

Statistical Process Optimization Through Multi-Response Surface Methodology

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Abstract—In recent years, response surface methodology (RSM) has brought many attentions of many quality engineers in different industries. Most of the published literature on robust design methodology is basically concerned with optimization of a single response or quality characteristic which is often most critical to consumers. For most products, however, quality is multidimensional, so it is common to observe multiple responses in an experimental situation. Through this paper interested person will be familiarize with this methodology via surveying of the most cited technical papers.

It is believed that the proposed procedure in this study can resolve a complex parameter design problem with more than two responses. It can be applied to those areas where there are large data sets and a number of responses are to be optimized simultaneously. In addition, the proposed procedure is relatively simple and can be implemented easily by using ready-made standard statistical packages.

Keywords—Multi-Response Surface Methodology (MRS), Design of Experiments (DOE), Process modeling, Quality improvement, Robust Design.

I. INTRODUCTION

RESPONSE Surface Methodology (RSM) is a well known up to date approach for constructing approximation models based on either physical experiments, computer experiments (simulations) (Box et al., [1] ; Montgomery, [2]) and experimented observations. RSM, invented by Box and Wilson, is a collection of mathematical and statistical techniques for empirical model building. By careful design of experiments, the objective is to optimize a response (output variable) which is influenced by several independent variables (input variables). An experiment is a series of tests, called runs, in which changes are prepared in the input variables in order to recognize the reasons for changes in the output response (Montgomery & Runger [3]). RSM involves two basic concepts:

- (1) The choice of the approximate model, and
- (2) The plan of experiments where the response has to be evaluated.

The performance of a manufactured product often characterize by a group of responses. These responses in general are correlated and measured via a different measurement scale. Consequently, a decision-maker must resolve the parameter selection problem to optimize each response. This problem is regarded as a multi-response optimization problem, subject to different response requirements. Most of the common methods are incomplete in such a way that a response variable is selected as the primary

one and is optimized by adhering to the other constraints set by the criteria. Many heuristic methodologies have been developed to resolve the multi-response problem. Cornell and Khuri [4] surveyed the multi-response problem using a response surface method. Tai et al. [5] assigned a weight for each response to resolve the problem. Pignatiello [6] utilized a squared deviation-from-target and a variance to form an expected loss function for optimizing a multiple response problem. Layne [7] presented a procedure capable of simultaneously considering three functions: weighted loss function, desirability function, and distance function. While providing a multi-response example in which Taguchi methods are used, Byrne and Taguchi [8] discussed an example involving a connector and a tube.

Logothetis and Haigh [9] also discussed a manufacturing process differentiated by five responses. In doing so, they selected one of the five response variables as primary and optimized the objective function sequentially while ignoring possible correlations among the responses. Optimizing the process with respect to any single response leads to non-optimum values for the remaining characteristics.

II. RESPONSE SURFACE METHODOLOGY

Often engineering experimenters wish to find the conditions under which a certain process attains the optimal results. That is, they want to determine the levels of the design parameters at which the response reaches its optimum. The optimum could be either a maximum or a minimum of a function of the design parameters. One of methodologies for obtaining the optimum is response surface technique.

Response surface methodology is a collection of statistical and mathematical methods that are useful for the modeling and analyzing engineering problems. In this technique, the main objective is to optimize the response surface that is influenced by various process parameters. Response surface methodology also quantifies the relationship between the controllable input parameters and the obtained response surfaces.

The design procedure of response surface methodology is as follows:

- (i) Designing of a series of experiments for adequate and reliable measurement of the response of interest.
- (ii) Developing a mathematical model of the second order response surface with the best fittings.
- (iii) Finding the optimal set of experimental parameters that produce a maximum or minimum value of response.

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- (iv) Representing the direct and interactive effects of process parameters through two and three dimensional plots.

If all variables are assumed to be measurable, the response surface can be expressed as follows:

$$y = f(x_1, x_2, \dots, x_k) \quad (1)$$

The goal is to optimize the response variable y . It is assumed that the independent variables are continuous and controllable by experiments with negligible errors. It is required to find a suitable approximation for the true functional relationship between independent variables and the response surface. Usually a second-order model is utilized in response surface methodology.

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^k \beta_{ij} x_i x_j + \varepsilon \quad (2)$$

where ε is a random error. The β coefficients, which should be determined in the second-order model, are obtained by the least square method. In general (2) can be written in matrix form.

$$\mathbf{Y} = \mathbf{bX} + \mathbf{E} \quad (3)$$

where \mathbf{Y} is defined to be a matrix of measured values, \mathbf{X} to be a matrix of independent variables. The matrixes \mathbf{b} and \mathbf{E} consist of coefficients and errors, respectively. The solution of (3) can be obtained by the matrix approach.

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \quad (4)$$

where \mathbf{X}^T is the transpose of the matrix \mathbf{X} and $(\mathbf{X}^T \mathbf{X})^{-1}$ is the inverse of the matrix $\mathbf{X}^T \mathbf{X}$.

The mathematical models were evaluated for each response by means of multiple linear regression analysis. As said previous, modeling was started with a quadratic model including linear, squared and interaction terms. The significant terms in the model were found by analysis of variance (ANOVA) for each response. Significance was judged by determining the probability level that the F-statistic calculated from the data is less than 5%. The model adequacies were checked by R^2 , adjusted- R^2 , predicted- R^2 and prediction error sum of squares (PRESS). A good model will have a large predicted R^2 , and a low PRESS. After model fitting was performed, residual analysis was conducted to validate the assumptions used in the ANOVA. This analysis included calculating case statistics to identify outliers and examining diagnostic plots such as normal probability plots and residual plots.

Maximization and minimization of the polynomials thus fitted was usually performed by desirability function method, and mapping of the fitted responses was achieved using computer software such as Design Expert.

III. THE SEQUENTIAL NATURE OF THE RESPONSE SURFACE METHODOLOGY

Most applications of RSM are sequential in nature and can be carried out based on the following phases.

Phase 0: At first some ideas are generated concerning

which factors or variables are likely to be important in response surface study. It is usually called a screening experiment. The objective of factor screening is to reduce the list of candidate variables to a relatively few so that subsequent experiments will be more efficient and require fewer runs or tests. The purpose of this phase is the identification of the important independent variables.

Phase 1: The experimenter's objective is to determine if the current settings of the independent variables result in a value of the response that is near 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 process variables that will move the process toward the optimum. This phase of RSM makes considerable use of the first-order model and an optimization technique called the method of steepest ascent (descent).

Phase 2: Phase 2 begins when the process is near the optimum. At this point the experimenter usually wants a model that will accurately approximate the true response function within a relatively small region around the optimum. Because the true response surface usually exhibits curvature near the optimum, a second-order model (or perhaps some higher-order polynomial) should be used. Once an appropriate approximating model has been obtained, this model may be analyzed to determine the optimum conditions for the process. This sequential experimental process is usually performed within some region of the independent variable space called the operability region or experimentation region or region of interest.

IV. MULTI-RESPONSE PROBLEM OVERVIEWS

Optimization of the multi-response problem is a challenge to optimize output responses all together. Among the simultaneous optimization methods, most of the authors used the approaches that combine all the different response requirements into one composite requirement. Hence, the compromise solution is obtained in a much simpler way. A simple weighting method was found in Ilhan et al. [10], as applied in an electrochemical grinding (ECG) process. Zadeh [11] normalized each response and then gave a simple weight for each response. The discussion regarding the assignments of weights can be found in [12].

Myers and Carter [13] proposed an algorithm for obtaining the optimal solutions of the dual-response surface system (DRSM). Their method assumed that the DRSM includes a primary response and a constraint response which both of them can be fitted as a quadratic model.

Lee-Ing Tong et al. [14] used the signal to noise (SN) ratio and system sensitivity are used to assess the performance of each response. They performed principal component analysis (PCA) on SN values and system sensitivity values to obtain a set of uncorrelated principle components, which are linear combinations of the original responses. Additionally, they used of variation mode chart to interpret the variation mode (or principal component variation) resulting from PCA. They suggested that based on engineering requirements, engineers can determine the optimization direction for each principal

component using the variation mode chart. Finally, technique for order preference by similarity to ideal solution (TOPSIS) applied to derive the overall performance index (OPI) for multiple responses. The optimal factor/level combination can be determined with the maximum OPI value and therefore, simultaneously reduces the quality variation and brings the mean to the target value.

Onur Koksoy and Tankut Yalcinoz [15] presented a methodology for analyzing several quality characteristics simultaneously using the mean square error (MSE) criterion when data are collected from a combined array. They proposed a genetic algorithm based on arithmetic crossover for the multi-response problem in conjunction with a composite objective function based on the individual MSE functions of each response.

Lee-Ing Tong et al. [16] proposed procedure used the desirability function and dual-response-surface method to optimize the multi-response problems in a dynamic system. They established a regression model to obtain the sensitivity and quality variation for each experimental run and the desirability function is used to obtain a total measurement for the multiple responses. Next, the dual-response-surface method was used to obtain a set of possible optimal factor-level combinations. The optimal factor-level setting proposed to maximize total desirability.

Liao and Chen [17] proposed data envelopment analysis ranking (DEAR) approach to optimize multi-response problem. The author states that Taguchi method can only be used to optimize single response problems and PCA, although considered to solve multi-response problem, itself has shortcomings. The new approach is capable of decreasing uncertainty caused by engineering judgment in the Taguchi method and overcoming the shortcomings of PCA.

In order to overcome the single response optimization problem of Taguchi method, Liao [18] proposed an effective procedure called PCR-TOPSIS that is based on process capability ratio (PCR) theory and on the theory of order preference by similarity to the ideal solution (TOPSIS) to optimize multi-response problems.

Hsu [19] presents an integrated optimization approach based on neural networks, exponential desirability functions.

Fung and Kang [20] used Taguchi method and PCA to optimize the given process. Initially Taguchi method was used followed by PCA to correspond to multi-response cases, for transforming the correlated friction properties to a set of uncorrelated components and evaluating the principal components. The appropriate number of the principle components, and the influence of the number on the optimum process condition, was subsequently studied by extracting more than one principal component and integrating it into a comprehensive index.

Jiju Antony et al. [21] used artificial intelligent tool (neuro-fuzzy model) and Taguchi method of experimental design to tackle problems involving multiple responses optimization. They proposed a single crisp performance index called Multi-Response Statistics (MRS) as a combined response indicator of several responses. MRS is computed for every run by

applying neuro-fuzzy model. ANOVA is carried out on the MRS values to identify the key factors/interactions having significant effect on the overall process. Finally, optimal setting of the control factors is decided by selecting the level having highest value of MRS.

V. DESIRABILITY FUNCTION

The desirability function was originally developed by Harrington [22] to simultaneously optimize the multiple responses and was later modified by Derringer and Suich [23] to improve its practicality. The desirability function approach is one of the most frequently used multi-response optimization techniques in practice. The desirability lies between 0 and 1 and it represents the closeness of a response to its ideal value. If a response falls within the unacceptable intervals, the desirability is 0, and if a response falls within the ideal intervals or the response reaches its ideal value, the desirability is 1. Meanwhile, when a response falls within the tolerance intervals but not the ideal interval, or when it fails to reach its ideal value, the desirability lies between 0 and 1. The more closely the response approaches the ideal intervals or ideal values, the closer the desirability is to 1. According to the objective properties of a desirability function, the desirability function can be categorized into the nominal-the-best (NB) response, the larger-the-better (LB) response and the smaller-the-better (SB) response. Interested persons can follow the expressed relevant desirability functions in [101]. The proposed desirability function transforms each response to a corresponding desirability value between 0 and 1. All the desirability can be combined to form a composite desirability function which converts a multi-response problem into a single-response one. The desirability function is a scale-invariant index which enables quality characteristics to be compared to various units. In such method the plant manager can easily determine the optimal parameters among a group of solutions.

Kun-Lin Hsieh et al. [24] believed that when desirability values lies more close to 0 or 1 may lead to a bad model's additive. To solve this problem, they referred to Taguchi suggestion in using the Omega (Ω) transformation which is employed to transfer the data into an additive mode. Ω transformation's philosophy is to simultaneously maximize the average of the system and minimize the variation via S/N. This transformation transfer the desirability data lying in $[0,1]$ to the range of $(-\alpha, +\alpha)$. This transformation can resolve the problem by summing up the control factor's effect when the data lie outside the interval $[0,1]$.

VI. SPECIAL CASE: DUAL-RESPONSE SURFACE METHOD

In practical cases, there are many situations where the researchers encounter to multi-responses. In such cases surveying two or more response variables are critical.

Over the last few years in many manufacturing organizations, multiple response optimization problems were resolved using the past experience and engineering judgment, which leads to increase in uncertainty during the decision-

making process.

Myers and Carter [25] proposed an algorithm for obtaining the optimal solutions of the dual-response surface method (DRSM). Their method assumed that the DRSM includes a primary response, y_p and a constraint response, y_s . Both y_p and y_s can be respectively fitted as a quadratic model as follows:

$$y_p = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^k \beta_{ij} x_i x_j + \varepsilon_p$$

$$y_s = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^k \beta_{ij} x_i x_j + \varepsilon_s \quad (4)$$

where the β 's and γ 's represent the unknown coefficients, and ε_p and ε_s denote the random errors, respectively. The random errors are assumed to possess a normal distribution with mean 0 and variance σ^2 .

The DRSM attempts to obtain a set of X , which can optimize \hat{y}_p subjected to the constraint $\hat{y}_s = c$, where C is a constant.

The desirability function simultaneously optimize the multiple responses and was later modified by Derringer and Such [23] to improve its practicality. The desirability function approach is one of the most frequently used multi-response optimization techniques in practice. The desirability lies between 0 and 1 and it represents the closeness of a response to its ideal value. If a response falls within the unacceptable intervals, the desirability is 0, and if a response falls within the ideal intervals or the response reaches its ideal value, the desirability is 1.

Meanwhile, when a response falls within the tolerance intervals but not the ideal interval, or when it fails to reach its ideal value, the desirability lies between 0 and 1. The more closely the response approaches the ideal intervals or ideal values, the closer the desirability is to 1. According to the objective properties of a desirability function, the desirability function can be categorized into three forms, nominal-the-best (NB), larger-the-better (LB) and smaller-the-better (SB).

The total desirability is defined as a geometric mean of the individual desirability:

$$D = (d_1 \times d_2 \times \dots \times d_k)^{1/k} \quad (5)$$

where D is the total desirability and d_i is the i^{th} desirability, $i = 1, 2, \dots, k$. If all of the quality characteristics reach their ideal values, the desirability d_i is 1 for all i . Consequently, the total desirability is also 1. If any one of the responses does not reach its ideal value, the desirability d_i is below 1 for that response and the total desirability is below 1. If any one of the responses cannot meet the quality requirements, the desirability d_i is 0 for that response. Total desirability will then be 0. The desirability function is a scale-invariant index which enables quality characteristics to be compared to various units. Therefore, the desirability function is an effective means of

simultaneously optimizing a multi-response problem.

VII. MODEL ADEQUACY CHECKING

To verify the derived mathematical model of each response, model adequacy is always necessary to:

1. Examine the fitted model to ensure that it provides an adequate approximation to the true system;
2. Verify that none of the least squares regression assumptions are violated. There are several techniques for checking model adequacy.

Residual Analysis: The residuals from the least squares fit, defined by $e_i = y_i - \hat{y}_i$, $i = 1, 2, \dots, n$, play an important role in judging model adequacy. Many response surface analysts prefer to work with scaled residuals, in contrast to the ordinary least squares residuals. These scaled residuals often convey more information than do the ordinary residuals.

The standardizing process scales the residuals by dividing them by their average standard deviation. In some data sets, residuals may have standard deviations that differ greatly. There is some other way of scaling that takes this into account. Let's consider this.

The vector of fitted values \hat{y}_i corresponding to the observed values y_i is

$$\hat{\mathbf{y}} = \mathbf{Xb} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{Hy} \quad (6)$$

The $n \times n$ matrix $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ is usually called the hat matrix because it maps the vector of observed values into a vector of fitted values. The hat matrix and its properties play a central role in regression analysis.

Since $e_i = y_i - \hat{y}_i$, there are several other useful ways to express the vector of residuals

$$\mathbf{e} = \mathbf{y} - \mathbf{Xb} = \mathbf{y} - \mathbf{Hy} = (\mathbf{I} - \mathbf{H})\mathbf{y} \quad (7)$$

The "prediction error sum of squares" (PRESS) proposed in [26, 27], provides a useful residual scaling

$$PRESS = \sum_{i=1}^n \left(\frac{e_i}{1 - h_{ii}} \right)^2 \quad (8)$$

From [27], it is easy to see that the PRESS residual is just the ordinary residual weighted according to the diagonal elements of the hat matrix h_{ii} . Generally, a large difference between the ordinary residual and the PRESS residual will indicate a point where the model fits the data well, but a model built without that point predicts poorly.

VIII. CONCLUSION

The RSM is one of the design of experiments (DOE) methods used to approximate an unknown function for which only a few values are computed. The RSM stems from science disciplines in which physical experiments are performed to study the unknown relation between a set of variables and the system output, or response, for which only a few experiment

values are acquired. These relations are then modeled using a mathematical model, called response surface.

There are many situations where the quality engineers encounter to several correlated responses simultaneously. In such cases decision making on optimum set of parameters is a complicated mathematical problem. In this paper an analysis of the most cited methods proposed and the.

Through this paper, readers could be familiar to multi-response optimization problem via the most cited methods. The residual analysis method and the prediction error sum of squares (PRESS) proposed for evaluating the capability of the designed models. Researcher could follow standard optimization techniques such as the differentiation, the operation research method to set their process in optimum conditions.

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