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수정된 Notz계획을 이용한 2차모형의 경제적 추정

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Economic Second-Order Modeling Using Modified Notz Design

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Abstract

Purpose: In this paper we propose modified Notz designs which are useful to experimenters who want to adopt the sequential experimentation strategy and to estimate second-order regression model with as few experimental points as possible.
Methods: We first present the design matrices and design points in two or three dimensional spaces for such small sized second-order designs as small composite, hybrid, and Notz designs. Modified Notz designs are proposed and compared with some response surface designs in terms of the total number of experimental points, the estimation capability criteria such as D- and A-optimality.
Results: When sequential experimentation is necessary, the modified Notz designs are recommendable.
Conclusion: The result of this paper will be beneficial to experimenters who need to do experiments more efficiently, especially for those who want to reduce the time of experimentation as much as possible to develop cutting-edge products.

Key Words : Response Surface Methodology, Second-Order Modelling, Modified Notz Design, Optimality Criteria, Sequential Experimentation

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1. INTRODUCTION

Designing high-quality products and processes at low cost is an economic and technological challenge to the design and development engineers. The objective of a product and process design is to produce drawings, specifications, and other related information needed to manufacture products that meet customer requirements. Knowledge of scientific phenomena and past engineering experience with similar product and process design form the basis of the engineering design activities. However, a number of new decisions related to the particular product of interest must be made regarding product architecture, parameters of the product design, the process architecture, and parameters of the manufacturing process. A large amount of engineering effort is consumed in conducting experiments to generate the information needed to guide these decisions (Phadke, 1989). Design of experiments is an efficient and effective tool in product realization. There are generally three steps in systematically applying design of experiments for product and process designs. Screening experiments is used to identify influential factors, then these factors are used to investigate better experimental region. When the experimenter reaches a region near the optimum, the response surface methodology for the second-order model estimation is implemented (Myers and Montgomery, 2002). Two standard response surface designs, central composite design and Box-Behnken design are very popular with practitioners (Box and Wilson, 1951, Box and Behnken, 1960). The run sizes of these designs are large enough to provide a comfortable margin for lack of fit. However, for the cutting-edge products such as semiconductor, liquidated crystal display, and light-emitting diode products it is crucial to reduce experimental times. Thus we should employ more time-reducing experimental designs for second-order model estimation. For this purpose, small sized second-order designs will be useful. Small sized second-order designs can be helpful to experimenters who want to estimate second-order models but are not able to afford enough number of experimental runs. There are several saturated or near-saturated small sized second-order designs.

Hartley(1959) proposed small composite designs from central composite designs, in which the factorial portion is a special resolution III fraction. Roquemore(1976) developed a set of saturated or near-saturated second-order designs called hybrid designs. Later, Notz(1982) proposed a modification of factorial designs which are based on factorial points and one-factor-at-a-time axial points.

Although these small sized second-order designs are somewhat inferior to standard response surface designs in terms of prediction capability, they have smaller experimental runs. When we develop cutting-edge products, we may think about adopting small sized second-order designs to reduce the time spent in experimentation.

In this paper we propose a set of modified Notz designs which consist of smaller number of design points and are useful for sequential experimentation in the circumstance where there is a curvature in the original design region and a favorable direction of improvement for the response. In section 2 we first present the design matrices and design points in two or three dimensional spaces for such small sized second-order designs as small composite, hybrid, and Notz designs. Then modified Notz designs are proposed and displayed for the two to four design variables case in section 3. The modified Notz designs are then compared with other designs in terms of the total number of experimental points, the estimation capability criteria such as D- and A-optimality in section 4, and a guideline of adopting the modified Notz designs are suggested in section 5.

2. SMALL-SIZED SECOND-ORDER DESIGNS

2.1. Small composite designs

Small composite design, which was proposed by Hartley(1959), stems from the central composite design(CCD). The small composite design differs from the CCD in that the factorial portion is of neither a complete 2k nor a resolution Ⅴ fraction, but a special resolution Ⅲ in which no four-letter word is among the defining relations. This type of fraction is often called resolution Ⅲ*. As a result, the total run size is reduced from that of the CCD, hence the term small composite design. In <Figure 1> the design matrices of small composite designs for k=2 and 3 are presented. The distance between the center point and axial points α is set to be 1 for ease of presentation. As shown in <Figure 1> below, for 3 factors, the fractional factorial portion is the fraction generated with I= −ABC. The alternative fraction would be also satisfactory as the fractional factorial portion of the small composite design. There are 11 design points; 4 factorial points, 6 axial points, and one center point. Since the number of second-order parameters, p, is 10, this design is nearly saturated. Multiple center runs can allow degrees of freedom for pure error, and if the fitted model is of second order, there will be one degree of freedom for lack of fit. In <Figure 1> we can see that in the factorial portion linear main effect terms are aliased with two-factor interaction terms. In spite of this, all coefficients in the second-order model are estimable because the linear coefficients can be identified from the axial points (Hartley, 1959). <Figure 2> shows the experimental points in two and three dimensional spaces.

$$
\begin{array}{cc} x_1 & x_2 \end{array} \qquad \begin{array}{ccc} x_1 & x_2 & x_3 \end{array}
$$

$$
D=\begin{bmatrix} -1 & -1 \\ 1 & 1 \\ -1 & 0 \\ 1 & 0 \\ 0 & -1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \qquad
D=\begin{bmatrix} -1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}
$$

Figure 1. Design matrices of small composite designs for k=2 and 3 factors

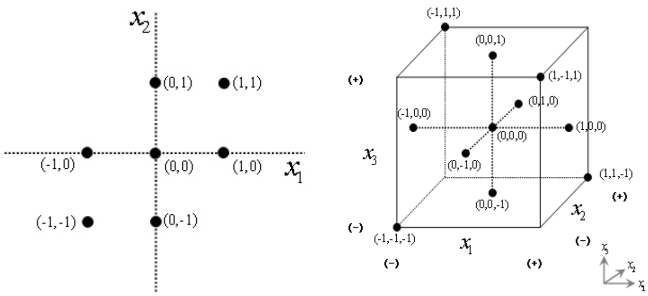

Figure 2. Small composite designs for k=2 and 3 factors

2.2. Hybrid designs

Roquemore(1976) developed a set of saturated or near-saturated second-order designs called hybrid designs. The hybrid designs are very efficient. They were created via an imaginative idea that involves the use of a central composite design for (k-1) variables, and the levels of the k-th variable are supplied in such a way as to create certain symmetries in the design. The result is a class of designs that are economical and either rotatable or near-rotatable. The design name D310 comes from the number of factors (k) equal to 3 and 10 distinct design points. Roquemore developed two additional k=3 hybrid designs D311A and D311B. These designs have 11 design points including a center point to avoid near-singularity. The design matrices of D310, D311A, D311B are shown in <Figure 3>. <Figure 4> shows the experimental points of the D311A design in the three dimensional spaces.

$$D_{310} = \begin{bmatrix} 0 & 0 & 1.2906 \\ 0 & 0 & -0.1360 \\ -1 & -1 & 0.6386 \\ 1 & -1 & 0.6386 \\ -1 & 1 & 0.6386 \\ 1 & 1 & 0.6386 \\ 1.736 & 0 & -0.9273 \\ -1.736 & 0 & -0.9273 \\ 0 & 1.736 & -0.9273 \\ 0 & -1.736 & -0.9273 \end{bmatrix} \quad (x_1, x_2, x_3)$$

$$D_{311A} = \begin{bmatrix} 0 & 0 & \sqrt{2} \\ 0 & 0 & -\sqrt{2} \\ -1 & -1 & 1/\sqrt{2} \\ 1 & -1 & 1/\sqrt{2} \\ -1 & 1 & 1/\sqrt{2} \\ 1 & 1 & 1/\sqrt{2} \\ \sqrt{2} & 0 & -1/\sqrt{2} \\ -\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & \sqrt{2} & -1/\sqrt{2} \\ 0 & -\sqrt{2} & -1/\sqrt{2} \\ 0 & 0 & 0 \end{bmatrix} \quad (x_1, x_2, x_3)$$

$$D_{311B} = \begin{bmatrix} 0 & 0 & \sqrt{6} \\ 0 & 0 & -\sqrt{6} \\ -0.7507 & 2.1063 & 1 \\ 2.1063 & 0.7507 & 1 \\ 0.7507 & -2.1063 & 1 \\ -2.1063 & -0.7507 & 1 \\ 0.7507 & 2.1063 & -1 \\ 2.1063 & -0.7507 & -1 \\ -0.7507 & -2.1063 & -1 \\ 2.1063 & 0.7507 & -1 \\ 0 & 0 & 0 \end{bmatrix} \quad (x_1, x_2, x_3)$$

Figure 3. Design matrices of hybrid designs for 3 factors (D310,D311A, D311B)

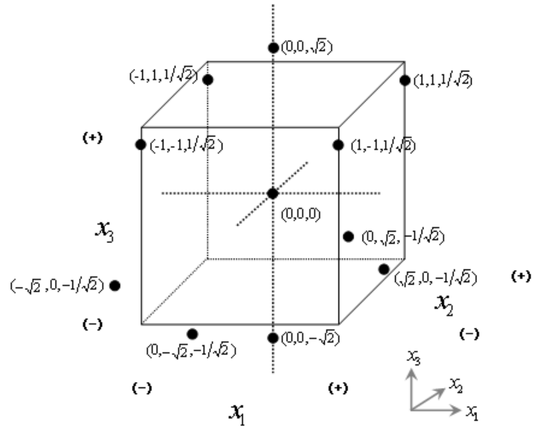

Figure 4. Hybrid design of D311A

2.3. Notz designs

Notz(1982) considered finding nearly D-optimal designs for second-order models on a cube which take as few observations as possible and still allow estimation of all parameters. For example, Notz 3-factor design involves seven design points from a factorial 23 excluding (1, 1, 1), plus three one-factor-at-a-time axial points, which is shown in <Figure 5>. Note that Notz design does not include the factorial point (1, 1, 1) and the center point. Notz design of the three variables case is shown in <Figure 6>.

$$D = \begin{array}{c} \begin{matrix} x_1 & x_2 \end{matrix} \\ \begin{bmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \end{array} \qquad D = \begin{array}{c} \begin{matrix} x_1 & x_2 & x_3 \end{matrix} \\ \begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{array}$$

Figure 5. Notz design matrices for k=2 and 3 factors

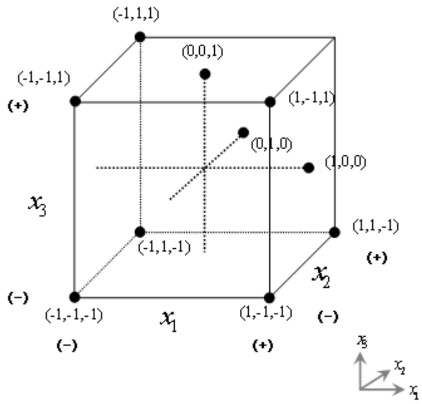

Figure 6. Notz design of k=3 factors

3. MODIFIED NOTZ DESIGNS

Most applications in response surface methodology are sequential in nature. At first some potential candidate factors are considered to be influential to the response variables. This usually leads to an experiment designed to investigate these factors with a view to select important ones. This type of experiment is usually called a screening experiment. The objective of factor screening is to reduce the number of candidate variables to a relatively few so that subsequent experiments will be more efficient and require fewer runs. Once the important independent variables are identified, the experimenter's objective is to determine if the current levels of the factors result in a value of the response that is near the optimum, or if the experimental region is remote from the optimum. If the current settings or levels of the independent variables are not consistent with optimum performance, then the experimenter must determine a set of adjustments to the variables that will move the process toward the optimum.

Since the empirical model based on the experimental data is first-order or second-order, we can start by adopting factorial design with center point. After the data is obtained and analyzed there will be three cases (Box, et al., 2005). First, the current experimental region is far from the point of optimal performance. In this case we need to move to the promising region based on the first-order model. Second, the optimal point is near the center point. Then some axial points can be added leading to the central composite design. By estimating second-order model we can reach to the optimal point. Third, the optimum can be achieved in vicinity of the boundary of the experimental region. In this case we need to build a second-order model. But we only need half of the axial points since we know favorable direction of each independent variable. For this third case we can employ a modified Notz design. Let's consider three independent variables case. Notz design for k=3 is different from the 23 factorial design in that it is without the factorial point (1, 1, 1) and that it is augmented with three axial points (1, 0, 0), (0, 1, 0), (0, 0, 1). We can construct a k=3 modified Notz design by augmenting the factorial point (1, 1, 1) and the center point (0, 0, 0) in the Notz design.

By adding center point to the factorial points, we can check whether there is a curvature effect of not. If there is a curvature effect in the design region we can augment some axial points to estimate second-order models. If the optimal seems to be in the near the center point, we should adopt central composite design by augment two axial points in each axis. However, if one direction of an axis is more preferable meaning that the response is better in one side of the axis, we can choose the modified Notz design by adding one axial point in each axis to reduce the number of experiment. The second design matrix of <Figure 7> is a k=3 modified Notz design when the direction (1, 0, 0), (0, 1, 0), (0, 0, 1) is preferable. The axial points added in the modified Notz design are dependent on the direction of preference. If the direction of preference is (−1, 0, 0), (0, 1, 0), (0, 0, −1), we can substitute these three points for the axial points (1, 0, 0), (0, 1, 0), (0, 0, 1). The third design matrix of <Figure 7> is a k=4 modified Notz design. In this matrix the first 8 rows are the resolution IV fractional factorial design 2_{IV}^{4-1}. The next 4 rows indicates semi-folded portion of factorial points which can separate the aliased linear main and interaction effects that are to be estimated from the fractional factorial design 2_{IV}^{4-1} (Mee and Peralta, 2000).

$$D = \begin{array}{c} \begin{matrix} x_1 & x_2 \end{matrix} \\ \begin{bmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \end{array} \quad D = \begin{array}{c} \begin{matrix} x_1 & x_2 & x_3 \end{matrix} \\ \begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \end{array} \quad D = \begin{array}{c} \begin{matrix} x_1 & x_2 & x_3 & x_4 \end{matrix} \\ \begin{bmatrix} -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

Figure 7. Modified Notz design matrices for k=2, 3 and 4

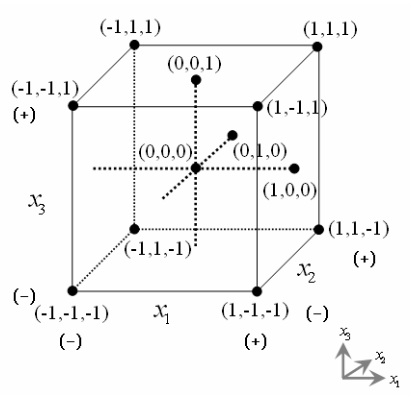

Figure 8. Modified Notz design for k=3 factors

4. COMPARISON OF SECOND-ORDER DESIGNS

4.1. Comparison Criteria

To compare the small sized second-order designs, we employ a couple of well-known design optimality criteria. The best known and most often used criterion is D-optimality. D-optimality is based on the notion that the experimental design should be chosen in order to achieve certain properties in the moment matrix $M = X'X/N$, where X is the design matrix and N is the number of experimental runs. $M^{-1} = N(X'X)^{-1}$ which is the dispersion matrix scaled by N/σ^2 contains variances and covariances of the regression coefficients. As a result, we can use this moment matrix to evaluate the designs by considering the variances and covariances of the dispersion matrix. An important norm on the moment matrix is the normalized determinant $M = (|X'X|/N^p)^{1/p}$, which is called as D1/p value, where p is the number of parameters in the model. Under the assumption of independent and identically normal errors, $|X'X|$ is inversely proportional to the square of the volume of the confidence region on the regression coefficients. The volume of the confidence region is relevant because it reflects how well the coefficients are estimated. A smaller $|X'X|$, that is, larger $|X'X|^{-1}$ implies poor estimation of the regression coefficients in the model (Myers and Montgomery, 2002).

The concept of A-optimality deals with the individual variances of the regression coefficients. Unlike D-optimality, it does not make use of covariances among coefficients; recall that the variances of regression coefficients appear in the diagonals of $(X'X)^{-1}$. A-optimality is defined as minimizing $tr(X'X)^{-1}$ where tr represents trace, that is, the sum of the variances of the coefficients (weighted by N/σ^2). To evaluate the efficiency of the designs the number of experimental points is also used as a comparison criterion.

4.2. Comparison of the Second-Order Designs

Comparison results of the second-order designs are shown in this subsection using Design Expert software (Stat-Ease, 2003), where the experimental run in the center point is set to be 1. For the small composite designs the distance from the center to the axial points is set to be $(n_f)^{(1/4)}$ to ensure rotatability where n_f is the number of factorial points. In <Table 1> it is seen that for the k=2 variables case the modified Notz design is better than the small composite design and quite comparable to the central composite design (CCD), considering that CCD has axial points with the axial distance of 1.414 while the modified Notz design has only the distance of 1. When we have k=3 factors, there are 10 or 11 design points for the small sized second-order designs, meaning that they are saturated or nearly saturated, since there are 10 parameters to be estimated, as seen in <Table 2>. Modified Notz design has 12 experimental points. The performance of the modified Notz design is very similar to that of Box-Behnken design (BBD), slightly better in terms of D-optimality and a little bit worse with respect to A-optimality, compared to BBD. It is moderately worse than the central composite design (CCD) in terms of D-optimality and performs much worse in view of A-optimality. Hybrid designs overall perform well with respect to the D- and A-optimality criteria, but they are not very favorable to the experimenters with more levels and lack of the possibility of sequential experimentation. As seen in <Table 3>, for the k=4 case, the performance of the modified Notz design is quite similar to that of the BBD, better in terms of D-optimality and worse with respect to A-optimality. It is worse than that of the CCD in terms of both the D- and A-optimality criteria. However, the number of design points of the modified design is only 17, compared with the 25 of the CCD and BBD.

Table 1. Comparison of second-order designs of k=2 factors

Second Order Designs	No. of Design Points	D1/p	A-optimality
Small composite design	7	0.417	4.174
Notz design	6	0.420	6.500
Modified Notz design	7	0.449	3.250
Central composite design	9	0.629	2.187

Table 2. Comparison of second-order designs of k=3 factors

Second Order Designs	No. of Design Points	D1/p	A-optimality
Small composite design	11	0.442	3.607
Hybrid design(D310)	10	0.616	2.279
Hybrid design(D311A)	11	0.514	2.984
Notz design	10	0.380	4.477
Modified Notz design	12	0.419	3.679
Central composite cesign	15	0.687	2.079
Box-Behnken cesign	13	0.379	3.438

Table 3. Comparison of second-order designs of k=4 factors

Second Order Designs	No. of Design Points	D1/p	A-optimality
Small composite design	17	0.526	3.000
Hybrid design(D416A)	16	0.608	2.488
Hybrid design(D416B)	16	0.568	2.075
Notz design	15	0.323	6.069
Modified Notz design	17	0.387	5.025
Central composite cesign	25	0.767	1.896
Box-Behnken cesign	25	0.253	4.250

5. CONCLUDING REMARKS

Modified Notz design is proposed which are efficiently implementable when the optimum can be achieved based on second-order model in vicinity of boundary of the experimental region with one direction more preferable in each axis. This design consists of factorial points, center point, and one axial point in each axis. This design is compared with other small-sized second-order designs and the traditional response surface designs such as central composite design and Box-Behnken design in terms of the number of design points and optimality criteria. Hybrid designs perform very well in terms of optimality criteria.

If we consider other aspects like ease of implementation and sequential nature of experimentation, hybrid designs are not easy-to-use, with many levels for each factor forcing the experimenter frequently to adjust the experimental conditions. When it is not easy to adjust factor levels or sequential experimentation is necessary, the modified Notz design is recommendable. The modified Notz design will be especially useful when the optimum lies in vicinity of boundary of the experimental region and time is very limited.

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