

ON SOME NEW SECOND ORDER ROTATABLE DESIGNS

T. K. GUPTA AND A. DEY

(Received Aug. 16, 1971; revised Jan. 17, 1975)

Summary

This paper presents a unified approach for the construction of Second Order Rotatable Designs (SORD) with factors each at four and six levels.

1. Introduction

Second Order Rotatable Designs (SORD) were introduced by Box and Hunter [4]. They obtained these designs through regular geometrical configurations. Subsequently, various authors, viz., Bose and Draper [1], Box and Behnken [2], [3], Draper [10], Das [6], Das and Narasimham [7] and others constructed these designs using different techniques. An examination of these works on SORD however, reveals that there is no design available with factors at four or six levels each. As designs with four or six levels of each of the factors are sometimes necessary, there is a need to investigate methods for constructing such designs. Some investigations in this direction have been made recently by Nigam and Dey [11] and Dey [8].

In the present paper, a unified method for the construction of four and six levels SORD has been presented.

2. SORD with factors at four levels each

Consider a Balanced Incomplete Block (BIB) design with usual parameters v, b, r, k, λ . Let $M=(m_{ij})$ be the incidence matrix of the BIB design, where

$$m_{ij} = \begin{cases} 1, & \text{if the } j\text{th treatment occurs in the } i\text{th block} \\ 0, & \text{otherwise; } i=1, 2, \dots, b; j=1, 2, \dots, v. \end{cases}$$

From the matrix M , we obtain another matrix D by omitting any column. Evidently D is $b \times (v-1)$ matrix. In D , replace the unity by α and zero by β , and call the resultant array as D^* . Next 'multiply' (in the sense of [7]) each of the rows of D^* by those of a 2^p factorial

with levels +1 and -1, where 2^p denotes the smallest fraction of 2^{v-1} factorial such that no interaction with four factors or less is confounded for obtaining the fraction. As a consequence of this operation, we obtain a set of $N=2^p$, $(v-1)$ -dimensional points. These points evidently satisfy the following conditions :

(A) $\sum_{u=1}^N \left\{ \prod_{i=1}^{v-1} x_{iu}^{x_i} \right\} = 0$, if any α_i is odd for $\alpha_i = 0, 1, 2$ or 3 and $\sum_i \alpha_i \leq 4$.

(B) $\sum_{u=1}^N x_{iu}^2 = \text{Constant} = 2^p[r\alpha^2 + (b-r)\beta^2] = N\lambda_2$ (say),

$\sum_{u=1}^N x_{iu}^4 = \text{Constant} = 2^p[r\alpha^4 + (b-r)\beta^4]$, for all $i = 1, 2, \dots, v-1$.

(C) $\sum_{u=1}^N x_{iu}^2 x_{ju}^2 = \text{Constant} = 2^p[\lambda\alpha^4 + (b-2r+\lambda)\beta^4 + 2(r-\lambda)\alpha^2\beta^2]$
 $= N\lambda_4$ (say); $i \neq j, i, j = 1, \dots, v-1$.

In the above expressions, x_{iu} denotes the i th coordinate in the u th point, $i = 1, 2, \dots, v-1, u = 1, 2, \dots, N$.

Now, in order that the $N, (v-1)$ -dimensional points form a SORD in $(v-1)$ factors, these points must satisfy two additional conditions, given below, apart from the conditions (A), (B) and (C):

(D) $3 \sum_u x_{iu}^2 x_{ju}^2 = \sum_u x_{iu}^4$

(E) $\lambda_4/\lambda_2^2 > k'/(k'+2)$, where k' denotes the number of factors in the design; in our case $k' = v-1$.

Condition (E) is evidently satisfied by the N points, as these points do not lie on a "Sphere."

Applying condition (D) on the N points obtained above, we have

$$r\alpha^4 + (b-r)\beta^4 = 3[\lambda\alpha^4 + (b-2r+\lambda)\beta^4 + 2(r-\lambda)\alpha^2\beta^2].$$

Simplifying, we have

(2.1) $(3\lambda-r)\alpha^4 + (2b-5r+3\lambda)\beta^4 + 6(r-\lambda)\alpha^2\beta^2 = 0.$

We now classify the BIB designs according as (i) $r=3\lambda$, (ii) $r < 3\lambda$ or (iii) $r > 3\lambda$. We treat these cases separately.

Case 1. $r=3\lambda$.

When $r=3\lambda$, (2.1) reduces to

(2.2) $(2b-4r)\beta^2 + 6(r-\lambda)\alpha^2\beta^2 = 0.$

From (2.2), it is clear that a positive solution for β^2/α^2 is possible if and only if

$$2b - 4r < 0 .$$

We now prove

LEMMA 2.1. *In a BIB design with parameters v, b, r, k, λ , if $r = 3\lambda$, $b \geq 2r$.*

PROOF. It has been shown in [9] that for any BIB design,

$$b \geq 3(r - \lambda) .$$

Thus, obviously for $r = 3\lambda$, $b \geq 2r$.

We thus see that a SORD with factors each at four levels cannot be constructed through a BIB design with $r = 3\lambda$, using the above technique.

Case 2. $r \neq 3\lambda$.

When $r \neq 3\lambda$, (2.1) may be written as

$$(2.3) \quad (2b - 5r + 3\lambda)x^2 + 6(r - \lambda)x + 3\lambda - r = 0 ,$$

where $x = \beta^2/\alpha^2$. Solving (2.3) for x , we obtain

$$(2.4) \quad x = \frac{-6(r - \lambda) \pm \sqrt{\{36(r - \lambda)^2 - 4(3\lambda - r)(2b - 5r + 3\lambda)\}}}{2(2b - 5r + 3\lambda)} .$$

From (2.4), it is clear that in order that x is real, we must have

$$(2.5) \quad 36(r - \lambda)^2 - 4(3\lambda - r)(2b - 5r + 3\lambda) > 0 .$$

From (2.5), we infer that if $(2b - 5r + 3\lambda) < 0$ and $r < 3\lambda$, a real positive solution for x will always exist. Further, if $r > 3\lambda$ and $(2b - 5r + 3\lambda) > 0$, a positive solution for x will always exist. It is also noted that the solution is not equal to unity.

We now prove

LEMMA 2.2. *For a BIB design with $r < 3\lambda$, $S < 0$ if $2v < 3k + 2$, where $S = 2b - 5r + 3\lambda$.*

PROOF. We have

$$(2.6) \quad S = 2b - 2r - 3(r - \lambda) .$$

Also,

$$(2.7) \quad r - \lambda = r - r(k - 1)/(v - 1) .$$

Substituting for $r - \lambda$ from (2.7) in (2.6) and after some simplification, we obtain,

$$(2.8) \quad k(v-1)S/r = (v-k)(2v-3k+2).$$

Hence the lemma.

It is easy to note that the following series of BIB designs satisfies (i) $r < 3\lambda$ and (ii) $2v < 3k+2$:

$$(2.9) \quad v=b, \quad r=k=v-1, \quad \lambda=v-2, \quad v \geq 3.$$

However, this series of designs does not exclude the possibility of existence of other BIB designs with $r < 3\lambda$ and satisfying $2v < 3k+2$. For instance, the following two BIB designs do not belong to the series (2.9) and still have $r < 3\lambda$ and $2v < 3k+2$:

- i) $v=5, b=10, r=6, k=3, \lambda=3$.
- ii) $v=6, b=15, r=10, k=4, \lambda=6$.

We may now summarise the above discussion in the following.

THEOREM 2.1. *If there exists a BIB design with parameters v, b, r, k, λ satisfying (i) $r < 3\lambda$ and (ii) $2v < 3k+2$, then we can construct a SORD for $(v-1)$ factors with factors each at four levels.*

It has been remarked earlier that if $r > 3\lambda$ and $(2b-5r+3\lambda) > 0$, a real positive solution for β^2/α^2 is always available. From (2.8) we find that if $2v > 3k+2$, then $(2b-5r+3\lambda) > 0$. We note that the following series of BIB designs have this property:

- (a) $v, b = \binom{v}{2}, k=2, r=v-1, \lambda=1, v > 4$.
- (b) $v=b=s^2+s+1, r=k=s+1, \lambda=1, s > 2$.
- (c) $v=b, r=k=1, \lambda=0$.

Thus, if there exists a BIB design satisfying $r > 3\lambda$ and $2v > 3k+2$, we can always construct a $(v-1)$ -factor SORD, using the BIB design. If the chosen BIB design is symmetrical the resultant SORD will obviously have minimum number of points.

3. SORD with factors at six levels each

In this section, we deal with a method of construction of SORD with factors at six levels each.

Let it be possible to find an $s \times k$ array D satisfying the following conditions:

- i) There are exactly three symbols in the array, denoted by 0, 1, 2 (say).
- ii) In each column of the array, the i th symbol occurs exactly r_i times ($i=0, 1, 2$).
- iii) In each row of the array, the i th symbol occurs exactly k_i times ($i=0, 1, 2$).

- iv) In any $s \times 2$ sub-array of D , the frequency of the pair (i, i) is λ_{ii} and is constant for any permutation of columns, $i=0, 1, 2$.
- v) If λ_{ij} denotes the frequency of the ordered pair (i, j) in any $s \times 2$ sub-array of D , then $\lambda_{ij} + \lambda_{ji}$ is constant for given (i, j) $i \neq j$, $i, j = 0, 1, 2$ and for any permutation of columns.

From D , we obtain another array D^* by omitting a column of D . It is easy to see then that D^* also satisfies all the conditions i), ii), iv) and v) of D but not iii).

Now, for constructing a six-level SORD replace in D^* , zero by α , 1 by β and 2 by γ . 'Multiply' each of those s combinations involving α , β and γ by those of a 2^p factorial with levels ± 1 , where 2^p is the smallest fraction of 2^{k-1} without confounding any interaction with four factors or less. Thus, we get $N (=s2^p)$, $(k-1)$ -dimensional points which satisfy the following relations :

$$(A') \quad \sum_{u=1}^N \left\{ \prod_{i=1}^{k-1} x_{iu}^{\alpha_i} \right\} = 0, \text{ if any } \alpha_i \text{ is odd for } \alpha_i = 0, 1, 2 \text{ or } 3 \text{ and } \sum_i \alpha_i \leq 4.$$

$$(B') \quad \sum_{u=1}^N x_{iu}^2 = \text{Constant} = 2^p [r_0 \alpha^2 + r_1 \beta^2 + r_2 \gamma^2] = N \lambda_2 \text{ (say),}$$

$$\sum_{u=1}^N x_{iu}^4 = \text{Constant} = 2^p [r_0 \alpha^4 + r_1 \beta^4 + r_2 \gamma^4]; \quad i = 1, 2, \dots, k-1.$$

$$(C') \quad \sum_{u=1}^N x_{iu}^2 x_{ju}^2 = \text{Constant} = 2^p [\lambda_{00} \alpha^4 + \lambda_{11} \beta^4 + \lambda_{22} \gamma^4 + (\lambda_{01} + \lambda_{10}) \alpha^2 \beta^2$$

$$+ (\lambda_{02} + \lambda_{20}) \alpha^2 \gamma^2 + (\lambda_{12} + \lambda_{21}) \beta^2 \gamma^2]$$

$$= N \lambda_4 \text{ (say); } i \neq j, \quad i, j = 1, 2, \dots, k-1.$$

Now, in order that the N points obtained above form a SORD, these points must satisfy the conditions (D) and (E) of Section 2, apart from (A'), (B'), (C') above. Condition (E) is satisfied by these N points, as they are not equidistant from the origin. Applying condition (D) on these N points, we obtain,

$$(3.1) \quad r_0 \alpha^4 + r_1 \beta^4 + r_2 \gamma^4 = 3[\lambda_{00} \alpha^4 + \lambda_{11} \beta^4 + \lambda_{22} \gamma^4 + \mu_1 \alpha^2 \beta^2 + \mu_2 \alpha^2 \gamma^2 + \mu_3 \beta^2 \gamma^2],$$

where

$$\mu_1 = \lambda_{01} + \lambda_{10}, \quad \mu_2 = \lambda_{02} + \lambda_{20}, \quad \mu_3 = \lambda_{12} + \lambda_{21}.$$

The equation (3.1) reduces, after simplification, to

$$(3.2) \quad (r_0 - 3\lambda_{00})u^2 + (r_1 - 3\lambda_{11})\omega^2 - 3\mu_1 u\omega - 3\mu_2 u - 3\mu_3 \omega + (r_2 - 3\lambda_{22}) = 0,$$

where

$$u = \alpha^2/\gamma^2, \quad \omega = \beta^2/\gamma^2.$$

Since (3.2) involves two unknowns u and ω , we may choose one of

them arbitrarily so that the solution of the other is real and positive. The value of γ can be determined from the relation

$$2^p[r_0u+r_1\omega+r_2]\gamma^2=N \text{ (fixing } \lambda_2=1) .$$

From the above discussions, it is clear that a six-level SORD can be constructed if we can find an array D , satisfying conditions i), ii), iii), iv) and v), which further permits real positive solutions for u and ω . In what follows, we shall demonstrate that if v ($=2t+1$), t a positive integer is a prime or a prime power, we can construct a six-level SORD for $(v-1)$ factors. Since t can be either even or odd, we take up these two cases separately.

Case 1. $t=2n$

Since $v=2t+1$ a prime power, $GF(v)$ exists. It has been shown by Saha and Gupta [12] that a three-symbol Partially Balanced Array [5] of strength two exists with $v=4n+1$ constraints and $8n+2$ assemblies. We describe their method of construction for the sake of completeness.

Let $0, 1, \dots, v-1$ be the elements of $GF(v)$ and x be a primitive element of $GF(v)$. Let R be a row vector containing all the v elements of $GF(v)$. From R , obtain another row vector R^* by replacing in R , zero by 1, the elements corresponding to even powers of x by 2 and the elements corresponding to odd powers of x by 0. Next, permute R^* cyclically to obtain a square matrix A_1 of order v . Let A_2 be another matrix whose rows are 'images' of the rows of A_1 , i.e. if $z_i^{(1)}$ is the i th row of A_1 , then the corresponding row of A_2 , say, $z_i^{(2)}$ is given by

$$z_i^{(1)}+z_i^{(2)}=(2, 2, \dots, 2) .$$

Then, $A=\begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$ is a three-symbol Partially Balanced Array involving v constraints, $2v$ assemblies, and strength two, where $v=4n+1$.

It is easy to see that A satisfies all the requirements of D . For this case, we have

$$\begin{aligned} r_0 &= 4n, & r_1 &= 2, & r_2 &= 4n, \\ \lambda_{00} &= 2n-1, & \lambda_{11} &= 0, & \lambda_{22} &= 2n-1, \\ \mu_1 &= 2, & \mu_2 &= 4n, & \mu_3 &= 2. \end{aligned}$$

Substituting these values in (3.2), we have

$$\begin{aligned} & -(2n-3)u^2+2\omega^2-6u\omega-12nu-6\omega-(2n-3)=0 \\ (3.3) \quad \text{or,} & \\ & (2n-3)u^2-2\omega^2+6u\omega+12nu+6\omega+2n-3=0 . \end{aligned}$$

Solving for u in terms of ω , we obtain

$$(3.4) \quad u = \frac{-(6\omega + 12n) \pm \delta}{(4n - 6)},$$

where

$$(3.5) \quad \delta^2 = 12\omega^2 + 128n^2 + 96n\omega + 48n + 16n\omega^2 + 72\omega - 36.$$

In order to make the value of u real and positive, we must have (for $n > 1$)

$$(3.6) \quad \begin{aligned} (a) \quad & \delta > 0 \\ (b) \quad & \delta - (6\omega + 12n) > 0. \end{aligned}$$

Thus, the problem now reduces to the choice of ω in such a manner that (3.6) is satisfied. Since ω is necessarily positive, (a) of (3.6) can readily be satisfied by a suitable choice of ω . Further, condition (b) of (3.6) is equivalent to the following condition:

$$(3.7) \quad -2\omega^2 + 6\omega + 2n - 3 < 0.$$

It may be remarked here that if (3.7) holds, then (a) of (3.6) also holds. Thus, we may choose ω in order to satisfy (3.7) only. It is easy to see that (3.7) is satisfied for all ω given by

$$(3.8) \quad \begin{aligned} \text{i) } & \omega < (3 - \sqrt{4n + 3})/2 \\ \text{ii) } & \omega > (3 + \sqrt{4n + 3})/2. \end{aligned}$$

The value of ω given in i) of (3.8) is however inadmissible for our purpose. Thus, we shall consider only the value of ω given in ii) of (3.8).

For $n=1$, it is seen that $\omega=2$ provides a positive solution for u . The following table gives the solutions of u and ω for $1 \leq n < 5$.

Table 1

n	No. of factors	No. of design points	Solution of*	
			u	ω
1	4	160	0.1244	2
2	8	1152	0.1454	4
3	12	6656	0.0830	4
4	16	8704	0.0415	4

* In the above table, only one solution of u and ω is given.

Case 2. $t = 2n + 1$

For this case also, one can get a three-symbol Partially Balanced

Array in the same manner as described for the case $t=2n$. However, when $t=2n+1$, the matrix A_1 , defined earlier, itself serves our purpose, as A_1 satisfies all the conditions of D . In this case, we have

$$\begin{aligned} r_0 &= 2n+1, & r_1 &= 1, & r_2 &= 2n+1, \\ \lambda_{00} &= n, & \lambda_{11} &= 0, & \lambda_{22} &= n, \\ \mu_1 &= 1, & \mu_2 &= 2n+1, & \mu_3 &= 1. \end{aligned}$$

Substituting these values in (3.2), we obtain

$$(3.9) \quad (n-1)u^2 + (6n+3\omega+3)u + 3\omega + (n-1) - \omega^2 = 0.$$

The equation (3.9) involves two unknowns u and ω (for a given value of n) and hence we fix ω arbitrarily so that a positive solution of u is obtained. In the following table, we have presented solutions of u and ω for $1 \leq n \leq 4$.

Table 2

n	No. of factors	No. of design points	Solution of*	
			u	ω
1	6	224	0.1905	4
2	10	704	0.1107	4
4	18	4864	0.0256	4

* Here also, only one solution of u and ω is reported.

Remark

It is clear from Table 1 that most of the designs for the cast $t=2n$ require a large number of points. However, designs with smaller number of points can be obtained by omitting a requisite number of columns from the designs for the case $t=2n+1$. For instance, the design in 8 factors given in Table 1 requires 1152 points whereas, an 8-factor design in only 704 points can be obtained by omitting any two columns from the 10-factor design given in Table 2.

Acknowledgements

Thanks are due to the referee for his helpful comments. The work of one of the authors (TKG) was supported by a Senior fellowship of the Indian Council of Agricultural Research.

INSTITUTE OF AGRICULTURAL RESEARCH STATISTICS*

* T. K. Gupta is now at University of Kalyani, India.

REFERENCES

- [1] Bose, R. C. and Draper, N. R. (1959). Second order rotatable designs in three dimensions, *Ann. Math. Statist.*, **30**, 1097-1112.
- [2] Box, G. E. P. and Behnken, D. W. (1960a). Simplex-sum designs: a class of second order rotatable designs derivable from those of first order, *Ann. Math. Statist.*, **31**, 835-864.
- [3] Box, G. E. P. and Behnken, D. W. (1960b). Some new three level designs for the study of quantitative variables, *Technometrics*, **2**, 455-475.
- [4] Box, G. E. P. and Hunter, J. S. (1957). Multifactor experimental designs for exploring response surfaces, *Ann. Math. Statist.*, **28**, 195-241.
- [5] Chakravarti, I. M. (1957). Fractional replication in asymmetrical factorial designs and partially balanced arrays, *Sankhya*, **17**, 143-164.
- [6] Das, M. N. (1961). Construction of rotatable designs from factorial designs, *J. Ind. Soc. Agril. Statist.*, **13**, 169-194.
- [7] Das, M. N. and Narasimham, V. L. (1962). Construction of rotatable designs through balanced incomplete block designs, *Ann. Math. Statist.*, **33**, 1421-1439.
- [8] Dey, A. (1971). On a class of four-level second order rotatable designs, *Proc. Ind. Sc. Congress*, 58th session, Bangalore, India.
- [9] Dey, A. and Das, M. N. (1970). On blocking second order rotatable designs, *Calcutta Statist. Assoc. Bull.*, **19**, 75-85.
- [10] Draper, N. R. (1960). Second order rotatable designs in four or more dimensions, *Ann. Math. Statist.*, **31**, 23-33.
- [11] Nigam, A. K. and Dey, A. (1970). Four and six level second order rotatable designs, *Calcutta Statist. Assoc. Bull.*, **19**, 155-157.
- [12] Saha, G. M. and Gupta, T. K. (1973). Three symbol partially balanced arrays, to appear.