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Optimal Third Order Rotatable Designs Constructed from Balanced Incomplete Block Design (BIBD)

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Authors' contributions

This work was carried out in collaboration between all authors. Author JCR developed the design matrix, moment matrix and the information matrix. Authors JCR, MKK and GKK evaluated the alphabetic optimality criteria and performed analysis on the final results. All authors read and approved the final manuscript.

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ABSTRACT

In the design of experiments for estimating statistical models, optimal designs allow parameters to be estimated without bias and with minimum variance. Optimal designs are experimental designs that are generated based on a particular optimality criterion and are generally optimal only for a specific statistical model. The purpose of this study therefore was to investigate the optimality criteria for third order rotatable designs (TORD) constructed from balanced incomplete block design (BIBD). Specifically the study obtained alphabetic optimality criteria for specific TORD in three, four, five and six factors. From the existing TORD constructed using BIBD, the design matrix, moment matrix and information matrix considering full parameter system were obtained. Evaluation of the alphabetic optimality criteria was done. However, all the designs under investigation were found to be E-optimal. E-optimality maximizes the minimum eigenvalue of the information matrix. Optimum TORD from BIBD can be applied in real life experiments

Keywords: TORD; BIBD; Optimality.

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1. INTRODUCTION

The concept of rotatability as a desirable quality of an experimental design was first put forward by [1]. This property is that the variances of estimates of the response made from the least squares estimates of the Taylors series are constant on circles, spheres or hyper-spheres about the centre of the design. Thus, a rotatable design, that is, a design which satisfies this property, could be rotated through any angle around its centre and the variances of responses estimated from it would be unchanged. Victorbabu [2] studied a new method of construction of second order slope rotatable design using balanced incomplete block designs.

In the design of experiments, optimal designs are a class of experimental designs that are optimal with respect to some statistical criterion. In practical terms, optimal experiments can reduce the costs of experimentation.

The class of rotatable designs is very rich in the sense that under many commonly used criteria, such as D-optimality, the optimal designs for polynomial regression models over hyper spherical regions may be found within this class [3]. It has been recognized in recent years that even in response surface designs the main interest of the experimenter may not always be in the response at individual locations. Sometimes, the differences between responses at various locations may be of greater interest [4].

According to [5], an incomplete block design is said to be a balanced incomplete block (BIB) design if it satisfies the following conditions:

(i) The experimental material is divided into b blocks of s units each, different treatments being applied to the units in the same block.
(ii) There are v treatments each of which occurs in r blocks.
(iii) Any two treatments occur together in exactly λ blocks.

The quantities v, b, r, s and λ are called the parameters of BIB design.

Third order rotatable designs can be group into sequential and non-sequential designs. Sequential designs are performed in parts or blocks while non-sequential experimentation all the runs must be run at one time to make a rotatable least square fitting possible. Draper [6] stated that sequential experiments are more useful in practice and are economical. Therefore third order rotatable designs may be run sequentially in three stages with three or four blocks depending on the model adequacy. Normally, the first part consisting of first order is run and the response function is approximated using a first order model. If the first order model is found to be adequate, as the representation of the unknown function by noting evidence of the goodness of fit, the experiment may be terminated at this stage. However, if the first model is found to be inadequate ,the trials of second order are run and ultimately, proceed to fit a third order if a second order model is also found to be inadequate. The first block may contain the k+1 runs, second block containing the second order runs and third block containing third order runs.

2. OPTIMALITY CRITERIA

Pukelsheim [7] gave methods of evaluating particular criteria. Morgan [8] has been working on design optimality for various classes of designs with blocking. Huda et al. [9] did a study on A- and D- rotatability of two dimensional third order designs. He obtained the expression for variance-covariance matrix of the estimated axial slopes at a point in the factor space for a symmetric balanced two dimensional third order design. Huda went ahead to derive the trace and the determinant of the matrix to show that symmetry and balance are not sufficient for either A-rotatability or D-rotatability of the design. Alphabetic optimality criteria under consideration in this study include D-, E-, A-, T- , I- and G-optimality criteria. D-optimality seeks to minimize $|(X'X)^{-1}|$, or equivalently maximize the determinant of the information matrix X'X of the design and A-optimality seeks to minimize the trace of the inverse of the information matrix. This criterion results in minimizing the average variance of the estimates of the regression coefficients. E-optimality maximizes the minimum eigenvalue of the information matrix while T-optimality maximizes the trace of the information matrix. G-optimality seeks to minimize the maximum entry in the diagonal of the hat matrix $X(X'X)^{-1}X'$. This has the effect of minimizing the maximum variance of the predicted values and I-optimality seeks to minimize the average prediction variance over the design space.

The problem is to obtain optimal third order rotatable designs constructed from BIBD. The third order rotatable designs under consideration were constructed by [10].

The information matrices for three, four, five and six factors are obtained and utilized to determine optimal third order rotatable designs constructed from BIBD.

Consider an arrangement of the design matrix in k dimensions given by x

$$x = \begin{bmatrix} 1 \\ x_{1u}^2 \\ x_{2u}^2 \\ \vdots \\ x_{ku}^2 \\ x_{1u}x_{2u} \\ x_{1u}x_{3u} \\ \vdots \\ x_{k-1}x_k \\ x_{1u}x_{2u}x_{3u} \\ x_{1u}x_{2u}x_{4u} \\ \vdots \\ x_{k-2u}x_{k-1u}x_{ku} \\ x_{1u} \\ x_{1u}^3 \\ x_{1u}x_{2u}^2 \\ \vdots \\ x_{1u}x_{ku}^2 \\ \vdots \\ x_{ku} \\ x_{ku}^3 \\ x_{ku}x_{1u}^2 \\ \vdots \\ x_{ku}x_{k-1u}^2 \end{bmatrix}$$

Then a general third order design can be expressed as;

$$\eta_\mu = \beta_o + \sum_{i=1}^{k}\beta_i x_{iu} + \sum_{i\le j=1}^{k}\beta_{ij}x_{iu}x_{ju} + \sum_{i\le j\le l=1}^{k}\beta_{ij}x_{iu}x_{ju}x_{lu}$$

Where u=1, 2,…, N

With parameters

$\beta_0, \beta_{11}, \beta_{22}, \dots, \beta_{kk}, \beta_1, \beta_2, \dots \beta_k, \beta_{12}, \dots, \beta_{k-1\,k}, \beta_{111}, \dots,$
$\beta_{kkk}, \beta_{112}, \dots, \beta_{k-1k-1k}, \beta_{122}, \dots,$
$\beta_{k-1kk}, \beta_{123}, \dots, \beta_{k-2k-1k}$

The independent variables $x_1, x_2, \dots, x_k$ have been coded so that

$$\sum_{u=1}^{N} x_{1u}^2 = \sum_{u=1}^{N} x_{2u}^2 = \cdots = \sum_{u=1}^{N} x_{ku}^2 = N$$

To standardize the moment matrix for ease in further investigation, each term is a moment of independent variables i.e. the term in the column headed by x_2^2 and the row labeled x_2^2 is a fourth moment of x_2.

That is;

$$\frac{1}{N}\sum_{u=1}^{N} x_{2u}^4 = 3\,\lambda_4$$

And the term in the column headed by $x_1x_2^2$ and the row, x_1^3, is a sixth order mixed moment of both x_1 and x_2, i.e.

$$\frac{1}{N}\sum_{u=1}^{N} x_{1u}^4 x_{2u}^2 = 3\,\lambda_6$$

Thus, the moment matrix according to [11], of a rotatable design of order 3 in k factors is given by

$$M_{\left[\substack{3+k\\k}\right]\times\left[\substack{3+k\\k}\right]} = N^{-1}(X^T X)$$

While the information matrix is given by the following expression

$$C_k(M) = \left[K_k^{'} M_k^{-1} K_k\right]^{-1}$$

Where k is the coefficient matrix of a full parameter system and M is the moment matrix.

We now utilize methods stated by [7] to obtain particular alphabetic optimality criteria in three, four, five and six factors.

3. RESULTS

The study shows that all the designs under consideration in the study were found to be E-optimal. It was found that the design D_3 is D-optimal, D_1 is A-optimal, D_4 is T-optimal and Designs D_1 and D_4 are I- and G-optimal respectively. As the number of factors increase the designs get less optimal for A-optimality criteria. For T-optimality and G-optimality criteria, designs with more factors are more optimal. The results are as shown in Table 1.

Table 1. Summary of particular criteria for the four designs

K	D	A	T	E	I	G
$D_1(3\ factors)$	0.03583	55.338	0.1383	0.0031	49.5917	0.2263
$D_2(4\ factors)$	0.02455	117.0680	0.0956	0.0063	-51454.9846	0.1442
$D_3(5\ factors)$	0.01939	216.188	0.0689	0.0033	176.014	0.1273
$D_4(6\ factors)$	0.0203	428.022	0.0607	0.0033	205.639	0.1005

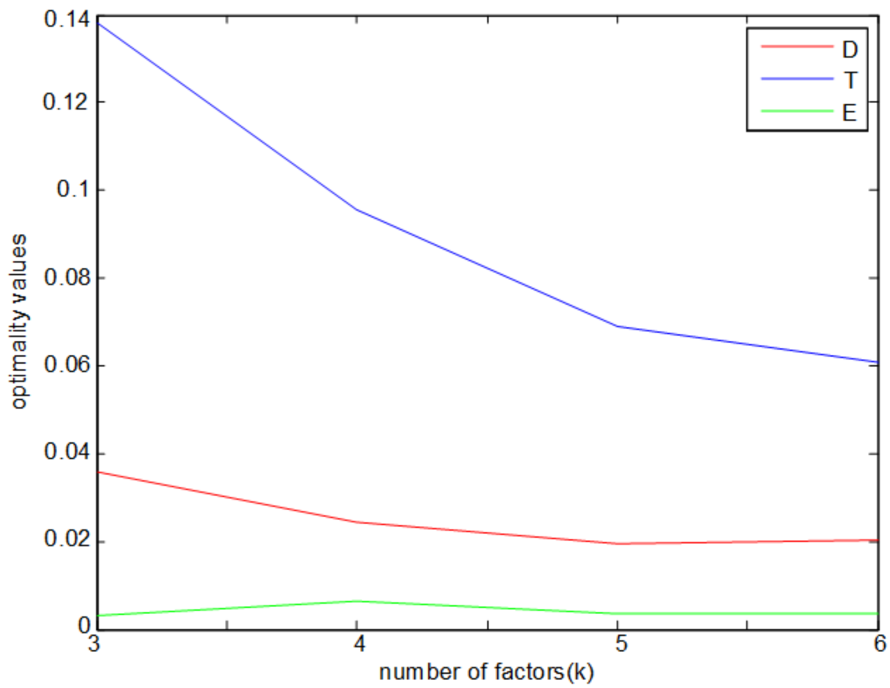

Fig. 1. Graph of optimal values vs number of factors

4. DISCUSSION

The behaviour of these values on different factors can be visualized well in Fig. 1. From the above results, it shows that the designs optimal values decrease with increase in the number of factors for D- and T- optimality. However, the decrease is significant for T-optimality. All the designs under consideration in the study were found to be E-optimal. The trend of I-optimality cannot be predicted.

5. CONCLUSION

Alphabetic optimality criteria for third order rotatable designs constructed from balanced incomplete block designs were determined hence optimal designs exist. Although D-optimality criteria are always recommended this study shows that other optimality criteria can play a role in cases where D-optimality is not suitable. Optimal TORD from BIBD can be applied in real life experiments.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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