Two Combined Alphabetic Optimality Criteria for Second Order Rotatable Designs Constructed Using Balanced Incomplete Block Design in Four Dimensions

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Abstract: The theory of optimal experimental designs is concerned with the construction of designs that are optimum with respect to some statistical criteria. Some of these criteria include the alphabetic optimality criteria such as D-, A-, E-, T-, G- and C- criterion. Compound optimality criteria are those that combine two or more alphabetic optimality criteria. Design that require optimality criteria have specific desired properties that do very well in one design and at the same time perform poorly in another design. Thus, a compound optimality criterion gives a balance to the desirability of any two or more alphabetic optimality criteria. The present paper aims to introduce CD- and DT- criteria which are compound optimality criteria for second order rotatable designs constructed using Balanced Incomplete Block Designs (BIBDs) in four dimensions.

Keywords: Optimality Criteria, Compound Criteria, DT-optimum and CD-optimum

1. Introduction

Design experts 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. In the field of life sciences optimal designs are required in order to cut on cost of experimentation. Kussmaul [15] introduced method that allows for an efficient consideration of nonlinear constraints.

An experimenter is therefore advised to make the choice of a design to be used prior to carrying out any experiment. In statistics, Response Surface Methodology (RSM) explores the relationships between several explanatory variables and one or more response variables. The method was introduced by George E. P. Box and K. B. Wilson [1]. The main idea of RSM is to use a sequence of designed experiments to obtain an optimal response. Box and Wilson [1] suggest using a second-degree polynomial model to do this. They acknowledge that this model is only an approximation, but they use it because such a model is easy to estimate and apply, even when little is known about the process. Statistical approaches such as RSM can be employed to maximize the production of a special substance by optimization of operational factors. In contrast to conventional methods, the interaction among process variables can be determined by statistical techniques [2].

According to Box and Draper [3], RSM is either used to explore response surfaces or to estimate the parameters of a model. Bose and Draper [4] 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 in 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.

The proper meaning of optimal depends on the situation and can include cost effective, minimum variance and minimum bias. Youdim [13] Correctly chosen D-optimum designs provide efficient experimental schemes when the aim of the investigation is to obtain precise estimates of parameters. The commonly used classical optimality criteria
which were introduced and widely discussed by Pukelsheim [5] includes, Determinant criterion (D-), the average variance criterion (A-), the smallest Eigen value (E-) and the trace criterion (T-). Many results on optimal designs of experiments are derived under the assumption that the statistical model is known at the design stage. Nguyen [14] proposed to use a compound optimality criterion based on the pure quadratic, the linear and the interaction effects. Consequently, the moment matrix is also partitioned as factors are four.

The vector in (3) is partitioned in the following order; the quadratic, the linear and the interaction effects. Consequently, the moment matrix is also partitioned as shown below.

\[ M = \begin{bmatrix} B & 0 & 0 \\ 0 & A_1 & 0 \\ 0 & 0 & A_2 \end{bmatrix} \]

where

\[ y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_i x_i^2 + \sum_{i<j}^{k} \beta_{ij} x_i x_j + \epsilon \quad (1) \]

$\beta_0$ is the intercept
$\beta_i$ is the linear coefficient for the $i^{th}$ factor
$\beta_{ii}$ is the quadratic coefficient for the $i^{th}$ factors
$\beta_{ij}$ is the cross product coefficient for the $i^{th}$ and $j^{th}$ factors
$x_i$ is the level of the $i^{th}$ factor
$x_i x_j$ is the level of the $i^{th}$ and $j^{th}$ factor

2. Evaluation of C-Criterion in Four Dimensions

The C-criterion for the second order rotatable design in four dimensions is obtained through minimizing the variance of the linear unbiased estimator of the integral function $w/(X'X)^{-1}w$. This was defined by Elfving [8] as;

\[ C\text{-Criterion} = \int \int \int \int w/(X'X)^{-1}w \\ dx_1 dx_2 ... dx_k. \quad (2) \]

where

\[ B = \begin{bmatrix} 1 & \lambda & \lambda & \cdots & \lambda \\ \lambda & 3\lambda & \lambda & \cdots & \lambda \\ \lambda & \lambda & 3\lambda & \cdots & \lambda \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda & \lambda & \lambda & \cdots & 3\lambda \end{bmatrix} \]

\[ A_1 = \begin{bmatrix} \lambda_2 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_2 \end{bmatrix} \]

\[ A_2 = \begin{bmatrix} \lambda_4 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_4 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_4 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_4 \end{bmatrix} \]

The inverse of (5) is;
\[ M^{-1} = \begin{bmatrix} B^{-1} & 0 & 0 \\ 0 & A_1^{-1} & 0 \\ 0 & 0 & A_2^{-1} \end{bmatrix} \]  \hspace{1cm} (6)

where,

\[ B^{-1} = \frac{1}{\Delta_1} \begin{bmatrix} \alpha & \beta & \beta & \cdots & \beta \\ \beta & \gamma & \mu & \cdots & \mu \\ \beta & \mu & \gamma & \cdots & \mu \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \beta & \mu & \mu & \cdots & \gamma \end{bmatrix} \]  \hspace{1cm} (7)

In which;

\[ \alpha = 2(k+2)^2, \beta = -2\lambda_2^4, \mu = (k+1)\lambda_4 - (k-1)\lambda_2^2 \]

\[ \Delta_1 = 2[(k+2)\lambda_4^2 - k\lambda_2^2 \lambda_4]; \]

\[ A_1^{-1} = \frac{1}{\Delta_2} \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix} \]  \hspace{1cm} (8)

The coefficient matrix \( K' \) is determined from a reduced parameters system, where the reduced pure quadratic and the interaction effect is that;

\[ \beta_i = \left( \begin{array}{c} \beta_0 \\ \sum_{j=1}^{k} \beta_i \\ \sum_{j=1}^{k} \sum_{j \neq i} \beta_{ij} \\ \vdots \\ \sum_{j=1}^{k} \sum_{j \neq i} \sum_{j \neq k \neq i} \beta_{ijk} \end{array} \right) \]  \hspace{1cm} (10)

Where

\[ \beta = \left( \beta_0, \beta_1, \beta_2, \ldots, \beta_k, \beta_{k-1} \right) \]

is the full parameter system and is the coefficient of the second order model

\[ y = \beta_0 + \beta_1 x_1 + \beta_2 x_2^2 + \ldots + \beta_k x_k + \beta_{k-1} x_k x_{k-1} + \ldots + \beta_k x_k x_{k-1} x_{k-2} + \ldots + \beta_k x_k x_{k-1} x_{k-2} \cdots x_1 \]

\[ K' = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 \end{bmatrix} \]  \hspace{1cm} (11)

is generalized coefficient matrix of the parameter system of interest.

The coefficients of \( w^j \) in (3) are the diagonal elements of a \( k \) matrix in the parameter system of interest.

4. Information Matrix

Mwan and Rambaei [9] used the moment matrix for second order model to determine the information matrix for the parameter system of interest. Its information matrix \( C \) is determined by

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

where \( M = \frac{1}{N} x'x \) and \( k \) is the number of factors and \( X \) is as defined in (4)
Using the elements of the inverse of the moment matrix in
(7), (8) and (9) respectively (3) is obtained.
The computation for the C- criterion was portioned into
three parts; the linear effects the pure quadratic and
the interaction effects which were denoted as \( \beta_{ij} \). For the 64 points
the parts are \( \beta_{11}, \beta_{12} \) and \( \beta_{13} \) with the help of matlab software.

5. D – Criterion for 2\textsuperscript{nd} Degree Design
with Sixty Four Points

For \( k = 4 \) factors, the information matrix is given as;
\[
C_4(M) = \begin{bmatrix}
1 & 4\lambda_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
4\lambda_2 & 24\lambda_4 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \lambda_2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \lambda_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \lambda_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \lambda_2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \lambda_4 & 6 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda_4 \\
\end{bmatrix}
\]

Thus the determinant criterion is
\[
\phi_0C_4(M) = \left[ \text{Det}C_4(M) \right]^{1/7} = \left[ 24\lambda_2^4\lambda_4^4 \left( 6\lambda_4 - 4\lambda_2^2 \right) \right]^{1/7}
\]

Now from (13), we have, for the designs with \( k = 4 \), we substitute the following to (14)
\[
\lambda_2 = 0.233258\rho^2 \text{ and } \lambda_4 = 0.06251\rho^4
\]
Thus,
\[
\phi_0C_4(M) = \left[ 24\lambda_2^4\lambda_4^4 \left( 6\lambda_4 - 4\lambda_2^2 \right) \right]^{1/7} = 0.3541807443
\]

6. T – Criterion for 2\textsuperscript{nd} Degree Design
with Sixty Four Points

The trace criterion is given as;
\[
\phi C_4(M) = \frac{1}{7} \text{trace}C_4(M)
\]

Thus,
\[
\phi C_4 = \frac{1}{7} \left[ 1 + 24\lambda_2 + 4\lambda_4 + 6\lambda_4 \right]
\] and by further
simplification we get;

\[
\phi C_4 = \frac{1}{7} \left[ 1 + 4\lambda_2 + 30\lambda_4 \right].
\]

Now from (17), we have, for the designs with \( k = 4 \),
Substituting for these values of \( \lambda_2 \) and \( \lambda_4 \) given in (15)
then;
The Trace criterion is
\[
\phi_1C_4 = 0.54440474286.
\]

7. C–Criterion for 2\textsuperscript{nd} Degree Design
with Sixty Four Points

Substituting \( \lambda_2 \) and \( \lambda_4 \) given in (15) to (7) yields the
information matrix given as;
\[
B^{-1} = \begin{bmatrix}
2.3825 & -1.4817 & -1.4817 & -1.4817 & -1.4817 & -1.4817 \\
-1.4817 & 7.5871 & -0.4116 & -0.4116 & -0.4116 & -0.4116 \\
-1.4817 & -0.4116 & 7.5871 & -0.4116 & -0.4116 & -0.4116 \\
-1.4817 & -0.4116 & -0.4116 & 7.5871 & -0.4116 & -0.4116 \\
-1.4817 & -0.4116 & -0.4116 & -0.4116 & 7.5871 & -0.4116 \\
-1.4817 & -0.4116 & -0.4116 & -0.4116 & -0.4116 & 7.5871 \\
\end{bmatrix}
\]

The vector \( \mathbf{w} \) expanded to include all terms of a second
order rotatable design in four dimensions was given by,
\[
\mathbf{w}^{[4]} = \begin{bmatrix}
\frac{1}{4}x_1^4 & \frac{1}{4}x_1^2x_2^2 & \frac{1}{4}x_1^2x_3^2 & \frac{1}{4}x_1^2x_4^2 & \frac{1}{4}x_2^4 & \frac{1}{4}x_2^2x_3^2 & \frac{1}{4}x_2^2x_4^2 & \frac{1}{4}x_3^4 & \frac{1}{4}x_3^2x_4^2 & \frac{1}{4}x_4^4 \\
\end{bmatrix}
\]

Taking only the pure quadratic terms from (21) then we
have;
\[
\mathbf{w}^{[3]} = \begin{bmatrix}
\frac{1}{4}x_1^2 & \frac{1}{4}x_1x_2^2 & \frac{1}{4}x_1x_3^2 & \frac{1}{4}x_1x_4^2 & \frac{1}{4}x_2^2 & \frac{1}{4}x_2x_3^2 & \frac{1}{4}x_2x_4^2 & \frac{1}{4}x_3^2 & \frac{1}{4}x_3x_4^2 & \frac{1}{4}x_4^2 \\
\end{bmatrix}
\]
Substituting (20) and (22) to integral function in (2) gives;

\[
\iiint_1^1 [2.3825 - 0.3704x_1^2 - 0.3704x_2^2 - 0.3704x_3^2 - 0.3704x_4^2 - 0.3704x_1x_2 + 0.4742 - 0.02573x_1^3 x_2^2 - 0.02573x_1^2 x_2^3 - 0.02573x_1 x_2^3 + 0.4742 x_2^4 - 0.02573x_1 x_2 x_3 + 0.02573 x_2 x_3^2 - 0.3704 x_1 x_3^2 - 0.3704 x_2 x_3^2 - 0.3704 x_3 x_4^2 - 0.02573 x_1 x_4^3 - 0.02573 x_2 x_4^3 - 0.02573 x_3 x_4^3 + 0.4742 x_4^4]d_1 d_2 d_3 d_4
\]

\[\beta_{11} = 3.8586. \quad (23)\]

Again by Substituting \(\lambda_2\) given in (15) to (8) gives

\[A_1^{-1} = \begin{bmatrix} 4.2871 & 0 & 0 & 0 \\ 0 & 4.2871 & 0 & 0 \\ 0 & 0 & 4.2871 & 0 \\ 0 & 0 & 0 & 4.2871 \end{bmatrix}, \quad (24)\]

Taking only the linear terms in (21) the outcome is;

\[w^{[4]} = [x_1, x_2, x_3, x_4] \quad (25)\]

Substituting sub matrix in (24) and the linear terms in (25) to the integral function in (2) gives;

\[
\iiint_1^1 [4.2871 x_1^2 + 2.3825 x_2^2 + 4.2871 x_3^2 + 4.2871 x_4^2] d_1 d_2 d_3 d_4
\]

\[\beta_{12} = 11.4323. \quad (26)\]

Substituting \(\lambda_4\) given in (15) to (9) gives

\[A_4^{-1} = \begin{bmatrix} 15.9974 & 0 & 0 & 0 & 0 \\ 0 & 15.9974 & 0 & 0 & 0 \\ 0 & 0 & 15.9974 & 0 & 0 \\ 0 & 0 & 0 & 15.9974 & 0 \\ 0 & 0 & 0 & 0 & 15.9974 \end{bmatrix} \quad (27)\]

Taking only the interactions terms of vector \(w\) in (21) we have;

\[w^{[3]} = [x_1, x_2, x_3, x_4^2, x_1 x_2, x_1 x_3, x_1 x_4, x_2 x_3, x_2 x_4, x_3 x_4] \quad (28)\]

Substituting (27) and (28) to the integral function in (2) yields;

\[
\iiiint_1^1 [15.9974 x_1^2 x_2^2 + 15.9974 x_1 x_2 x_3^2 + 15.9974 x_1 x_2 x_4^2 + 15.9974 x_2 x_3 x_4^2 + 15.9974 x_1 x_3 x_4^2 + 15.9974 x_1 x_4 x_2^2 + 15.9974 x_2 x_3 x_4^2 + 15.9974 x_2 x_4 x_3^2 + 15.9974 x_3 x_2 x_4^2 + 15.9974 x_3 x_4 x_2^2 + 15.9974 x_4 x_2 x_3^2 + 15.9974 x_4 x_3 x_2^2] d_1 d_2 d_3 d_4 d_5
\]

\[\beta_{13} = 21.33. \quad (29)\]

The C-criterion for a design with 64 points is;

\[\beta_{11} + \beta_{12} + \beta_{13} = 36.62092 \quad (30)\]

### 8. DT-Optimality

This paper combines two alphabetic optimality criteria D- and T- by using the concept that was introduced by Atkinson [10], where DT-optimality criterion is a combination of D-optimality criterion for parameter estimation with the T-optimality criterion for discriminating between models. The DT- criterion provides a specified balance between model discrimination and parameter estimation.

The Generalized Determinant and Trace Criteria are given as;

\[
\phi_D (M) = \frac{1}{k+4} \left[ \lambda_4^{k+2} \lambda_2 - k \lambda_2^2 \right] \quad (31)
\]

\[
\phi_T (M) = \frac{1}{k+3} \left[ 1 + (k+2) k \lambda_4 + k \lambda_2 + \frac{k}{2} \lambda_4 \right] \quad (32)
\]

The DT-criterion is given by the formula;

\[
\phi_{DT} (M) = (1-k) \log \Delta_1 (\epsilon) + \left( \frac{k}{p_1} \log |m_1 (\epsilon)| \right) \quad (33)
\]

where \(\phi_{DT} (M)\) is a convex combination of two design criteria, the first criterion is \(\log \Delta_1 (\epsilon)\) which is the logarithm of T-optimality and the second \(\log |m_1 (\epsilon)|\) is also the logarithm of D-optimality.

Designs maximizing (33) are called DT-optimum. The quantities in (31) and (32) are substituted in (33) to obtain the DT-optimality criterion.

For \(k=4\), the determinant criterion is given in (16) and the trace criterion in (19) substituting it in the compound formula given in (33) results to the DT-compound optimality criteria is;

\[
\phi_{DT} (M) = (1-k) \log \Delta_1 (\epsilon) + \left( \frac{k}{p_1} \log |m_1 (\epsilon)| \right) = (1-k) \log \Delta_1 (\epsilon) + \left( \frac{k}{p_1} \log |m_1 (\epsilon)| \right)
\]

\[\Delta_1 (\epsilon) = \frac{1}{4} \log 0.5440474286 \quad (34)\]

### 9. CD-Criterion for 64 Points in Four Dimension

The CD-optimality that combines C-optimality for a model selection and D-optimality for parameter estimation which was introduced by Atkinson [11], provides a specified balance between model discrimination and parameter estimation too. The criterion to be maximized was;

\[
\phi_{CD} (M) = \left( \frac{k}{p_1} \log |m_1 (\epsilon)| \right) - (1-k) \log w^T M^{-1} (\epsilon) w \quad (35)
\]

where \(\phi_{CD} (M)\) is a convex combination of two design criteria, the first criterion is \(\log |m_1 (\epsilon)|\) which is the logarithm of D-
optimality and the second log $w^TM^{-1}w$ is the logarithm of C- optimality.

The designs maximizing (35) are called CD-optimality. The quantities in (2) and (31) were substituted in (35) to obtain the CD-optimality criterion.

The Determinant criterion was given in (16) and the C criterion in (30) for $k = 4$ using the compound formula stated in (35) gave the CD- compound optimality criterion as;

$$\Phi^{CD}(e) = \frac{4}{7} \log 0.3541807443 + 3 \log 36.62092$$

$$\Phi^{CD}(e) = - 0.257585745 + 4.691187752$$

$$\Phi^{CD}(e) = 4.4336.$$  (36)

10. Conclusion

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 alphabetic optimality design in four factors constructed by Mwan, kosgei and Rambaei [9]. The D-, T- and DT- optimality criteria are compared and there is a clear balance brought by the DT-combination. Again the analysis of the two alphabetic criteria and the compound criterion above show that design experts will prefer characteristics from the D- optimality criteria. However, when the experiment requires the utilization of the two properties the compound optimality serves the deal. This is from the result obtained above for the D- criterion the value was 0.3541807443, the T- criterion become 0.5440474286 but the combination of the two gave a value of 0.5355039691 which is in between the two criteria. Hence, a balance between parameter estimation and model discrimination is achieved. Again, the result obtained above for the D- criterion the value was 0.3541807443, the C- criterion become 36.62092 but the combination of the two gave a more homogenous value tending to zero 4.4336 as compared to single optimality criterion. This clearly brought a balance between parameter estimation and model discrimination.

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