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SOME THIRD-ORDER ROTATABLE DESIGNS IN THREE DIMENSIONS

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Summary

Some new third-order rotatable designs in three dimensions are derived from some of the available third-order rotatable designs in two dimensions. When these designs are used the results of the experiments performed according to the two-dimentional designs need not be discarded. Some of these designs may be performed sequentially in all three factors, starting with a one-dimensional design. Further, these third-order rotatable designs require a smaller number of points than most of the available three-dimensional third-order rotatable designs.

1. Introduction

For a rotatable design, the variance of the estimated response is constant at points equidistant from the centre of the design (Box and Hunter [2]) and further, the variance of the difference between the estimated responses at any two points is a function of the distances of the points from the centre of the design and the angle subtending the points at the centre (Herzberg [11]).

The problem considered in this paper is that of constructing third-order rotatable designs in three dimensions from those in two dimensions such that the experiments performed according to the two-dimensional designs need not be discarded when analysing the three-dimensional designs (a dth order design permits all the coefficients in a polynomial of order d to be estimated).

The designs constructed allow experiments to be performed 'sequentially' in the factors by starting with experiments involving two factors only. After performing a two-dimensional design the experiments may be stopped if it is felt that the third factor is not really needed, while if it is felt that another factor should have been included, the ex-

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perimenter may proceed by the method presented without discarding the original results. The number of additional experiments required to convert the two-dimensional designs into three-dimensional designs is smaller than the number of experiments required by the designs with minimum number of experiments among the available three-dimensional third-order rotatable designs which are all non-sequential in the factors. The designs presented may therefore be more economic.

The moment requirements of a rotatable design were derived by Box and Hunter [2]. The necessary and sufficient conditions for a k-dimensional point-set to be a non-singular third-order rotatable design were obtained by Gardiner, Grandage and Hader [8] and the geometrical interpretation of these conditions was derived by Draper [4]. For the sake of brevity, these conditions are not to be restated here.

2. Available third-order rotatable designs

Gardiner, Grandage and Hader [8], Draper [4], [5], [7], Thaker and Das [15], Das and Narasimham [3], Herzberg [9], Tyagi [17], Nigam [14] and Huda [13] have considered the problem of constructing third-order rotatable designs. In particular, Gardiner, Grandage and Hader [8], Draper [4], [7] and Das and Narasimham [3] provided a large number of three-dimensional third-order rotatable designs. However, none of these designs can be performed 'sequentially' in the factors. The designs with the minimum number of points among these require 32 points (Herzberg and Cox [12]), others requiring 42 or more points.

3. The construction of three-dimensional designs from two-dimensional designs

It is known from Box and Hunter [2], Bose and Carter [1] and Gardiner, Grandage and Hader [8] that a set of N' ($\geqq 7$) points equally spaced on a circle centred at the origin satisfies the moment requirements of a third-order rotatable set and hence, two-dimensional third-order rotatable designs may be constructed by combining such point-sets associated with two or more distinct circles. Suppose such a design is given by the points $(x_{1u}^{(i)}, x_{2u}^{(i)})$ $(i=1, 2;\ u=1, \cdots, N')$ where for each i the points are equally spaced on the circle of radius ρ_i $(i=1, 2)$. Further, let $A=(N'/2)(\rho_1^2+\rho_2^2)$, $B=(N'/8)(\rho_1^4+\rho_2^4)$ and $C=(N'/48)(\rho_1^6+\rho_2^6)$.

Now consider a three-dimensional point-set given by the $2N'+22$ points

$$(x_{1u}^{(i)}, x_{2u}^{(i)}, 0) \qquad (u=1, \cdots, N';\ i=1, 2)\,,$$

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

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

(1) $$(\pm v,\ \pm v,\ \pm a)\ ,$$

$$(0,\ 0,\ \pm\alpha)\ ,$$

$$(0,\ 0,\ \pm\beta)\ ,$$

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

For this set of points the following conditions hold:

$$\sum_{u=1}^{N} x_{iu}^2 = A+4d^2+8v^2 \qquad (i=1,\ 2)\ ,$$

$$\sum_{u=1}^{N} x_{iu}^4 = 3B+4d^4+8v^4 \qquad (i=1,\ 2)\ ,$$

$$\sum_{u=1}^{N} x_{1u}^2 x_{2u}^2 = B+8v^4\ ,$$

$$\sum_{u=1}^{N} x_{iu}^6 = 15C+4d^6+8v^6 \qquad (i=1,\ 2)\ ,$$

$$\sum_{u=1}^{N} x_{iu}^4 x_{ju}^2 = 3C+8v^6 \qquad (i\neq j;\ i,\ j=1,\ 2)\ ,$$

$$\sum_{u=1}^{N} x_{3u}^2 = 8b^2+8a^2+2(\alpha^2+\beta^2+\gamma^2)\ ,$$

$$\sum_{u=1}^{N} x_{3u}^4 = 8b^4+8a^4+2(\alpha^4+\beta^4+\gamma^4)\ ,$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{3u}^2 = 4b^2d^2+8v^2a^2 \qquad (i=1,\ 2)\ ,$$

$$\sum_{u=1}^{N} x_{3u}^6 = 8b^6+8a^6+2(\alpha^6+\beta^6+\gamma^6)\ ,$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{3u}^4 = 4b^4d^2+8a^4v^2 \qquad (i=1,\ 2)\ ,$$

$$\sum_{u=1}^{N} x_{iu}^4 x_{3u}^2 = 4b^2d^4+8a^2v^4 \qquad (i=1,\ 2)\ ,$$

$$\sum_{u=1}^{N} x_{1u}^2 x_{2u}^2 x_{3u}^2 = 8v^4a^2\ ,$$

and all other sums of powers and products up to order six are zero. It follows that this set of points forms a third-order rotatable design in three dimensions if

$$d^2=2v^2\ , \qquad b^2=a^2=\frac{3}{2}v^2\ ,$$

and

$$v^4=\frac{B}{16}\,,\qquad v^6=\frac{3C}{28}\,,\tag{2}$$

with

$$\alpha^2+\beta^2+\gamma^2=\frac{1}{2}(A-8v^2)\,,\quad \alpha^4+\beta^4+\gamma^4=18v^4\,,\quad \alpha^6+\beta^6+\gamma^6=63v^6\,.\tag{3}$$

Let $\rho_2^2=t\rho_1^2$ $(1\neq t\geqq 0)$. Then the two equations in (2) are simultaneously satisfied if there exists a nonnegative t such that

$$\frac{(1+t^2)^3}{(1+t^3)^2}=\frac{512}{49N'}\,,\tag{4}$$

and then $v^2=\{N'(1+t^2)/128\}^{1/2}\rho_1^2$. Clearly such a t exists for $N'\leqq 10$.

Consider the case $N'=7$. Then the solution to (4) is given by $t=0.46945$ whence $\rho_2^2=0.46945\rho_1^2$, $v^2=0.25834\rho_1^2$. Therefore, (3) is replaced by

$$\begin{aligned}\alpha^2+\beta^2+\gamma^2&=1.53818\rho_1^2\,,\\ \alpha^4+\beta^4+\gamma^4&=1.20131\rho_1^4\,,\\ \alpha^6+\beta^6+\gamma^6&=1.08622\rho_1^6\,.\end{aligned}\tag{5}$$

Let $\alpha^2=p\rho_1^2$, $\beta^2=q\rho_1^2$, $\gamma^2=r\rho_1^2$. It follows that p, q, r have to be nonnegative real roots of the cubic equation

$$g(z)=z^3-z^2(p+q+r)+z(pq+qr+rp)-pqr=0$$

which may, due to (5), be written as

$$g_1(z)=z^3-z^2(1.53818)+z(0.58234)-0.04471=0\,.\tag{6}$$

Now from the theory of cubic equations (see Turnbull [16]) it is known that the 3 roots of the cubic equation,

$$z^3+a_1z^2+a_2z+a_3=0\,,\tag{7}$$

are all real if

$$\Delta=\frac{\Delta_1^3}{27}+\frac{\Delta_2^2}{4}<0\,,\tag{8}$$

where

$$\Delta_1=\left(a_2-\frac{1}{3}a_1^2\right)\,,\qquad \Delta_2=\frac{2}{27}a_1^3-\frac{1}{3}a_1a_2+a_3\,.\tag{9}$$

Further, the three real roots of (7) are then given by

$$z=2\left(-\frac{\Delta_1}{3}\right)^{1/2}\cos\left(\frac{\theta+2j\pi}{3}\right)-\frac{1}{3}a_1 \qquad (j=0, 1, 2)$$

where $\theta=\text{Arc}\cos\{-\Delta_2/2(-\Delta_1^3/27)^{1/2}\}$.

Clearly, the conditions for having 3 real roots are satisfied by $g_1(z)$ in (6). Further, since $g_1(z)<0$ for $z\leqq 0$, all the roots are strictly positive. Thus nonnegative p, q, r and hence, nonnegative $\alpha^2, \beta^2, \gamma^2$ satisfying (3) exist. Therefore, when $N'=7$, the 36 points described in (1) form a third-order rotatable design in three dimensions if ρ_1^2, ρ_2^2, v^2, a^2, b^2, d^2, α^2, β^2 and γ^2 are appropriately chosen in the manner described.

Consider the case $N'=8$. Then the solution to (4) is given by $t=0.3537$ whence $\rho_2^2=0.3537\rho_1^2$ and $v^2=0.26518\rho_1^2$. Therefore, (3) is replaced by

$$\alpha^2+\beta^2+\gamma^2=1.64669\rho_1^2\ ,$$

$$\alpha^4+\beta^4+\gamma^4=1.26574\rho_1^4\ ,$$

$$\alpha^6+\beta^6+\gamma^6=1.17476\rho_1^6\ .$$

Let $\alpha^2=p\rho_1^2$, $\beta^2=q\rho_1^2$, $\gamma^2=r\rho_1^2$. The p, q, r have to be nonnegative real roots of

$$g_2(z)=z^3-z^2(1.64669)+z(0.72292)-0.09364=0\ . \tag{10}$$

It can readily be seen from (7), (8) and (9) that (10) has 3 positive real roots. Therefore, when $N'=8$, the 38 points described in (1) form a third-order rotatable design in three dimensions if ρ_1^2, ρ_2^2, v^2, a^2, b^2, d^2, α^2, β^2 and γ^2 are suitably chosen.

4. Comments

When $N'=10$, a third-order rotatable design in three dimensions with 42 points may be constructed in the manner described. However, when $N'=9$, the solution to (4) is given by $t=0.2485$ and then surprisingly, (3) cannot be satisfied since calculations show that nonnegative real p, q, r of the desired type do not exist. This is rather an unexpected result. However, some variation of the method might work.

Draper [6] presented a method of constructing a second-order rotatable design in k dimensions from a second-order rotatable design in $(k-1)$ dimensions. Herzberg [10] presented an alternative method for which the results of the experiments performed according to the $(k-1)$-dimensional design need not be discarded. The three-dimensional third-order rotatable designs presented here share some of the features of the designs constructed by Herzberg's method. These designs allow the experiments to be performed 'sequentially' in the factors by starting with experiments involving two factors rather than all three factors and this can result in saving of resources. The 38-point and the 42-point designs derived are particularly interesting since these may be performed sequentially, beginning with symmetric one-dimensional designs.

It may be possible to derive designs sequential in the factors from two-dimensional designs other than those considered here.

The method described may be extended to construct higher-dimensional designs which are sequential in the factors.

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