 0 & \text{if any } \alpha_j \text{ odd } (j = 1, \dots, k), \\ \lambda \frac{\left(\prod_{j=1}^k \alpha_j! \right)}{2^{\alpha/2} \prod_{j=1}^k \left(\frac{1}{2} \alpha_j \right)!} & \text{all } \alpha_j \text{ even } (j = 1, \dots, k), \end{cases} \quad (4.10.6)$$

all α_j even ($j = 1, \dots, k$),

where

$$\lambda_{\sum_{j=k_0+1}^{k_1} \alpha_j, \dots, \sum_{j=k_{m-1}+1}^{k_m} \alpha_j} = a_{\sum_{j=k_0+1}^{k_1} \alpha_j, \dots, \sum_{j=k_{m-1}+1}^{k_m} \alpha_j} 2^{\alpha/2} \frac{(2d-\alpha)!}{(2d)!} \prod_{i=1}^m \left(\frac{1}{2} \sum_{j=k_{i-1}+1}^{k_i} \alpha_j \right)! \quad (4.10.7)$$

is constant for any design and any $\sum_{j=k_{i-1}+1}^{k_i} \alpha_j$ ($i = 1, \dots, m$).

The design points have to be chosen in a way such that the variance-covariance matrix of the estimated parameters is non-singular.

The cylindrically rotatable designs are likely to be most useful when the number of experiments required by such designs are relatively smaller than the number of experiments required by rotatable designs of the same order and dimensions. Any method of construction of rotatable designs of order d can also be used for the construction of cylindrically rotatable designs of the same order. However, those methods which yield these designs with small number of points are of greater interest. One such method of construction of second-order m -grouped-cylindrically rotatable designs of type 3 is presented here along with some examples.

For second-order designs, the condition (4.10.6) reduce to

$$\sum_{u=1}^N x_{ju}^2 = A_i \quad (k_{i-1}+1 \leq j \leq k_i; i = 1, \dots, m),$$

$$\sum_{u=1}^N x_{ju}^4 = 3B_i \quad (k_{i-1}+1 \leq j \leq k_i; i = 1, \dots, m), \quad (4.10.8)$$

$$\sum_{u=1}^N x_{ju}^2 x_{\ell u}^2 = \begin{cases} B_i (k_{i-1}+1 \leq j \neq \ell \leq k_i; i = 1, \dots, m), \\ C_{is} (k_{i-1}+1 \leq j \leq k_i; k_{s-1}+1 \leq \ell \leq k_s; i \neq s; i, s = 1, \dots, m), \end{cases}$$

with all other sums of powers and products up to order four being zero.

Note that (4.10.8) does not guarantee non-singularity of the design.

For example, if any of the C_{is} 's is zero then the design is singular for the full second-order model since the coefficients of the products of factors from the i -th group and s -th group cannot then be estimated using the design. For the design to be non-singular all the A_i 's, B_i 's and C_{is} 's must be non-zero.

Consider a $\text{BIB}(t, b, r, s, \lambda)$. Associate with each block a point $(h_1, \dots, h_t)$, where each h_i has the value a_i or 0 corresponding to the presence or absence of the i -th treatment in the block. Now consider the balanced incomplete block designs with $t = m$ and $s \geq 2$. Then from each block a k -dimensional point set $(S(h_1, \dots, h_1), \dots, S(h_m, \dots, h_m))$ is obtained by replacing each h_i with the vectors $S(h_i, \dots, h_i)$ of size $1 \times (k_i - k_{i-1})$ in $(h_1, \dots, h_m)$. Take any one of the smallest 2^{-q} Resolution V' fractions of the k -dimensional point set. The collection of b such fractional factorial designs, one corresponding to each block of $\text{BIB}(m, b, r, s, \lambda)$, along with the $2k$ axial points $(\pm b_1, 0, \dots, 0), \dots, (0, 0, \dots, 0, \pm b_k)$, where $b_j = d_i$ ($k_{i-1} + 1 \leq j \leq k_i$; $i = 1, \dots, m$), forms a second-order m -grouped cylindrically rotatable design of type 3 if the a_i 's and d_i 's are suitably chosen.

Example 4.10.1: Consider $m = 3$, $k_1 = 4$, $k_2 = 8$, $k = 12$. The design points derived by the method described using a $\text{BIB}(3, 3, 2, 2, 1)$ are

$$\begin{aligned} & 2^{-2}(\pm a_1, \pm a_1, \pm a_1, \pm a_1, \pm a_2, \pm a_2, \pm a_2, \pm a_2, 0, 0, 0, 0), \\ & 2^{-2}(\pm a_1, \pm a_1, \pm a_1, \pm a_1, 0, 0, 0, 0, \pm a_3, \pm a_3, \pm a_3, \pm a_3), \\ & 2^{-2}(0, 0, 0, 0, \pm a_2, \pm a_2, \pm a_2, \pm a_2, \pm a_3, \pm a_3, \pm a_3, \pm a_3), \\ & (\pm d_1, 0, 0, \dots, 0, 0, 0), \\ & \vdots \\ & (0, 0, 0, \dots, 0, 0, \pm d_3). \end{aligned}$$

Therefore, for $d_i = 2^{7/4} a_i$ ($i = 1, 2, 3$), these 216 points form a second-order 3-grouped cylindrically rotatable design of type 3.

Example 4.10.2: Consider $m = 4$, $k_1 = 3$, $k_2 = 6$, $k_3 = 9$, $k = 12$. By using a BIB(4,6,3,2,1) the 192 points derived are

$$\begin{aligned}
 &2^{-1}(\pm a_1, \pm a_1, \pm a_1, \pm a_2, \pm a_2, \pm a_2, 0, 0, 0, 0, 0, 0), \\
 &2^{-1}(\pm a_1, \pm a_1, \pm a_1, 0, 0, 0, \pm a_3, \pm a_3, \pm a_3, 0, 0, 0), \\
 &2^{-1}(\pm a_1, \pm a_1, \pm a_1, 0, 0, 0, 0, 0, 0, \pm a_4, \pm a_4, \pm a_4), \\
 &2^{-1}(0, 0, 0, \pm a_2, \pm a_2, \pm a_2, \pm a_3, \pm a_3, \pm a_3, 0, 0, 0), \\
 &2^{-1}(0, 0, 0, \pm a_2, \pm a_2, \pm a_2, 0, 0, 0, \pm a_4, \pm a_4, \pm a_4), \\
 &2^{-1}(0, 0, 0, 0, 0, 0, \pm a_3, \pm a_3, \pm a_3, \pm a_4, \pm a_4, \pm a_4).
 \end{aligned}$$

These points along with the 24 axial points

$$\begin{aligned}
 &(\pm d_1, 0, \dots, 0, 0), \\
 &\vdots \\
 &(0, 0, \dots, 0, \pm d_4),
 \end{aligned}$$

form a second-order 4-grouped cylindrically rotatable design of type 3 if $d_i = (96)^{1/4} a_i$ ($i = 1, 2, 3, 4$). The designs with the smallest number of points among all the second-order rotatable designs in 12 dimensions need 224 points.

Example 4.10.3: Let $m = 3$, $k_1 = 3$, $k_2 = 6$, $k = 8$. By using a BIB(3,3,2,2,1) the points derived are

$$\begin{aligned}
 &2^{-1}(\pm a_1, \pm a_1, \pm a_1, \pm a_2, \pm a_2, \pm a_2, 0, 0), \\
 &2^{-1}(\pm a_1, \pm a_1, \pm a_1, 0, 0, 0, \pm a_3, \pm a_3), \\
 &2^{-1}(0, 0, 0, \pm a_2, \pm a_2, \pm a_2, \pm a_3, \pm a_3).
 \end{aligned}$$

These 64 points and the 16 axial points

$$\begin{aligned}
 &(\pm d_1, 0, \dots, 0), \\
 &\vdots \\
 &(0, \dots, 0, \pm d_3),
 \end{aligned}$$

form a second-order 3-grouped cylindrically rotatable design of type 3 if $d_i = (48)^{1/4} a_i$ ($i = 1, 2$) and $d_3 = 2^{5/4} a_3$.

Example 4.10.4: Let $m = 3$, $k_1 = 3$, $k_2 = 3$, $k = 9$. Consider BIB(3,3,2,2,1). Then the 114 points

$$\begin{aligned} & 2^{-1}(\pm a_1, \pm a_1, \pm a_1, \pm a_2, \pm a_2, \pm a_2, 0, 0, 0), \\ & 2^{-1}(\pm a_1, \pm a_1, \pm a_1, 0, 0, 0, \pm a_3, \pm a_3, \pm a_3), \\ & 2^{-1}(0, 0, 0, \pm a_2, \pm a_2, \pm a_2, \pm a_3, \pm a_3, \pm a_3), \\ & (\pm d_1, 0, \dots, 0), \\ & \vdots \\ & (0, \dots, 0, \pm d_3), \end{aligned}$$

form a second-order 3-grouped cylindrically rotatable design of type 3 if $d_i^2 = a_i^{3/2}$ ($i = 1, 2, 3$). The smallest 9-dimensional second-order rotatable design known so far requires 146 points.

There are many other methods that may be used to generate grouped cylindrically rotatable design of type 3 with small number of points, depending upon the particular grouping of factors. For example the 112 points

$$\begin{aligned} & (\pm a_1, \pm a_1, \pm a_1, \pm a_1, 0, 0, 0, 0, 0), \\ & 2^{-1}(0, 0, 0, 0, \pm a_2, \pm a_2, \pm a_2, \pm a_2, \pm a_2), \\ & (S(d_1, 0, 0, 0), S(d_2, 0, 0, 0, 0)), \end{aligned}$$

form a second-order 2-grouped cylindrically rotatable design of type 3 in 9 dimensions if $d_1^2 = (\frac{8}{5})^{1/2} a_1^2$ and $d_2^2 = 2^{1/2} a_2^2$.

CHAPTER 5

ROTATABLE DESIGNS FOR NON-IDENTICALLY DISTRIBUTED AND CORRELATED OBSERVATIONS

5.1 Introduction

The assumption of independent and identically distributed observations, that is, the second-order distributional assumption is restrictive and often unrealistic. When this second-order assumption is not true but the variance-covariance function of the observations is completely known it may be preferable to construct designs that are rotatable in terms of the best linear unbiased estimates. However, more often than not, the variance-covariance function is not completely known and hence it is usual to restrict to the least squares estimates. Departures from the second-order distributional assumption may cause a given rotatable design to lose its rotatability. Hence it may be desirable to construct robust rotatable designs, that is, designs which are rotatable when the observations are independent and identically distributed and which remain rotatable in terms of the least squares estimates under slight perturbations in the variance-covariance structure from this simple idealistic structure. It may also be of interest to locate families of variance-covariance functions which do not affect the rotatability of any given ordinary rotatable design.

It is assumed that the expected value of the response is given by the polynomial regression model considered in (4.1.1) and (4.1.2). Let $\underline{S}$ be the $N \times N$ positive definite variance-covariance matrix of the observation. If $\underline{S} \neq \sigma^2 \underline{I}$ and if the coefficients are estimated by the method of least squares then from the least squares theory it is known that (4.1.3) is replaced by

$$\text{Var}\{\hat{y}(\underline{x})\} = \underline{x}'^{[d]}(\underline{X}'\underline{X})^{-1}(\underline{X}'\underline{S}\underline{X})(\underline{X}'\underline{X})^{-1}\underline{x}^{[d]}. \quad (5.1.1)$$

Therefore, the necessary and sufficient condition for rotatability in terms of the least squares estimates is given by

$$\underline{M}'^{[d]}(\underline{X}'\underline{X})^{-1}(\underline{X}'\underline{S}\underline{X})(\underline{X}'\underline{X})^{-1}\underline{M}^{[d]} = (\underline{X}'\underline{X})^{-1}(\underline{X}'\underline{S}\underline{X})(\underline{X}'\underline{X})^{-1}, \quad (5.1.2)$$

or equivalently

$$\begin{aligned} (\underline{M}'^{[d]}\underline{X}'\underline{X}\underline{M}^{[d]})^{-1}(\underline{M}'^{[d]}\underline{X}'\underline{S}\underline{X}\underline{M}^{[d]})(\underline{M}'^{[d]}\underline{X}'\underline{X}\underline{M}^{[d]})^{-1} \\ = (\underline{X}'\underline{X})^{-1}(\underline{X}'\underline{S}\underline{X})(\underline{X}'\underline{X})^{-1}, \end{aligned} \quad (5.1.3)$$

for every orthonormal matrix $\underline{M}$ of the form described in Section 4.2.

In what follows it will be the convention to have $\underline{M}^{[0]} = \underline{I}$.

When $\underline{S} \neq \sigma^2 \underline{I}$ and the coefficients are estimated by the method of best linear unbiased estimation, (4.1.3) is replaced by

$$\text{Var}\{\hat{y}(\underline{x})\} = \underline{x}'^{[d]}(\underline{X}'\underline{S}^{-1}\underline{X})^{-1}\underline{x}^{[d]}. \quad (5.1.4)$$

Therefore, a necessary and sufficient condition for rotatability in terms of the best linear unbiased estimates is

$$\underline{M}'^{[d]}\underline{X}'\underline{S}^{-1}\underline{X}\underline{M}^{[d]} = \underline{X}'\underline{S}^{-1}\underline{X} \quad (5.1.5)$$

for every orthonormal matrix $\underline{M}$ of the form under consideration.

When $\underline{S} = \sigma^2 \underline{I}$ conditions (5.1.3) and (5.1.5) reduce to the condition (4.2.2) derived by Box and Hunter (1957). From these conditions it can be seen that when $\underline{S} \neq \sigma^2 \underline{I}$ and the variance-covariance function of the observations is completely known it might be easier to construct designs rotatable in terms of the best linear unbiased estimates than the designs which are rotatable in terms of the least squares estimates.

5.2 Uncorrelated observations with nonconstant variance

In general, for uncorrelated observations with nonconstant variances, the construction of a design rotatable in terms of the least squares estimates or the best linear unbiased estimates may be difficult. However, if the variances are functions of the distances of the observation points from the origin of the design region then these difficulties may be overcome. This particular variance function of the observations is of interest because in many situations it may be quite realistic. Herzberg and Andrews (1976) suggest the use of the assumption of such a variance function in formulating measures of robustness of a design against missing observations.

From Box and Hunter (1957) and Draper (1960a), a set of points equidistant from the origin is called an 'equiradial rotatable set of order d ' if the condition (4.2.2) is satisfied for the set. It is well-known that no single set can provide a non-singular design of order greater than one. However, as the following lemma shows, by taking combinations of such sets robust rotatable designs may be obtained.

Lemma 5.2.1. Any design of order d which is rotatable when the observations are independent and identically distributed and which consists of only equiradial rotatable sets of order d , remains rotatable in terms of the least squares estimates and the best linear unbiased estimates when the observations are uncorrelated but have variances dependent on distances from the origin.

The proof of the Lemma 5.2.1 follows from the results of Box and Hunter (1957).

It is interesting to note that if a rotatable design for independent and identically distributed observations is constructed by combining arbitrary point sets or even equiradial rotatable sets of lower orders,

then this design would not necessarily retain its rotatability under the kind of distributional departures considered here. Only the designs constructed from equiradial rotatable sets of the same order would necessarily retain their rotatability.

For two dimensions, Box and Hunter (1957) construct rotatable designs by combining sets of points equally spaced on concentric circles, i.e. by combining equiradial rotatable sets of the same order. In higher dimensions also, it may be possible to construct rotatable designs of order d by combining equiradial rotatable sets of the same order. The third-order rotatable design of Draper (1960c) in four dimensions and the new eight-dimensional designs displayed in Table 4.4.4 are typical examples. Lemma 5.2.1 provides justification for the use of such designs.

When the observations are uncorrelated but not identically distributed and when the exact form of the non constant variance function $f(\cdot)$ is known, designs rotatable in terms of the best linear unbiased estimates may be constructed by combining equiradial rotatable sets of lower orders. These designs can be obtained from the well-known designs by making slight alterations in the relative distances from the origin of their component point sets without changing the relative orientation. The so-called 'Cube + Cross polytope' second-order rotatable designs are typical examples. Using the notation of Chapter 4 the vertices of a measure polytope (hyper cube) and the vertices of a cross polytope (Octahedra) may be denoted by $\frac{\rho_1}{\sqrt{k}} S(\pm 1, \dots, \pm 1)$ and $\rho_2 S(\pm 1, 0, \dots, 0)$, respectively, where k is the dimension of the space. The distances ρ_1 and ρ_2 are the radii of the corresponding hyperspheres circumscribing these regular figures. Each set of vertices forms an equiradial rotatable set, and hence a design, of the first order. Box and Hunter (1957) showed that these two sets

may be combined, with $\rho_2/\rho_1 = 2^{k/4}/k^{1/2}$, to provide a second-order rotatable design when the observations are independent and identically distributed. When $k = 2$ or 4 , centre points have to be added in order to have a nonsingular design. It can be seen that when the observations have a non-constant variance function $f(\cdot)$ of the form described, these point sets, with

$$\frac{\rho_2}{\{f(\rho_2)\}^{1/4}} = \frac{2^{k/4}}{k^{1/2}} \frac{\rho_1}{\{f(\rho_1)\}^{1/4}}$$

form a second order rotatable design in terms of the best linear unbiased estimates. When $k = 2$ or 4 , centre points have to be added in order to obtain a non-singular design.

The example shows that when the nonconstant variance function $f(\cdot)$ of the uncorrelated observations is completely known there is no additional difficulty in constructing rotatable designs by combining equiradial rotatable sets of lower order. But the function $f(\cdot)$ is seldom completely known. Hence in order to guard against all such $f(\cdot)$ under consideration it may be better to obtain designs by combining equiradial rotatable sets of the same order.

5.3 Effects of correlation on rotatability

When a rotatable design is constructed under the assumption of independent and identically distributed observations and parameters are estimated by least squares estimators, any departure from the distributional assumption usually destroys the rotatability of the design. However, there are variance-covariance functions which do not affect the rotatability of a design at all. These functions seem to belong to the family of functions in which the variances and covariances of the observations are invariant under rotations of the factor space. In

order to prove the main results of this section the following lemmata are needed.

Lemma 5.3.1. If a set of N points, $\underline{x}_u = (x_{1u}, \dots, x_{ku})$ ($u = 1, \dots, N$), satisfies the condition

$$\underline{M}^{[d]'} \left(\sum_{u=1}^N \underline{x}_u^{[d]} \underline{x}_u^{[d]'} \right) \underline{M}^{[d]} = \sum_{u=1}^N \underline{x}_u^{[d]} \underline{x}_u^{[d]'} ,$$

for every matrix $\underline{M}$ (see Section 4.2), the set also satisfies the condition that

$$\underline{M}^{[c]'} \left(\sum_{u=1}^N \underline{x}_u^{[c]} \underline{x}_u^{[\ell]'} \right) \underline{M}^{[\ell]} = \sum_{u=1}^N \underline{x}_u^{[c]} \underline{x}_u^{[\ell]'} ,$$

for every c, ℓ with $c + \ell \leq 2d$ and for every orthogonal matrix $\underline{M}$ under consideration.

Lemma 5.3.2. For any given (ℓ, w) there exist $\binom{\ell+k}{k} \times \binom{w+k}{k}$ matrices $\underline{V}^{(\ell, w)}$ such that

$$\underline{M}^{[\ell]'} \underline{V}^{(\ell, w)} \underline{M}^{[w]} = \underline{V}^{(\ell, w)}$$

for every orthogonal matrix $\underline{M}$ of the form described in Section 4.2.

Lemma 5.3.1 is a consequence of the results of Box and Hunter (1957). The matrices $\underline{V}^{(\ell, w)}$ ($\ell, w = 1, \dots, d$) have to satisfy far less restrictive conditions than the moment matrix of the same order corresponding to a rotatable design and hence these always exist. For example, when $k = 2$, $\ell = 2$ and $w = 2$ any matrix of the form

$$\begin{bmatrix} A & 0 & 0 & B & B & 0 \\ 0 & C & 0 & 0 & 0 & 0 \\ 0 & 0 & C & 0 & 0 & 0 \\ B & 0 & 0 & E+F & E & 0 \\ B & 0 & 0 & E & E+F & 0 \\ 0 & 0 & 0 & 0 & 0 & F \end{bmatrix}$$

satisfies the required conditions. It is not necessary to have $B = C$.

In a moment matrix, $B = C$ would be necessary.

From these lemmata follows a simple but interesting property of the rotatable designs stated in the following theorem.

Theorem 5.3.1. Any design of order d which is rotatable when the observations are independent and identically distributed, retains rotatability in terms of the least squares estimates when the observations have a variance covariance function of the form

$$\text{cov}(y(\underline{x}), y(\underline{z})) = b\delta_{\underline{x}, \underline{z}} + \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \underline{x}^{[\ell]'} \underline{v}^{(\ell, w)} \underline{z}^{[w]} \quad (5.3.1)$$

with $b_{\ell w} = b_{w\ell}$, $\underline{v}^{(w, \ell)} = \underline{v}^{(\ell, w)}$ and as considered in Lemma 5.3.2, $\delta_{\underline{x}, \underline{z}}$ being the Kronecker δ .

Proof: When the variance-covariance structure is as in (5.3.1) the variance covariance matrix $\underline{S}$ is given by

$$\underline{S} = b\underline{I} + \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} [\underline{x}_1^{[\ell]}, \dots, \underline{x}_N^{[\ell]}]' \underline{v}^{(\ell, w)} [\underline{x}_1^{[w]}, \dots, \underline{x}_N^{[w]}]$$

Since by the assumption

$$\underline{M}'^{[d]} \underline{X}' \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{X},$$

it is only necessary to show that

$$\underline{M}'^{[d]} \underline{X}' \underline{S} \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{S} \underline{X},$$

for every orthogonal matrix M of the form under consideration (see, Section 4.2). Now, since

$$\underline{X}'\underline{S}\underline{X} = b\underline{X}'\underline{X} + \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \left(\sum_{u=1}^N \underline{x}_u^{[\ell]} \underline{x}_u^{[w]'} \right) \underline{v}^{(\ell, w)} \left(\sum_{u=1}^N \underline{x}_u^{[w]} \underline{x}_u^{[\ell]'} \right),$$

by applying Lemma 5.3.1 the desired result and hence the theorem are obtained.

The class of variance-covariance functions covered in the theorem is fairly large. In effect it is being assumed that the covariance between $y(\underline{x})$ and $y(\underline{z})$ is an arbitrary polynomial in $(\underline{x}'\underline{x})$, $(\underline{z}'\underline{z})$ and $(\underline{x}'\underline{z})$ of degree d or less. In practice, subclasses of this large class of functions may be of interest. Particularly interesting may be the situations where

$$\text{cov}(y(\underline{x}), y(\underline{z})) = b\delta_{\underline{x}\underline{z}} + \sum_{\ell=0}^d b_{\ell\ell} \underline{x}^{[\ell]} \underline{v}^{(\ell, \ell)} \underline{z}^{[\ell]},$$

or, equivalently,

$$\text{cov}(y(\underline{x}), y(\underline{z})) = b\delta_{\underline{x}\underline{z}} + \sum_{\ell=0}^d b_{\ell\ell} \underline{x}^{[\ell]} \underline{z}^{[\ell]}.$$

From Kiefer (1975b), a square matrix is called completely symmetric if all its diagonal elements are the same and if all its off-diagonal elements are the same. A variance-covariance structure is called completely symmetric if for all choices of design points a completely symmetric variance-covariance matrix of the observations is obtained. It can be seen from the theorem that a completely symmetric variance-covariance structure does not affect the rotatability of the design.

It is interesting to note that the theorem does not hold if the summation in (5.3.1) over ℓ and w is from zero to some value greater than d .

Although Lemma 5.3.1 and Theorem 5.3.1 are consequences of the results of Box and Hunter (1957) these are useful in the investigation of the effects of more complex variance-covariance functions on the rotatability of designs. For example, it may be more realistic to assume variances dependent on distances from the origin and covariances dependent on distances between the observation points. The next theorem provides a result for such a variance-covariance function.

Theorem 5.3.2. The rotatability of a design of order d consisting of equiradial rotatable sets of the same order is unaffected when the observations have a variance-covariance structure given by

$$\begin{aligned} \text{var}\{y(\underline{x})\} &= f(|\underline{x}|), \\ \text{cov}\{y(\underline{x}), y(\underline{z})\} &= f(|\underline{x}-\underline{z}|), \end{aligned} \tag{4.3.2}$$

where $f(\cdot)$ is a positive definite polynomial of degree $2d$ or less.

Proof: It is assumed that the design satisfies the condition that

$$\underline{M}^{[d]'} (\underline{X}' \underline{X}) \underline{M}^{[d]} = \underline{X}' \underline{X}$$

for every matrix $\underline{M}$ under consideration (see Section 4.2). Hence, it is sufficient to show that if $\underline{S}$ is the variance-covariance matrix of the observations then $(\underline{X}' \underline{S} \underline{X})$ is also invariant under every rotation of the factor space. To show this, positive definiteness of the function $f(\cdot)$ is not necessary. This restriction on $f(\cdot)$ is needed since the observations may not have negative variances.

It can readily be seen that under the assumptions of the theorem

$$f(|\underline{x}|) = \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \underline{x}^{[\ell]'} \underline{v}^{(\ell, w)} \underline{x}^{[w]},$$

with $b_{\ell,w}$'s and $\underline{v}^{(\ell,w)}$'s suitably chosen, satisfying the conditions of Theorem 5.3.1. This implies that the variance-covariance matrix $\underline{S}$ may be written as

$$\underline{S} = \underline{S}_1 + \underline{S}_2 ,$$

where

$$\underline{S}_1 = \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \begin{bmatrix} \underline{x}_1^{[\ell]'} \underline{v}^{(\ell,w)} \underline{x}_1^{[w]} & & & \\ & \ddots & & \\ & & \ddots & \\ \underline{Q} & & & \underline{x}_N^{[\ell]'} \underline{v}^{(\ell,w)} \underline{x}_N^{[w]} \end{bmatrix} ,$$

$$\underline{S}_2 = \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} [\underline{A}^{(\ell,w)} + \underline{A}'^{(\ell,w)} - \underline{B}^{(\ell,w)} - \underline{B}'^{(\ell,w)}] ,$$

with

$$\underline{A}^{(\ell,w)} = j [\underline{x}_1^{[\ell]'} \underline{v}^{(\ell,w)} \underline{x}_1^{[w]}, \dots, \underline{x}_N^{[\ell]'} \underline{v}^{(\ell,w)} \underline{x}_N^{[w]}] ,$$

$$\underline{B}^{(\ell,w)} = \begin{bmatrix} \underline{x}_1^{[\ell]'} \\ \vdots \\ \underline{x}_N^{[\ell]'} \end{bmatrix} \underline{v}^{(\ell,w)} [\underline{x}_1^{[w]}, \dots, \underline{x}_N^{[w]}] .$$

Here, j is the $N \times 1$ column vector of 1's.

Let the points $\underline{x}_{i,j}$ ($j = 1, \dots, n_i$) belong to the i -th equiradial rotatable set of order d ($i = 1, \dots, m$). Then

$$\underline{X}' \underline{S}_1 \underline{X} = \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \sum_{i=1}^m \sum_{j=1}^{n_i} (\underline{x}_{i,j}^{[\ell]'} \underline{v}^{(\ell,w)} \underline{x}_{i,j}^{[w]}) \underline{x}_{i,j}^{[d]} \underline{x}_{i,j}^{[d]'} .$$

Since $\underline{M}^{[\ell]'} \underline{v}^{(\ell,w)} \underline{M}^{[w]} = \underline{v}^{(\ell,w)}$ for each $\underline{v}^{(\ell,w)}$, it follows that for

each i ($i = 1, \dots, m$), $\tilde{x}_{ij}^{[l]'} \tilde{v}^{(\ell, w)} \tilde{x}_{ij}^{[w]}$ ($j = 1, \dots, n_i$) is a constant. Therefore,

$$\tilde{M}^{[d]'} \tilde{X}' \tilde{S}_1 \tilde{X} M^{[d]} = \tilde{X}' \tilde{S}_1 \tilde{X}$$

for every orthogonal matrix $\tilde{M}$ under consideration. Also

$$\tilde{X}' \tilde{A}^{(\ell, w)} \tilde{X} = \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \left(\sum_{i=1}^m \sum_{j=1}^{n_i} \tilde{x}_{ij}^{[d]} \right) \left\{ \sum_{i=1}^m \sum_{j=1}^{n_i} (\tilde{x}_{ij}^{[l]'} \tilde{v}^{(\ell, w)} \tilde{x}_{ij}^{[w]}) \tilde{x}_{ij}^{[d]'} \right\}.$$

Hence by Lemma 5.3.1,

$$\tilde{M}^{[d]'} \tilde{X}' \tilde{A}^{(\ell, w)} \tilde{X} M^{[d]} = \tilde{X}' \tilde{A}^{(\ell, w)} \tilde{X}.$$

Similarly,

$$\tilde{X}' \tilde{B}^{(\ell, w)} \tilde{X} = \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \left(\sum_{i=1}^m \sum_{j=1}^{n_i} \tilde{x}_{ij}^{[d]} \tilde{x}_{ij}^{[l]'} \right) \tilde{v}^{(\ell, w)} \left(\sum_{i=1}^m \sum_{j=1}^{n_i} \tilde{x}_{ij}^{[w]} \tilde{x}_{ij}^{[d]'} \right),$$

and by Lemma 5.3.1.

$$\tilde{M}^{[d]'} \tilde{X}' \tilde{B}^{(\ell, w)} \tilde{X} M^{[d]} = \tilde{X}' \tilde{B}^{(\ell, w)} \tilde{X}.$$

Therefore,

$$\tilde{M}^{[d]'} \tilde{X}' \tilde{S}_2 \tilde{X} M^{[d]} = \tilde{X}' \tilde{S}_2 \tilde{X},$$

and hence the theorem follows.

Theorem 5.3.1 applies to all rotatable designs whereas Theorem 5.3.2 applies only to the rotatable designs consisting of equiradial rotatable sets of the same order. Theorem 5.3.2 shows that designs constructed from equiradial rotatable sets are highly robust against wide classes of departures from the 'second order' distributional assumptions.

In many ways the variance-covariance function considered in Theorem 5.3.2 may be more realistic than that in Theorem 5.3.1. In practice, $f(\cdot)$ as a polynomial of degree 2, may be sufficient to approximate any realistic situation. In all cases, it might be better to use rotatable designs based on equiradial rotatable sets of the same order provided that the number of points required by such a design is not excessively large. However, these designs do not necessarily exhaust all possible designs whose rotatability remain unaffected. There may be other designs with this property.

5.4 Best linear unbiased estimates

When dealing with the best linear unbiased estimates, the variance-covariance matrices need to be inverted. The following lemmata are useful for inverting well-patterned matrices.

Lemma 5.4.1: If $\underline{S} = [\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}]' [\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}]$ then $\underline{\bar{S}} = [\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}]' \left(\sum_{i=1}^N \underline{x}_i^{[l]} \underline{x}_i^{[l]'} \right)^{-1} [\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}]$ is a g-inverse of $\underline{S}$ and if $\underline{S}$ is nonsingular then $\underline{\bar{S}} = \underline{S}^{-1}$.

Lemma 5.4.2: If $\underline{S} = a\underline{D} + b[\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}]' [\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}]$

where $\underline{D}$ is diagonal matrix then the inverse of $\underline{S}$ is given by

$$\underline{S}^{-1} = \frac{1}{a} \underline{D}^{-1} - \frac{b}{a^2} \underline{D}^{-1} \begin{bmatrix} \underline{x}_1^{[l]'} \\ \vdots \\ \underline{x}_N^{[l]'} \end{bmatrix} \left(\underline{I} + \frac{b}{a} [\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}] \underline{D}^{-1} \begin{bmatrix} \underline{x}_1^{[l]'} \\ \vdots \\ \underline{x}_N^{[l]'} \end{bmatrix} \right)^{-1} \\ \times [\underline{x}_1^{[l]}, \dots, \underline{x}_N^{[l]}] \underline{D}^{-1}.$$

Lemma 5.4.3: If $S_0 = aI + b_0J$ and $S_i = S_{i-1} + b_i [x_1^{[i]}, \dots, x_N^{[i]}]' \times [x_1^{[i]}, \dots, x_N^{[i]}]$ ($i = 1, \dots, d$) then the inverses of the matrices S_i 's are given iteratively by

$$S_i^{-1} = S_{i-1}^{-1} - b_i S_{i-1}^{-1} \begin{bmatrix} x_1^{[i]}' \\ \vdots \\ x_N^{[i]}' \end{bmatrix} (I + b_i [x_1^{[i]}, \dots, x_N^{[i]}] S_{i-1}^{-1} \begin{bmatrix} x_1^{[i]}' \\ \vdots \\ x_N^{[i]}' \end{bmatrix})^{-1} \\ \times [x_1^{[i]}, \dots, x_N^{[i]}] S_{i-1}^{-1} \quad (i = 1, \dots, d).$$

Lemma 5.4.4: If $S_0 = aI + b_0J$ and $S_i = S_{i-1} + b_i [x_1^{[i]}, \dots, x_N^{[i]}]' v^{(i,i)} \times [x_1^{[i]}, \dots, x_N^{[i]}]$ where the $v^{(i,i)}$'s satisfy $M^{[i]}' v^{(i,i)} M^{[i]} = v^{(i,i)}$ ($i = 1, \dots, d$) then the inverses of the matrices S_i are given iteratively by

$$S_i^{-1} = S_{i-1}^{-1} - b_i S_{i-1}^{-1} \begin{bmatrix} x_1^{[i]}' \\ \vdots \\ x_N^{[i]}' \end{bmatrix} (v^{(i,i)} + b_i [x_1^{[i]}, \dots, x_N^{[i]}] S_{i-1}^{-1} \begin{bmatrix} x_1^{[i]}' \\ \vdots \\ x_N^{[i]}' \end{bmatrix})^{-1} \\ \times [x_1^{[i]}, \dots, x_N^{[i]}] S_{i-1}^{-1} \quad (i = 1, \dots, d).$$

The proofs of the above lemmata involve standard matrix algebra [See Graybill (1969), Rao (1973) or Rao and Mitra (1971)]. By using these lemmata it is easy to see how the rotatability of a design in terms of the best linear unbiased estimates may be affected by simple departures from the 'second-order' distributional assumptions.

Theorem 5.4.1: Any design of order d , rotatable when the observations are independent and identically distributed, remains rotatable in terms of the best linear unbiased estimates when the observations have a variance-covariance function given by

$$(i) \quad \text{cov}(y(\underline{x}), y(\underline{z})) = b\delta_{\underline{x}\underline{z}} + \sum_{\ell=0}^d b_{\ell\ell} \underline{x}^{[\ell]'} \underline{v}^{(\ell,\ell)} \underline{z}^{[\ell]} \quad (5.4.1a)$$

or, more generally

$$(ii) \quad \text{cov}(y(\underline{x}), y(\underline{z})) = b\delta_{\underline{x}\underline{z}} + \sum_{\ell=0}^d \sum_{w=0}^d b_{\ell w} \underline{x}^{[\ell]'} \underline{v}^{(\ell,w)} \underline{z}^{[w]}, \quad (5.4.1b)$$

where $b_{\ell w}$ and $\underline{v}^{(\ell,w)}$ satisfy conditions mentioned in Theorem 5.3.1.

Proof: In case (i) the result can be proved directly since it is easy to obtain the inverse of the variance-covariance matrix $\underline{S}$ explicitly. In this case $\underline{S}$ is the matrix $\underline{S}_d$ of Lemma 5.4.4. Because of the particular dependence of $\underline{S}_i^{-1}$ on $\underline{S}_{i-1}^{-1}$ it follows that $\underline{M}^{[d]'} \underline{X}' \underline{S}_i^{-1} \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{S}_i^{-1} \underline{X}$ if

$$\underline{M}^{[d]'} \underline{X}' \underline{S}_{i-1}^{-1} \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{S}_{i-1}^{-1} \underline{X},$$

$$\underline{M}^{[d]'} \underline{X}' \underline{S}_{i-1}^{-1} [\underline{x}_1^{[i]}, \dots, \underline{x}_N^{[i]}]' \underline{M}^{[i]} = \underline{X}' \underline{S}_{i-1}^{-1} [\underline{x}_1^{[i]}, \dots, \underline{x}_N^{[i]}],$$

and

$$\underline{M}^{[i]'} [\underline{x}_1^{[i]}, \dots, \underline{x}_N^{[i]}] \underline{S}_{i-1}^{-1} \begin{bmatrix} \underline{x}_1^{[i]'} \\ \vdots \\ \underline{x}_N^{[i]'} \end{bmatrix} \quad \underline{M}^{[i]} = [\underline{x}_1^{[i]}, \dots, \underline{x}_N^{[i]}] \underline{S}_{i-1}^{-1} \begin{bmatrix} \underline{x}_1^{[i]'} \\ \vdots \\ \underline{x}_N^{[i]'} \end{bmatrix}.$$

Since the design is rotatable of order d under independent and identically distributed observations, these requirements are satisfied for $i = 1$ and hence it can be seen, iteratively, that they are satisfied for all $i \leq d$. Hence the result.

In case (ii) the more general variance-covariance function of Theorem 5.3.1 is under consideration. The inversion of the variance-covariance matrix may be messy. However, results from estimation theory may be used to avoid the algebra completely. Kruskal (1968), Rao (1967), Watson (1967) and Zyskind (1967) have investigated the situations under which the least squares estimates and the best linear unbiased estimates

are equivalent. In particular, from Rao (1967) and Watson (1967) it is known that the two types of estimates are equivalent when

$$\mathcal{R}[\underline{S}\underline{X}(\underline{X}'\underline{X})^{-1}] \subset \mathcal{R}(\underline{X}),$$

where $\mathcal{R}(\underline{X})$ is the column space of the matrix $\underline{X}$. Clearly, this is true in both case (i) and case (ii) under consideration. Hence the theorem follows.

If the variance-covariance function of the observations is completely known a priori, it is always possible, in principle, to construct a design rotatable in terms of the best linear unbiased estimates. It may even be possible to obtain such a design by combining lower order rotatable sets. For example, consider the variance covariance function given by

$$\begin{aligned} \text{var}(y(\underline{x})) &= \sigma^2 \underline{x}'\underline{x}, \\ \text{cov}(y_1(\underline{x}_1), y_2(\underline{x}_2)) &= \sigma^2(\underline{x}_1 - \underline{x}_2)'(\underline{x}_1 - \underline{x}_2). \end{aligned} \quad (5.4.2)$$

Without loss of generality one may assume that $\sigma^2 = 1$. Then the variance covariance matrix $\underline{S}$ for the observations at $\underline{x}_1, \dots, \underline{x}_N$, is given by

$$\begin{aligned} \underline{S} &= \begin{bmatrix} \underline{x}_1'\underline{x}_1 & \underline{0} \\ \underline{0} & \underline{x}_N'\underline{x}_N \end{bmatrix} - 2 \begin{bmatrix} \underline{x}_1' \\ \vdots \\ \underline{x}_N' \end{bmatrix} [\underline{x}_1, \dots, \underline{x}_N] \\ &+ \begin{bmatrix} \underline{x}_1'\underline{x}_1 \\ \vdots \\ \underline{x}_N'\underline{x}_N \end{bmatrix} \underline{j}' + \underline{j} [\underline{x}_1'\underline{x}_1, \dots, \underline{x}_N'\underline{x}_N], \end{aligned}$$

where $\underline{j}$ is the column vector of 1's.

This decomposition of $\underline{S}$ renders the inversion of $\underline{S}$ a simple exercise and aids in deriving the sufficient conditions on $\underline{x}_i$'s ($i = 1, \dots, N$) so as to satisfy the condition (5.1.5). Now, suppose

$$\underline{S}_0 = \begin{bmatrix} \underline{x}_1' \underline{x}_1 & & & 0 \\ & \ddots & & \\ 0 & & & \underline{x}_N' \underline{x}_N \end{bmatrix},$$

$$\underline{S}_1 = \underline{S}_0 - 2[\underline{x}_1, \dots, \underline{x}_N]' [\underline{x}_1, \dots, \underline{x}_N],$$

$$\underline{S}_2 = \underline{S}_1 + [\underline{x}_1' \underline{x}_1, \dots, \underline{x}_N' \underline{x}_N]' \underline{j}'.$$

Then

$$\underline{S} = \underline{S}_2 + \underline{j}[\underline{x}_1' \underline{x}_1, \dots, \underline{x}_N' \underline{x}_N].$$

It follows that

$$\underline{S}_1^{-1} = \underline{S}_0^{-1} + 2\underline{S}_0^{-1} \begin{bmatrix} \underline{x}_1' \\ \vdots \\ \underline{x}_N' \end{bmatrix} (\underline{I} - 2[\underline{x}_1, \dots, \underline{x}_N] \underline{S}_0^{-1} \begin{bmatrix} \underline{x}_1' \\ \vdots \\ \underline{x}_N' \end{bmatrix})^{-1} [\underline{x}_1, \dots, \underline{x}_N] \underline{S}_0^{-1},$$

$$\underline{S}_2^{-1} = \underline{S}_1^{-1} - \underline{S}_1^{-1} \begin{bmatrix} \underline{x}_1' \underline{x}_1 \\ \vdots \\ \underline{x}_N' \underline{x}_N \end{bmatrix} \underline{j}' \underline{S}_1^{-1} / (1 + \underline{j}' \underline{S}_1^{-1} \begin{bmatrix} \underline{x}_1' \underline{x}_1 \\ \vdots \\ \underline{x}_N' \underline{x}_N \end{bmatrix}),$$

and

$$\underline{S}^{-1} = \underline{S}_2^{-1} - \underline{S}_2^{-1} \underline{j}[\underline{x}_1' \underline{x}_1, \dots, \underline{x}_N' \underline{x}_N] \underline{S}_2^{-1} / (1 + [\underline{x}_1' \underline{x}_1, \dots, \underline{x}_N' \underline{x}_N] \underline{S}_2^{-1} \underline{j}).$$

Hence the design is rotatable if

$$\underline{M}^{[d]'} \underline{x}' \underline{S}_2^{-1} \underline{X} \underline{M}^{[d]} = \underline{x}' \underline{S}_2^{-1} \underline{X}, \quad (5.4.3a)$$

$$\underline{M}^{[0]'} [\underline{x}_1' \underline{x}_1, \dots, \underline{x}_N' \underline{x}_N] \underline{S}_2^{-1} \underline{X} \underline{M}^{[d]} = [\underline{x}_1' \underline{x}_1, \dots, \underline{x}_N' \underline{x}_N] \underline{S}_2^{-1} \underline{X}. \quad (5.4.3b)$$

Also from the form of S_2^{-1} it follows that for (5.4.3a) to hold a sufficient condition is

$$\underline{M}^{[d]'} \underline{X}' \underline{S}_1^{-1} \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{S}_1^{-1} \underline{X} , \quad (5.4.4a),$$

$$\underline{M}^{[d]'} \underline{X}' \underline{S}_1^{-1} \begin{bmatrix} \underline{x}_1' \underline{x}_1 \\ \vdots \\ \underline{x}_N' \underline{x}_N \end{bmatrix} \underline{M}^{[0]} = \underline{X}' \underline{S}_1^{-1} \begin{bmatrix} \underline{x}_1' \underline{x}_1 \\ \vdots \\ \underline{x}_N' \underline{x}_N \end{bmatrix} . \quad (5.4.4b).$$

Further, since $\underline{S}_1^{-1}$ is symmetric, the sufficient conditions for (5.4.3b) are implied by (5.4.4). Similarly from the form of $\underline{S}_1^{-1}$ it follows that a sufficient condition for (5.4.4a) to hold is

$$\underline{M}^{[d]'} \underline{X}' \underline{S}_0^{-1} \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{S}_0^{-1} \underline{X} \quad (5.4.5a)$$

since (5.4.5a) implies that

$$\begin{aligned} \underline{M}^{[d]'} \underline{X}' \underline{S}_0^{-1} [\underline{x}_1, \dots, \underline{x}_N]' \underline{M}^{[1]} &= \underline{X}' \underline{S}_0^{-1} [\underline{x}_1, \dots, \underline{x}_N]' , \\ \underline{M}^{[1]'} [\underline{x}_1, \dots, \underline{x}_N] \underline{S}_0^{-1} [\underline{x}_1, \dots, \underline{x}_N]' \underline{M}^{[1]} &= [\underline{x}_1, \dots, \underline{x}_N] \underline{S}_0^{-1} [\underline{x}_1, \dots, \underline{x}_N]' . \end{aligned}$$

Finally, it can readily be seen that for (5.4.4b) to hold it is sufficient to have (5.4.5a) coupled with

$$\underline{M}^{[d]'} \underline{X}' \underline{j} \underline{M}^{[0]} = \underline{X}' \underline{j} . \quad (5.4.5b)$$

Conditions (5.4.5a) and (5.4.5b) suggest that even though the observations have nonconstant variances and are correlated it would be possible to construct rotatable designs of order d from lower order rotatable sets, in particular from rotatable sets of order $d-1$. As a specific example consider the quadratic model, that is, the case with $d = 2$. It was shown in Section 5.2 that if there is no correlation but variances are as assumed in (5.4.2) then a measure polytope of radius ρ_m and a cross-polytope of radius ρ_c with $\rho_c^4 / (1 + \rho_c^2) = \frac{2^k}{k^2} \rho_m^4 / (1 + \rho_m^2)$ may be combined in their standard relative orientation

to give a design of order two rotatable in terms of the best linear unbiased estimates. Clearly, for such an arrangement of points conditions (5.4.5a) and (5.4.5b) are both satisfied. Hence this design is also rotatable when the variance-covariance function is of the form considered in (5.4.2). As in the case of uncorrelated observations, centre points need to be added when $k = 2$ or 4 in order to obtain a non-singular design.

The example suggests that if a design is known to be rotatable when the observations are independent and identically distributed, it may quite easily be possible to construct designs rotatable in terms of the best linear unbiased estimates when the observations are correlated. It may be necessary only to change the relative distances from the origin without altering the relative orientation of the various point sets involved. However, prior knowledge of the exact form of the variance-covariance function is needed for constructing such designs.

5.5 Robust designs in two dimensions

In Section 5.3 it has been shown that the rotatability of rotatable designs built up from equiradial rotatable sets of the same order are robust against wide classes of departures from the 'second-order' distributional assumptions. From Carter (1957) or Bose and Carter (1959) it is known that it is not necessary, although it may be usual to construct rotatable designs in 2 dimensions by combining sets of points equally placed on concentric circles. If d is the order of the design then there must be at least $2d+1$ equally spaced points on each circle for such a design. The minimum number of such circles required is to be determined by the order d . The relative radii of the circles may be determined by the necessity to have the parameter estimates free

from block effects when the experiment is of a sequential nature. Within this class of designs there is a subclass whose rotatability is robust against even wider classes of variance-covariance functions than those considered earlier. This subclass of designs are obtained by having the same number n ($\geq 2d+1$) of equally spaced points on each circle and the circles having relative orientations such that the angle subtended at the origin by any two design points is an integral multiple of $\frac{\pi}{n}$. The robustness of these designs is shown in the following theorem.

Theorem 5.5.1: The rotatability of the two-dimensional designs described is unaffected by variance-covariance structures of the form given by

$$\text{cov}(y_1(\underline{x}_1), y_2(\underline{x}_2)) = \sigma^2 \{ a \delta_{\underline{x}_1 \underline{x}_2} g(\underline{x}_1' \underline{x}_1) + h(\underline{x}_1' \underline{x}_2) + f(|\underline{x}_1 - \underline{x}_2|) \} ,$$

where $g(\cdot)$, $h(\cdot)$ and $f(\cdot)$ may be arbitrary functions except that $\{ag(z) + h(z) + f(0)\}$ is positive definite for every real z .

Proof: Suppose there are c circles, each with n points. Then the ' $\underline{X}$ ' matrix may be written as

$$\underline{X} = \begin{bmatrix} \underline{x}_1^{[d]} \\ \vdots \\ \underline{x}_c^{[d]} \end{bmatrix} ,$$

where

$$\underline{x}_i^{[d]} = [x_{i1}^{[d]}, \dots, x_{in}^{[d]}]' \quad (i = 1, \dots, c).$$

Also, for each i ($i = 1, \dots, c$),

$$\underline{M}^{[d]'} = \sum_{j=1}^n \underline{x}_{ij}^{[d]} \underline{x}_{ij}^{[d]'} \quad \underline{M}^{[d]} = \sum_{j=1}^n \underline{x}_{ij}^{[d]} \underline{x}_{ij}^{[d]'} .$$

Hence, if $\underline{S}$ is the variance-covariance matrix of the observations, it is sufficient to show that

$$\underline{M}^{[d]'} \underline{X}' \underline{S} \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{S} \underline{X}.$$

Now $\underline{S}$ may be written as

$$\underline{S} = \underline{G} + \underline{H} + \underline{F},$$

where the matrices $\underline{G}$, $\underline{H}$ and $\underline{F}$ correspond to the functions $g(\cdot)$, $h(\cdot)$ and $f(\cdot)$, respectively. These are partitioned matrices given by

$$\underline{G} = \begin{bmatrix} \underline{G}_{11} & & \underline{Q} \\ & \ddots & \\ \underline{Q} & & \underline{G}_{cc} \end{bmatrix},$$

$$\underline{H} = \begin{bmatrix} \underline{H}_{11} & \cdot & \cdot & \cdot & \underline{H}_{1c} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \underline{H}_{c1} & \cdot & \cdot & \cdot & \underline{H}_{cc} \end{bmatrix},$$

$$\underline{F} = \begin{bmatrix} \underline{F}_{11} & \cdot & \cdot & \cdot & \underline{F}_{1c} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \underline{F}_{c1} & \cdot & \cdot & \cdot & \underline{F}_{cc} \end{bmatrix}.$$

Each $\underline{G}_{ii}$ is a $n \times n$ diagonal matrix with, say, g_i , as diagonal elements ($i = 1, \dots, c$). Therefore, by Lemma 5.2.1,

$$\underline{M}^{[d]'} \underline{X}' \underline{G} \underline{X} \underline{M}^{[d]} = \underline{X}' \underline{G} \underline{X}.$$

Now, since there are at most $\lfloor \frac{n}{2} \rfloor + 1$ distinct inner products of the points on any two circles, each $\underline{H}_{ij}$ has at most $\lfloor \frac{n}{2} \rfloor + 1$ distinct elements corresponding to these inner products. This implies that regardless of what the function $h(\cdot)$ actually is, it is possible to have a simple decomposition of the matrices $\underline{H}_{ij}$ given by

$$\underline{H}_{ii} = \alpha_{ii} \underline{I} + \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor - 1} \alpha_{ii\ell} (\underline{X}_i^{[\ell]} \underline{X}_i^{[\ell]'}) \quad (i = 1, \dots, c),$$

and

$$H_{ij} = \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor} \alpha_{ij\ell} (X_i^{[\ell]} X_j^{[\ell]})' \quad (i, j = 1, \dots, c; i \neq j),$$

where

$$X_i^{[\ell]} = [x_{i1}^{[\ell]}, \dots, x_{in}^{[\ell]}]'$$

Therefore,

$$\begin{aligned} X'HX &= \sum_{i=1}^c \sum_{j=1}^c X_i^{[d]'} H_{ij} X_j^{[d]}, \\ X_i^{[d]'} H_{ii} X_i^{[d]} &= \alpha_{ii} X_i^{[d]'} X_i^{[d]} + \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor - 1} \alpha_{ii\ell} (X_i^{[d]'} X_i^{[\ell]})(X_i^{[\ell]'} X_i^{[d]}), \\ X_i^{[d]'} H_{ij} X_j^{[d]} &= \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor} \alpha_{ij\ell} (X_i^{[d]'} X_i^{[\ell]})(X_j^{[\ell]'} X_j^{[d]}). \end{aligned}$$

But since $2d \leq n-1$, by Lemma 5.3.1 it follows that

$$M^{[d]'} X_i^{[d]'} X_i^{[\ell]} M^{[\ell]} = X_i^{[d]'} X_i^{[\ell]} \quad (\ell = 0, 1, \dots, \lfloor \frac{n}{2} \rfloor; i = 1, \dots, c),$$

and hence

$$M^{[d]'} X' H X M^{[d]} = X' H X.$$

In the same way, since there are at most $\lfloor \frac{n}{2} \rfloor + 1$ distinct interpoint distances for the points on any two circles, each F_{ij} has at most $\frac{n}{2} + 1$ distinct elements corresponding to these distances. Thus, regardless of what the function $f(\cdot)$ actually is, it is possible to have a simple decomposition of the matrices F_{ij} in exactly the same way as obtained for the H_{ij} . Hence, by similar arguments it follows that

$$M^{[d]'} X' F X M^{[d]} = X' F X.$$

This completes the proof of the theorem.

It is interesting to note that the functions $g(\cdot)$, $h(\cdot)$ and $f(\cdot)$ in the theorem are completely arbitrary. If these were to be polynomials, no restriction is needed on their degrees. The two dimensional designs obtained, therefore, have highly desirable features as far as the robustness of their rotatability is concerned.

If similar robust designs are to be obtained in higher dimensions, in analogy with the two-dimensional situation the designs would be required to be such that there are no more than $d+2$ distinct interpoint distances or inner products for the points belonging to each equiradial rotatable set of order d . If a design is to comprise of several equiradial rotatable sets of order d then in addition it is required that the relative orientation of these sets be such that the same holds for inter-point distances and inner products of points from any two sets. The upper bound $d+2$ may be increased to $d+3$ if the $(2d+1)$ -th moments vanish for a design in the first case and for each of the equiradial rotatable sets in the second case. If on the other hand a design of order d is constructed by combining equiradial rotatable sets of order $d-1$ then the upper bound is decreased to $d+1$ if the $(2d-1)$ -th moments vanish for each set. For example, in 3 dimensions when $d = 1$, that is, among the first-order designs those comprising of the vertices of regular tetrahedron or cube or octahedron have their rotatability robust against the kind of distributional departures considered here. In higher dimensions, only the tetrahedron and the octahedron seem to have this property. Among the second-order three-dimensional designs, the design consisting of the vertices of an icosahedron have this property whereas that consisting of, say, the vertices of a dodecahedron does not. This can be seen by looking at the co-ordinates of the vertices of these regular figures [see, Coxeter (1948)]. These examples show how

restrictive this class of desired designs is. This restrictiveness is not surprising since the rotatable designs searched for are to be robust against almost arbitrary departures from the second-order distributional assumptions.

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