International Journal of Statistics and Applied Mathematics

ISSN: 2456-1452
Maths 2024; 9(1): 44-47

https://www.mathsjournal.com
Received: 17-10-2023
Accepted: 14-11-2023

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Series of asymmetrical second order partially rotatable designs

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DOI: https://dx.doi.org/10.22271/maths.2024.v9.i1a.1581

Abstract
Response Surface Methodology (RSM) is commonly employed to establish connections between factors and responses, aiming to identify the optimal variables for maximizing desired outcomes. The excessive use of nitrogen, particularly when compared to phosphate and potassium, poses agronomic and environmental challenges. Soil potassium and phosphorus levels are declining, and unbalanced fertilizer application may result from diverse response curves for individual optimal doses. Consequently, determining the balanced N, P, and K amounts for various crops is a significant challenge. RSM offers a solution by allowing the adjustment and optimization of fertilizer dosage. While RSM typically addresses quantitative factors, it can also be applied to qualitative factors like soil type, seed varieties, and irrigation methods. In such cases, research has demonstrated the effectiveness of RSM. A rotatable design is crucial as it guarantees equal in formativeness in all directions. This article introduces a series of cost-effective asymmetrical second-order partially rotatable designs, achieved through a reduced number of runs utilizing main effect plans.

Keywords: Asymmetric factors, g-efficiency, response surface methodology, rotatable design

1. Introduction

Factorial design, by simultaneously examining multiple factors, reduces the required number of trials. It allows the identification of main effects (from each independent factor) and interaction effects (when both factors jointly influence the outcome). However, factorial design provides only relative values; actual numerical values require regressions, involving the minimization of a sum of values. Nonetheless, it proves valuable in designing trials for both laboratory and commercial settings. When each factor has an equal number of levels, it's termed a symmetric factorial design; otherwise, it is referred to as an asymmetric factorial design. Factorial experiments play a crucial role in response surface design, which holds extensive significance within the realm of experimental design. RSM finds application across diverse sectors such as manufacturing, agriculture, electronics, and medicine. It is employed when optimal responses are sought.

Let x_1, $x_2 \ldots x_v$ be v independent variables or factors, y be the response variable and there be N observations. The response function can be approximated in some region of polynomial model given by $y_u = f(x_{1u}, x_{2u}, x_{3u}, \ldots, x_{vu}) + e_u$.

Where u = 1,2,…,N (total number of observations), y_u is the response from u^{th} treatment combination and x_{iu} is the level of the i^{th} (i = 1,2,…,v) factor in the u^{th} combination. The function of describes the form in which the response and the input variables are related. e_u is the random error associated with the u^{th} observation that is independently and normally distributed with mean zero and common variance σ^2.

Response surface models are polynomial models that accurately depict the real dose-response relationship. Response surface designs are those that enable the fitting of response surfaces and offer a way to gauge how effective they are. For details on RSM, one can refer to Myers (1971) [10], Khuri and Cornell (1996) [8] and Myers *et al.* (2009) [11].

First order response surface, function is defined as follows:

$$f(x_u) = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} \quad , u = 1,\ldots,N \qquad \ldots(1.1)$$

It is a polynomial of degree 1 and used to find whether there is curvature or not.

A response surface function of second degree is written as follows:

$$f(x_u) = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} + \sum_{i=1}^{v} \beta_{ii} x_{iu}^2 + \sum_{i=1}^{v-1} \sum_{i'=i+1}^{v} \beta_{ii'} x_{iu} x_{i'u}$$

u=1,…,N …(1.2)

In response surface methodology (RSM), a design is considered rotatable when the variance of the estimated response is constant in all directions from the center of the design space. This property is desirable because it ensures that the design is equally informative in all directions. Box and Hunter (1957) [3] established the class of designs known as rotatable designs. When a second order design satisfy this condition, then design is called second order rotatable design. For more detail please refer Bose and Draper (1959) [1], Das (1963) [5], Draper (1960) [6], Mehta and Das (1968) [9]. However, in some cases, achieving a fully rotatable design may be impractical or unnecessary for various reasons, such as resource constraints or specific constraints on the experimental factors. In such situations, a partially rotatable design is employed, where only a portion of the design space exhibits rotas ability. A partially rotatable response surface design refers to an experimental design in which only a subset of the design points or factor combinations is rotatable or when considering design points equidistant from the design center, we observe the variance of the estimated response yielding two or more values. A partially rotatable response surface design aids in achieving a well-distributed experimental design with fewer runs. A fractional factorial design is of resolution R if no p-factor is aliased with another effect containing R-p factors, this definition is due to Box and Hunter (1961) [4]. An orthogonal plan is a fractional factorial design that allows the estimation of all pertinent effects with zero correlation. Main effects plans refer to designs that guarantee the estimability of the mean and all main effects, assuming the absence of all interactions.

2. Material and Methods: Series of asymmetrical second order partially rotatable designs

2.1. The model considered here is the second order model without interaction term given as follows:

$$f(x_u) = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} + \sum_{i=1}^{v} \beta_{ii} x_{iu}^2 \qquad \ldots(2.1)$$

The designs have been obtained using orthogonal main effect plans of asymmetrical factorial of resolution III derivable from Hadamard Matrices.

Series 2.1.1: Using main effect plans for 4.2^{2n-4} // 2n Experiments

Consider H as a Hadamard matrix of order n, where n is a multiple of 4, and assume H is in its semi-normal form. To obtain matrix B of dimensions n×(n-1) from H, eliminate the first column containing all units. Let B = [b_1: B_2], where b_1 is any one column of B and B_2 is n×(n-2) matrix of remaining columns of B. Consider the matrix D_1 as given below.

$$D_1 = \begin{bmatrix} b_1 & B_2 & B_2 \\ 3b_1 & B_2 & -B_2 \end{bmatrix}$$

D_1 is a fraction of $4 \times 2^{2n-4}$ in 2n runs where one factor is at 4 levels (-3, -1, 1, 3) and 2n-4 factors are at 2 levels (1, -1) each. Augment D_1 with axial points ($\sqrt{v}$, 0,..,0) × 2 and center points. Design so obtained is $7 \times 5^{2n-4}$ in $2n + 2v + n_c$ runs where v = 2n-3, total number of factors. The designs obtained are partially rotatable with five different variances of estimated response.

Example 2.1.1: Consider a main effect plan 4×2^4 in 8 runs. Augment it with axial points ($5^{1/2}$, 0,..,0) × 2 and center points. The design so obtained is 7×5^4 in 23 runs with 10 axial runs and 5 center runs. Design matrix X with column X_1, X_2, X_3, X_4 and X_5 is as follows:

1	1	1	1	1
-1	1	-1	1	-1
1	-1	-1	-1	-1
-1	-1	1	-1	1
3	1	1	-1	-1
-3	1	-1	-1	1
3	-1	-1	1	1
-3	-1	1	1	-1
2.23607	0	0	0	0
-2.23607	0	0	0	0
0	2.23607	0	0	0
0	-2.23607	0	0	0
0	0	2.23607	0	0
0	0	-2.23607	0	0
0	0	0	2.23607	0
0	0	0	-2.23607	0
0	0	0	0	2.23607
0	0	0	0	-2.23607
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

The variances of estimated response are $0.15487\sigma^2$, $0.2709\sigma^2$, $0.29845\sigma^2$, $0.62468\sigma^2$ and $0.74891\sigma^2$. One factor is at 7 levels (-3, -2.23607, -1, 0, 1, 2.23607, 3) and four factors are at 5 levels (-2.23607, -1, 0, 1, 2.23607) each. The G-Efficiency of the design is obtained as 0.63861. The design is thus partially rotatable design.

Series 2.1.2: Using main effect plans for $4^3 \times 2^{2n-10}$ // 4n experiments

Consider the method given in 4.1.1.1 above. Writing **B** in the following form:

$$\mathbf{B} = \begin{bmatrix} b_1 & b_2 & b_3 & B_4 \end{bmatrix}$$

Where b_i (i= 1,2,3) are any three distinct columns of B and B_4 is the n×(n-4) matrix of remaining columns of B. Define B_i (i=1,2,3) as

$$\mathbf{B}_i = \begin{bmatrix} \mathbf{b}_i & \mathbf{B}_4 \end{bmatrix}$$

Then plan D_1 is given by

$$\mathbf{D}_1 = \begin{bmatrix} \mathbf{b}_1 & \mathbf{3b}_2 & \mathbf{3b}_3 & \mathbf{B} & \mathbf{B}_1 & \mathbf{B}_2 & \mathbf{B}_3 \\ \mathbf{3b}_1 & \mathbf{-3b}_2 & \mathbf{-b}_3 & \mathbf{B} & \mathbf{-B}_1 & \mathbf{B}_2 & \mathbf{-B}_3 \\ \mathbf{-b}_1 & \mathbf{-b}_2 & \mathbf{b}_3 & \mathbf{B} & \mathbf{B}_1 & \mathbf{-B}_2 & \mathbf{-B}_3 \\ \mathbf{-3b}_1 & \mathbf{b}_2 & \mathbf{-3b}_3 & \mathbf{B} & \mathbf{-B}_1 & \mathbf{-B}_2 & \mathbf{B}_3 \end{bmatrix}$$

The first three columns of D_1 represent three, four level (-3, -1, 1, 3) factors and remaining (4n-10) columns, the levels of 2-level (-1, 1) factors. D_1 is orthogonal main effect plan for a $4^3 \times 2^{2n-10}$ experiments in 4n runs. Augment D_1 with axial points $(\sqrt{v},0,..,0) \times 2$ and center points. Design so obtained is $7^3 \times 5^{2n-10}$ in $4n + 2v + n_c$ runs where v= 2n-9, total number of factors. The designs obtained are partially rotatable with five kind of variances of estimated response.

Series 2.1.3: Augmenting Orthogonal Main Effect Plans for $n \times 2^n$ // 2n Experiments with axial point $(\sqrt{v},0,..,0) \times 2$ and center points. Design so obtained is $(n+3)\times5^n$ in $2n + 2v + n_c$ runs where v= n+1, total number of factors. Obtained designs are partially rotatable with 9 kind of variances of estimated response.

2.2. The next series of designs are obtained using orthogonal main effect plans of asymmetrical factorial of resolution IV derivable from Hadamard Matrices and the model considered is second order model with interaction term:

$$f(x_u) = \beta_0 + \sum_{i=1}^{v}\beta_i x_{iu} + \sum_{i=1}^{v}\beta_{ii}x_{iu}^2 + \sum_{i=1}^{v-1}\sum_{j=i+1}^{v}\beta_{ij}x_{iu}x_{ju} \quad \ldots(2.2)$$

Series 2.2.1: Design is obtained by using main effect plans for $4^2 \times 2^{2n-4}$ // 8n Experiments and augmenting with axial points $(\sqrt{v},0,..,0) \times 2$ and center points. Design so obtained is$7^2\times5^{2n-4}$ in $8n + 2v + n_c$ runs where v=2n-2, total number of factors. Obtained design is partially rotatable.

Series 2.2.2: Another series of design is obtained by using Main Effect Plans for $4^3 \times 2^{4n-12}$ // 16n Experiments, augment with axial points $(\sqrt{v}, 0,..,0) \times 2$ and center points. Design so obtained is $7^3 \times 5^{4n-12}$ in $16n + 2v + n_c$ runs where v=2n-2, total number of factors. Obtained design is partially rotatable.

Series 2.2.3: Using main effect plans for $4^m \times 2^n$ Experiments These designs are derived based on main effect orthogonal plans designed for 2^m experiments, where m is a power of 2. The resultant plan achieves resolution IV for a 4×2^v experiment with 16 runs, considering the subset involving v effects.Add axial points $(\sqrt{v}, 0,..,0) \times 2$ and center points to the obtained plan. The design as obtained is $7^m \times 5^n$, which is partially rotatable.

Series 2.2.4: Using asymmetrical factorial $4^m \times 2^n$ of resolution V from Orthogonal Arrays by choosing the right subset of a $(2^v -1)$ effects of a 2^v factorial and swapping sets of three 2 level factor representations for 4 level factors, $4^m \times 2^n$ can be achieved. Augment obtained plan with axial points $(\sqrt{v}, 0,..,0) \times 2$ and center points. Design so obtained is $7^m\times5^n$ which is partially rotatable.

3. Results and Discussion

A list of asymmetrical second order partially rotatable designs (ASOPRD) is prepared and presented in Table 3.1 along with variance of estimated response and G-efficiency.

Table 3.1: List of ASOPRD along with variance of estimated response and G-efficiency

Factors	Runs	Design	Variance of Estimated Response	G-Efficiency
$7 \times 5^{2n-4}$ in $2n + 2v + n_c$ runs where v= 2n-3				
v = 5 (7×5^4)	$8 + 10 + n_c$	$4 \times 2^4 + (\sqrt{v}, 0,..,0) \times 2$	0.15487 0.27092 0.29845 0.62468 0.74891	0.63861
v = 13 (7×5^{12})	$16 + 26 + n_c$	$4 \times 2^{12} + (\sqrt{v}, 0,..,0) \times 2$	0.07538 0.32923 0.33596 0.47750 0.78872	0.63394
v = 29 (7×5^{28})	$32 + 58 + n_c$	$4 \times 2^{28} + (\sqrt{v}, 0,..,0) \times 2$	0.04306 0.34373 0.45434 0.51714 0.75143	0.74073
$7^3 \times 5^{2n-10}$ in $4n + 2v + n_c$ runs where v = 2n-9				
v = 25 $7^3\times5^{22}$	$32 + 50 + n_c$	$4^3\times2^{22} + (\sqrt{v}, 0,..,0) \times 2$	0.03052 0.29488 0.41392 0.42721 0.80064	0.56874
$(n+3) \times 5^n$ in $2n + 2v + n_c$ runs where v= n+1				
v = 13 15×5^{12}	$24 + 26 + n_c$	$12\times2^{12} + (\sqrt{v}, 0,..,0) \times 2$	0.17148 0.20377 0.26793 0.27131 0.28299 0.31202 0.37110 0.47655 0.74912	0.66745
$7^m \times 5^n$ Resolution IV				
v = 4 7×5^3	$16 + 8 + n_c$	$4\times2^3 + (\sqrt{v}, 0,..,0) \times 2$	0.20710 0.23332 0.56388 0.60306 0.72283	0.76858
$7^m \times 5^n$ Resolution V				
v = 5 $7^2\times5^3$	$64 + 10 + n_c$	$4^2\times2^3 + (\sqrt{v}, 0,..,0) \times 2$	0.12362 0.16357 0.20356 0.21716 0.32415 0.93029	0.29316

Note: G-Efficiency

$$\text{G-Eff.} = \frac{p}{N\times \max(v(x))_{x\epsilon R}}$$

Where $\max(v(x))_{x\epsilon R}$ is the maximum of prediction variance over the design space? The goal of the G-efficiency criterion is to minimize the variances of the predicted values, which maximizes a design's ability to predict.

4. Summary and Conclusion

Methods of constructing designs for fitting response surfaces for asymmetric factors under second order model setups have been developed. Series of asymmetrical second order partially rotatable designs have been obtained using orthogonal main effect plans of asymmetrical factorial in minimal runs under a second order model with or without interaction term.

Response surface methodology finds application in diverse agricultural fields, including fisheries experiments, animal husbandry, and determining optimal fertilizer doses. Employing second order partially rotatable response surface designs proves advantageous as it minimizes resource utilization due to less number of runs and enhances cost-effectiveness.

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