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Development of a Dual Response Optimization Model under Non-standard Experimental Design Situations

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Abstract **–** The design of experiments is a highly effective offline quality improvement method to optimize the existing and new processes or products. In the literature, standard experimental situations have been paid a lot of attention. In a number of non-standard experimental situations, special experimental design techniques should be considered in order to conduct an experiment for design factors. Indeed, an *I*-optimal design, a computer-generated special experimental design, is a good choice to predict the mean and variance responses under non-standard experimental design situations. In this research work, an *I*-optimal design is selected to generate experimental design points for a non-standard experimental situation. Then, an *I*-optimal design-based dual response optimization model is proposed in order to obtain an optimum operating condition for design factors while minimizing the process variance as small as possible. Comparison studies are also conducted. Finally, a numerical example is conducted in order to illustrate the effectiveness of the proposed optimization model.

Keywords *– Quality improvement, Dual Response Model, Non-standard Experimental Design, I-optimal design, Optimization*

I. Introduction

An alphabetic design, *I*-optimality, was offered by Box and Draper [1]. The *I*-optimality criterion is also known as the I_V-, *Q*-, and *V*-optimality criteria in the literature. Box and Draper [1, 2] used the integrated variance function over a selected design region for the *I*-optimality criterion. Draper [3], Borkowski [4] and Allen and Tseng [5] conducted further studies in the context of the *I*-optimality criterion. In addition, Toro Diaz et al. [6] and Myers et al. [7] provided comprehensive discussions on more theoretical aspects of optimal designs, including the *I*-optimality criterion.

Taguchi [8] introduced the term robust parameter design (RPD) to optimize design factors using the signal-to-noise ratio. Taguchi [8] has introduced that the process mean is at the desired target value while the process variance is as small as possible. Vining and Myers [9] performed one of the earliest research attempts to propose an alternative to Taguchi's method which was the integration of response surface methodology (RSM). This alternative, called the dual response approach, is to minimize the process standard deviation of the response while the process mean of the response equals the target value. Fathi [10] and Del Castillo and Montgomery [11] conducted further improvements of the dual response approach. Lin and Tu [12] used the mean-squared error (MSE) model while allowing the process bias. Therefore, Lin and Tu [12] improved the dual response model while minimizing more variance reduction. Along the same lines, Copeland and Nelson [13] enhanced the MSE model considering a desired upper bound for the process bias. Further work in the area of RPD has been reviewed by Steinberg and Bursztyn [14], Robinson et al. [15], Park et al. [16] and Arvidsson and Gremyr [17]. Ouyang et al. [18], Ozdemir and Cho [19, 20, 21], Tsai and Liukkonen [22], Hot et al. [23], Lu et al. [24] and Chatterjee et al. [25] conducted the recent studies in the context of the RSM-based RPD problems.

The aim of this paper is three-fold. First of all, the I-optimality criterion is selected for prediction purposes. Therefore, an *I*-optimal design is generated using the *I*-optimality criterion under a non-standard experimental situation. Second, the process mean and variance responses are obtained. Third, an *I*-optimal design-based dual response optimization model is developed to obtain optimum operating conditions for design factors.

This paper is organized as follows. Firstly, the proposed methodology development section is presented in Section 2. Secondly, a numerical example is given in Section 3. Finally, the concluding remarks are drawn in Section 4.

II. Proposed Methodology Development

The proposed methodology development consists of the four main phases: (1) the *I*-optimality criterion, (2) the rotatability issue, (3) the modeling step, (4) an *I*-optimal design-based dual response optimization model.

A. The I-Optimality Criterion

The *I*-optimality criterion, $I(\zeta)$, is the average of the scaled prediction variance, $V[\mathbf{x}]$, and it is:

$$\min_{\zeta} \int_R V[\mathbf{x}] d[\mathbf{x}] \Big/ \int_R d[\mathbf{x}]$$

$$\Rightarrow \min_{\zeta} \frac{N}{K} \int_R [\mathbf{x}]^{(m)\prime} (\mathbf{X}'\mathbf{X})^{-1} [\mathbf{x}]^{(m)} d[\mathbf{x}]$$

where $V[\mathbf{x}] = N[\mathbf{x}]^{(m)'}\left(\mathbf{X}'\mathbf{X}\right)^{-1}[\mathbf{x}]^{(m)}$, $\mathbf{x}$ is the vector of design factors, $\mathbf{X}$ represents the model matrix, N is the number of design points, and K is a constant. The goal of the *I*-optimality criterion is to minimize the average prediction variance through the feasible design region. It is also noted that the number of design points is specified by the experimenter.

B. Rotatability Issue

The design rotatability is one of the design properties for the design of experiments [7]. An experimental design is rotatable if the prediction variance is constant and all experimental design points are equidistant from the center point of the experiment. *I*-optimal experimental designs are not rotatable because $[i] = \sum_{a=1}^{n} x_{ia} \Big/ n \neq 0 \ \left(i, j = 1, 2, ..., m \text{ and } i \neq j\right)$ where $[i]$ is the first moments, and $\frac{[iiii]}{[iijj]} = \frac{\sum_{a=1}^{n} x_{ia}^4 \Big/ n}{\sum_{a=1}^{n} x_{ia}^2 x_{ja}^2 \Big/ n} = \frac{\sum_{a=1}^{n} x_{ia}^4}{\sum_{a=1}^{n} x_{ia}^2 x_{ja}^2} \neq 3$ where $[iiii]$ and $[iijj]$ represent the fourth pure moments and the fourth mixed moments, respectively. All experimental design points are not equidistant from the center point of the *I*-optimal experimental design due to non-standard experimental design situations. However, the *I*-optimality criterion provides high-quality predictions over the design space and this criterion does not need to use experimental points outside the original design factor range, such as axial points. In addition, missing corner points could be a good property when the researcher should not deal with the combined factor extremes. Therefore, this property avoids the loss of data in these situations. Finally, it is concluded that the rotatability is not a priority for the *I*-optimal experimental design.

C. Modeling Step

In this paper, the estimated process mean response is found as follows:

$$\hat{\mu}(\mathbf{x}) = \hat{\alpha}_0 + \mathbf{x}'\mathbf{a} + \mathbf{x}'\mathbf{A}\mathbf{x} \text{ where } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ \cdots \\ \cdots \\ x_n \end{bmatrix}, \ \mathbf{a} = \begin{bmatrix} \hat{\alpha}_1 \\ \hat{\alpha}_2 \\ \cdots \\ \cdots \\ \cdots \\ \hat{\alpha}_n \end{bmatrix},$$

$$\text{and } \mathbf{A} = \begin{pmatrix} \hat{\alpha}_{11} & \hat{\alpha}_{12}/2 & \cdots & \hat{\alpha}_{1n}/2 \\ \cdots & & \cdots & \cdots \\ \cdots & & \cdots & \cdots \\ \cdots & & \cdots & \cdots \\ \hat{\alpha}_{n1}/2 & \hat{\alpha}_{n2}/2 & \cdots & a_{nn} \end{pmatrix}$$

where $\hat{\alpha}_i$ is the i^{th} regression coefficient. Vector **a** and matrix **A** represent the estimated regression coefficients of the process mean.

The estimated process standard deviation response is:

$$\hat{\sigma}(\mathbf{x}) = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \text{ where } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ \cdots \\ \cdots \\ x_n \end{bmatrix}, \ \mathbf{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \cdots \\ \cdots \\ \cdots \\ \hat{\beta}_n \end{bmatrix},$$

$$\text{and } \mathbf{B} = \begin{pmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \cdots & \hat{\beta}_{1n}/2 \\ \cdots & & \cdots & \cdots \\ \cdots & & \cdots & \cdots \\ \cdots & & \cdots & \cdots \\ \hat{\beta}_{n1}/2 & \hat{\beta}_{n2}/2 & \cdots & \hat{\beta}_{nn} \end{pmatrix}$$

where $\hat{\beta}_i$ is the i^{th} regression coefficient. Vector **b** and matrix **B** represent the estimated regression coefficients of the process standard deviation.

In a similar way, the estimated process variance response is denoted as follows:

$$\hat{\sigma}^2(\mathbf{x}) = \hat{\gamma}_0 + \mathbf{x}'\mathbf{c} + \mathbf{x}'\mathbf{C}\mathbf{x} \text{ where } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ \cdots \\ \cdots \\ x_n \end{bmatrix}, \ \mathbf{c} = \begin{bmatrix} \hat{\gamma}_1 \\ \hat{\gamma}_2 \\ \cdots \\ \cdots \\ \cdots \\ \hat{\gamma}_n \end{bmatrix},$$

$$\text{and } \mathbf{C} = \begin{pmatrix} \hat{\gamma}_{11} & \hat{\gamma}_{12}/2 & \cdots & \hat{\gamma}_{1n}/2 \\ \cdots & & \cdots & \cdots \\ \cdots & & \cdots & \cdots \\ \cdots & & \cdots & \cdots \\ \hat{\gamma}_{n1}/2 & \hat{\gamma}_{n2}/2 & \cdots & \hat{\gamma}_{nn} \end{pmatrix}$$

where $\hat{\gamma}_i$ is the i^{th} regression coefficient. Vector **c** and matrix **C** represent the estimated regression coefficients of the process standard deviation.

D. Optimization Step

The objective is to minimize the process variance as small as possible in quality engineering problems. Therefore, the objective function of the optimization model is

$$\text{minimize } \hat{\gamma}_0 + \mathbf{x}'\mathbf{c}^* + \mathbf{x}'\mathbf{C}^*\mathbf{x}$$

where $\mathbf{c}^*$ and $\mathbf{C}^*$ are the estimated regression coefficients of the process variance after *I*-optimal design points.

The process mean may be desired at the target value for some cases. Therefore, the constraint is defined as follows:

$$\hat{\alpha}_0 + \mathbf{x}'\mathbf{a}^* + \mathbf{x}'\mathbf{A}^*\mathbf{x} = \mu_\tau$$

where μ_τ is the desired target value, $\mathbf{a}^*$ and $\mathbf{A}^*$ are the estimated regression coefficients of the process mean after *I*-optimal design points.

The boundary requirements for design factors are

$$LB \leq x_i \leq UB$$

where x_i is the i^{th} design factor, LB and UB are lower and upper bounds, respectively.

The proposed optimization scheme is able to achieve more variance reduction based on *I*-optimal design points and collected data.

III. NUMERICAL EXAMPLE

A numerical example is conducted to show how to apply the proposed methodology. The numerical example is modified from Myers et al. [7]. The two design factors and their levels are shown in Table 1.

Table 1. Design factors and their levels

Level	Temperature (^{0}C) (x_1)	Concentration (%) (x_2)
High (+1)	250	25
Center (0)	225	20
Low (-1)	200	15

An *I*-optimal design is generated using the coordinate exchange algorithm. The number of design points is twelve, and the number of design points is specified by the experimenter. If an orthogonal CCD is used, the number of design points is sixteen. Therefore, the number of design points could be decreased with the *I*-optimality criterion. Table 2 shows the collected data for the *I*-optimal design.

Table 2. The collected data for the *I*-optimal design

Run	x_1	x_2	y_1	y_2	y_3	$\bar{y}$	s	s^2
1	0	0	52	58	55	55.0	3.0	9.0
2	1	-1	46	48	50	48.0	2.0	4.0
3	0	-1	48	47	53	49.3	3.2	10.3
4	0	0	47	45	59	50.3	7.6	57.3
5	-1	1	52	56	58	55.3	3.1	9.3
6	-1	-1	28	33	29	30.0	2.6	7.0
7	0	1	68	60	67	65.0	4.4	19.0
8	-1	0	47	52	51	50.0	2.6	7.0
9	1	0	54	45	38	45.7	8.0	64.3
10	0	0	50	60	52	54.0	5.3	28.0
11	0	0	50	55	54	53.0	2.6	7.0
12	1	1	51	53	51	51.7	1.2	1.3

Note that $\bar{\mathbf{y}}$ is the vector for the mean of each design run, $\mathbf{s}$ is the vector for the standard deviation of each design run, $\mathbf{s}^2$ is the vector for the variance of each design run.

The estimated mean and variance responses are

$$\hat{\mu}(\mathbf{x}) = 54.0 + 1.7x_1 + 7.5x_2 - 5.4x_1x_2 - 8.1x_1^2 + 1.2x_2^2$$

$$\hat{\sigma}^2(\mathbf{x}) = 28.6 + 7.7x_1 + 1.4x_2 - 1.3x_1x_2 + 0.5x_1^2 - 20.5x_2^2$$

The proposed optimization model is denoted as follows:

$$\text{Minimize } Z = 28.6 + 7.7x_1 + 1.4x_2 - 1.3x_1x_2 + 0.5x_1^2 - 20.5x_2^2$$

subject to

$$54.0 + 1.7x_1 + 7.5x_2 - 5.4x_1x_2 - 8.1x_1^2 + 1.2x_2^2 = 55$$

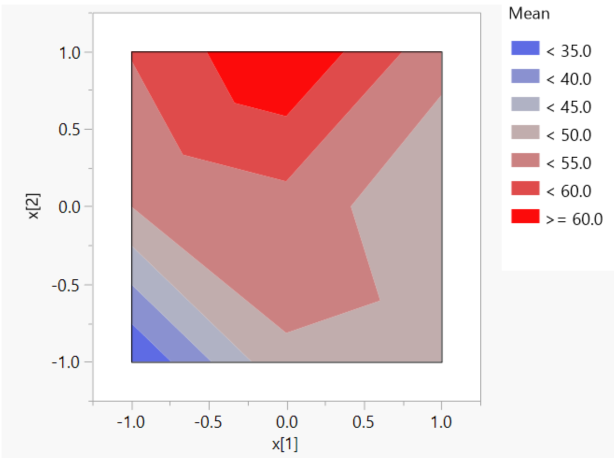
$$-1 \le x_1, x_2 \le +1 \text{ and } x_1, x_2 \in R$$

where $\mu_\tau = 53$. In Table 3, the results of the proposed optimization model are shown.

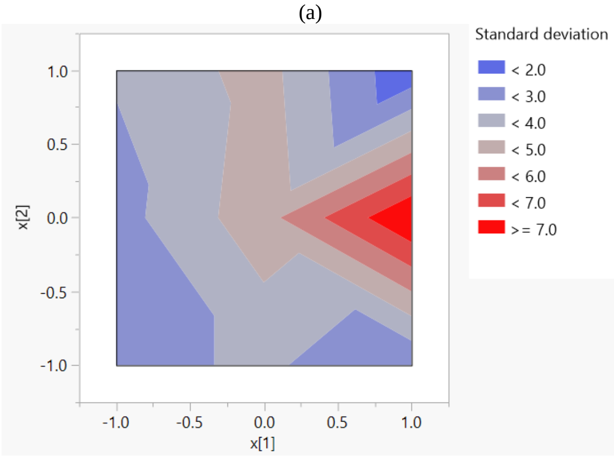
Fig. 1 shows the contour plots for the mean response, the standard deviation response, and the variance response, respectively. It is also noted that the contour plots are important to describe the estimated relationship between design factors and responses.

Table 3. The results of the proposed optimization model for the experiment

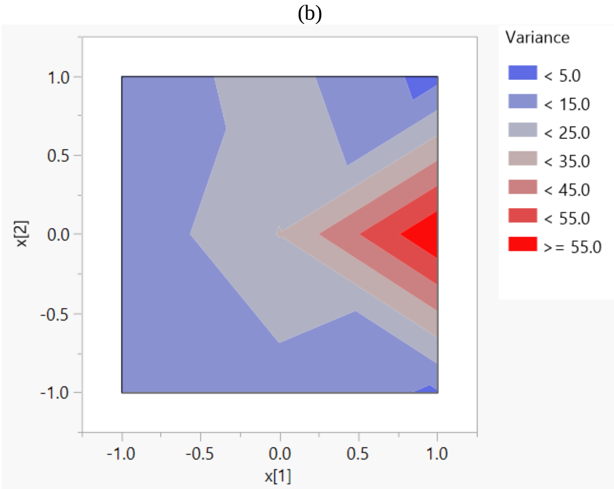
Model	x_1*	x_2*	Min Z $\hat{\sigma}^2(\mathbf{x}^*)$
Proposed model using the *I*-optimality criterion	0.890	1.000	15.597



(a)



(b)



(c)

Fig. 1 (a) Contour plot for the mean response; (b) Contour plot for the standard deviation response; (c) Contour plot for the variance response

The results of the proposed model are based on the desired target value. If the target value changes, the objective function value changes as well. The objective function value denotes the estimated process variance for the collected data. The optimum design factors for the *I*-optimal design are found as 247.25 ^{0}C and 25 %, respectively.

IV. CONCLUDING REMARKS

In this paper, an *I*-optimal design-based robust design optimization model is proposed to find optimum levels of design factors. The results of the numerical example show that optimum levels of design factors are found using the proposed optimization model. In addition, the proposed optimization model is effective to reduce the process variance. It is also noted that the *I*-optimality criterion is a suitable choice for a prediction purpose, a non-standard design region, and less number of design points.

For further studies, a multi-objective optimization model could be proposed in order to optimize two or more mean response functions at the same time. This paper just focuses on controllable design factors. Therefore, both controllable and noise design factors could be considered for *I*-optimal designs.

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