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OBTAINING DESIGNS TO SATISFY THE MOMENT AND NON-SINGULARITY CONDITIONS FOR ROTATABILITY

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ABSTRACT
In this study, the aim was to obtain designs to satisfy the moment and non-singularity conditions for rotatability. Rotatability is a property that requires that the variance of estimates of responses at points equidistant from the centre of the design is constant on circles or spheres or hyper-spheres. The study of rotatable designs mainly emphasises the estimation of the absolute response. Using a balanced incomplete block design in three, four, five, six, and k-factors where each factor will contain two treatments, factorial combinations were obtained. An incidence matrix of Balanced Incomplete Block Design is suitably chosen and must satisfy the necessary Balanced Incomplete Block Design conditions. It should also satisfy the non-singularity conditions for a second-order design to be rotatable. A set of points $s(a,a,a)$ was also suitably chosen and used to denote the symmetric point sets associated with an appropriate, balanced incomplete design. In conclusion, some new second-order rotatable designs in three, four, five and six factors and their generalisation in K factors was obtained through balanced incomplete block designs.

KEYWORDS: Rotatability, Non-singularity, Designs

INTRODUCTION
Response surface methodology (RSM) is a collection of statistical and mathematical techniques useful for developing, improving and optimising processes. The goal of most response surface research is to find a suitable approximating function for the purpose of predicting future response and to find levels of the input variables for which in some sense the response is optimised. The aim is actually to determine optimum operating conditions or to define a region in the space of the input variables where certain operating specifications are met.

A rotatable design is a series of response surface designs with the property that the variance of estimates of response at points equidistant from the centre of the design is constant. These designs ensure equal precision on the response estimates. The study of rotatable designs mainly emphasised on the estimation of absolute response.

Rotatability of designs has been studied by a number of researchers, Box and Hunter (1957) introduced rotatable designs for the exploration of response surfaces. He emphasised the estimation of absolute response, Victorbabu and Vasundharadevi (2009) studied on the efficiencies of second-order response surface designs for the estimation of response and slopes using symmetrical unequal block arrangement two unequal block sizes, VictorBabu (2006) constructed rotatable design using a pair of incomplete block design, Huda (1987) constructed third-order rotatable design from design of lower dimension. Some new third-order rotatable design in five dimensions through balanced incomplete block (BIB) designs has also been suggested by Koske, Mutiso and Kosgei (2011). In this study, some new second-order rotatable designs are obtained through a balanced incomplete block (BIB) designs. The method of construction will share some features proposed by Koske et al. (2011). Here the experimenter will start with three factors then four, five and six factors and later give a generalisation using k factors.

Balanced incomplete block (BIB) designs
According to Victorbabu (2006) and Victorbabu and Surekha (2011), a balanced incomplete block (BIB) design denoted by (v, b, r, s, λ) is an arrangement of v-treatments in b-blocks each containing s(< v) treatments and satisfying the following conditions.

a) Every treatment occurs at most once in a block
b) Every treatment occurs in exactly r-blocks
c) Every pair of treatments occurs together in λ blocks

The quantities v, b, r, s and λ are called the parameters of a BIB design
The basic conditions for the existence of a BIB design are;-

(i) $rv = sb$
(ii) $(r-1) = r(s-1)$
(iii) $r > \lambda$
(iv) $b \geq v$

Second-Order Rotatable Designs

Suppose we want to use a second response surface $D = x_{iu}$ to fit the surface

$$Y_u = b_o + \sum_{i=1}^{v} b_i x_{iu} + \sum_{i=1}^{v} b_{ii} x_{iu}{}^2 + \sum_{i \prec j} \sum b_{ij} x_{iu} x_{ju} + \ell_u$$

Where x_{iu} denotes the level of the i^{th} factor ($i = 1,2,......v$ in the u^{th} run ($u = 1,2,......N$ of the experiment e_u s are uncorrelated random errors with mean zeros and variance σ^2

b_0, b_i, b_{ii}, b_{ij} are the parameters of the model and y_u is the response observed at the u^{th} design point.

Then the surface is said to be a second-order rotatable arrangement if it satisfies the following two moment conditions.

(i) $$\sum_{u=1}^{N} x_{iu}{}^2 = N\lambda_2 = A$$

(ii) $$\sum_{u=1}^{N} x_{iu}{}^4 = 3\sum_{u=1}^{N} x_{iu}{}^2 x_{ju}{}^2 = 3N\lambda_4 = 3B$$

Where λ_2 and λ_4 are constants, $A = \frac{N}{K}$ $B = \frac{N}{K(K+2)}$

A necessary condition for the existence of a non-singular second-order design is

$$\frac{\lambda_4}{\lambda_2{}^2} > \frac{K}{K+2} \text{ i.e } \frac{NB}{A^2} > \frac{K}{K+2}$$

LITERATURE REVIEW

Response surface methodology (RSM) is a statistical technique very useful in the design and analysis of experiments. It involves a dependent variable y_u such as yield and is called the response variable.

In general $y_u = f(x_{1u}, x_{2u}, ...x_{ku}) + e_u$, where $u = 1,2,\cdots\cdots.N$ represents the N-observations and x_{iu} is the level of the i^{th} factor in the u^{th} observation and y_u is the response, e_u is the random error with mean zero and variance σ^2. Response surface method is useful where several independent variables influence a dependent variable.

The concept of rotatability, which is very important in response to surface second-order designs, was proposed by Box and Hunter (1957). The study emphasises on the estimation of absolute response. The k-dimensional point set forms a second-order rotatable arrangement in k- factors if the following conditions hold

$$\sum_{u=1}^{N} x_{iu}^{2} = A \qquad i = (1,2 \cdots\cdots k\ )$$

$$\sum_{u=1}^{N} x_{iu}^{4} = 3\sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2} = 3B \qquad (1)$$

and all other sums of powers and products up to order four are zero i.e. $\sum_{u=1}^{N}\prod_{i=1}^{v} x_{iu}\alpha_u = 0$

if any α is odd for $\sum \alpha_i \leq 4$ and $A = N\lambda_2$, $B = N\lambda_4$

This arrangement of the points forms a non-singular second order rotatable designs if it satisfies the necessary condition of a second-order rotatable non-singular design, i.e. $\frac{NB}{A} \succ \frac{k}{k+2}$ which is the condition required for a second-order arrangement of points to form a second-order rotatable design, where also

$$A = \frac{N}{K} \text{ and } B = \frac{N}{K(K+2)} \qquad (2)$$

According to Victorbabu and Vasundharaderi (2009), a design for fitting a response surface consists of a number of suitable combinations of levels of several input factors. He considered v factors and N combinations in the design, each having a constant number of levels. A response surface design can be written as v - rows and N columns each. Each row being a combination of v - levels codes on from each of v - ordered factors. This combination of level codes he called a design point, and the combination with 0- code for each factor is called a central point. They were considering the efficiencies of various second-order response surface designs. Victorbabu (2005) studied modified slope rotatable central composite designs (SRCCD). Victorbabu (2006) studied second order rotatable designs using a pair of incomplete block designs. He considered a second order rotatable design by taking combinations with unknown constants and associated 2^k factorial combinations or a suitable fraction of it with factors each at ± 1 levels to make the level codes equidistant to form a design. Victorbabu and Narasimham (1991) constructed second-order slope rotatable designs (SOSRD) using a balanced incomplete block design. Victorbabu (2009) also reviewed the modified SOSRDs. He also presented different methods of construction of modified SOSRDs using central composite designs, Balanced incomplete block design, and pairwise balanced designs symmetrical unequal block arrangement with two unequal block sizes. Victorbabu and Surekha (2011) constructed a SOSRD using a balanced incomplete block design. The study of rotatable designs is mainly emphasised on the estimation of differences of yields and its precision. Estimation of differences in responses at two different points in the factor space is of great importance. Park (1987) studied the estimations of local slope (rate of change) of the response. He gave an example of the rate of change in the yield of the crop to various fertilizer doses. Das and Narasimham (1962) constructed many third-order rotatable designs by taking appropriate combinations of the symmetric point set or their suitably balanced subset obtained through balanced incomplete block designs and fractional replications. Huda (1987) constructed third-order rotatable designs in k-dimensions from those in lower dimensions. Koske et al. (2011) constructed a third-order rotatable design five-dimensions from a third-order rotatable design in lower dimensions through balanced incomplete block designs (BIBDs). Das et al. (1999) studied response surface design, symmetrical and asymmetrical rotatable and modified. Victorbabu (2011) explored a new method of construction of second order-slope-rotatable design using incomplete block designs with unequal block sizes. Victorbabu and Rajyalakshmi (2012) studied a new method of construction of robust second order rotatable designs using balanced incomplete block designs. Furthermore, Mutai, Koske and Mutiso (2012) constructed some new four-dimensional third-order rotatable design through balanced incomplete design.

The method used by Huda (1987) and Koske, et al. (2011),(2012) can be used to obtain a generalised method of constructing designs.

METHODOLOGY

To construct a second-order rotatable design, a combination with unknown constants is taken and associated with 2^k factorial combinations of factors each at ± 1 levels to make level codes equidistant. All such combinations form a design. An incidences matrix of BIB is chosen suitable to satisfy the moment of rotatability i.e.

(i) $\sum_{u=1}^{N} x_{iu}^{2} = N\lambda_2 = A$ and

(ii) $\sum_{u=1}^{N} x_{iu}^{4} = 3\sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2} = 3N\lambda_4 = 3B$

Where all other sums of odd powers and cross products up to order four are zeros i.e.

$\sum_{u=1}^{N}\prod_{i=1}^{v} x_{iu}\alpha_i = 0$ if any α_i is odd for $\sum \alpha_i \leq 4$

These arrangements of points are said to form a rotatable design of second-order only if it forms a non-singular second-order design. These points should give rise to a non-singular $X'X$ matrix.

Moment and Non- singularity conditions

A review of the moment and non-singularity conditions is done where a given set of points is said to be second-order rotatable arrangement if it satisfies the moment conditions $\sum_{u=1}^{N} x_{iu}^{2} = N\lambda_2 = A$ and

$\sum_{u=1}^{N} x_{iu}^{4} = 3\sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2} = 3N\lambda_4 = 3B$

The second-order rotatable arrangement becomes a second-order rotatable design where the arrangement of points also satisfy the non-singularity condition $\frac{\lambda_4}{\lambda_2^{2}} \geq \frac{K}{K+2}$

A matrix X of order $(N \times K)$ is considered

$$X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix}$$

Where X' is the transpose of X $N^{-1}(X'X)$ and is the moment matrix of the arrangement of N points in $K-$ dimensional factor space. The determinant of M is obtained, and this gives the non-singularity conditions for a second-order experimental design to be rotatable. Box and Hunter (1957) give the necessary non-singularity condition as $\frac{\lambda_4}{\lambda_2^{2}} > \frac{K}{K+2}$ and the arrangement forms a non-singular second order rotatable design. The strict inequality is achieved by the addition of centre points.

RESULTS AND ANALYSIS

Non-singularity conditions

These are the conditions that must be satisfied in order for a second-order experimental design to be rotatable. From the moment matrix of second-order its polynomial determinant is determined and this will give the non-singularity conditions. The response surface approximated is a second-order polynomial and is given by;

$$y_u = b_0 + \sum_{i=1}^{v} b_i x_{iu} + \sum_{i=u}^{v} b_{ii} x_{iu}^2 + \sum_{i<j} \sum b_{ij} x_{iu} x_{ju} \quad \text{where } u = 1,2,\cdots,N \tag{3}$$

From least squares estimations $X'X\underline{\beta} = X'\underline{Y}$, let M be the moment matrix, $M = \frac{1}{N} X'X$ then we have

$$M_{(K+1)\times(K+1)} = \begin{matrix} E & 0 & 0 \\ & F & 0 \\ sym & & G \end{matrix} \tag{4}$$

where

$$E = \begin{bmatrix} 1 & \lambda_2 & \lambda_2 & . & . & . & \lambda_2 \\ & 3\lambda_4 & \lambda_4 & . & . & . & \lambda_4 \\ & & 3\lambda_4 & . & . & . & \lambda_4 \\ & & & . & & & . \\ & & & & . & & . \\ Symmetric & & & & & . & . \\ & & & & & & 3\lambda_4 \end{bmatrix} \tag{5}$$

$$F = \begin{bmatrix} \lambda_4 & 0 & . & . & . & 0 \\ & \lambda_4 & . & . & . & 0 \\ & & . & & & . \\ & & & . & & . \\ & & & & . & . \\ Symmetric & & & & & \lambda_4 \end{bmatrix} \tag{6}$$

$$G = \begin{bmatrix} \lambda_2 & 0 & . & . & . & 0 \\ & \lambda_2 & . & . & . & 0 \\ & & . & & & . \\ & & & . & & . \\ & & & & . & . \\ Symmetric & & & & & \lambda_2 \end{bmatrix} \tag{7}$$

Their inverses and determinants are;

$$E^{-1} = \frac{1}{[2\lambda_4][k\lambda_2^2 - (k+2)\lambda_4]} \begin{bmatrix} -(k+2)\lambda_4^2 & 2\lambda_2\lambda_4 & 2\lambda_2\lambda_4 & . & . & 2\lambda_2\lambda_4 \\ & (k-1)\lambda_2^2 - (k+1)\lambda_4 & \lambda_4 - \lambda_2^2 & . & . & \lambda_4 - \lambda_2^2 \\ & & (k-1)\lambda_2^2 - (k+1)\lambda_4 & . & . & \lambda_4 - \lambda_2^2 \\ & & & . & . & . \\ & symmetric & & . & . & . \\ & & & & & (k-1)\lambda_2^2 - (k+1)\lambda_4 \end{bmatrix}_{k+1\times k+1} \tag{8}$$

Which gives, $$|E| = [2\lambda_4][k\lambda_2^2 - (k+2)\lambda_4]$$

$$F^{-1} = \begin{bmatrix} \lambda_4^{-1} & 0 & 0 & . & . & . & 0 \\ & \lambda_4^{-1} & 0 & . & . & . & \lambda_4 \\ & & \lambda_4^{-1} & . & . & . & \lambda_4 \\ & & & . & & & . \\ & & & & . & & . \\ Symmetric & & & & & . & . \\ & & & & & & \lambda_4^{-1} \end{bmatrix} \qquad (9)$$

Which gives $|F| = \lambda_4 I_k$

and

$$G^{-1} = \begin{bmatrix} \lambda_2^{-1} & 0 & 0 & . & . & . & 0 \\ & \lambda_2^{-1} & 0 & . & . & . & 0 \\ & & \lambda_2^{-1} & . & . & . & 0 \\ & & & . & & & . \\ & & & & . & & . \\ Symmetric & & & & & . & . \\ & & & & & & \lambda_2^{-1} \end{bmatrix} \qquad (10)$$

which gives $|G| = \lambda_2 I_k$

The determinant $|M|$ was given as the product of $|E|$ $|F|$ $|G|$

Therefore,

$$|M| = \left[2\lambda_2\lambda_4^{\ 2}\right]\left[k\lambda_2^{\ 2} - (k+2)\lambda_4\right] \qquad (11)$$

From the equation(11),

$$\left[2\lambda_2\lambda_4^{\ 2}\right] \neq 0 \ \text{ and } \ \left[k\lambda_2^{\ 2} - (k+2)\lambda_4\right] \neq 0$$

then the non-singularity condition is obtained, i.e., $\frac{\lambda_4}{\lambda_2^{\ 2}} \geq \frac{k}{k+2}$ i.e $\frac{NB}{A^2} \geq \frac{k}{k+2}$. where $A = N\lambda_2$ and $B = N\lambda_4$

CONCLUSION AND RECOMMENDATION

Conclusion

The non-singularity condition for a second-order design to be rotatable were reviewed and obtained from equation 11 where the condition is

$$\frac{\lambda_4}{\lambda_2^{\ 2}} \geq \frac{k}{k+2}$$

The designs satisfying this condition were also obtained where for a second-order design to be rotatable the following moment condition holds

$$\sum_{u=1}^{N} x_{iu}^{\ 2} = A \qquad i = (1,2\cdots\cdots k\ )$$

$$\sum_{u=1}^{N} x_{iu}^{\ 4} = 3\sum_{u=1}^{N} x_{iu}^{\ 2} x_{ju}^{\ 2} = 3B$$

Recommendation

The experimental designs that were obtained in this study ensure equal precision on the response to cut down on cost. The design can be useful in agriculture, textile industry, motor vehicle industry and all other types of industry that make use of experimental designs to manufacture their products.

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