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METHODS FOR THE CONSTRUCTION OF SOGDRD

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Abstract

Since the introduction of second order rotatable designs (SORD) by Box and Hunter (1957) some authors have proposed to get new series of second order response surface designs. One such attempt was made by Das and Dey (1967) to get an alternative series of response surface designs by modifying the restrictions imposed on the levels of the factors in a second order rotatable design. Such designs are termed as second order group divisible rotatable designs (SOGDRD). They also proposed some methods for the construction of SOGDRD. In this paper, a remark on Das and Dey (1967) SOGDRD is noted and some modifications are made in the methods of Das and Dey (1967) to derive the SOGDRD. A new method of construction of CCD type SOGDRD is also derived. In addition to these methods, general formula for A- and D- optimality for SOGDRD are also deduced.

Keywords: rotatable design, group divisible rotatable design, central composite design, BIBD.

1. INTRODUCTION

Let there be v factors $X_1, X_2, \ldots, X_v$ which influence the response variable Y. Then the design matrix $D_{N\times v}$, is

$$D = ((X_{u1}, X_{u2}, \ldots, X_{uv})) \quad (1.1)$$

where X_{ui} be the level of the i^{th} factor in the u^{th} treatment combination (i=1,2, ... v; u =1,2…N), and let Y_u denote the response at the u^{th} combination, then the corresponding vector of observations are

$$\underline{Y} = (Y_1, Y_2, \ \ldots, Y_N)' \qquad (1.2)$$

Divide the v factors $X_1, X_2, \ldots, X_v$ into two groups, viz.,

$$S_1 = (X_1, \ldots, X_p) \text{ and } S_2 = (X_{p+1}, \ldots, X_v) \qquad (1.3)$$

Suppose it is required to fit a second order response surface model in v factors, given by

$$\underline{Y} = X\underline{\beta} + \underline{\boldsymbol{\varepsilon}} \qquad (1.4)$$

Where $\underline{Y} = (Y_1, Y_2, \ \ldots, Y_N)'$ is the vector of observations,

$X_u = (1, X_{u1}, X_{u2}, \ldots X_{uv}, X^2_{u1}, X^2_{u2}, \ldots X^2_{uv}, X_{ul}X_{u2}, \ldots X_{uv-1}X_{uv})$ is the u^{th} row of X

$\underline{\beta} = (\beta_0, \beta_1, \beta_2, \ldots \beta_v, \beta_{11}, \beta_{22}, \ldots \beta_{vv}, \beta_{l2}, \ldots \beta_{v\text{-}1v})'$ is the vector of parameters

$\underline{\boldsymbol{\varepsilon}} = (\varepsilon_1, \varepsilon_2, \ldots \varepsilon_N)'$ is the vector of random errors.

Assume that $E(\underline{\boldsymbol{\varepsilon}})=0$, $D(\underline{\boldsymbol{\varepsilon}})= \sigma^2 I$ and $\underline{\boldsymbol{\varepsilon}} \sim N(0,\sigma^2)$.

If the design D satisfies the following conditions

$$\left.\begin{array}{l}
1.\ \Sigma\, x_{ui}^{\delta 1}\, x_{uj}^{\delta 2}\, x_{uk}^{\delta 3}\, x_{ul}^{\delta 4} = 0 \ \text{ when ever } \delta_i \text{ is odd and } \Sigma\, \delta_i \leq 4;\ i\neq j\neq k\neq l = 1, 2, \ldots v \\
2.\ \Sigma\, x^2_{ui} = N\,\mu_2;\ \ \Sigma\, x^4_{ui} = 3N\mu_4;\ \ \Sigma\, x^2_{ui}\, x^2_{uj} = N\mu_4 \ \ (\text{for } i= 1, 2, \ldots, p) \\
3.\ \Sigma\, x^2_{ui} = N\,\lambda_2;\ \Sigma\, x^4_{ui} = 3N\lambda_4;\ \ \ \ \Sigma\, x^2_{ui}\, x^2_{uj} = N\lambda_4 \ (\text{for } j= p+1, \ldots, v) \\
4.\ \Sigma\, x^2_{ui}\, x^2_{uj} = N\theta \ \ \ (\text{for } i= 1, 2, \ldots, p;\ \ j= p+1, \ldots, v)
\end{array}\right\} \qquad (1.5)$$

Then, the pattern of the Moment Matrix $N^{-1}(X'X)$ is

$$\begin{pmatrix}
1 & 0 & 0 & \mu_2 J_{1,p} & \lambda_2 J_{1,v\text{-}p} & 0 & 0 & 0 \\
0 & \mu_2 I_v & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \lambda_2 I_v & 0 & 0 & 0 & 0 & 0 \\
\mu_2 J_p & 0 & 0 & \mu_4[2I+J] & \theta J & 0 & 0 & 0 \\
\lambda_2 J_{v\text{-}p,\,1} & 0 & 0 & \theta J & \lambda_4[2I+J] & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \mu_4 I_p & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \lambda_4 I_{v\text{-}p} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \theta I
\end{pmatrix} \qquad (1.6)$$

The variance of the estimated response at any u^{th} design point X_u is

$$V(\hat{Y}_u) = V(\beta_0) + [V(\beta_i) + 2Cov(\beta_0, \beta_{ii})] \rho_1^2 + V(\beta_{ii})\rho_1^4 + [V(\beta_j) + 2Cov(\beta_0, \beta_{jj})] \rho_2^2 + V(\beta_{jj})\rho_2^4 + 2Cov(\beta_{ii}, \beta_{jj})\rho_1^2\rho_2^2 \quad (1.7)$$

Hence, we have

$$V(\hat{Y}_u) = N^{-1}\sigma^2 [\mathbf{a}_0 + [(1/\mu_2) + 2\mathbf{a}_1]\rho_1^2 + [(1/\lambda_2) + 2\mathbf{a}_2)] \rho_2^2 + [C_1+C_2]\rho_1^4 + [C_4+C_5]\rho_2^4 + [(1/\theta) + 2C_3] \rho_1^2\rho_2^2] \quad (1.8)$$

Where

$\mathbf{a}_0 = [1 - \mathbf{a}_1\mu_2 p - \mathbf{a}_2 \lambda_2(v-p)]$

$\mathbf{a}_1 = \{ \mu_2 - \mathbf{a}_2[\lambda_2\mu_2(v-p) - \theta(v-p)] \} / [\mu_2^2 - \mu_4(p+2)]$

$\mathbf{a}_2 = [-\mu_2\theta p + \mu_4(p+2)] / \{[\lambda_2\mu_2(v-p) - \theta(v-p)] [\lambda_2\mu_2 p - \theta p] - [\lambda_2^2(v-p) - \lambda_4(v-p+2)] [\mu_2^2 p - u_4(p+2)]\}$

$C_1 = 1 / 2\lambda_4$

$C_4 = 1 / 2\lambda_2$

$C_3 = [a_1\lambda_2 \mu_2 - \theta a_1] / [\lambda_2\theta(v-p) - \lambda_2\mu_4(v-p+2)]$

$C_2 = [-a_1\lambda_2 - C_1\theta - C_3\lambda_4(v-p+2)] / p\theta$

$C_5 = [-a_2 - \mu_2 p C_3 - \lambda_2 C_4] / [\lambda_2(v-p)]$

Thus, from (1.8), Variance of $\hat{Y}_u$ is a function of ρ_1^2, ($= \Sigma X_{ui}^2$; summation is over i= 1, 2, ... , p) and ρ_2^2 ($= \Sigma X_{ui}^2$; summation is over i= p+1, p+2, ... , v) only. If the $V(\hat{Y}_u)$ is a function of ρ_1^2 and ρ_2^2 only then the design D is said to be second order group divisible rotatable design (SOGDRD).

Das and Dey (1967), Adhikary and Sinha (1976), Adhikary and Panda (1983) and several authors gave the different methods of constructions of SOGDRD. In this paper, SOGDRD are derived suggesting some modifications to the methods of Das and Dey in section 2.1 & 2.2. A new method of construction of CCD type SOGDRD is also derived. In addition to these methods, general formula for A- and D- optimality and estimated responses for SOGDRD are presented.

2. METHODS OF CONSTRUCTION OF SOGDRD

Das and Dey (1967) made an attempt to construct the SOGDRD and proposed two methods one through factorials and another through BIBD. Constructional methods given by these authors are also incorrect. Because in all these designs $\Sigma x_{ui} x^2_{uj} \neq 0$ when i and j belong to different groups. In this section, the methods for the construction of SOGDRD through factorial design and BIBD are suggested by making certain modifications to Das and Dey (1967).

2.1 METHODS OF CONSTRUCTION OF SOGDRD THROUGH FACTORIALS

Consider a set of combinations of 2^v factorial design points with the levels $\pm\alpha$ for v factors. Divide the v factors into two groups, one containing the p factors and the remaining containing (v-p) factors. Consider a set $\mathbf{S_1}$, of 2p combinations of the type $(\pm\gamma, 0, \dots, 0), \dots, (0,0, \dots, \pm\gamma)$ and a set $\mathbf{S_2}$ of 2(v-p) combinations of type $(\pm\beta, 0, \dots, 0), \dots, (0, \dots, \pm\beta)$. Generate 4p(v-p) combinations by taking 2(v-p) combinations of $\mathbf{S_2}$ with each of the combinations of $\mathbf{S_1}$. Take n_0 central points if necessary. Thus the total number of design points are $N=2^v + 4p(v-p) + n_0$.

Obtain the unknown levels $\pm\alpha$, $\pm\beta$, $\pm\gamma$ such that they satisfy the relations

$$\Sigma x^4_{ui} = 3 \Sigma x^2_{ui} x^2_{uj} \quad \text{(for i = 1,2, ..., p)} \quad (2.1.1)$$

$\Sigma x^4_{ui} = 3 \Sigma x^2_{ui} x^2_{uj}$ (for j = p+1, ... v) (2.1.2)

The resulting design provides a v-dimensional SOGDRD with N= 2^v+ 4p(v-p) +n_0 design points. For the N design points, we have

$$\left.\begin{aligned} &1.\ \Sigma x^2_{ui} = N \mu_2 = 2^v \alpha^2 + 4(v-p) \gamma^2 \\ &\Sigma x^4_{ui} = 3N\mu_4 = 2^v \alpha^4 + 4(v-p) \gamma^4 \\ &\Sigma x^2_{ui} x^2_{uj} = N\mu_4 = 2^v \alpha^4 \end{aligned}\right\} \quad \text{(for i=1,2, ..., p)} \quad (2.1.3)$$

$$\left.\begin{aligned} &2.\ \Sigma x^2_{ui} = N \lambda_2 = 2^v \alpha^2 + 4p \beta^2 \\ &\Sigma x^4_{ui} = 3N\lambda_4 = 2^v \alpha^4 + 4p \beta^4 \\ &\Sigma x^2_{ui} x^2_{uj} = N\lambda_4 = 2^v \alpha^4 \end{aligned}\right\} \quad \text{for j = p+1, ... v)} \quad (2.1.4)$$

3. $\Sigma x^2_{ui} x^2_{uj} = N\theta = 2^v \alpha^4 + 4p \beta^2\gamma^2$ (for i= 1, 2, ..., p; j = p+1, ...,v) (2.1.5)

Using the relations in (2.3) and (2.4), we obtain

$$\left.\begin{aligned} \beta^4/\alpha^4 &= 2^{v-1}/ p \\ \gamma^4/\alpha^4 &= 2^{v-1}/(v-p) \end{aligned}\right\} \quad (2.1.6)$$

From (2.1.6), it can be easily seen that, if we fix any one of the values (either α or β or γ) arbitrarily we can obtain the values of the other two parameters. The method is illustrated in the example 2.1.1.

EXAMPLE 2.1.1: Consider a set of combinations for four factors with the levels and these four factors are divided into two groups such that each group consists of two factors. Then the SOGDRD in four factors with 33 design points.

$$\left(\begin{array}{cc|cc} \pm\alpha & \pm\alpha & \pm\alpha & \pm\alpha \\ \pm\gamma & 0 & \pm\beta & 0 \\ 0 & \pm\gamma & 0 & \pm\beta \\ \pm\gamma & 0 & 0 & \pm\beta \\ 0 & \pm\gamma & \pm\beta & 0 \\ 0 & 0 & 0 & 0 \end{array}\right)$$

Then, from (2.1.6), we have β^4/α^4 =4 and γ^4/α^4=4. For λ_2=μ_2 =1, we can obtain α=1, β= √2 and γ=√2. λ_4= 4.64062= μ_4, θ= 5.15625.

2.2 METHOD OF CONSTRUCTION OF SOGDRD THROUGH BIBD

Consider a balanced incomplete block design (BIBD) with the parameters v, b, r, k and λ such that $r<3\lambda$. Let N_{bxv} be its incidence matrix consists of zeros and unities as elements. Replace the unities in N_{bxv} with a 2^k factorial or with a suitable fraction of 2^k with the levels +1 and –1. Divide the v factors into two groups one containing the p factors and the other containing (v-p) factors.

Consider a set $\mathbf{S_1}$ of 2p combinations f the type $(\pm\gamma, 0, \ldots, 0), \ldots, (0,0, \ldots, \pm\gamma)$ and a set $\mathbf{S_2}$ of 2(v-p) combinations of type $(\pm\beta, 0, \ldots, 0), \ldots, (0, \ldots, \pm\beta)$. Generate 4p(v-p) combinations by taking 2(v-p) combinations of $\mathbf{S_2}$ with each of the combinations of $\mathbf{S_1}$. Add n_0 central points if necessary. Thus the total number of the design points are $b.2^k + 4p(v-p)$.

Obtain the unknown levels $\pm\alpha$, $\pm\beta$, $\pm\gamma$ such that they satisfy the relations

$$\Sigma x^4_{ui} = 3\, \Sigma x^2_{ui}\, x^2_{uj} \quad \text{(for } i = 1,2, \ldots, p) \qquad (2.2.1)$$

$$\Sigma x^4_{ui} = 3\, \Sigma x^2_{ui}\, x^2_{uj} \quad \text{(for } j = p+1, \ldots v) \qquad (2.2.2)$$

The resulting design provides a v-dimensional SOGDRD with $N= b2^k+ 4p(v-p) +n_0$ design points. For the N design points, we have

1. $$\left.\begin{aligned} \Sigma x^2_{ui} &= N\mu_2 = 2^k .r.\alpha^2 + 4(v\text{-}p)\,\gamma^2 \\ \Sigma x^4_{ui} &= 3N\mu_4 = 2^k\, \alpha^4 + 4(v\text{-}p)\,\gamma^4 \\ \Sigma x^2_{ui}\, x^2_{uj} &= N\mu_4 = 2^k\, \lambda.\alpha^4 \end{aligned}\right\} \quad \text{(for } i=1,2, \ldots, p) \qquad (2.2.3)$$

2. $$\left.\begin{aligned} \Sigma x^2_{ui} &= N\lambda_2 = 2^k .r.\alpha^2 + 4p\,\beta^2 \\ \Sigma x^4_{ui} &= 3N\lambda_4 = 2^v\, \alpha^4 + 4p\,\beta^4 \\ \Sigma x^2_{ui}\, x^2_{uj} &= N\lambda_4 = 2^k .\lambda.\alpha^4 \end{aligned}\right\} \quad \text{(for } j = p+1, \ldots v) \qquad (2.2.4)$$

3. $$\Sigma x^2_{ui}\, x^2_{uj} = N\theta = 2^k\, \lambda\alpha^4 + 4p\, \beta^2\gamma^2 \quad \text{(for } i=1,2, \ldots,p;\ j = p+1, \ldots,v) \qquad (2.2.5)$$

Using the relations of (2.2.1) and (2.2.2), we obtain

$$\left.\begin{aligned} \beta^4/\alpha^4 &= 2^{k-1}(3\lambda - r)/4(v\text{-}p) \\ \gamma^4/\alpha^4 &= 2^{k-1}(3\lambda - r)/4p \end{aligned}\right\} \qquad (2.2.6)$$

If we fix any of them (either α or β or γ) arbitrarily so that other two give a positive solution. The method is illustrated in the example 2.2.1

EXAMPLE 2.2.1: Consider a BIBD with the parameters v=4=b, λ=2 and r=3=k so that $r < 3\lambda$. Using the above method, we can obtain a SOGDRD in four factors with 48 design points such that each factor consisting of five levels.

$$\left(\begin{array}{cc|cc} \pm\alpha & \pm\alpha & \pm\alpha & 0 \\ \pm\alpha & \pm\alpha & 0 & \pm\alpha \\ \pm\alpha & 0 & \pm\alpha & \pm\alpha \\ 0 & \pm\alpha & \pm\alpha & \pm\alpha \\ \pm\gamma & 0 & \pm\beta & 0 \\ 0 & \pm\gamma & 0 & \pm\beta \\ \pm\gamma & 0 & 0 & \pm\beta \\ 0 & \pm\gamma & \pm\beta & 0 \\ 0 & 0 & 0 & 0 \end{array}\right)$$

Then from (2.11), we have, $\beta^4/\alpha^4 = 3$, $\gamma^4/\alpha^4 = 3$. For $\lambda_2 = \mu_2 = 1$, we can obtain, $\alpha^2 = 6/(3+\sqrt{3})$, $\beta^2 = 6/(1+\sqrt{3}) = \gamma^2$ and $\lambda_4 = \mu_4 = 0.53898$, $\theta = 0.93782$.

REMARKS:

1. The number of design points got by Das and Dey for the methods are $N=2^v + 2p(v-p) + n_0$ and $N= b2^k + 2p(v-p) + n_0$, where as in the above methods are $N=2^v + 4p(v-p) + n_0$ and $N= b2^k + 4p(v-p) + n_0$.
2. Das and Dey methods are not satisfying the condition $\Sigma\, x_{ui}\, x^2_{uj} = 0$ when i and j belong to different groups where as the above methods are satisfying the condition.

3. CONSTRUCTION OF CENTRAL COMPOSITE TYPE SOGDRD

In this section, a new method of construction of SOGDRD through factorial design, which is of central composite type, is suggested.

METHOD 3.1: Consider the treatment combinations of the type (α, α, ... , α, β, β, ... , β) with the first p elements as α's and the next (v-p) elements as β's for v factors. Associate the set with a 2^v factorial or with a suitable fraction of 2^v with the levels +1 and –1. Take the 2v additional axial points [2p points of the type (±γ, ... , 0, ... , 0) ... (0, ... , ±γ, 0, ... , 0) and 2(v-p) points of the type (0, ... , 0, ±δ, ... , 0) ... (0, ... , 0, 0, ... , ±δ,) in v-dimensions]. Complete the design by taking n_0 central point if necessary.

Obtain the unknown levels ±α, ±β, ±γ and ±δ such that they satisfy the relations.

$$\Sigma\, x^4_{ui} = 3\,\Sigma\, x^2_{ui}\, x^2_{uj} \quad (\text{for } i \neq j = 1,2, ..., p) \tag{3.1}$$

$$\Sigma\, x^4_{ui} = 3\,\Sigma\, x^2_{ui}\, x^2_{uj} \quad (\text{for } i \neq j = p+1, ... v) \tag{3.2}$$

The resulting design provides a v-dimensional SOGDRD with $N= 2^v + 2v + n_0$ design points.

For the N design points, we have

1. $\Sigma x^2_{ui} = N\mu_2 = 2^v \alpha^2 + 4(v\text{-}p)\gamma^2$

   $\Sigma x^4_{ui} = 3N\mu_4 = 2^v \alpha^4 + 4(v\text{-}p)\gamma^4$ (3.3)

   $\Sigma x^2_{ui} x^2_{uj} = N\mu_4 = 2^v \alpha^4$ (for i=1,2, ..., p)

2. $\Sigma x^2_{ui} = N\lambda_2 = 2^v \beta^2 + 4p\,\delta^2$

   $\Sigma x^4_{ui} = 3N\lambda_4 = 2^v \beta^4 + 4p\,\delta^4$ (3.4)

   $\Sigma x^2_{ui} x^2_{uj} = N\lambda_4 = 2^v \beta^4$ for j = p+1, ... v)

3. $\Sigma x^2_{ui} x^2_{uj} = N\theta = 2^v \beta^2\alpha^2$ (for i=1,2, ...,p; j = p+1, ...,v) (3.5)

Using the relations in (3.3) and (3.4), we obtain

$$\left.\begin{aligned} \delta^4/\beta^4 &= 2^v \\ \gamma^4/\alpha^4 &= 2^v \end{aligned}\right\} \quad (3.6)$$

By fixing any two unknown levels say α and β) arbitrarily the other two unknown levels of γ and δ can be obtained. The resulting design is a SOGDRD. This design is termed as CCD type SOGDRD for v-dimension. This method is illustrated in the Example 3.1.

REMARKS:

1. The number of the design points in this design is less than the number of the design points in the design given by the Das and Dey (1967) through factorials.
2. In the above design, if α=β (it implies that γ=δ) then the resulting design provides a central composite rotatable design.

EXAMPLE 3.1: Consider a combination of the type (α, α, β, β) with the first two elements as α and the next elements as β for four factors. Then using the above method we can obtain a SOGDRD in four factors design points such that each factors with five levels.

$$\left(\begin{array}{cc|cc} \pm\alpha & \pm\alpha & \pm\beta & \pm\beta \\ \pm\gamma & 0 & 0 & 0 \\ 0 & \pm\gamma & 0 & 0 \\ 0 & 0 & \pm\delta & 0 \\ 0 & 0 & 0 & \pm\delta \\ 0 & 0 & 0 & 0 \end{array}\right)$$

From the relations, we can obtain the values of levels. Suppose α=1 and β=2, then we get γ=2 and δ =4. In this case λ_2=3.84, μ_2=0.96, λ_4= 10.24, μ_4=0.64, θ=2.56.

4. OPTIMALITY CRITERIA AND VARIANCE OF ESTIMATED RESPONSE

In this section, an optimality criteria and variance of estimated response are studied. The A- and D-optimality for SOGDRD are derived from the moment matrix (1.6) as

A-optimality for a SOGDRD is:

$$\text{Trace }(X'X)^{-1} = N^{-1} \left[a_0 + \{p/\mu_2\} + \{(v-p)/\lambda_2\} + \{p(p-1)/2\mu_4\} + \{(v-p)(v-p-1)/2\lambda_4\} + \{p(v-p)/\theta\} + (C_1+C_2)p + (C_4+C_5)(v-p) \right]$$

D-optimality for a SOGDRD is

$$\text{Det }(X'X)^{-1} = 1 / [\, 2^{v-1} N^K \mu_2{}^p \lambda_2{}^{v-p} \mu_4{}^J \lambda_4{}^L \theta^{p(v-p)} \Delta_1 W \,]$$

$\Delta_2 = \lambda_4(v-p+2) - \lambda_2^2(v-p)$; $\Delta_1 = \mu_4(v+2) - \mu_2^2 p$

$W = \Delta_2 - p(v-p)(\theta - \lambda_2\mu_2)^2$; $K = (v+1)(v+2)/2$; $L = (v-p)(v-p-+1)/2$; $J = (p-1)(p+2)/2$

A comparison table of the above three methods is presented below.

Example	A-Optimality	D-Optimality	Variance of estimated Response $V(\hat{Y}_u)$
2.1.1	0.17815	6.684×10^{-35}	$0.0352 + 0.0279(\rho_1^2+\rho_2^2) + 0.0029(\rho_1^4+\rho_2^4) + 0.0465\,\rho_1^2\rho_2^2$
2.2.1	3.6839	1.550×10^{-22}	$2.6613 + 1.2994(\rho_1^2+\rho_2^2) + 0.1933(\rho_1^4+\rho_2^4) + 0.3178\,\rho_1^2\rho_2^2$
3.1	0.41896	1.548×10^{-31}	$0.1067 - 0.0117\rho_1^2 - 0.0029\rho_2^2 + 0.383\,\rho_1^4 + 0.0014\rho_2^4 + 0.0112\rho_1^2\rho_2^2$

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