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Calculus Optimum Values Optimality Criteria for Twenty Four Points Specific Second Order Rotatable Design in Three Dimensions

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Abstract: This study uses the existing second order rotatable design to obtain optimum design based on the known classical optimality criteria that is the determinant criterion, the average-variance criterion, the smallest-Eigen value criterion and the trace criterion. These criteria measure the desirability of a design, D-optimum design minimizes the content of the ellipsoidal confidence region for the parameters of the linear model, A-optimum design minimizes the sum (or average) of the variances of the parameter estimates, E-criterion reduces the variance of each individual parameter estimate and T-criterion is one that has not enjoyed much use because of the linearity aspect of T-criterion. This study considers the already existing twenty four points three dimensional specific rotatable design of order two. The information matrices C_1, for this design is obtained from the moment matrix M, for the second order model for three factors using the relation $C=(K^1M^{-1}K)^{-1}$, where $M=1/N(X^1X)$, is the moment matrix, K is the coefficient matrix of the parameter sub system of interest. Our parameter system of interest is that of the linear and pure quadratic factors only. The optimality criteria for the design with the corresponding information matrix C_1, is determined as A-optimal.

Keywords: Rotatable Design, Moment Matrix, Optimality Criteria, Order

1. Introduction

The theory of optimal experimental designs has its origins in a paper [1]. She was among the first to state a criterion and obtain optimal experimental designs for regression problems. For polynomial regression of order $p-1$ in one variable over the design region $X=(-1,1)$, she proposed the criterion

$$\hat{y}(x)=\min\{\max xM^{-1}x\}\ (x_i, i=1,2...n), x_i \in X \quad (1)$$

This criterion was later called the G-optimality and it has assumed considerable importance in the theory and constructions of optimum designs [2]. Using this criterion Smith obtained designs for various values of p. For a polynomial of degree p-1, the allocation of points according to min max criterion in equation (1) could be obtained by finding the zeroes of the derivative of a Legendre polynomial [1, 3]. In the study of efficient design of statistical investigations, Wald [4] proposed the criteria of maximizing the determinant of X^lX as a means of maximizing the local power of the F-ratio for testing a linear hypothesis on the parameters of certain fixed-effects, in the analysis of variance of models. The same criterion was proposed for obtaining weighing designs [5]. This criterion was later called D-optimality and its use was extended to regression models in general by minimizing the trace of $(X^lX)^{-1}$ to obtain regression designs [2, 6]. Study done by De la Garza showed that, for a polynomial of degree p-1there exist a design with p distinct points which has the same X^lX matrix as a design with more than p distinct points [7]. The proof of this theorem was subsequently corrected, and can be found in [8]. Maximizing the minimum eigenvalue of X^lX was suggested as the efficient criterion for experimental designs [9], while the optimal allocation for a polynomial of degree $p-1$ can be done using both the minimum-maximum criterion and the determinant criterion. The two criteria gave the same results, thus hinting at the equivalence theorem [10]. Various other properties of the $X^I X$ matrix were suggested as being an appropriate criterion for a design. An extensive review of D-optimality for weighing problems and for analysis of variance problems was given in the study of D-Optimality for regression models [11]. In the early 1970's the core of the theory was crystallized in the papers by [12, 13] and [14]. In the process of development, two parallel approaches took place, one concerned more with developing methods for tackling applied problems and the other vested with the general mathematical theory. The former is associated with the name Box and the work is reported in papers by [15-19]. The latter is associated with the name Kiefer. Although their aims were different there is considerable overlap in ideas between what might be called Kiefer-type theory and the Box approaches, and this overlap has become more apparent in recent years when there has been more emphasis on developing tools for applying the Kiefer-type theory and the Box approaches, a seminar paper in this context being that which of constructed calculus optimum designs of order two in three dimensions [20, 21]. Draper [22], gave the six second order rotatable design classes in letter pronouncements from which were specified by Mutiso [21], with coded levels into natural levels [23, 24].

2. Particular Criteria

2.1. D –Criterion

The most intensively studied criterion is the D-criterion for which

$$\emptyset o(M) = \begin{cases} log\ det(M), \text{if M is non} - \text{singular} \\ -\infty, \text{otherwise} \end{cases}$$

The determinant criterion $\emptyset \circ (C)$ differs from the determinant det C by taking the 7th root, whence both functions induce the same preordering among information matrices. For comparing different criteria, and for applying the theory of information functions, the version $\emptyset \circ (C) = (\det C)^{1/7}$ is appropriate.

Maximizing the determinant of information matrices is the same as minimizing the determinant of dispersion matrices, because of the formula.

$$(det\ C)^{-1} = det(C^{-1})$$

2.2. A-Criterion

This is the average of the standardized variances of the optimal estimators for the scalar parameter systems $C_1\ddot{\Theta}, \dots, C_5\ddot{\Theta}$ formed from the columns of K. the average variances of optimal criterion $\emptyset_{-1}(C)$ is given by:

$$\emptyset_{-1}(C) = \frac{1}{s}(trace\ C^{-1})^{-1}$$

if C is positive definite.

Maximizing the average-variance criterion among information matrices is the same as minimizing the average of the variance given above.

2.3. E-Criterion

The eigen value criterion $\emptyset$-∞ is one extreme member of the matrix mean family $\emptyset_p$, corresponding to the parameter $p = -\infty$ This criterion involves the evaluation of the smallest eigenvalue. The smallest eigenvalue criterion,

$$\emptyset - \infty(C) = \lambda\_\min(C)$$

It is the same as minimizing the largest eigenvalue of the dispersion matrix,

$$\frac{1}{\emptyset} - \infty\big(C_k(A)\big) = \lambda_{max}\big(C_k(A)\big) = \max Z^1K^1A^{-1}KZ$$

minimizing this expression guards against the worst possible variance among all one-dimensional subsystem $Z^1K^1\beta^1$with a vector Z of norm 1. In terms of variance, it is a minimax approach, in terms of information a maximum minimum approach. This criterion plays a crucial role in the admissibility investigations.

2.4. T-Criterion

The trace-criterion is one of the extreme members of the $\emptyset_{-1}$ family; however, the trace criterion by itself is rather meaningless because of its linearity property which makes it susceptible to interpolation [25]. It is worth noting that the weaknesses of the T-criterion are an exception in the matrix mean family with $\emptyset_p\ p \in \{-\infty; 1\}$. The other matrix means are concave without being linear.

The evaluation of the trace criterion is

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

3. Specific Designs

3.1. The Twenty Four Points Three Dimensional Specific Rotatable Design of Order Two

We consider the design,

$$M_1 = S(f, f, 0) + S(C_1, 0,0) + S(C_2, 0,0)$$

This gives the following set of points

(f, f, 0) (f, 0, f) (0, f, f)

(-f, f, 0) (-f, 0, f) (0, -f, f)

(f, -f, 0) (f, 0, -f) (0,f, -f)

(-f, -f, 0) (-f, 0, -f) (0, -f, -f)

(C_1, 0, 0) (0, 0, C_1) (0, C_1, 0)

(-C_1, 0, 0) (0, 0, -C_1) (0, -C_1, 0)

(C_2, 0, 0) (0, 0, C_2) (0, C_2, 0)

(-C_2, 0, 0) (0, 0, -C_2) (0, -C_2, 0)

The moment conditions that the set of twenty-four points should satisfy to form a rotatable arrangement of order two are:

$$\sum_{u=i}^{24} x_{iu}^2 = 2(C_1^2 + C_2^2 + 4f^2) = 24\lambda_2 \quad (2)$$

$$\sum_{u=i}^{24} x_{iu}^4 = 2(C_1^4 + C_2^4 + 4f^4) = 72\lambda_4 \quad (3)$$

$$\sum_{u=i}^{24} x_{iu}^2 x_{ju}^2 = 4f^4 = 24\lambda_4 \quad (4)$$

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

The excess of $\sum_{u=i}^{24} x_{iu}^4 = 3\sum_{u=i}^{24} x_{iu}^2 x_{ju}^2$ is given by

$$\text{Ex (S(f,f,0)+ S(c}_1\text{,0,0) + S(c}_2\text{,0,0))} = \sum_{u=i}^{24} x_{iu}^4 - 3\sum_{u=i}^{24} x_{iu}^2 x_{ju}^2 = 2c_1^4+2c_2^4+8f^4-12f^4=0$$

Simplifying we get;

$$C_1^4 + C_2^4 - 2f^4 = 0$$

Letting $C_1^2 = xf^2$ and $C_2^2 = yf^2$ we $x^2 + y^2 - 2 = 0$
Implying

$$y = \sqrt{(2 - x^2)}, 0 < x < \sqrt{2}$$

Specifically, when $x = 0.5$
we have,

$$y = 1.3228757$$

Therefore,

$$C_1^2 = 0.5f^2, C_1 = 0.7071067$$

$$C_2^2 = 1.3228757, C_2 = 1.1501633f$$

The points form a second order specific rotatable arrangement in three dimensions in the twenty-four points if the non-singularity condition of rotatability
$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$ is satisfied. From equation (2 – 4) we have, $\lambda_2 = 0.4852396f^2$ and $\lambda_4 = 0.1666666667f^4$ respectively.
Therefore $\frac{\lambda_4}{\lambda_2^2} := \beta_2 = 0.707842267 > \frac{k}{k+2}$

3.2. The Estimation of the Free Parameter in the Twenty Four Points Design

Theorem
The arrangements M_1 form an optimum rotatable designs of order two
Proof

$$\beta_2 = 0.7078418, \beta_{22} = 0.50104, \lambda_4 = 0.485239\sigma f^2,$$

$$\lambda_2^2 = 0.2354574f^4, \lambda_2\beta_2^2 = 0.2431244f^2$$

$$k\lambda_2 = 3 \times 0.4852396f^2 = 1.4557188f^2$$

$$k(k-1)\lambda_4 = 3 \times 2 \times 0.166667f^4 = 1.2f^4$$

$$3k\lambda_4 = 3 \times 3 \times 0.166667f^4 = 1.53f^4$$

Where k is the dimension or the number of factors.

$$\delta = \frac{\lambda_2^4}{2\lambda_4((k+2)\lambda_4 - k\lambda_{2)}^2} = \frac{1}{2\beta_2((k+2)\beta_2 - k},$$

$$\delta = \frac{1}{2\text{x}0.7078418(5\text{x}0.70784183)} = 1.3100162$$

Recalling to N = 24, we shall obtain

$$Var(\hat{y}_u) = 0.054584\sigma^2\left(2 \times 5 \times 0.50104 + \frac{5\text{x}0.7078418-2}{0.2354574f^4}(1.50000\,f^4) - \frac{4\times0.7078418}{0.4852396f^2} \times (1.4557188f^2) - \frac{2\times(0.7078418-1)}{(0.2354574f^4)}(1.000002f^4) - \frac{1.4557188f^2}{0.2354574f^4} - \frac{1.0000002f^4}{0.2431244f^2}\right)$$

$$Var(\hat{y}_u) = 0.054584\sigma^2(5.0104+9.8056547-8.494106+2.4816231-6.1825145f^{-2}-4.1131215f^2$$

$$Var(\hat{y}_u) = 0.054584\,\sigma^2(8.8035762 - 6.1825145f^{-2} - 4.1131215f^2)$$

$$Var(\hat{y}_u) = 0.4805344\sigma^2 - 0.3374663\sigma^2 f^{-2} - 0.02245106\sigma^2 f^2 \tag{5}$$

Hence

$$\frac{d}{df}Var(\hat{y}_u) = 0.6749326\,\sigma^2 f^{-3} - 0.4490212\,\sigma^2 f$$

Equating to zero implies that

$$0.6749326 = 0.4490212 f^4$$

$$f = 1.107256886$$

thus $f = 1.1072569$ makes the design M_1 optimal.

$$M_1 = S(1.1072569, 1.1072569, 0) + S(0.7829487, 0, 0) + S(1.2735263, 0, 0)$$

The information matrix for the design M_1 is given as,

$$\begin{bmatrix} 1 & 0.5949 & 0.5949 & 0.5949 & 0 & 0 & 0 \\ 0.5949 & 0.7516 & 0.2505 & 0.2505 & 0 & 0 & 0 \\ 0.5949 & 0.2505 & 0.7516 & 0.2505 & 0 & 0 & 0 \\ 0.5949 & 0.2505 & 0.2505 & 0.7516 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.5949 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5949 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5949 \end{bmatrix}$$

The X matrix for the design M_1 is given as:

$$\begin{bmatrix} 1 & 1.11 & 1.11 & 0 & 1.23 & 1.23 & 0 \\ 1 & -1.11 & 1.11 & 0 & 1.23 & 1.23 & 0 \\ 1 & 1.11 & -1.11 & 0 & 1.23 & 1.23 & 0 \\ 1 & -1.11 & -1.11 & 0 & 1.23 & 1.23 & 0 \\ 1 & 0.78 & 0 & 0 & 0.61 & 0 & 0 \\ 1 & -0.78 & 0 & 0 & 0.61 & 0 & 0 \\ 1 & 1.27 & 0 & 0 & 1.61 & 0 & 0 \\ 1 & 1.27 & 0 & 0 & 1.61 & 0 & 0 \\ 1 & 1.11 & 0 & 1.11 & 1.23 & 0 & 1.23 \\ 1 & -1.11 & 0 & 1.11 & 1.23 & 0 & 1.23 \\ 1 & 1.11 & 0 & -1.11 & 1.23 & 0 & 1.23 \\ 1 & -1.11 & 0 & -1.11 & 1.23 & 0 & 1.23 \\ 1 & 0 & 0 & 0.78 & 0 & 0 & 0.61 \\ 1 & 0 & 0 & -0.78 & 0 & 0 & 0.61 \\ 1 & 0 & 0 & 1.27 & 0 & 0 & 0.61 \\ 1 & 0 & 0 & -1.27 & 0 & 0 & 0.61 \\ 1 & 0 & 1.11 & 1.11 & 0 & 1.23 & 1.23 \\ 1 & 0 & -1.11 & 1.11 & 0 & 1.23 & 1.23 \\ 1 & 0 & 1.11 & -1.11 & 0 & 1.23 & 1.23 \\ 1 & 0 & -1.11 & -1.11 & 0 & 1.23 & 1.23 \\ 1 & 0 & 0.78 & 0 & 0 & 0.61 & 0 \\ 1 & 0 & -0.78 & 0 & 0 & 0.61 & 0 \\ 1 & 0 & 1.27 & 0 & 0 & 1.61 & 0 \\ 1 & 0 & -1.27 & 0 & 0 & 1.61 & 0 \end{bmatrix}$$

A-Criterion $= 0.005366$, D-Criterion $= 0.398647$, E-Criterion $= 0.072085$, T-Criterion $= 0.565103$

A practical hypothetical example

We shall discuss the hypothetical production of Katumani hybrid maize to illustrate the use of the specific optimum second order rotatable design of twenty four points

$$D = \left\{\tfrac{1}{2}G(1.1072569, 1.1072569, 0) + \tfrac{1}{4}G(0.7829487, 0, 0) + \tfrac{1}{4}G(1.2735263, 0, 0)\right\}$$

Suppose the initial three factors are Potassium (ψ_{1u}), sodium (ψ_{2u}), and calcium (ψ_{3u}) as a result of soil mapping investigations which indicated deficiencies of these mineral elements in the Kibwezi loam soils. We wish to point out that the original letters f, c_1 and c_2 represent the variation in quantity application of a factor due to soil fertility gradient culminating in several radii manifestations of rotatability criterion. The criterion can revert the mineral elements to its natural levels denoted by ψ_{iu} [15]. Scaling condition fixes a particular design when $\lambda_2 = 1$ [26]. Whence

$$\chi_{iu} = \frac{\psi_{iu} - \psi_{i*}}{S_i}$$

$$\psi_{i*} = \frac{1}{N}\sum_{u=1}^{N}\psi_{iu}$$

$$S_i = \left[\frac{1}{N}\sum_{u=1}^{N}(\psi_{iu} - \psi_{i*})^2\right]^{0.5}$$

$$\psi_{iu} = \chi_{iu}S_{i*} + \psi_{i*}$$

For $\sum_{u=1}^{N}\chi_{iu}^2 = N$ and $\sum_{u=1}^{N}\chi_{iu} = 0$, the design matrix can then be constituted but the evaluation of the inverse will be a major computational project to estimate the coefficients of the second order rotatable design model which give the optimum response or yield. This requires a separate discourse but the actual response or yields can be obtained if a field experiment is conducted as explained. Let the scale parameter, S_i, assume $S_1 = 0.5, S_2 = 0.3$ and $S_3 = 1$. Suppose that

Potassium (K): $\psi_{1*} = 20$ milligrams

Sodium (Na): $\psi_{2*} = 15$ milligrams

Calcium (Ca): $\psi_{3*} = 30$ milligrams

Are the hoe hole average quantities of the levels of the mineral elements recommended by the soil mapping team. For D we have the following coded and natural levels respectively as treatments:

$(\chi_{1u}, \chi_{2u}, \chi_{3u}); (\psi_{1u}, \psi_{2u}, \psi_{3u})$

(1.1072569, 1.1072569, 0); (20.553628, 15.332177, 30)

(-1.1072569, 1.1072569, 0);(19.446372, 15.332177, 30)

(1.1072569, -1.1072569, 0);(20.553628, 14.667823, 30)

(-1.1072569, -1.1072569, 0);(19.446372, 14.667823, 30)

(1.1072569, 0, 1.1072569);(20.553628, 15, 31.107257)

(-1.1072569, 0, 1.1072569);(19.446372, 15, 31.1072569)

(1.1072569, 0, -1.1072569);(20.553628, 15, 28.892743)

(-1.1072569, 0, -1.1072569);(19.446372, 15, 28.892743)

(0, 1.1072569, 1.1072569); (20, 15.332177, 31.1072569)

(0, -1.1072569, 1.1072569); (20, 15.332177, 31.1072569)

(0, 1.1072569, -1.1072569); (20, 15.332177, 28.892743)

(0, -1.1072569, -1.1072569); (20, 14.667823, 28.892743)

(0.7829487, 0, 0); (20.391474, 15, 30)

(-0.7829487, 0, 0); (19.608526, 15, 30)

(0, 0, 0.7829487); (20, 15, 30.782949)

(0, 0, -0.7829487); (20, 15, 29.217051)

(0, 0.7829487, 0); (20, 15.234885, 30)

(0, -0.7829487, 0); (20, 14.765115, 30)

(1.2735263, 0, 0); (20.636763, 15, 30)

(-1.2735263, 0, 0); (19.363237, 15, 30)

(0, 0, 1.2735263); (20, 15, 31.273526)

(0, 0, -1.2735263); (20, 15, 28.726474)

(0, 1.2735263, 0); (20, 15.382058, 30)

(0, -1.2735263, 0); (20, 14.617942, 30)

to estimate the coefficients

$\beta_0, \beta_1, \beta_2, \beta_3, \beta_{11}, \beta_{22}, \beta_{33}, \beta_{12}, \beta_{13}$ and β_{23}.

In the expected second order rotatable design model in three dimensions

$$y_u = \beta_0 x_{0u} + \beta_1 x_{1u} + \beta_2 x_{2u} + \beta_3 x_{3u} + \beta_{11} x_{1u}^2 + \beta_{22} x_{2u}^2 + \beta_{33} x_{3u}^2 + \beta_{12} x_{1u} x_{2u} + \beta_{13} x_{1u} x_{3u} + \beta_{23} x_{2u} x_{3u} + \varepsilon_u$$

We require field observations of the yield $y_u, u = 1,2,\ldots,24$ as alluded to earlier.

4. Conclusion

Because of flexibility, easy estimation of the parameters (the β's) and practicability of solving real response surface problems, the second-order model is widely used in response surface methodology. The criteria discussed and determined for the six specific designs are all functions of the information matrix. The information matrix for the second order model with the linear and the pure quadratic factors only are determined for the respective designs considered. Estimation of the design moments λ_2 and λ_4 is done using calculus optimum values.

In this study, the matrix means for the six specific second order rotatable designs in three dimensions were obtained using the methods of evaluating the optimality criteria presented in [24]. It is noticed that, the design M_1 is A-optimal, and does not actually comply with the usual notion that the most often used criterion is D-optimality.

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