GROUP DIVISIBLE ROTATABLE DESIGN WHICH MINIMIZE THE MEAN SQUARE BIAS

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SUMMARY

A class of group divisible rotatable designs in its general from has been considered and its optimality properties in the sense of minimisation of mean square bias has been studied. The constructional aspects of these designs are being considered in a separate paper.

INTRODUCTION

The class of rotatable designs was first introduced by Box and Wilson (1951) and its mathematical theory in full details was developed by Box and Hunter (1957). Herzberg (1967) relaxed the restrictive conditions for rotatability and introduced the concept of cylindrical rotatability of types 1, 2 and 3 (1967). Das and Dey (1967) introduced the concept of group divisible rotatability. This concept, though introduced independently of Herzberg, is essentially the same as that of type 3 cylindrically rotatable designs. Later Adhikari and Sinha (1976) considered the problem more elaborately.

Das and Dey (1967) and also Adhikari and Sinha (1976) in their group divisible rotatable designs deal with two groups, which can without much difficulty be extended to any number of groups and that is done in the present paper.

We consider the class of group divisible rotatable designs in its general form and study its optimality properties in the sense of minimisation of mean square bias in the line of Draper and Lawrence (1967) in the present paper and discuss the constructional aspects of these designs in a separate paper.

Definitions and notations

Let the observed response Y_x be composed of two parts, viz., $\eta_{(x)}$, a d-th degree polynomial in x, representing the true response and ε, the error.

Let, $y(x)=\eta(x)+\varepsilon$

where, $$\eta(x)=\beta_o+\beta_1x_1+\beta_2x_2+\ldots$$
$$+\beta_{11}x_1^2+\beta_{22}\,x_2^2+\ldots+\beta_{12}\,x_1\,x_2+\ldots$$
$$E(\varepsilon)=0 \text{ and } V(\varepsilon)=\sigma^2$$

Group divisible rotatable designs (m groups).

Let $\hat{Y}(x)$ be the least square estimate of $\eta(x)$.

A design is said to be group divisible rotatable of order d, if the variance of the estimated response at a point x, estimated by a d-th degree polynomial remains unchanged for all orthogonal rotations of the form

$$R=\text{Diag}\,[R_1,\,R_2,\ldots R_m] \qquad \ldots(2.2)$$

where each $R_i\,(n_i\,xn_i)$ is an orthogonal matrix and $\sum_{i=1}^{m} n_i=k$ i.e., the factors are divided into m groups and if the vector $x^{(i)}$ denote the levels of the factors belonging to the i-th group, then $V(\hat{Y}(x))$, remains unchanged as long as $(x^{(i)})'\,x^{(i)}$ remains unchanged for $i=1,2,\ldots,m$.

We observe the following particular cases of group divisible rotatability:

(*i*) $m=1$ leads to the rotatable designs of Box and Hunter (1957)

(*ii*) $m=2$ leads to the cylindrically rotatable designs of type 3, defined by Herzberg (1967).

(*iii*) $n_1>1$ and $n_2=n_3=\ldots=n_m=1$
lead to the cylindrically rotatable design of type 2 of Herzberg (1967).

Moment conditions for group divisible rotatable designs

Let the design D consisting of N observation be denoted by N design points $(x_{1u},\,x_{2u}\ldots x_{ku})$, $u=1,2,\ldots N$.

Let us denote the moment

$$N^{-1} \quad \sum_{u=1}^{N} x_{1u}^{d_1}\,x_{2u}^{d_2}\,\ldots x_{ku}^{d_k} \text{ by } [1^{d_1}\ldots k^{d_k}]$$

Let $S_i=\{j : j\text{-}th \text{ factor belongs to the } i\text{-}th \text{ group}\}$

Then, proceeding exactly in the same manner as Box and Hunter (1957), we arrive at the following moment conditions for a d-th order group divisible rotatable design.

$$[1^{d_1} \ldots k^{d_k}]=0 \text{ if any } \alpha_j \text{ is odd}$$

$$=\lambda_{r_1}, \ldots r_m. \, 2^{-\frac{\alpha}{2}} \left(\prod_{j=1}^{k} (\alpha_j)\,!\right)/\left(\prod_{j=1}^{k} (\tfrac{1}{2}\alpha_j)\,!\right) \text{ otherwise} \tag{3.1}$$

where
$$\alpha=\sum_{j=1}^{k}\alpha_j \leqslant 2d,$$

$$r_i=\sum_{j \varepsilon s_i}\alpha_j, \; i=1,2,\ldots,m$$

and $\lambda_{r_1,\ldots,\, r_m}$ is a constant depending only on r_i's but not on α_j's individually.

The moments of a second order group divisible rotatable design can thus be written as

$$[1^{\alpha_1}\ldots k^{\alpha_k}]=0 \text{ if any } \alpha_j \text{ is odd and } \sum_j \alpha_j \leqslant 4$$

$$=\lambda_2^{(i)}, \text{ if } \alpha_j+2, \alpha_{j'}=0, i\neq j, j \varepsilon^s s_i, i=1, 2,\ldots m$$

$$=3\, \lambda_4^{(i)}, \text{ if } \alpha_j=4, \alpha_{j'}=0, j' \neq j, j \varepsilon s_i, i=1, 2,\ldots m$$

$$=\lambda_4^{(i)}, \text{ if } \alpha_j=\alpha_j'=2, \alpha_j+0, j''\neq j, j', j\neq j', j. \, j' \varepsilon s_i, i=1, 2,\ldots m$$

$$=\theta_{ii'}, \text{ if } \alpha_j=\alpha_{j'}=2, \alpha_j''=0, j'',\neq j, j',$$
$$j \varepsilon s_i, j \varepsilon s_i, i\neq i', i, i'=1, 2,\ldots m.$$

Estimation of parameters of a second order GDR design and the variance function

The expression for moments of a second order GDR designs are given in (3.2). From that we can write the moment matrix using the notation of Box and Hunter (1957). $S=N^{-1}(X' \; X)$ in the form

$$S=\begin{bmatrix} A & O & B' & O \\ O & C & O & O \\ B & O & D & O \\ O & O & O & E \end{bmatrix}$$

where $A=1$, $B'=(\lambda_2^{(1)}\ J_{1\times n_{11}}\ \ldots,\ \lambda_2^{(m)}\ J_{1\times n_m})$,

$$c=\text{diag}\ [\lambda_2^{(1)}\ I_{n_1}'\ \ldots,\ \lambda_2^{(m)}\ I_{n_m}],$$

$$D=\begin{bmatrix} D_{ll} & \cdots\cdots\cdots & \cdots & D_{lm} \\ \vdots & & & \vdots \\ D_{ml} & \cdots\cdots\cdots\cdots & & D_{mm} \end{bmatrix}$$

where $D_{ii}=2\ \lambda_4^{(i)}\ I_{n_i}+\lambda_4^{(i)}\ J_{n_i\times n_i}$, $i=1, 2, \ldots$

and $D_{ii}'=\theta_{ii'}\ N_{n_i}\times n_i'$, $i\neq i'$, i, $i'=1, 2, \ldots m$

$$E=\text{diag}\ (E_l \ldots E_m)$$

where $E_i\quad =\text{diag}\ (E_{ii}', \ldots E_{im})$

where $\quad E_{ii}=\lambda_4^{(i)}\ \binom{I_{n_i}}{2}$

and $\quad E_{ii}'=\theta_{ii}'\ I_{n_i}\times n_i'$,

$i'>i$, $i=1, 2\ldots m$ ...(4.1.)

Let us consider the nonsingularity conditions for S and its inverse.

For estimation of the parameters in the response function, we need to derive the nonsingularity conditions for S and then obtain S^{-1} in case it exists.

Let $\bar{D}=D-BB'$ where D and B are as defined in (5.1).

Then the nonsingularity condition in the general case of GDR designs is $|\ \bar{D}\ | > 0$, since $\lambda_2^{(i)}$' s and $\lambda_4^{(i)}$' s must be > 0.

For $m=2$, this condition can be written in the simple form

$$0<\theta_{12}<1+2\ \lambda_4^{(2)}/(n_2\ A)+(\lambda_4^{(2)}-1)/A$$

where

$$A=n_1/2\lambda_4^{(1)}+n_1\ (\lambda_4^{(1)}-1)/(\ (n_1+2)\lambda_4^{(2)}-n_1) \qquad \ldots(4.2)$$

For $m>2$ (the case $m=2$ has been considered in details by Adhikari and Sinha (1976) without the non-singularity condition explicitly stated) although it is possible to give recurrence formulae for evaluation of $|\ \bar{D}\ |$ and obtaining $\bar{D}^1$ and hence S^{-1} in stages, it seems rather tedious to derive explicit algebraic expressions for both $|\ \bar{D}\ |$ and $\bar{D}^{-1}$. But the form of $\bar{D}$ becomes extremely simple in the special case $\theta_{ii'}=1$, $i=i'$, $i,i'=1, 2, \ldots m$, so that $|\ \bar{D}\ |$ and $\bar{D}^{-1}$ can easily be obtained there. This case corresponds exactly to the groupwise spherical weight density, which is the product of m spherical densities (considered in section 5).

If we standardise the variables, *i e.*, $\lambda_2^{(i)}=1$, $i=1, 2 \ldots m$, we arrive at the nonsingularity condtion in this special case as

$$\lambda_4^{(i)} > n_i/(n_i+2),\ i=1, 2, \ldots, m$$

and S^{-1} as

$$S^{-1}=\begin{bmatrix} a_o & O & -(B^*)' & O \\ O & I_k & O & O \\ -B^* & O & D & O \\ O & O & O & E^{-1} \end{bmatrix} \quad \ldots(4.3)$$

where $a_o=1+\sum_{i=1}^{m} n_i\ (\lambda_4^{(i)}-1)/(\lambda_4^{(i)}\ \mu_i)$,

$(B^*)'=(b_1\ J1\times n_1,\ \ldots\ b_m\ J_1\times n_m)$

with $b_i=\mu_i^{-1}$,

$D^*=\text{diag}\ (D^*_{11},\ \ldots\ D^*_{mm})$, ...(4.4)

where $D^*_{ii}=p_i\ In_i+q_i\ Jn_i\times n_i$,

with $p_i=(2\lambda_4^{(i)})^{-1}$ and

$q_i=(\lambda_4^{(i)}-1)/\mu_i$,

and $\mu_i=\lambda_4^{(i)}\ (n_i+2-n_i:$

Now we know that the least square estimates for the parameters (β) are given by

$$\hat{\beta}=S^{-1}\ (N^{-1}\times x'y)$$

and the covariance matrix of $\hat{\beta}$ is

$$D(\hat{\beta})=o^2\ S^{-1},$$

which can now be obtained, since S^{-1} is unknown.

The variance function for this simple case is given by $v(\rho_1,\ldots\rho_m)$

$$=(N/o^2)\ V(\hat{Y}(x))$$

$$=a_o+\sum_{i=l}^{m}(1-2b_i)\ \rho_i^2+\sum_{i=1}(p_i+q_i-1)\rho_i^4+\sum_{i=1}^{m}\rho_i^2$$

where $\rho_i^2=\sum_{i\epsilon s_i}(x_j^{(i)})^2$ and a_o, b_i, p_i, q_i are as given in ...(4.4).

Minimisation of weighted mean square bias with respect to a particular type of weight densities

The result proved by Draper and Lawrence (1967) gives an important property of the rotatable designs, the bias minimising property, in a sense.

While measuring the bias due to the inadequacy of the chosen polynomial (of degree d_1 say) in representing the actual response function (of degree d_2 say, $d_2>d_1$), one may be interested in an weighted mean square error of the estimated response with respect to a certain weight density. Box and Draper (1959, 1963) have shown that weighted mean square bias is the principal contributor to this weighted mean square error and as such minimising the weighted mean square bias may be a good criterion for obtaining a good response surface design. Draper and Lawrence (1967) have shown that this criterion is satisfied by any design having moments equal to those of the chosen weight density upto and including order d_1+d_2.

The moments of a group-wise spherical distribution :

Let $X=(x'^{(l)}_{l\times n_l}, \ldots\ldots x'^{(m)}_{l\times n_m})$ be a vector of variables having its p.d.f. a function of the quantities $x'^{(l)}\, x^{(l)}, \;..\; x'^{(m)}\, x^{(m)}$. This distribution, a generalization of spherical distribution has been termed group-wise spherical in the present paper.

Now from the definition, the moment generating function of this distribution is invariant under any orthogonal transformation of the form (2.2). Using this fact, the moments of a groupwise spherical distribution are found to be precisely of the same form as those given in (3.1).

We see that the moments of order upto 2d of GDR design of order d coincide with the corresponding moments of a groupwise spherical density.

From the result proved by Draper and Lawrence (1967), if the weight density assumed is groupwise spherical, then the optimum design (in the sense that it has got minimum weighted mean square bias) will be such that its moments of order $\leqslant d_1+d_2$ will equal those of the chosen groupwise spherical weight density. Such a design is as we see, a group divisible rotatable one of order $(d_1+d_2)/2$ with moments of order d_1+d_2 zero (if d_1+d_2 is odd). This fact emphasizes the importance of GDR designs with preassigned moments, specified by a groupwise spherical weight density chosen.

A special case of group wise spherical density

Let us consider a groupwise spherical distribution which has got its density as the product of m spherical densities. For this type of a distribution

$$E[(x_j^{(i)})^2 (x_{j'}^{(i')})^2] = E(x_j^{(i)})^2 . E(x_{j}'^{(i')})^2$$
$$J=1, 2, \ldots n_i, J'=1, 2, \ldots, n_i',$$
$$i \neq i', i, i'=1, 2, \ldots m \qquad (5.2.1)$$

Standardising the variables by dividing them by the square root of the second moments (*i.e.* $\lambda_2^{(i)}$), when the weight density is the product of m spherical densities, we have

$$\theta_{ii'}=1, \; i \neq i', \; i,i'=1,2, \ldots m \text{ using (5.2.1).}$$

This is the case considered in detail in section 4.

In practice, the experimenter may be interested in a bounded region within R^k, termed operability region by Mukhopadhyay (1969), rather than in the whole of the factor space R^k- It may be noted that for a group-wise spherical weight density, defined in a bounded region, the operability region for the experiment has to be also the same bounded region.

Method of construction for GDR designs defined over suitable operability regions will be taken up in a forthcoming article.

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