



Optimal Sequential Third Order Rotatable Designs in Three, Four and Five Dimensions

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Abstract: Response surface methodology (RSM) is a statistical technique used to evaluate the relationship between multiple input variables and one or more response variables with the aim of optimizing the response variables. Sequential experiments are very economical and useful in practice. Therefore, rotatable designs such as the third order rotatable design (TORD) may be run sequentially in three stages with three or four blocks depending on the model adequacy. Normally, the first section 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 the evidence of the goodness of fit, the experiment may be stopped at this stage. However, if the first model is found to be unfit, the trials of the second order are run and ultimately, proceed to fit a third order if a second order model is also found to be inadequate. In this paper, two sets of second order rotatable designs are combined to form sequential third order rotatable designs (TORD) in three, four and five dimensions. The TORDs are then evaluated on their alphabetic optimality criteria with the aim of reducing the costs of experimentation. The classical optimality criteria includes; D-criterion, A-criterion, T-criterion and E-criterion.

Keywords: Response Surface Methodology, Third Order Rotatable Designs, Optimality Criteria

1. Introduction

The concept of rotatability as a desirable quality of an experimental design was first discussed by [1]. In this property, the variances of estimates of the response are constant on circles, spheres or hyperspheres about the Centre of the design. Thus a rotatable design which satisfies this property could be rotated through any angle around its center and the variances of the responses estimated from it could be unchanged [1]. The moment conditions and the non-singularity conditions for third order rotatability was developed by [8]. The TORDs can be grouped into sequential and non-sequential designs [13]. Sequential designs are performed in parts or blocks while in non-sequential experimentation, all the runs must run at one time to make a rotatable least square fitting possible [7]. Sequential experiments are more economical and useful in practice. Therefore, TORDs may be run sequentially in three stages with three or four blocks depending on the model adequacy [7]. Normally, the first section 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 the evidence of the goodness of fit, the experiment may be terminated at this stage [12, 14 & 15]. However, if the first model is found to be inadequate, the trials of the second order are run and ultimately, proceed to fit a third order if a second order model is also found to be inadequate [15]. According to Draper [7], third order rotatable designs can be constructed by combining the existing second order rotatable designs in three dimensions. Third order rotatable designs in three, four and five dimensions can be obtained by combining pairs of second order rotatable designs in three, four and five dimensions [2-6].

In design of experiments, a class of experimental designs that are optimal with respect to some statistical criterion constitutes an optimal design. Optimal experiments are known to 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 [10]. It has been recognized in recent years that even in response surface designs, the main interest of the experimenter may not always be in response at individual locations. Sometimes, the differences between responses at various locations may be of greater interest [9]. Optimality criteria for second order rotatable designs in three dimensions was obtained by [11].

2. Methods

2.1. Moment Conditions and Non-singularity Conditions for Third Order Rotatability

The following moment conditions must be satisfied for a set of points to form a third order rotatable design.

$$\sum_{u=1}^N x_{iu}^2 = N\lambda_2, i = 1, 2, \dots, k \quad (1)$$

$$\sum_{u=1}^N x_{iu}^4 = 3 \sum_{u=1}^N x_{iu}^2 x_{ju}^2 = 3N\lambda_4 \quad i \neq j = 1, 2, \dots, k \quad (2)$$

$$\sum_{u=1}^N x_{iu}^6 = 5 \sum_{u=1}^N x_{iu}^4 x_{ju}^2 = 15 \sum_{u=1}^N x_{iu}^2 x_{ju}^2 x_{lu}^2 = 15\lambda_6 \quad i \neq j \neq l = 1, 2, \dots, k \quad (3)$$

The non-singularity conditions are given as;

$$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2} \text{ For } k = 3, 4, 5 \quad (4)$$

$$\frac{\lambda_2 \lambda_6}{\lambda_4^2} > \frac{k+2}{k+4} \text{ For } k = 3, 4, 5 \quad (5)$$

2.2. Construction of Sequential Rotatable Designs in Three, Four and Five Dimensions

The sequential third order rotatable designs are obtained by either combining two second order specific rotatable designs or adding sets of points to an existing second order rotatable design.

Let,

$$s_1 = S(f, f, 0), \quad (6)$$

$$s_2 = s(a, a, a) + s(c_1, 0, 0) + s(c_2, 0, 0), \quad (7)$$

$$s_3 = s(f, f, 0) + s(a, a, a) + s(c, 0, 0), \quad (8)$$

$$s_4 = s(f, f, 0, 0), \quad (9)$$

$$s_5 = s(a, a, a, a) + s(c_1, 0, 0, 0) + s(c_2, 0, 0, 0), \quad (10)$$

$$s_6 = s(f, f, 0, 0) + s(a, a, a, a) + s(c, 0, 0, 0), \quad (11)$$

$$s_7 = s(a, a, a, a, a) + s(c_1, 0, 0, 0, 0) + s(c_2, 0, 0, 0, 0), \quad (12)$$

$$s_8 = s(f, f, 0, 0, 0) + s(a, a, a, a, a) + s(c, 0, 0, 0, 0). \quad (13)$$

In this case, s_2 and s_3 in (7) and (8) above represent the existing second order rotatable designs of twenty and twenty six points respectively.

The thirty two points third order rotatable design in three

dimensions is obtained by adding a set of twelve points given by s_1 in (6) to a second order rotatable design of twenty points given by s_2 in (7) to give;

$$D_1 = s(a, a, a) + s(c_1, 0, 0) + s(c_2, 0, 0) + s(f, f, 0) \quad (14)$$

The sets s_2 and s_3 in (7) and (8) respectively are combined to give forty six points third order rotatable designs in three dimensions given by;

$$D_2 = s(a, a, a) + s(c_1, 0, 0) + s(c_2, 0, 0) + s(f, f, 0) + s(a, a, a) + s(c, 0, 0) \quad (15)$$

The sets s_4 and s_5 in (9) and (10) respectively which represent two existing second order rotatable designs in four dimensions are combined to give fifty six points third order rotatable designs in four dimensions given by;

$$D_3 = s(a, a, a, a) + s(c_1, 0, 0, 0) + s(c_2, 0, 0, 0) + s(f, f, 0, 0) \quad (16)$$

Similarly, The sets s_5 and s_6 in (10) and (11) respectively are combined to form eighty points third order rotatable designs in three dimensions given by;

$$D_4 = s(a, a, a, a) + s(c_1, 0, 0, 0) + s(c_2, 0, 0, 0) + s(f, f, 0, 0) + s(a, a, a, a) + s(c, 0, 0, 0) \quad (17)$$

Finally, the sets s_7 and s_8 in (12) and (13) which represent two existing second order rotatable designs in five factors are

combined to give hundred and thirty four points third order rotatable design in five dimensions given by;

$$D_4 = s(a, a, a, a, a) + s(c_1, 0, 0, 0, 0) + s(c_2, 0, 0, 0, 0) + s(f, f, 0, 0, 0) + s(a, a, a, a, a) + s(c, 0, 0, 0, 0) \quad (18)$$

These sets of points form third order rotatable designs since the moment conditions in (1), (2), (3) and the non-singularity conditions in (4) and (5) are satisfied as shown in [14].

2.3. Optimality Criteria for Third Order Rotatable Designs

The moment matrices of sequential third order rotatable designs in three, four and five dimensions are utilized in obtaining the optimality criteria. The; D -, A -, E -, & T - optimality criteria are considered. The D - criterion is obtained by finding the determinant of the moment matrix,

the A - criterion is obtained by finding the trace of the inverse of the moment matrix, and the E - criterion is obtained by finding the smallest Eigen value of the moment matrix.

2.3.1. D - Optimality

This is the most studied criterion. It seeks to minimize $|(X'/X)^{-1}|$, or equivalently maximize the determinant of the information matrix X'/X of the design [11]. For comparing different criteria and for applying the theory of information functions, the D - criterion can be given by;

$$D - \text{Criterion} = |M|^{\frac{1}{s}} \quad (19)$$

Where

$$|M| = |M_1| |M_2| |M_3| |M_4| \quad (20)$$

For third order rotatability,

$$|M_1| = [(K+2)\lambda_4 - K\lambda_2^2] (2\lambda_4)^{K-1} \quad (21)$$

$$|M_2| = [3\lambda_2(2\lambda_6)^K [(k+4)\lambda_2\lambda_6 - (K+2)\lambda_4^2]]^K \quad (22)$$

$$|M_3| = (\lambda_4)^{\binom{K}{2}}, \quad (23)$$

And

$$|M_4| = (\lambda_6)^{\binom{K}{3}} \quad (24)$$

Substituting (21), (22), (23) and (24) to 20 gives;

$$|M| = \cap \lambda_2^K \lambda_6^{(K^2+K)} \lambda_4^{(2K-1)} [(k+4)\lambda_2\lambda_6 - (k+2)\lambda_4^2]^k [(k+2)\lambda_4 - K\lambda_2^2] \quad (25)$$

$$\text{For } \cap = 2^{k^2+k-1} \times 3^k \quad (26)$$

2.3.2. A -optimality Criterion for Third Rotatability

The A -criterion is also called average variance criterion. It is used to minimize the average variance of the parameter estimates. The A -criterion for TORD can be given by;

$$A\text{-criterion} = \left[\frac{1}{s} \text{tr}(M^{-1}) \right]^{-1} \quad (27)$$

Where

$$\text{tr}(M^{-1}) = \text{tr}(M_1^{-1}) + \text{tr}(M_2^{-1}) + \text{tr}(M_3^{-1}) + \text{tr}(M_4^{-1}) \quad (28)$$

For,

$$\text{tr}(M_1^{-1}) = \frac{2(K+2)\lambda_4^2 + K(K+1)\lambda_4 - K(K-1)\lambda_2^2}{2\lambda_4[(K+2)\lambda_4 - K\lambda_2^2]} \quad (29)$$

$$\text{tr}(M_2^{-1}) = \frac{6(K+4)\lambda_6^2 + K(3K^2+7K-8)\lambda_2\lambda_6 - K(K-2)(2K+10)\lambda_4^2}{6\lambda_6[(K+4)\lambda_2\lambda_6 - (K+2)\lambda_4^2]} \quad (30)$$

$$\text{tr}(M_3^{-1}) = \frac{K(K-1)}{2\lambda_4} \quad (31)$$

$$\text{tr}(M_4^{-1}) = \frac{K(K-1)(K-2)}{6\lambda_6} \quad (32)$$

2.3.3. T-optimality Criteria for Third Order Rotatability

T-optimality is also known as trace criterion. By itself, the trace criterion is rather meaningless because of its linearity aspect which makes it exposed to interpolation. the weakness of the T-criterion is an exception in the matrix mean family

ϕ_p , with the $p \in [-\infty, 1]$ and the other matrix means are concave without being linear.

Mathematically, the definition of T-criterion can be given by;

$$T - \text{Criterion} (M) = \frac{1}{s} \text{tr}(M) \quad (33)$$

Where M in 4.15 is equivalent to

$$\text{tr}(M_1) + \text{tr}(M_2) + \text{tr}(M_3) + \text{tr}(M_4) \quad (34)$$

The traces of the sub-matrices which form $\text{tr}(M)$ in (35) are given by;

$$\text{tr}(M_1) = 1 + K(3\lambda_4) \quad (35)$$

$$\text{tr}(M_2) = K(\lambda_2 + 15\lambda_6 + 3\lambda_6(K - 1)) \quad (36)$$

$$\text{tr}(M_3) = \lambda_4 \begin{bmatrix} K \\ 2 \end{bmatrix} \quad (37)$$

$$\text{tr}(M_4) = \lambda_6 \begin{bmatrix} K \\ 3 \end{bmatrix} \quad (38)$$

2.3.4. E-Optimality Criterion for Third Order Rotatability

E- Optimality is also known as Eigen value criterion. The procedure for using the Eigenvalue criterion is that each component should explain at least one variables worth of the

variability. Therefore, the eigenvalue criterion states that only components with eigenvalues greater than one should be retained. For a TORD, the Eigen values of the determinant of the information matrix is given by;

$$|M^*| = |M_1^*||M_2^*||M_3^*||M_4^*| \quad (39)$$

Where,

$$|M_1^*| = (1 - \alpha)^2 [(K + 2)\lambda_4 - K\lambda_2^2 - \alpha][2\lambda_4 - \alpha]^{K-1}, \quad (40)$$

$$|M_2^*| = (\lambda_2 - \alpha(6\lambda_6 - \alpha)(2\lambda_6 - \alpha)^{K-2}(2\lambda_6[(K + 4)\lambda_6(\lambda_2 - \alpha) - (K + 2)\lambda_4^2 - \alpha(\lambda_2 - \alpha)])^K, |M_3^*| = (\lambda_4 - \alpha)^{\begin{bmatrix} K \\ 2 \end{bmatrix}}, \quad (41)$$

And

$$|M_4^*| = (\lambda_4 - \alpha)^{\begin{bmatrix} K \\ 3 \end{bmatrix}}. \quad (42)$$

Substituting 4.22, 4.23, 4.24 and 4.25 to 4.21, and equating the result to zero, we obtain the characteristic polynomial as,

$$\phi_{-\infty}(M) = \alpha^2 - [(K + 4\lambda_6 + \lambda_2)]\alpha + [(K + 4)\lambda_2\lambda_6 - (K + 2)\lambda_4^2] = 0 \quad (43)$$

The quadratic equation in (44) is solved and the smallest value of α is taken as the smallest Eigen value of the moment matrix which is the E-criterion.

3. Results and Discussions

The results for evaluation of the optimality for the designs under investigation are summarized in the table below.

Table 1. A Summary of the particular optimality criteria for the five designs.

| Designs | Number of points | Number of factors | D-criterion | A-criterion | E-criterion | T-criterion |
|---------|------------------|-------------------|-------------|-------------|-------------|-------------|
| D_1 | 32 | 3 | 0.33440772 | 0.00024640 | 0.045364831 | 1.087552604 |
| D_2 | 46 | 3 | 0.52794634 | 0.00051466 | 0.032326560 | 1.458000000 |
| D_3 | 56 | 4 | 0.45315748 | 0.00012838 | 0.013265214 | 1.064750337 |
| D_4 | 80 | 4 | 0.57495106 | 0.00009299 | 0.007160400 | 1.443935885 |
| D_5 | 134 | 5 | 0.74132797 | 0.00006425 | 0.025359870 | 1.520279261 |

From table 1 above, D_1 and D_2 represents the third order rotatable designs whereas D_3 and D_4 represents the sequential

third order rotatable designs in four dimensions. D_5 represents a sequential third order rotatable design in five dimensions. All

the designs considered in this paper were A-optimal. In a similar study by [15], all their designs were found to be E-Optimal. This implies that the TORs are uniquely optimal. On determinant criterion, the thirty two points third order rotatable design in three dimensions with 0.33 was more optimal compared to the forty six points third order rotatable design in three dimensions with 0.53. Similarly, the fifty six points third order rotatable design in four dimensions with 0.45 was found to be better than the eighty points third order rotatable designs in four dimensions with 0.57. The same trend was observed on the other optimality criteria. It is important to note that for a given number of factors, the design with a relatively lower number of points was more optimal than its counterpart of more points as confirmed in [15].

4. Conclusion

Each of the A-, D-, E-, and T- optimality criteria demands a specific statistical property of the best linear unbiased estimator and it amounts to the minimization of a particular convex function of the information matrix. Taking the smallest value among the matrix means does the identification of the optimality criteria. There is a clear indication that the more homogenous the design is, the larger the information matrix as evidenced by the values of the information functions.

D-optimum designs minimize the content of the ellipsoidal confidence region for the parameters of the linear model. Eigen values minimizes the generalized variance of the parameter estimates. A – Optimality minimizes the sum or average of the variance of parameter estimates, Atkinson and Donev (1992). The eigenvalues of the inverse of the information matrix are proportional to the squares of lengths of the axes of the confidence ellipsoid. Thus the variance of each individual parameter estimate may be reduced to insignificant size when we take the smallest value. E-Optimum designs reduces the variance of each individual parameter estimate. However, the T-optimality criterion has not enjoyed much use because of its linearity aspect.

5. Recommendations

We recommend that the third order rotatable design be evaluated on their robustness against missing data.

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