

Original Research Article

Optimal third order rotatable designs constructed from BIBD

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. The methods proposed by Pukelsheim (1993) were then utilized to evaluate the alphabetic optimality for the designs from their information matrices. However, all the designs under investigation were found to be E-optimal. Optimum TORD from BIBD can be applied in real life experiments.

Key words: TORD, BIBD, Optimality

1.0: Introduction

The concept of rotatability as a desirable quality of an experimental design was first put forward by Box and Hunter in 1957. 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.

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 optimality of a design depends on the statistical model and is assessed with respect to a statistical criterion, which is related to the variance matrix of the estimator. Under design of experiments for estimating statistical models, optimal designs allow parameter to be estimated without bias and with minimum variance. A non-optimal design requires a greater number of experimental runs to estimate the parameter with the same precision as an optimal design.

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 (Kiefer (1960)). It has been

38 recognized in recent years that even in response surface designs the main interest of the
 39 experimenter may not always be in the response at individual locations. Sometimes, the
 40 differences between responses at various locations may be of greater interest (Herzberg
 41 (1967)).

42 2.0: Optimality criteria

43 Pukelsheim (1993) gave methods of evaluating particular criteria. The problem is to obtain
 44 optimal third order rotatable designs constructed from BIBD. The third order rotatable
 45 designs under consideration were constructed by Mutai (2012).

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

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

$$49 \quad x = \begin{bmatrix} 1 \\ x_{1u}^2 \\ x_{2u}^2 \\ \vdots \\ x_{ku}^2 \\ x_{1u}x_{2u} \\ x_{1u}x_{3u} \\ \vdots \\ x_{k-1u}x_{ku} \\ x_{1u}x_{2u}x_{3u} \\ x_{1u}x_{2u}x_{4u} \\ \vdots \\ x_{k-2u}x_{k-1u}x_{ku} \\ x_{1u}^3 \\ x_{1u}^2x_{2u} \\ \vdots \\ x_{1u}^2x_{ku} \\ \vdots \\ x_{ku}^3 \\ x_{ku}^2x_{1u} \\ \vdots \\ x_{ku}^2x_{k-1u} \end{bmatrix}$$

50 Then a general third order design can be expressed as;

$$51 \quad \eta_\mu = \beta_o + \sum_{i=1}^k \beta_i x_{iu} + \sum_{i \leq j=1}^k \beta_{ij} x_{iu} x_{ju} + \sum_{i \leq j \leq l=1}^k \beta_{ijl} x_{iu} x_{ju} x_{lu} , \text{ where } u=1, 2, \dots, N$$

52 with parameters

$$53 \quad \beta_0, \beta_{11}, \beta_{22}, \dots, \beta_{kk}, \beta_1, \beta_2, \dots, \beta_k, \beta_{12}, \dots, \beta_{k-1,k}$$

$$54 \quad , \beta_{111}, \dots, \beta_{kkk}, \beta_{112}, \dots, \beta_{k-1k-1k}, \beta_{122}, \dots, \beta_{k-1kk}, \beta_{123}, \dots, \beta_{k-2k-1k}$$

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

$$\sum_{u=1}^N x_1^2 = \sum_{u=1}^N x_2^2 = \dots = \sum_{u=1}^N x_k^2 = N$$

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

59 That is;

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

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

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

62 Thus, the moment matrix (according to Gardiner (1959)), of a rotatable design of order 3 in k
63 factors is given by

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

65 While the information matrix is given by the following expression

66

$$C_k(M) = [K'_k M_k^{-1} K_k]^{-1}$$

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

68 We now utilize methods stated by Pukelsheim (1993) to obtain particular alphabetic
69 optimality criteria in three, four, five and six factors.

70 3.0: Results

71 The study shows that all the designs under consideration in the study were found to be E-
72 optimal. It was found that the design D_3 is D-optimal, D_1 is A-optimal, D_4 is T-optimal and
73 Designs D_1 and D_4 are I- and G-optimal respectively. The results are as shown in table 3.1.

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

Table 3.1: A summary of particular criteria for the four designs

74 4.0: Discussion

75 The behaviour of this the optimal values on different factors can be visualized well in figure
76 4.1

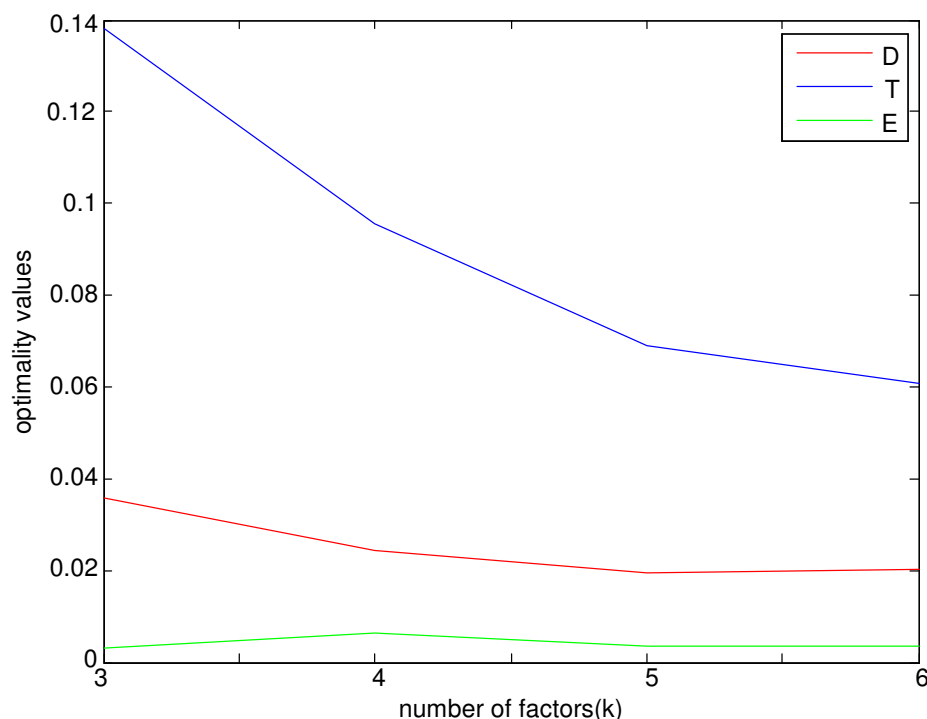


Figure 4.1: Graph of optimal values vs number of factors

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.

4.0: Conclusion

Alphabetic optimality criteria for third order rotatable designs constructed from balanced incomplete block designs were determined hence optimal designs exist. Optimal TORD from BIBD can be applied in real life experiments.

Reference

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