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Department of Statistics and Computer Science, Moi University, Eldoret, Kenya

ABSTRACT
The technique of fitting a response surface design is useful in modelling of experimental designs. Response surface is used in situations where the response of interest is influenced by several experimental variables. The objective of fitting a response surface design is to reduce cost of experimentation and to obtain optimal designs. The property of rotatability is a desirable quantity of experimental design and requires the variance of the fitted design to be constant on circles or spheres about the centre of the design. In this article, a construction technique of fitting modified non-sequential third order rotatable design (TORD) using Pairwise Balanced Design (PBD) is presented. The variance function of a third order response surface design and the properties of Pairwise Balanced Design are utilised for the construction.

1. Introduction

Response surface methodology is as a collection of mathematical and statistical technique useful for the modelling and analysis of experimental designs in which the response of interest is influenced by several variables. The objective of response surface modelling is to obtain an optimal response. Rotatable designs for the exploration of response surface were introduced by Box and Hunter (1957). The property of rotatability implies that the variances of the estimated response are constant on circles or spheres centred at the origin of the design.

Construction of rotatable designs using Balanced Incomplete Block Designs (BIBD) was done by Das and Narasimham (1962). Modified third order rotatable designs using BIBD was constructed by Kosgei et al. (2013). In this paper, a new method has been suggested for constructing modified non-sequential third order rotatable designs.

2. Third order rotatable designs

The fitting of a second order response surface design sometimes becomes inadequate and unrealistic due to lack of fit caused by the presence of third order terms. The use of third order model provides an opportunity to estimate third order terms and therefore solves the problem of lack of fit. The experimental runs of a third order model are relatively more than the runs of a second order model but the number of experimental runs are significantly reduced by use of fractional replicates of the design.

The $D = ((x_{iu}))$ model for fitting a third order response surface design is represented as

$$y_u = b_o x_{ou} + \sum_{i=1}^{v} b_i x_{iu}$$
$$+ \sum_{i \le j=1}^{v} b_{ij} x_{iu} x_{ju}$$
$$+ \sum_{i \le j \le l=1}^{v} b_{ijl} x_{iu} x_{ju} x_{lu} + \varepsilon_u.$$

where x_{iu} – denote level of the ith factor $i = (1, 2, \ldots, v)$ in the uth run $(u = 1, 2, \ldots, N)$ of the experiment. ε_u is uncorrelated random error with mean zero and variance δ^2. $b_o, b_i, b_{ii}, b_{ij}, b_{iii}, b_{ijj}, b_{ijl}$ are the parameters of the model.

3. Conditions for third order rotatability

Third order rotatability was explored by Gardiner et al. (1959) and they developed the following moments and non-singularity condition of rotatability.

The moment's conditions are summarised as follows:

(i) $\sum_{u=1}^{N} \prod_{i=1}^{v} x_{iu}^{\alpha_i} = 0$ if anl α_i is odd $\sum_{i}^{v} \alpha_i = 6$
(ii) $\sum_{i=1}^{N} x_{iu}^2 = N\lambda_2$ for $i = 1, 2, \ldots, v$
(iii) $\sum_{i=1}^{N} x_{iu}^4 = c \sum_{i=1}^{N} x_{iu}^2 x_{ju}^2 = cN\lambda_4$

CONTACT Haron Mutai Ng'eno ✉ haronmutaingeno@yahoo.com 🌐 Department of Statistics and Computer Science, Moi University, P.O Box 3900-30100, Eldoret, Kenya

(iv) $\sum_{i=1}^{N} x_{iu}^6 = 5\sum_{i=1}^{N} x_{iu}^4 x_{ju}^2 = 5c \sum_{i=1}^{N} x_{iu}^2 x_{ju}^2 x_{lu}^2$
$= 5cN\lambda_6$

where $c, \lambda_2, \lambda_4, \lambda_6$ are constants.

The variances and covariance of the design are obtained by applying the least squares techniques and are listed below

$$Var(b_o) = \frac{(c+v-1)\lambda_4}{N[(c+v-1)\lambda_4 - v\lambda_2^2]}\delta^2$$

$$Var(b_{ii}) = \frac{(c+v-2)\lambda_4 - (v-1)\lambda_2^2}{(c-1)N\lambda_4[(c+v-1)\lambda_4 - v\lambda_2^2]}\delta^2$$

$$Var(b_{ij}) = \frac{1}{N\lambda_4}\delta^2 Var(b_i)$$

$$= \frac{(c+v+1)\lambda_6}{N[(c+v+1)\lambda_6\lambda_2 - (v+2)\lambda_4^2]}\delta^2$$

$$Var(b_{iii}) = \frac{(c+v-2)\lambda_6\lambda_2 - (v-1)\lambda_4^2}{c(c-1)N\lambda_6\lambda_2[(c+v+1)}\delta^2$$
$$\lambda_6\lambda_2 - (v+2)\lambda_4^2]$$

$$Var(b_{ijj}) = \frac{(c+v)\lambda_6\lambda_2 - (v+1)\lambda_4^2}{(c-1)N}\delta^2$$
$$\lambda_6\lambda_2[(c+v+1)\lambda_6\lambda_2 - (v+2)\lambda_4^2]$$

$$Var(b_{ijl}) = \frac{1}{N\lambda_6}\delta^2$$

$$Cov(b_o, b_{ii}) = \frac{-\lambda_2}{N[(c+v-1)\lambda_4 - v\lambda_2^2]}\delta^2$$

$$Cov(b_{ii}, b_{jj}) = \frac{\lambda_2^2 - \lambda_4}{(c-1)N\lambda_4[(c+v-1)\lambda_4 - v\lambda_2^2]}\delta^2$$

$$Cov(b_i, b_{iii}) = \frac{-\lambda_4}{N[(c+v+1)\lambda_6\lambda_2 - (v+2)\lambda_4^2]}\delta^2$$

$$Cov(b_{iii}, b_{ijj}) = \frac{\lambda_4^2 - \lambda_6\lambda_2}{(c-1)N}\delta^2.$$
$$\lambda_6\lambda_2[(c+v+1)\lambda_6\lambda_2 - [v+2]\lambda_4^2]$$

An inspection of the variances shows that for it to be positive definite the following must hold.

$$(c+v-1)\lambda_4 - v\lambda_2^2 > 0$$

$$(c+v+1)\lambda_6\lambda_2 - (v+2)\lambda_4^2 > 0$$

This leads to

$$\frac{\lambda_4}{\lambda_2^2} > \frac{v}{c+v-1} \qquad (1)$$

$$\frac{\lambda_6\lambda_2}{\lambda_4^2} > \frac{v+2}{c+v+1}. \qquad (2)$$

Equations (1) and (2) above are referred to as non-singularity conditions.

Hader and Park (1978) studied estimates in response at two points in a factor space and introduced the concept slope rotatability. The technique used partial derivatives to estimate the response surface at two different points in a factor space. Hader and Park (1978) and Park (1987) stated that the necessary and sufficient condition for slope rotatability is $4Var(b_{ii}) = Var(b_{ij})$. The condition was simplified by Victorbabu and Narasimham (1991) and they developed the equation below which is the necessary and sufficient condition for a design to be slope rotatable.

$$\lambda_4[v(5-c) - ((c-3)^2] + \lambda_2^2[v(c-5) + 4] = 0$$

4. Modified third order rotatable designs

A design is third order rotatable if it satisfies both the moments and non-singularity conditions. The usual method of constructing third order rotatable design is by putting some restrictions indicating some relations among third order moments. The paper explores modified condition of rotatability which is obtained by solving the equation below which is the necessary and sufficient condition for slope rotatability

$$\lambda_4[v(5-c) - (c-3)^2] + \lambda_2^2[v(c-5) + 4] = 0.$$

The equation gives a solution of $c = 5$ if and only if $\lambda_2^2 = \lambda_4$. In particular, we investigate the restriction

$$\lambda_2^2 = \lambda_4 \text{ i.e.} \left(\sum_{u=1}^{N} x_{iu}^2\right)^2 = N\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2.$$

The restriction $\lambda_2^2 = \lambda_4$ and $c = 5$ are similar conditions and gives another series of rotatable designed called modified Third order rotatable designs.

The modified symmetry condition therefore becomes

$$\sum_{u=1}^{N} x_{iu}^4 = 5\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = 5N\lambda_4$$

$$\sum_{u=1}^{N} x_{iu}^6 = 5\sum_{u=1}^{N} x_{iu}^4 x_{ju}^2 = 25\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 x_{lu}^2 = 25N\lambda_6.$$

5. Construction of the design

Das and Narasimham (1962) presented a construction method of second and third order rotatable design. In constructing the design, they considered each point in the design as essentially a combination of levels of different factors. First, we have unknown level denoted by a, b, c etc. Secondly, we have another design in v factors of the form 2^v where the two levels each are ± 1. Thirdly, we get another combination by associating the two designs by multiplication.

Definition 5.1: Let $(v, b, r, k_1, k_2, \ldots, k_p, \lambda)k = Sup$ $(k_1, k_2, \ldots, k_p)$ denote a pairwise balanced design, and $2^{t(k)}$ denote a fractional replicate of 2^k in $\pm$ levels, in which no interaction with less than seven factors are confounded. Let $[1 - (v, b, r, k_1, k_2, \ldots, k_p, \lambda)]2^{t(k)}$ and $b2^{t(k)}$ be the design points generated from PBD by multiplication. Let $(a, a, \ldots, a)2^v$ denote the design points generated from $(a, a, \ldots, a)$ point set. Repeat this set of additional points says n_a times (Victorbabu (2011)).

The design points generate the following design matrix

$$
\begin{bmatrix}
\pm & \pm & \cdots & \pm \\
\pm & \pm & \cdots & \pm \\
\vdots & \vdots & \ddots & \vdots \\
\pm & \pm & \cdots & \pm \\
\pm a & \pm a & \cdots & \pm a \\
\pm a & \pm a & \cdots & \pm a \\
\vdots & \vdots & \ddots & \vdots \\
\pm a & \pm a & \cdots & \pm a
\end{bmatrix}.
$$

6. Non-sequential third order rotatable design

Third order rotatable design can either be sequential or non-sequential. The design is non-sequential if the design points satisfy all the moments and non-singularity conditions of rotatability in one occasion. Sequential designs are performed in blocks and in most cases takes more than one trial. In this section, a construction method of non-sequential third order rotatable design using PBD is developed.

Theorem 6.1: *Consider a PBD with parameters $(v, b, r, k_1, k_2, \ldots, k_p, \lambda)k = Sup(k_1, k_2, \ldots, k_p)$*

The design point, $[1 - (v, b, r, k_1, k_2, \ldots, k_p, \lambda)]2^{t(k)}$ $un_a(a, a, \ldots, a)2^{t(v)}un_o$ will generate modified non-sequential TORD with $N = b2^{t(k)} + n_a2^{t(v)} + n_o$ design points if

$$
a^6 = \frac{2^{t(k)-t(v)}[r - 5\lambda]}{4n_a}, N = \frac{[r2^{t(k)} + n_a2^{t(v)}a^2]^2}{\lambda2^{t(k)}} \text{ and}
$$

$$
n_o = \frac{[r2^{t(k)} + n_a2^{t(v)}a^2]^2}{\lambda2^{t(k)}} - b2^{t(k)} - n_a2^{t(v)}.
$$

Proof: The design point of PBD and modified condition of rotatability generates the following equations.

(i) $\sum_{u=i}^{N} x_{iu}^2 = r2^{t(k)} + n_a2^{t(v)}a^2 = N\lambda_2$
(ii) $\sum_{u=i}^{N} x_{iu}^4 = r2^{t(k)} + n_a2^{t(v)}a^4 = 5N\lambda_4$
(iii) $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = \lambda2^{t(k)} + n_a2^{t(v)}a^4 = N\lambda_4$
(iv) $\sum_{u=i}^{N} x_{iu}^6 = r2^{t(k)} + n_a2^{t(v)}a^6 = 25N\lambda_6$
(v) $\sum_{u=1}^{N} x_{iu}^4 x_{ju}^2 = \lambda2^{t(k)} + n_a2^{t(v)}a^6 = 5N\lambda_6$

Using (iv) and (v) we have

$$
r2^{t(k)} + n_a2^{t(v)}a^6 = 5[\lambda2^{t(k)} + n_a2^{t(v)}a^6]
$$

and on simplification we obtain

$$
a^6 = \frac{2^{t(k)-t(v)}[r - 5\lambda]}{4n_a}.
$$

The modified symmetry condition under investigation is

$$
\lambda_2^2 = \lambda_4 \text{i.e.} \left(\sum_{u=1}^{N} x_{iu}^2\right)^2 = N\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2.
$$

$$
N = \frac{\left(\sum_{u=1}^{N} x_{iu}^2\right)^2}{\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2} = \frac{[r2^{t(k)} + n_a2^{t(v)}a^2]^2}{\lambda2^{t(k)} + n_a2^{t(v)}a^4}.
$$

But, $N = b2^{t(k)} + n_a2^{t(v)} + n_o$, implying that $n_o = N - b2^{t(k)} - n_a2^{t(v)}$ and therefore,

$$
n_o = \frac{[r2^{t(k)} + n_a2^{t(v)}a^2]^2}{\lambda2^{t(k)} + n_a2^{t(v)}a^4} - b2^{t(k)} - n_a2^{t(v)}.
$$

∎

Example: Suppose we want to construct an experimental design with a maximum of three factors and five treatments. Let consider a pairwise balanced design with $v = 5, k_1 = 2, k_2 = 3, r = 6, b = 10, \lambda = 1$. In this example,

$$
a^6 = \frac{2^{t(k)-t(v)}[r - 5\lambda]}{4n_a} = \frac{2^{3-5}(6 - 5)}{4} = 0.0625
$$

Non- sequential experimental designs are tried at once meaning that $n_a = 1$

$$
\sum_{u=i}^{N} x_{iu}^6 = r2^{t(k)} + n_a2^{t(v)}a^6 = 6(2^3) + 2^5(0.0625) = 50
$$

$$
\sum_{u=1}^{N} x_{iu}^4 x_{ju}^2 = \lambda2^{t(k)} + n_a2^{t(v)}a^6 = 2^3 + 2^5(0.0625) = 10
$$

$$
\frac{\sum_{u=1}^{N} x_{iu}^6}{\sum_{u=1}^{N} x_{iu}^4 x_{ju}^2} = \frac{50}{10} = 5.
$$

Hence the design forms a rotatable arrangement.
Also,

$$
N = \frac{[r2^{t(k)} + n_a2^{t(v)}a^2]^2}{\lambda2^{t(k)} + n_a2^{t(v)}a^4} = \frac{3684.39}{13.03968} = 283 \text{ points.}
$$

$$
n_o = N - b2^{t(k)} - n_a2^{t(v)} = 283 - 80 - 32
$$
$$
= 172 \text{ Centre points.}
$$

For rotatability, we need to check if the non-singularity conditions are also satisfied

(i) $\frac{\lambda_4}{\lambda_2^2} > \frac{v}{c+v-1}$

(ii) $\frac{\lambda_6\lambda_2}{\lambda_4^2} > \frac{\nu+2}{c+\nu+1}$.

In this case,

$$\lambda_4 = \frac{\lambda 2^{t(k)} + n_a 2^{t(\nu)}a^4}{N} = 0.04608$$

$$\lambda_2 = \frac{r2^{t(k)} + n_a 2^{t(\nu)}a^2}{N} = 0.21448$$

$$\lambda_6 = \frac{\lambda 2^{t(k)} + n_a 2^{t(\nu)}a^6}{5N} = 7.067 \times 10^{-3}$$

$$\frac{\lambda_4}{\lambda_2^2} = \frac{0.04608}{0.21448^2} = 1.0017$$

$$\frac{\nu}{c+\nu-1} = \frac{5}{9} = 0.5556.$$

Since $1.0017 > 0.5556$ condition (i) is satisfied.
Also,

$$\frac{\lambda_6\lambda_2}{\lambda_4^2} = \frac{7.067 \times 10^3 \times 0.21448}{0.04608^2} = 0.71383$$

$$\frac{\nu+2}{c+\nu+1} = \frac{7}{11} = 0.6364$$

Since $0.71383 > 0.6364$, condition (ii) is satisfied. Therefore, the non-singularity conditions are satisfied.

The design points form non-sequential third order rotatable design because both the moments and non-singularity conditions of third order rotatability are satisfied in one trial. The method allows the fitting of third order rotatable response surface with 283 design points. The full list of third order rotatable designs constructed using Pairwise Balanced Design is as tabulated in the Appendix.

Disclosure statement

No potential conflict of interest was reported by the author(s).

Notes on contributor

Haron Mutai Ng'eno is a PHD student at MOI University. He holds Master of Science Biostatistics degree and is currently pursuing PHD in statistics. His research interests are in response surface methodology and has authored four published papers on second order rotatability.

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Appendix

Table A1. Third order rotatable designs constructed using PBD for $6 \leq v \leq\leq 12$

$(v, k_1, k_2, r, b, \lambda, n_a$	$2^{t(k)}$	$2^{t(v)}$	a	n_0	N
5, 3, 2, 6, 10, 1, 1	8	32	0.62996	172	283
6, 3, 2, 6, 20, 1, 1	$\frac{1}{2}$ replicate $= 4$	$\frac{1}{2}$ replicate $= 32$	0.56123	113	209
7, 4, 2, 10, 35, 1, 2	$\frac{1}{4}$ replicate $= 4$	$\frac{1}{4}$ replicate $= 32$	0.65383	85	289
8, 4, 3, 7, 28, 1, 2	$\frac{1}{4}$ replicate $= 4$	$\frac{1}{4}$ replicate $= 64$	0.50000	60	300
9, 3, 2, 14, 42, 2, 2	$\frac{1}{4}$ replicate $= 2$	$\frac{1}{4}$ replicate $= 128$	0.44545	101	441
10, 4, 3, 12, 30, 2, 2	$\frac{1}{8}$ replicate $= 2$	$\frac{1}{8}$ replicate $= 128$	0.39689	84	400
11, 5, 3, 15, 33, 2, 1	$\frac{1}{8}$ replicate $= 4$	$\frac{1}{8}$ replicate $= 256$	0.51894	241	629
12, 6, 4, 11, 22, 1	$\frac{1}{8}$ replicate $= 4$	$\frac{1}{8}$ replicate $= 256$	0.53496	207	551