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Group Divisible Variance – Sum Third Order Rotatable Design through Balanced Incomplete Block Designs in Four Dimensions

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Authors' contributions

This work was carried out in collaboration between all authors. Author NC designed the study, performed the statistical analysis and wrote the first draft of the manuscript. Authors MK and GK managed the analyses of the study and the literature searches. All authors read and approved the final manuscript.

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ABSTRACT

In the study of rotatable designs, the variance of the estimated response at a point is a function of the distance of that point from a particular origin. Group divisible Rotatable Designs have been evolved by imposing conditions on the levels of factors in a rotatable design. In Group Divisible Third Order Rotatable Designs (GDTORD), the v-factors are split into two groups of p and (v-p) factors such that the variance of a response estimated at a point $(x_{1,0}, x_{2,0}, ... x_{v,0})$ equidistant from the centre of the designs is a function of the distances d_1^2 and d_2^2 from a suitable origin for each group respectively. Where d_1^2 and d_2^2 denotes the distances of the projection of the points in each of the group from a suitable origin respectively. In this paper, a four dimensional Group Divisible Variance-Sum Third Order Rotatable Design is constructed using a balanced incomplete block design.

Keywords: Third order rotatable designs; BIBD; group divisible third order rotatable designs; group divisible variance- sum third order rotatable designs.

1. INTRODUCTION

study of rotatable designs mainly The emphasized on the estimation of absolute response. [1] introduced rotatable designs for the exploration of response surfaces. In rotatable designs, the variance of the estimated response at a point is a function of the distance of that point from origin. In Group divisible rotatable designs the variance of a response estimated at the point is a function of the distances d_1^2 and d_2^2 from a suitable origin for group one and two respectively. As the factors get divided into two groups, thus these might be called "Group -Divisible Rotatable Designs" such that for the factors within each group the designs are certainly rotatable when the level of factors in the other group is held constant. [2] independently studied some generalization of SORD and introduced Group-Divisible Second Order Rotatable Designs (GDSORD). They introduced GDSORD by modifying the restrictions on the levels of the factors in a second order rotatable design. [3] identified some practical grouping of the set of factors and introduced group divisible response surface designs both of second and third order and gave methods for their construction. [4] introduced and constructed Variance Sum Group Divisible Second Order Slope Rotatable Designs. [5] constructed a Variance Sum second order and third order slope rotatable designs. [6] introduced a Variance-Sum Group Divisible Third Order Slope Rotatable Designs. Now we introduce in this paper a construction of a four dimensional Group Divisible Variance-Sum Third Order Rotatable Designs using a balanced incomplete block designs.

2. METHODOLOGY

The construction of Group Divisible Third Order Rotatable Designs can in many occasions be made to depend on known solutions for BIB designs. To construct a (p, v - p) GDTORD in four factors we consider a BIBD with parameter parameters (v = 4, b = 6, r = 3, k = 2, $\lambda = 1$) with $r \ge 3\lambda$, which is then divided to form two groups of factors, one of p-dimension and the other (v - p) dimension with $p \ge 2$ and $(v - p) \ge 2$ 2.We will first start by writing the transpose of incidence matrix of the four factor BIBD Design with unknown level a and zero, where a takes the place of 1 in the above matrix which generates b combinations. From these design points we get b combinations each containing k a's and (v - k)zeros. Then by combining the points above with their suitably chosen points set of S(c,0,0...,0), 2S(d,0,0...,0) and 2S(b,b,b...,b) levels with $d^2 = tc^2$ for $t \ge 0$ where unique solutions is obtainedbyassuming function а t = $\frac{\left(1+2t^2\right)^3}{\left(1+2t^3\right)^2}$ chosen suitably for four factors so that $t \ge 0$. The equations obtained are satisfied for t = 0.4544 solution forming a four dimensional GDTORD.

All the unknown levels is determined by the moment conditions for Group Divisible Third Order Rotatable Designs [7].

Let $\lambda = f(d)$ be a function of the radius of a rotatable design,

Where d = radius and λ a scaling parameter . Also let $d^2 = \sum_{i=1}^4 x_{iii}^2$, such that Where $d_1^2 = \sum_{i=1}^2 x_i^2$,

$$d_2^2 = \sum_{j=3}^4 x_j^2$$

 $\begin{array}{ll} \text{(b) (i)} & \sum x_i^2 x_j^4 = 5N\lambda_6 & \text{for } i \neq j \text{ for } i = 1,2 \\ & & j = 3,4 \\ \text{(ii)} & \sum_{j\neq j'} x_j^2 x_j^4 = 5N\lambda_6 & \text{for } j,j' = 3,4 \\ \text{(iii)} & \sum_{i\neq i'} x_i^2 x_i^4 = 5N\lambda_6 & \text{for } i,i' = 1,2 \\ \text{(3)} & \sum \sum \sum x_i^2 x_i^2 x_k^2 = N\lambda_6 & \text{for } i\neq j\neq k \\ \end{array}$

We have all odd order moments equal to Zero in both the groups.

Non-singularity conditions

1.
$$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$$

2.
$$\frac{\lambda_2 \lambda_6}{\lambda_4^2} > \frac{k+2}{k+4}$$

The above summations are taken over all design points.

2.1 Method of obtaining a Variance – Sum Group Divisible Third Order Rotatable Designs

From the design points generated through GDTORD; we obtain a VSGDTORD in four dimensions meaning, the sum of variance of the response estimates in the direction of any factor axis in each group of mutually orthogonal spaces, one of p-dimension and the other of (v-p)-dimension given any point must be a function of the distances d_1^2 and d_2^2 respectively from the design origin. Let $D = ((x_{ik}))$ be a set of N design points and $y_1, y_2, ..., y_N$ be the N responses to fit the following third order response surface,

$$\begin{split} Y(X) &= b_0 + \sum b_i x_i + \sum b_j x_j \\ &+ \sum \sum b_{ij} x_i x_j \\ &+ \sum \sum b_{ij'} x_i x_{i'} \\ &+ \sum \sum b_{jj'} x_j x_{j'} + \sum b_{ii} x_i^2 + \sum b_{jj} x_j^2 + \sum b_{iii} x_i^3 + \sum b_{jjj} x_j^3 \\ &+ \sum \sum b_{ijj} x_i x_j^2 + \sum \sum b_{ii'i'} x_i x_{i'}^2 + \sum \sum b_{jj'j'} x_j x_j^2 + \sum \sum b_{jj'j'} x_j x_j^2 + \sum \sum b_{ijk} x_i x_j x_k + e \end{split}$$

The Taylor series approximation is of the form

where *y* is the response, x_i and x_i is a *p* factor group, x_j and x_j is the (v-p) factor group, β 's are the regression coefficients at both the *p* factor levels and (v-p) factor levels. For a complete third-order model, including the intercept, we can express the total number of model terms, *L*, as

$$L = \binom{k+3}{3}.$$

We then consider the linear model as

$$y_i = f'(x_i)B + \mathcal{E}_i$$

i=1,2,...n

Which can be expressed in matrix notation as

$$\underline{Y} = \underline{X'}\underline{\beta} + \underline{\varepsilon}$$

The vector \underline{Y} is an n×1 vector of observations; \underline{X} is an n×p matrix; $\underline{\beta}$ is a p×1 vectors of unknown parameters; $\underline{\varepsilon}$ is an n×1 vector of independently distributed random variables, with mean zero and variance σ^2 . By the method of least squares the estimates of the parameters $\underline{\beta}$ will be obtained. These are given by

$$\underline{\beta} = (X'X)^{-1}X'Y$$

let M be the moment matrix,

where
$$M = \frac{1}{N} X' X$$

With the help of MATLAB software, the determinant of M is obtained, which gives the non-singularity conditions for third order design to be rotatable. Then the inverse of M will be determined which enables the variances to be obtained. For a third order full model we have,

$$f'(x) = [f_1'(x), f_2'(x), f_3'(x), f_4'(x)],$$

Where v=4, the total number of factors in a four-dimensional factor space, then we have

$$f_{1}^{t}(x) = (1, x_{1}^{2}, x_{2}^{2}, x_{3}^{2}, x_{4}^{2})$$

$$f_{2}^{t}(x) = (x_{1}x_{2}, x_{1}x_{3}, x_{1}x_{4}, x_{2}x_{3}, x_{2}x_{4}, x_{3}x_{4}),$$

$$f_{3}^{t}(x) = (x_{1}x_{2}x_{3}, x_{1}x_{2}x_{4}, x, x_{1}x_{3}x_{4}, x_{2}x_{3}x_{4})$$
and
$$f_{4}^{t}(x) = (g_{1}^{t}(x), g_{2}^{t}(x), g_{3}^{t}(x), g_{4}^{t}(x)) where$$

$$g_{1}^{t}(x) = (x_{1}, x_{1}^{3}, x_{1}x_{2}^{2}, x_{1}x_{3}^{2}, x_{1}x_{4}^{2}), g_{2}^{t}(x) = (x_{2}, x_{2}^{3}, x_{2}x_{1}^{2}, x_{2}x_{3}^{2}, x_{2}x_{4}^{2}),$$

$$g_{3}^{t}(x) = (x_{3}, x_{3}^{3}, x_{3}x_{1}^{2}, x_{3}x_{2}^{2}, x_{3}x_{4}^{2}), g_{4}^{t}(x) = (x_{4}, x_{4}^{3}, x_{4}x_{1}^{2}, x_{4}x_{2}^{2}, x_{4}x_{3}^{2})$$

Thus for a third order design ξ , the partitioned matrix of the moment matrix $M(\xi)$ is given by

$$M(\xi) = \begin{bmatrix} M_{11}(\xi) & 0 & 0 & 0 \\ 0 & M_{22}(\xi) & 0 & 0 \\ 0 & 0 & M_{33}(\xi) & 0 \\ 0 & 0 & 0 & M_{44}(\xi) \end{bmatrix}$$

Where $M_{ij}(\xi) = \int_{x} f_i(x) f_j^t(x) \xi(dx) \ (i, j = 1, 2, 3, 4)$

Considering the symmetric designs only we will be in a position to obtain the inverse of $M(\xi)$. For a symmetric design ξ , $M_{ii}(\xi)(i \neq j)$ are null matrices thus $M(\xi)$ is reduced to a block diagonal matrix

of $M(\xi) = Diag\{M_{11}(\xi), M_{22}(\xi), ..., M_{vv}(\xi)\}$. Note that for a symmetric design ξ , $M_{11}(\xi), M_{22}(\xi), ..., M_{vv}(\xi)$ are diagonal matrices and further $M_{vv}(\xi)$ in itself is a block diagonal matrix given by

$$M_{\nu\nu}(\xi) = \text{Diag} \{ M_{1}^{*}(\xi), ..., M_{k}^{*}(\xi) \},$$

where $M_i^*(\xi) = \int_x g_i(x)g_i^*(x)\xi(dx)$ (*i*=1,2). Then for a symmetric design $M(\xi)$, it is seen that

variances is given as,

$$V(\xi) = \sum_{i=1}^{4} V_i(\xi)$$

where $V_i(\xi) = x' [M_{ii}(\xi)]^{-1} x$ (i=1, 2, 3, 4).

Summing the above variances we get expression which is a function of

$$d_1^2, d_2^2, \sum_{i < j} x_i^2 x_{i'}^2, \sum_{i' < j'} x_j^2 x_{j'}^2 \sum_{i < j} x_i^2 x_{i'}^4 \sum_{i < j} x_i^4 x_{i'}^2, \sum_{i' < j'} x_{i'}^2 x_{j'}^4, \sum_{i, i' < j'} x_i^2 x_{i'}^2 x_{j'}^2, \sum_{i < j, i'} x_i^2 x_j^2 x_{i'}^2 x_$$

In order to achieve the variance in a GDTORD, the variance must be a function of d_1^2 , d_2^2 only. Therefore we need to cancel all the interactions by equating them to zero.

Then at the point $x \in \chi$ the response is

$$V(\hat{y}(\mathbf{x})) = f'(\mathbf{x})\hat{\beta}$$

With variances for the two groups being

$$V(\hat{y}(x_i)) = \sigma^2 f'(x_i) (X'X)^{-1} f(x_i)$$

$$V(\hat{y}(x_j)) = \sigma^2 f'(x_j) (X'X)^{-1} f(x_j)$$

Where the Variance Sum will be a function of distances d_1^2 and d_2^2 only as shown below

$$\sum_{i=1}^{4} V(\hat{y}(\mathbf{x})) = f(d_1^2, d_2^2)$$
, Where $d_1^2 = \sum_{i=1}^{2} x_i^2$, $d_2^2 = \sum_{j=3}^{4} x_j^2$

3. RESULTS AND DISCUSSION

3.1 Group Divisible Variance-Sum Third Order Rotatable Designs in Four Dimensions

From the 80 design points of a four dimensional GDTORD generated through BIB designs, the moment matrix of a four dimensional GDTORD is given by;

Moment matrix
$$M = \frac{1}{N} x' x$$

Where N = 80 design points for $v = 4, x_1, x_2$ forms the p factor group whereas x_3, x_4 forms the (v-p) factor group. Then for the full third order model in four factors we have,

$$f'(x) = [f_1'(x), f_2'(x), f_3'(x), f_4'(x)],$$

The design space is divided into two groups of two factors each, the p- factor and (v-p) factor space satisfying $d_1^2 = \sum_{i=1}^2 x_i^2$ and $d_2^2 = \sum_{j=3}^4 x_j^2$ with the corresponding variances $V([\hat{y}(x_i)])$ and $V([\hat{y}(x_j)])$ respectively, thus the design is called a Group Divisible Variance-Sum third order rotatable design in four dimensions.

3.1.1 <u>Group one: Variance $V([\hat{y}(x_i)])$ for p dimensional space</u>

For a symmetric design $M(\xi)$ as generated through MATLAB software, it is seen that variances for p-factor group is given as,

$$\begin{split} M_{11}(\xi) &= \begin{bmatrix} 1 & x_1^2 & x_2^2 \\ x_1^4 & x_1^2 x_2^2 \\ (symm) & x_2^4 \end{bmatrix} = \begin{bmatrix} 1.0000 & 1.0051 & 1.0051 \\ 1.0051 & 2.1524 & 0.7175 \\ 1.0051 & 0.7175 & 2.1524 \end{bmatrix}. \\ M_{22}(\xi) &= \begin{bmatrix} 0.7175 & 0 \\ 0 & 0 \end{bmatrix} \\ M_{22}(\xi) &= \begin{bmatrix} 0.7175 & 0 \\ 0 & 0 \end{bmatrix} \\ M_{44(1)} &= \begin{bmatrix} x_1^2 & x_1^4 & x_1^2 x_2^2 \\ x_1^6 & x_1^4 x_2^2 \\ symm & x_1^2 x_2^4 \end{bmatrix} = \begin{bmatrix} \lambda_2 & 3\lambda_4 & \lambda_4 \\ 15\lambda_6 & 3\lambda_6 \\ symm & 3\lambda_6 \end{bmatrix} = \begin{bmatrix} 1.0051 & 2.1524 & 0.7175 \\ 2.1524 & 6.0000 & 1.2000 \\ 0.7175 & 1.2000 & 1.2000 \end{bmatrix} \end{split}$$

For the variances we have,

$$V_{11}(\xi) = f_1' [M_{11}(\xi)]^{-1} f_1$$
Let (M_{11}^{-1}) be represented by $\begin{bmatrix} a & b & b \\ b & c & d \\ b & d & c \end{bmatrix}$ such that
$$V_{11}(\xi) = \begin{bmatrix} a + 2bx_1^2 + 2bx_2^2 + cx_1^4 + cx_2^4 + 2dx_1^2x_2^2 \end{bmatrix}$$

$$V_{22}(\xi) = f_2' [M_{22}(\xi)]^{-1} f_2$$
Let (M_{22}^{-1}) be represented by $\begin{bmatrix} n & 0 \\ 0 & 0 \end{bmatrix}$ such that
$$V_{22}(\xi) = \begin{bmatrix} nx_1^2x_2^2 \end{bmatrix}$$

$$V_{44(1)}(\xi) = g_1' [M_{44(1)}(\xi)]^{-1} g_1$$

Let
$$(M_{44(1)}^{-1})$$
 be represented by $\begin{bmatrix} e & f & g \\ f & h & k \\ g & k & l \end{bmatrix}$ such that
 $V_{44(1)}(\xi) = \begin{bmatrix} ex_1^2 + 2fx_1^4 + hx_1^6 + 2gx_1^2x_2^2 + 2kx_1^4x_2^2 + lx_1^2x_2^4 \end{bmatrix}$
 $V_{44(1)}(\xi) = V_{44(2)}(\xi)$

The variance $V([\hat{y}(x_i)]) = \sum_{i=1}^{2} V(x_i)$

Summing the above variances we get expression which is a function of $\sum x_1^2$, $\sum x_2^2$, $\sum x_1^2 x_2^2$, $\sum x_2^4 x_1^2$, $\sum x_1^4 x_2^2$ and in cancelling the interactions we;

$$\begin{split} &V\big([\hat{y}(x_i)]\big) = \Big(ax_0^2 + (2b+e)x_1^2 + (2f+c)x_1^4 + hx_1^6 + (2b+e)x_2^2 + (2f+c)x_2^4 + hx_2^6\Big) \text{being a} \\ &\text{function of } \sum x_1^2, \sum x_2^2 \text{ only }. \\ &\text{Let } d_1^2 = \sum_{i=1}^2 x_i^2 \text{ such that } \\ &V\big([\hat{y}(x_i)]\big) = \text{f} (d_1^2) \text{ only} \end{split}$$

3.1.2 <u>Group Two: Variance</u> $V([\hat{y}(x_j)])$ for (v-p) dimensional space

For a symmetric design $M(\xi)$, it is seen that variances for (v-p)-factor group is given as,

$$M_{11}(\xi) = \begin{bmatrix} 1 & x_3^2 & x_4^2 \\ x_3^4 & x_3^2 x_4^2 \\ (symm) & x_4^4 \end{bmatrix} = \begin{bmatrix} 1.0000 & 1.0051 & 1.0051 \\ 1.0051 & 2.1524 & 0.7175 \\ 1.0051 & 0.7175 & 2.1524 \end{bmatrix}.$$
$$M_{22}(\xi) = \begin{bmatrix} 0.7175 & 0 \\ 0 & 0 \end{bmatrix}$$
$$M_{44(3)} = \begin{bmatrix} x_3^2 & x_3^4 & x_3^2 x_4^2 \\ x_3^6 & x_3^4 x_4^2 \\ symm & x_3^2 x_4^4 \end{bmatrix} = \begin{bmatrix} \lambda_2 & 3\lambda_4 & \lambda_4 \\ 15\lambda_6 & 3\lambda_6 \\ symm & 3\lambda_6 \end{bmatrix} = \begin{bmatrix} 1.0051 & 2.1524 & 0.7175 \\ 2.1524 & 6.0000 & 1.2000 \\ 0.7175 & 1.2000 & 1.2000 \end{bmatrix}$$

$$M_{44(4)} = M_{44(3)}$$

 $V_{11}(\xi) = f_1' [M_{11}(\xi)]^{-1} f_1 =$

$$\begin{split} & \text{Let}\Big(M_{11}^{-1}\Big) \text{be represented by} \begin{bmatrix} a & b & b \\ b & c & d \\ b & d & c \end{bmatrix} \text{such that} \\ & V_{11}\left(\xi\right) = \begin{bmatrix} a + 2bx_3^2 + 2bx_4^2 + cx_4^4 + 2dx_3^2x_4^2 \end{bmatrix} \\ & V_{22}(\xi) = \int_2^r \left[M_{22}(\xi)\right]^{-1} f_2 \\ & \text{Let}\Big(M_{22}^{-1}\Big) \text{be represented by} \begin{bmatrix} n & 0 \\ 0 & 0 \end{bmatrix} \text{such that} \\ & V_{22}\left(\xi\right) = \begin{bmatrix} nx_3^2x_4^2 \end{bmatrix} \\ & V_{44(3)}(\xi) = g_3^r \left[M_{44(3)}(\xi)\right]^{-1}g_3 \\ & \text{Let}\Big(M_{44(3)}^{-1}\Big) \text{be represented by} \begin{bmatrix} e & f & g \\ f & h & k \\ g & k & l \end{bmatrix} \text{such that} \\ & V_{44(3)}\left(\xi\right) = \begin{bmatrix} ex_3^2 + 2fx_3^4 + hx_3^6 + 2gx_3^2x_4^2 + 2kx_3^4x_4^2 + lx_3^2x_4^4 \\ & V_{44(3)}\left(\xi\right) = V_{44(4)}(\xi) = g_4^r \left[M_{44(4)}(\xi)\right]^{-1}g_4 \\ & \text{The variance } V\left(\left[\hat{y}(x_j)\right]\right) = \sum_{j=3}^4 V(x_j) \end{split}$$

Summing the above variances we get expression which is a function of $\sum x_3^2$, $\sum x_4^2$, $\sum x_3^2 x_4^2$, $\sum x_3^2 x_4^2$, $\sum x_4^4 x_3^2$, $\sum x_4^4 x_3^2$ and in cancelling the interactions we;

$$\begin{split} &V\left([\hat{y}(x_{j})]\right) = \left(ax_{0}^{2} + (2b+e)x_{3}^{2} + (2f+c)x_{3}^{4} + hx_{3}^{6} + (2b+e)x_{4}^{2} + (2f+c)x_{4}^{4} + hx_{4}^{6}\right) \text{ a function of} \\ &\sum x_{3}^{2}, \sum x_{4}^{2} \text{ only.} \\ &\text{Let}d_{2}^{2} = \sum_{j=3}^{4} x_{j}^{2} \text{ such that} \\ &V\left([\hat{y}(x_{j})]\right) = \text{f}(d_{2}^{2}) \text{ only} \end{split}$$

With variances for the two groups being

$$V(\hat{y}(x_{i})) = \sigma^{2} f'(x_{i}) (X'X)^{-1} f(x_{i})$$

$$V([\hat{y}(x_{i})]) = \sigma^{2} f(d_{1}^{2})$$

$$V(\hat{y}(x_{j})) = \sigma^{2} f'(x_{j}) (X'X)^{-1} f(x_{j})$$

$$V([\hat{y}(x_{j})]) = f(d_{2}^{2})$$

Thus the variance Sum is the function of distances $d_1^2 \, {\rm and} \, d_2^2 {\rm only}.$

 $\sum_{i=1}^{4} \mathbb{V}(\hat{\mathcal{Y}}(\mathbf{x})) = f(d_{1}^{2}, d_{2}^{2}),$

Thus the considered response surface is a Group Divisible Variance - Sum Third Order Rotatable Designs in four dimensions through a BIBDS.

4. PRACTICAL APPLICATION

GDVSTORD is potentially useful in measuring of data, for example in clinical data where the cause of lung cancer in relation to lifestyle, age,

environmental and hereditary factors is determined given a case study of a particular region. Given such a combination of factors, we can visualize the best combination (group) which gives the optimum value of the response.

5. CONCLUSION

A four dimensional Group divisible Variance sum third order rotatable designs constructed here gave 80 design points compared to 120 design points of a four dimensional TORD constructed using BIBDS (Mutai et al. 2012) thus the cost effective. Therefore GDVSTORD gave less number of design points than the corresponding rotatable designs constructed using BIBDS. Further, the number of normal equations for estimating the parameters estimates is reduced by adopting this method since all the interactions are equated to zeros. Other investigation on the construction of a Group divisible Variance sum TORD for k number of groups is recommended.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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