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DT- optimality Criteria for Second Order Rotatable Designs Constructed Using Balanced Incomplete Block Design

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Authors' contributions

This work was carried out in collaboration between all authors. Author DMM designed the study, wrote the protocol and wrote the first draft of the manuscript. Authors MKK and SKR managed the computation of the study and the literature searches. All authors read and approved the final manuscript.

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Abstract

Experimenters have come to a realization that a design can perform very well in terms of a particular statistical characteristic and still perform poorly in terms of a rival characteristic. Due to this studies have narrowed down to the area of optimality criteria. Some of these criteria include the alphabetic optimality criteria and compound optimality criteria. Compound optimality criteria are those that combine two or more alphabetic optimality criteria in one particular design. In this paper two alphabetic optimality D- and T- criteria are combined to obtain DT- compound optimality criteria for the existing second order rotatable designs using Balanced Incomplete Block Designs. The purpose of this paper is to bring a balance between to statistical properties; parameter estimation and model discrimination. This will aid those researchers who are interested in more than two desired traits in one design. In this analysis, we note that the more homogenous the design is the more optimal it becomes.

Keywords: Optimality criteria; rotatability; compound criteria.

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1 Introduction

In many life sciences, optimal designs are required in order to cut on the cost of experimentation. An experimenter is therefore advised to make the choice of a design to be used prior to carrying out any experiment. Response surface methodology (RSM) is a collection of statistical and mathematical techniques that are useful in analyzing, developing, improving and optimizing processes. According to [1], RSM is either used to explore response surfaces or to estimate the parameters of a model. [1] point out that the technique of fitting a response surface is one widely used to aid in the statistical analysis of experimental work in which the response of a product depends on some unknown factors on one or more controllable variables. A particular selection of settings or factor levels at which observations are to be taken is called a design. Designs are usually selected to satisfy some desirable criteria chosen by the experimenter.

Regression models in general. [1] gave an extensive review of D-optimality for weighing problems and for analysis of variance problems. In the early 1970s, the core of the theory was crystallized in the papers by[2] and [3]. The family of matrix means, $0_p$with $-\infty \leq p \leq 1$ was introduced by [3]and is discussed in detail in [4]. [5] discussed on the duality of optimal designs for discrimination and parameter estimation. T-optimal design is a plan where the optimality is obtained by discriminating between two or more models, one of which is true. [6] introduced experimental designs for discriminating between two models and also between several models. [7]defined compound criterion as a weighted product of the efficiencies that is to be maximized and they introduced DT- and CD-optimality criteria. [8]combined D-optimality with T-optimality to get DT-optimality which provides a specified balance between model discrimination and parameter estimation. There are essentially two ways for the construction of design criteria which incorporate different purposes of the experimenter. One approach is the construction of a new optimality criterion by averaging several competitive design criteria. Alternatively one could try to maximize one primary optimality criterion subject to constraints for specific minimum efficiencies of other criteria, [9] and[10] constructed optimum designs of order two in three dimensions but the optimality criteria for their designs were not identified. [11] gave the optimality criteria for the construction of designs [12-14] gave practical examples and evaluated the efficiencies for the optimum designs respectively. In this paper, we construct a new optimal second order rotatable design in four dimensions, evaluate its determinant and trace criterion and combine them to obtain DT- criterion.

2 Conditions for Second Order Rotatability

Consider the model of second order response surface design

$\boldsymbol{D= (x_{iu})}$ to fit the model:

$$y_u = \theta_o x_{ou} + \varepsilon_{i=1}^{k} \theta_{ii} x_{iu}^2 + \sum\sum_{i<j}^{k} \theta_{ij} x_{iu} x_{ju} + \varepsilon_u \tag{1}$$

Where $\boldsymbol{x_{iu}}$ denotes the level of the i^{th} factor $(i = l,2,3,4)$ in the u^{th} run $(u = l,2,\ldots,32)$ of the experiment, ε_u are uncorrected random errors with mean zero and variance σ^2.The model is said to be SORD if the variance of the estimate of the response y_u is only a function of the distance $d^2 = \sum_{i=1}^{k} x_i^2$of the point $(x_1, x_2, x_3\ and\ x_4)$from the origin of the design.

The spherical variance function of the estimated second order response surface is achieved if the design points satisfy the following moments and non- singularity conditions;

$$\sum_{u=1}^{k} x_{iu}^2 = Constant = N\lambda_2$$

$$\sum_{u=1}^{k} x_{iu}^4 = Constant = 3N\lambda_4\ for\ alli,$$

$\sum_{u=1}^{k} x_{iu}^2 x_{ju}^u = constant = N\lambda_4, i \neq j$ (2)

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

3 Construction of the optimum Second Order Rotatable Design in Four Dimensions

We add a factor to each set of points that formed the twenty points constructed by [10], we consider the design,

$$m_1 = S\ (a, a, a, a) + S(c_1, o, o, o) + S\ (c_2, o, o, o) \quad (3)$$

The above set of 32 points form a second order rotatable arrangement in four dimensions if the following moment conditions holds:

i. $\sum_{u=1}^{32} x_{iu}^2 = 16a^2 + 2c_1^2 + 2c_2^2 = 32\lambda_2$
ii. $\sum_{u=1}^{32} x_{iu}^4 = 16a^4 + 2c_1^4 + 2c_2^4 = 96\lambda_4$
iii. $\sum_{u=1}^{32} x_{iu}^2 x_{ju}^2 = 16a^4 = 32\lambda_4$ (4)

For $i \neq j = 1, 2, 3$ with all other sums and products including order four being zero.

The excess of

$$\sum_{u=1}^{32} x_{iu}^4 = \sum_{u=1}^{32} x_{iu}^2 x_{ju}^2$$

Is given by,

$$\text{Ex}[S\ (a, a, a, a) + S\ (c_1, o, o, o) + S(c_2, o, o, o)] = \sum_{u=1}^{32} x_{iu}^4 - 3\sum_{u=1}^{32} x_{iu}^2 x_{ju}^2 = 0 \quad (5)$$

Therefore,

$$c_1^4 + C_2^4 - 16a^2 = 0$$

$$Let\ c_1^2 = x\ a^2\ and\ c_2^2 = y\ a^2$$

$$x^2 + y^2 = 16 \quad (6)$$

$$\text{X} = \sqrt{16 - y^2}\ \text{ for } 0 < y < 4$$

We shall need to look at the behavior of the optimum value of y at various points specifically, when $y = 3$, $x = 2.645751311$ hence $c_1 = 1.626576562a\ and\ c_2 = 1.732050808a$

Our point set now becomes

M_1= S (a, a, a, a) + S (1.626576562a, 0, 0, 0) + S (1.732050808a, 0, 0, 0)

The set of points in m_1 forms a second order rotatable arrangement in four dimensions if y = 3. For the set of points in m_1 to form a second order rotatable design the non- singularity conditions given in (2) must be satisfied.

$\lambda_2 = 0.852859456a^2$ and $\lambda_4 = 0.5a^4$ (7)

$$\frac{\lambda_4}{\lambda_2^2} = \frac{0.5}{0.727369251} > \frac{k}{k+2} = \frac{4}{6},$$

$$\frac{\lambda_4}{\lambda_2^2} = 0.69 > \frac{\lambda_4}{\lambda_2^2} = 0.67$$

The non- singularity conditions of rotatability of a second order design are satisfied [10] shows that the expansion of;

$$\text{Var}(y_u) = \beta\sigma^2 N^{-1}\big[2(k+2)\beta_2^2 + \langle(k+2)\beta_2 - (k-1)\rangle 3k\beta_2 - 4k\beta_2 - 2(\beta_2 - 1)\beta_2 k(k - 1 - k\lambda 2 - 1k\,(k-1) \quad (8)$$

Where $\beta = [\beta_2\,((k+2)\beta_2 - k]^{-1}$

And $\beta_2 = \frac{\lambda_4}{\lambda_2^2} \neq \frac{k}{(k+2)}$

Now substituting the values given equations (5) and (6) and taking k=4, we obtain;

$$\text{Var}\,((y_u) = 52.74609895\sigma^2 - 27.17198727\sigma^2 a^{-2} - 86.25465236\sigma^2 a^2$$

To obtain the free parameter a, we optimize var (y_2) where

$$\frac{\partial}{\partial_a}\big(var\ (y_u)\big) = 54.34397454a^{-3} - 172.5093047a = 0$$

a= 0.749177487

Now the variables c_1 and c_2 becomes;

c_1= 1.218594541 and c_2= 1.297613472

Hence from (1) the resulting design is then given by

M_1 = S (0.7491749, 0.7491749, 0.7491749, 0.7491749) + S (1.218594541, 0, 0, 0) + S (1.29761347, 0, 0, 0). (9)

4 Classical Optimality Criteria

The ultimate purpose of any optimality criteria is to measure the largeness of a non- negative definite information matrix, [4]. The implications of the general principles that a reasonable design must meet are well known from the existing literature. We now outline specific criteria which submit themselves to these principles and which enjoy a great popularity in practice. D and T- optimality criteria are some of the most prominent criteria in practice and are given by;

The Determinant criteria, $\emptyset_0(C) = (\det c)\ \frac{1}{s,}$

The trace criterion, T -$\emptyset_1(C) = \frac{1}{s}\ trace\ (c)$ (10)

Whereas is the number of parameters and c is the information matrix.

The information matrix for the second order rotatable design in four dimensions is subdivided into three sub-matrices as given below;

$$\beta_1 = \begin{bmatrix} 1 & \lambda_2 & \lambda_2 & \lambda_2 & \lambda_2 \\ \lambda_2 & 3\lambda_4 & \lambda_4 & \lambda_4 & \lambda_4 \\ \lambda_2 & \lambda_4 & 3\lambda_4 & \lambda_4 & \lambda_4 \\ \lambda_2 & \lambda_4 & \lambda_4 & 3\lambda_4 & \lambda_4 \\ \lambda_2 & \lambda_4 & \lambda_4 & \lambda_4 & 3\lambda_4 \end{bmatrix} = \begin{bmatrix} 10.64 & 0.64 & 0.64 & 0.64 & 0.64 \\ 0.64 & 1.12 & 0.37 & 0.37 & 0.37 \\ 0.64 & 0.37 & 1.12 & 0.37 & 0.37 \\ 0.64 & 0.37 & 0.37 & 1.12 & 0.37 \\ 0.64 & 0.37 & 0.37 & 0.37 & 1.12 \end{bmatrix} \quad (11)$$

$$\beta_2 = \begin{bmatrix} \lambda_2 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_2 & 0 \\ 0 & 0 & 0 & \lambda_2 \end{bmatrix} = \begin{bmatrix} 0.64 & 0 & 0 & 0 \\ 0 & 0.64 & 0 & 0 \\ 0 & 0 & 0.64 & 0 \\ 0 & 0 & 0 & 0.64 \end{bmatrix} \quad (12)$$

$$\beta_{23} = \begin{bmatrix} \lambda_4 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda_4 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_4 \end{bmatrix} = \begin{bmatrix} 0.37 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.37 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.37 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.37 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.37 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.37 \end{bmatrix} \quad (13)$$

4.1 Determinant criterion (D- optimality)

We determine the determinant of the information matrix c_1. For $\lambda_2 = 0.638943104 \; and \; \lambda_4 = 0.374588743$

$$\emptyset_o(C) = (\det c)^{\frac{1}{s}}$$

$$|(m_\varepsilon)| = (|\beta_1||\beta_2||\beta_3|)^{\frac{1}{s}}$$

$$= (0.2496 * 0.1678 * 0.0026)^{\frac{1}{s}}$$

$$= (0.0001074)^{\frac{1}{s}}$$

$$= 0.544252783 \quad (14)$$

4.2 Trace criterion (T- optimality)

We determine the trace of the information matrixc_1. For $\lambda_2 = 0.638943104 \; and \; \lambda_4 = 0.374588743$

$$\emptyset_1(C) = \frac{1}{s}\, trace\ (C)$$

Tr $(\beta) = \frac{1}{s}\ (tr\ (\beta_1) +\ tr\ (\beta_2) +\ tr\ (\beta_3))$ where s is the number of parameters of the design.

$= \frac{1}{s}\ (10.2600)$

$= 0.684$ (15)

5 DT- Optimality

[8] introduced DT-optimality which is a combination of D- optimality and T-optimality. The formulae for DT-optimality were given as;

$$\emptyset_{\mathbf{1}}^{\boldsymbol{DT}}(\boldsymbol{\varepsilon}) =\ (\mathbf{1}-\boldsymbol{k})\ \boldsymbol{log}\,\Delta_1(\boldsymbol{\varepsilon}) +\ \left(\frac{\boldsymbol{k}}{\boldsymbol{p_1}}\right)\boldsymbol{log}|\boldsymbol{m_1}(\boldsymbol{\varepsilon})|. \quad (16)$$

Where $\emptyset_{\mathbf{1}}^{\boldsymbol{DT}}(\boldsymbol{\varepsilon})$is a convex combination of two design criteria, the first criterion is log$\Delta_{\mathbf{1}}(\boldsymbol{\varepsilon})$, the logarithm of that T-optimality and the second $|m_1(\boldsymbol{\varepsilon})|$ is also the logarithm of D-Optimality.

Designs maximizing equation (16) are called DT-optimum and are denoted by $\boldsymbol{\varepsilon}^*_{DT}$.

Whence, $\emptyset_{\mathbf{1}}^{\boldsymbol{DT}}(\boldsymbol{\varepsilon}) = (\mathbf{1}-\boldsymbol{k})\boldsymbol{Log}\mathbf{0.684} +\ \left(\frac{\boldsymbol{k}}{\boldsymbol{p_1}}\right)\ \boldsymbol{log}\mathbf{0.544252783}$

$= (1\text{-}4)\ \log 0.684 + \frac{\mathbf{4}}{\mathbf{15}}\boldsymbol{log}(\mathbf{0.544252783})$

$= 0.494831694 - 0.070453157$

$= 0.424378536$ (17)

6 Concluding Remarks

There are two ways of constructing second order rotatable designs in four or more dimensions. One is by using the formula $n' = 2n + 4$, where $n'$is the number of points in the next dimension whereas n is the number of design points in the current dimension and the other one is by adding a factor to the sets of points of the design to extend it to the next dimension. [10] constructed 20 points specific second order rotatable design in three factors and extended it to 44 points in four factors using the first method. In our case, we extend the same design of 20 points second order rotatable design in three factors to 32 points second order rotatable design in four factors using the second method. We also evaluate the design's D-and T- optimality criteria. The study concludes by combining D- and T-optimality to get DT-(compound optimality). The design under consideration is said to be better than the 44 points optimal second order rotatable design in four factors constructed by [10] since the number of points are economical as compared to the other. The D-, T-, and DT- optimality criteria are compared and the least determines the optimality criteria, whence the 32 points second order rotatable design is DT-optimum. Again the analysis of the two alphabetic criteria and the compound criterion above show that the more the homogenous a design is the more optimal it becomes, this is the result obtained above for the D- criterion the value was 0.544232783, the T- criterion become 0.684 but the combination of the two gave a more homogenous value tending to zero 0.4243785. This clearly brought a balance between parameter estimation and model discrimination.

Competing Interests

Authors have declared that no competing interests exist.

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