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IRANIAN JOURNAL OF OPTIMIZATION

Volume 3, issue 1, Winter 2011,189-200
Research Paper

Islamic Azad University
Rasht Branch

Important Issues in Multiple Response Optimization

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Abstract

There have been many productive methods developed so far for optimization of multiple response surface (MRS) problems. This paper tends to review the most seminal approaches in MRS and discuss the strength and weakness of each of the approaches through existing aspects in MRS. A numerical example is included to compare results by different methods. Finally some of the prominent areas for future research discussed by different researchers are presented.

Keywords: Experimental Design; Multiple – Response Surface; Response Surface Methodology; Optimization.

1. Introduction

In today's highly competitive market, companies are impelled to constantly improve the quality of their products. Off- line quality control is a cost – effective means of optimizing product and process design in support of on – line quality control. Control parameters are factors which can be controlled by the designer and noise parameters are factors which can not be controlled. Optimization means finding the optimal setting of the control factors in such a manner that the product characteristic or response attains its target with minimum variation. Response surface methodology (RSM) is a collection of mathematical and statistical techniques used in empirical study of response and control factors. Detailed description of various response surface techniques can be found on Myers and Montgomery, khuri and cornell.[9,6]. However, many processes involve more than one quality characteristic which are called multiple – response surface (MRS) and can be formulated as follows:

$$\text{Optimize} \quad [\hat{y}_1(x), \hat{y}_2(x), ..., \hat{y}_r(x)] \quad i = 1,2,\ldots,r$$

$$\text{s.t.} \quad x \in \Omega,$$

where $\hat{y}_i(x)$ denotes the estimated i–th response, x is an input vector and Ω is experimental region. The optimization phase of multiple – response problem can result in trade - offs between different responses. Eventually, the goal is to find a possible solution that leads to the best combination of responses.

In this article, we review and categorize different approaches developed so far in MRS.

2. Classification of Existing Approaches in MRS

There have been many productive methods for multiple – response optimization which have been discussed in the literature. Pignatiello categorized the existing methods in three basic categories; herein, we will classify them in four basic categories [12]. Approaches developed so far mostly started by building regression models to estimate the responses of interest; however, in some other approaches model building is done at other stages.

1.2Building regression models

Polynomial regression models are aimed to estimate the relation between each of the responses and control factors. The models can whether estimate the relation between location or dispersion of each of the responses and control factors. The most common algorithm in building regression models is ordinary least square (OLS); however, Ortiz proposed using zellner's seemingly unrelated regression (SUR) for multiple – response problems with correlated responses [11].

In the next steps each of the three mentioned categories follows different procedure. Herein, we will discuss steps which are followed in each category.

2.2First Category: Overlaying Contour Plots

This graphical category consists of overlaying contour plots of responses to find the region of interest. The contour plots achieved from regression models developed to estimate the location of the responses. Region of interest is a region in the problem space all of the responses are simultaneously satisfied. An explanation for this category is available in Myers and Montgomery which obviously include its ease of use. However, there are two main problems to this category [9]. First, this category fails to recognize the most dominant solution in the problem space. Second, its usage can be quite difficult to analyze in problems with three or more control factors (high dimension).

3.2Second Category: Constrained Optimization Problem

This category is classified in Kim as priority – based approach. Different approaches have been proposed in this category [7]. The most common approach selects the most important response and uses it as the objective function and employs the rest of responses as constrains.

Optimize Primary Response

s.t. Requirments for other Responses

$x \in \Omega$

It should be noted that choosing one of the responses as the objective function may not be easy in all cases. Furthermore, this approach does not conform to the basic idea of simultaneously consider all the responses [7]. This approach could be considered to be contrary to the never – ending goal of continual quality improvement since no explicit effort would be made for improving the secondary responses. An example to this approach can be found in Del Castillo and Montgomery through with they solved a dual response problem [2].

Kim and Lin proposed using "minimum" operator for aggregating all the responses on both location and dispersion effects [8]. Their optimization can be formulated as follows

$$\underset{x}{\text{Maximize}} \quad \lambda$$

$$\text{s.t.} \quad d_{\mu_j}\left(\hat{y}_{\mu j}(x)\right) \geq \lambda \quad , \quad j = 1,2,\ldots,r$$

$$d_{\sigma j}\left(\hat{y}_{\sigma j}(x)\right) \geq \lambda \quad , \quad j = 1,2,\ldots r$$

$$x \in \Omega$$

Where λ is the minimum operator, $d_{\mu_j}\left(\hat{y}_{\mu j}(x)\right)$ is the DM's[1] degree of satisfaction from estimated mean of the j^{th} response and $d_{\sigma_j}\left(\hat{y}_{\sigma j}(x)\right)$ is the DM's degree of satisfaction from estimated standard deviation of the j^{th} response. This approach has the advantage of considering both location and dispersion effect of all

[1] - Decision Maker

responses. Generally, approaches available in this category have the advantage of utilizing the existing optimization methods.

4.2Third Category: Combination of Response Surfaces one

Similar to other categories, mentioned before, different approaches in this category start their procedure by building appropriate models to estimate the responses locations. These models are then combined into a single value response surface and solved as a single objective problem by an optimization technique. Various approaches are so far developed in this category through different combination techniques and different optimization techniques. Next we will discuss different approaches in this category.

5.2Desirability Function Approach

In this approach an estimated jth response $(\hat{y}_j, j=1,2,...,r)$ is transformed to a scaled free value in the interval 0 to 1 called individual desirability ($d_j(\hat{y}_j(x))$). Individul desirabilities for different responses are then combined to form the overall desirability (D). The most dominant solution is then determined by optimizing D [4].

Derringer and Suich extended Harrington's idea by developing a new transform function as individual desirability functions and aggregate them through geometric mean. Individual desirability function for the case of the target the better is as follows [4].

$$d_j(\hat{y}_j(x)) = \begin{cases} \left(\dfrac{\hat{y}_j - y_{\min j}}{T_j - y_{\min j}}\right)^s & \text{if} \quad y_{\min j} \le \hat{y}_j(x) \le T_j, \\ \left(\dfrac{\hat{y}_j - y_{\max j}}{T_j - y_{\max j}}\right)^t & \text{if} \quad T_j \le \hat{y}_j(x) \le y_{\max j}, \\ 0 & \textit{otherwise,} \end{cases}$$

where $y_{\min j}$,$y_{\max j}$ are minimum, maximum acceptable values for $\hat{y}_j$ and T_j is its target value. “t” and “s” are parameters that define the shape of desirability functions. Weighting of different responses to account for their relative importance can be achieved through elevating the peaks of individual desirability functions. A problem that arises in optimization of single value response surface D is that only search methods can be employed in optimization (e. g., the Hooke – Jeeves method as in Derringer and suich or Nelder – Mead simplex [10]. This is due to the fact that gradient – based methods need the first derivative function to be continuous through the domain. Desirability functions defined in Derringer and suich have points where their first derivative does not exist [10]. Del Castillo, Montgomery and Mccarville fitted polynomial of degree four in the small neighborhood of these breakpoints [3]. Hence, they used a gradient – based method (GRG[2]) to do the optimization.

Pignatiello discussed that neither gradient-based nor search methods are able to find the most dominant solution in badly behaved, multimodal and complex combined response surface [11]. They proposed using genetic algorithm as a heuristic search method to do the optimization. As the desirability function defined by Derringer and suich was unable to differentiate between infeasible and undesirable point and since an infeasible point may have some useful information for the algorithm, they added a penalty term to the total desirability to form an unconstrained desirability function (for detailed information refer to pignatiello) [11].

6.2Distance function Approach

Distance function approach is developed by Khuri and Conlon [5]. This approach aimes to find the most dominant solution by minimizing a distance function defined below:

$$p[\hat{y}(x),\phi]=\left[(\hat{y}(x)-\phi)'\{\mathrm{var}[\hat{y}(x)]\}^{-1}(\hat{y}(x)-\phi)\right]^{1/2}$$

Where $\hat{y}(x)$ is the vector of estimated responses, ϕ is a fixed non –stochastic target vector and var $[\hat{y}(x)]$ is the variance – covariance matrix of the estimated responses. Optimization of the distance function can either be done through gradient based or search methods.

7.2Loss Function Approach

The loss function approach was originally developed by pignatiello squared error loss function is as follows [12].

$$\text{Loss }(y(x))=(y(x)-\tau)'c(y(x)-\tau)$$

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[2] - *Generalized Reduced Gradient*

Where $\hat{y}(x)$ is the vector of responses, τ is the target vector and C is the cost matrix representing the relative importance of responses. He defined the objective of optimization the minimization of expected loss that can be derived as:

$$E[loss(y(x))] = trace(C\Sigma(x)) + (\eta(x) - \tau)' c(\eta(x) - \tau),$$

where $\Sigma(x)$ is the variance – covariance matrix and $\eta(x)$ the vector of expected value of the responses. It can be seen that the approach considers responses and not their estimation; hence, no prior model building is required. Pignatiello then discussed some strategies on minimization of the expected loss. Since this approach uses variance – covariance matrix of the responses, it does not consider the quality of prediction. Vinning proposed using the following loss function which accounts for quality of prediction as well [1].

$$\hat{E}(L) = [\hat{y}(x) - \tau]' C[\hat{y}(x) - \tau] + trace[C\Sigma_{\hat{y}}(x)],$$

where $\Sigma_{\hat{y}}(x)$ is the variance – covariance matrix of the predicted responses. It is obvious that prior model building is required in this approach. This approach produces Khuri and Conlons distance function as a special case.[5]

8.2Forth Category: Proportion of Conformance approach

This category includes a potent approach developed by Chiao and Hamada [1]. This approach considers the variance- covariance matrix as dependant on experimental factors as suggested by pignatiello [12]. The approach considers multiple response as a multivariate normal distribution models parameters in term experimental factors. Given a specification region, a measure of quality is the probability that m component responses simultaneously meeting their respection which is called proportion of conformance.

$$P\ (Y \in S),$$

where S is specification region and Y is multivariate normal distribution. The approach do the optimization through finding setting of control factors that maximizes the proportion of conformance.

3. Different aspects in MRS

Different approaches developed so far in the literature of MRS are viewed through three points of view: 1) Consideration of Correlation 2) Consideration of Process Economics
3) Quality of Response Models. In this section, we will discuss existing approaches through these aspects. Graphical approach discussed in the first

category is not an optimization method; hence, we will not classify it through these view points. However, it should be noted that this approach is a powerful tool in detecting the region of interest.

1.3Correlation among the Responses

The correlation means the strength of relationship among different responses. Not considering the correlation among the responses will result in erroneous results. In different categories correlation structure can be considered in different ways. However, as they all share prior model building stage, correlation can be considered through using more efficient methods of model building (e. g. seemingly unrelated regression.[11]

Approaches developed so far in the second category do not consider the correlation structure. However, proportion of conformance approach classified in the forth category is highly applicable for conditions where there exist high correlation among responses of interest. In the third category, correlation structure can considered through the stage in which different response surfaces are combined into one (In addition to model building stage discussed above). Distance function and loss function approaches consider the correlation structure through utilizing variance – covariance matrix. Desirability function approach using OLS method for building models for different responses does not consider correlation structure.

2.3Process Economics

By considering process economics we mean that whether an approach is capable of weighing different responses according to their importance or not.

Existing approaches in the second category are not capable of considering the process economics. In the third category, desirability function approach considers the process economics through assigning different weights on each response and also through defining the shape of desirability function. The loss function approach does consider the process economics by properly choosing C matrix. The distance function approach is incapable of considering the process economics and it lets the correlation structure and the design dictate the sensitivity of the distance measure. In addition, proportion of conformance approach classified in the forth category, is unable to consider the process economics.

3.3Quality of Response Models

The quality of response models refers to how reliable the estimated response models are. Usually, the quality of response models is discussed from two aspects: 1) The quality of description 2) The quality of prediction. The quality of description refers to how well the response models predict data. Mean square error (MSE), R^2 or adjusted R^2 are measures for quality of description. The quality of prediction means how large the variance of a model is at a specific setting control factors [7].

The approaches developed so far in the second category do not consider the quality of prediction. In the third category, the distance function approach considers the quality of prediction through Variance – Covariance matrix of predicted responses. The loss function approach developed by pignatiallo does not consider the quality of prediction; on the other hand, the Vinning's approach takes into account the quality of prediction through Variance – covariance matrix of predicted responses [12].

4. An Example

To illustrate the application of different approaches, an example of a multiple response problem is solved with some of the mentioned approaches. An example concerning a wire bonding process in semiconductor industry is gotten from Del Castillo et al [3]. Three control factors that influence six responses of and their levels in a Box – Behenken design are as Table 1.

Table 1: Factors and Their Levels in the Box – Behenken Experimental Design.

Factor	Neme	Units	Low Level	High Level
A	Flow Rate	SCFM	40.0	120.0
B	Flow Temp	˚C	200.0	450.0
C	Block Temp	˚C	150.0	350.0

Four responses are the bond temperature of two different positions at the beginning and finishing of the process and two others are the maximum bond temperature of these two positions during the process. The objective of the optimization is to make the response variables $Y_{1,}$ $Y_{2,}$ $Y_{3,}$ $Y_{4,}$ $Y_{5,}$ $Y_{6,}$ as close as possible to target Values 190, 185, 185, 190, 185, 185, respectively. The experimental results are shown in Table 2.

Table 2: Experimental Runs.

Flow Rate	Flow Temp	Block Temp	Y_1	Y_2	Y_3	Y_4	Y_5	Y_6
40	200	250	139	103	110	110	113	126
120	200	250	140	125	126	117	114	131
40	450	250	184	151	133	147	140	147
120	450	250	210	176	169	199	169	171
40	325	150	182	130	122	134	118	115
120	325	150	170	130	122	134	118	115
40	325	350	175	151	153	143	146	164
120	325	350	180	152	154	152	150	171
80	200	150	132	108	103	111	101	101
80	450	150	206	143	138	176	141	135
80	200	350	183	141	157	131	139	160
80	450	350	181	180	184	192	175	190
80	325	250	172	135	133	155	138	145
80	325	250	190	149	145	161	141	149
80	325	250	180	141	139	158	140	148

Regression models were first fitted to six responses of interest using the OLS estimation. The models computed in Del Castillo et al. in form of coded are as follows [3].

$$\hat{Y}_1 = 174.93 + 23.38x_2 + 3.62x_3 - 19.00x_2x_3$$

$$\hat{Y}_2 = 141.00 + 6.00x_1 + 21.02x_2 + 14.12x_3$$

$$\hat{Y}_3 = 139.53 + 7.25x_1 + 16.00x_2 + 19.75x_3$$

$$\hat{Y}_4 = 154.90 + 10.10x_1 + 30.60x_2 + 6.30x_3 - 11.20x_1^2 + 11.30x_1x_2$$

$$\hat{Y}_5 = 139.29 + 4.63x_1 + 19.75x_2 + 16.13x_3 - 5.41x_1^2 + 7.00x_1x_2$$

$$\hat{Y}_6 = 146.86 + 4.87x_1 + 15.62x_2 + 27.00x_2 - 3.98_1^2 + 4.75x_1x_2$$

The six contour plots associate with responses of interest are shown in Figure 1.

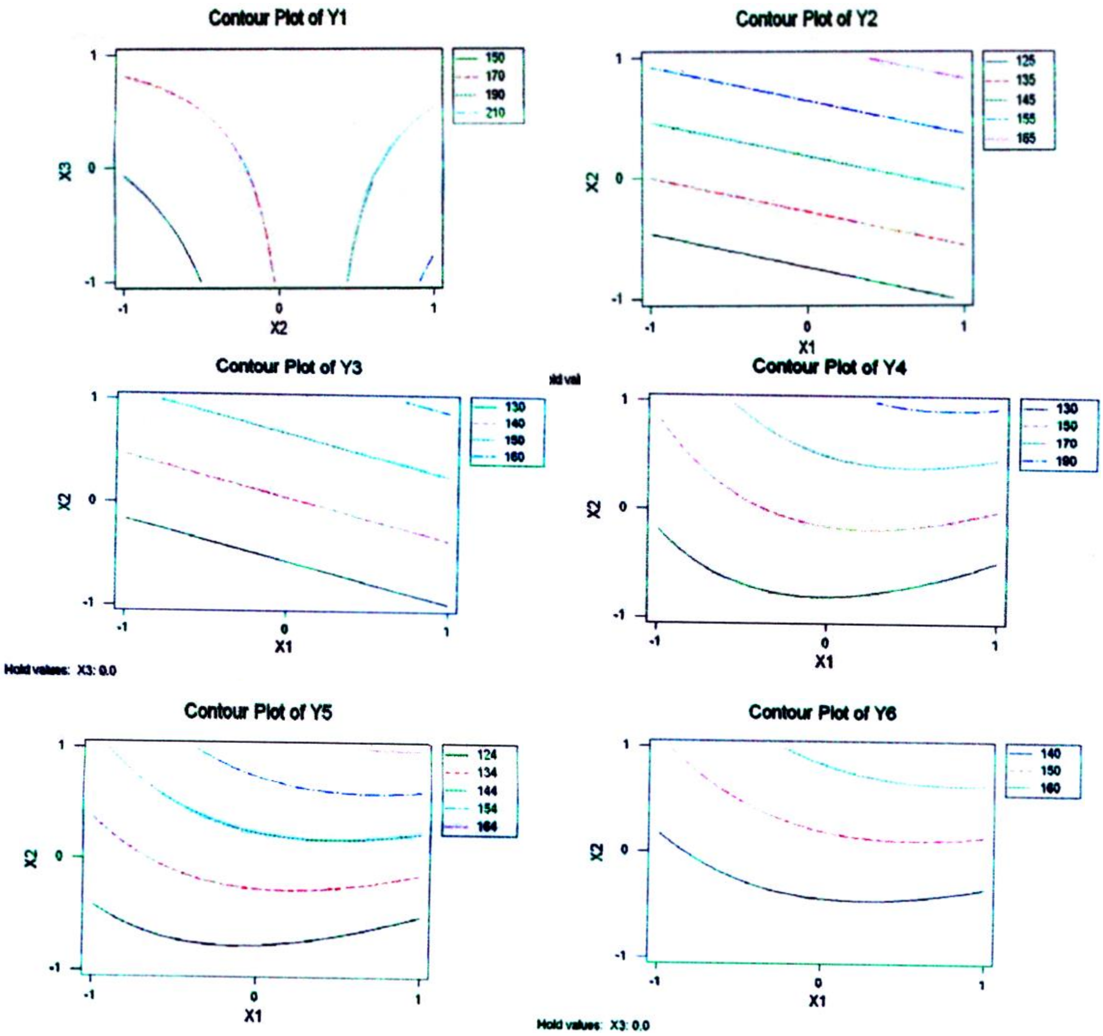

Figure (l): Contour plost for the six responses.

The problem is optimized using the priority – based approach, modified desirability approach and the approach developed in pignatiello et al. [11]. Since the X matrix for the six response models are different approach. The proportion of conformance approach requires the design matrix to include replication to estimate models for variances; therefore, the approach is not performed to this problem. Final results are shown in Table 3.

Table 3: Comparison of the final solutions.

Approach	X	Y_1	Y_2	Y_3	Y_4	Y_5	Y_6
Priority - based	(90.16, 445.95,327.33)	192.1	184.1	181.0	193.7	180.3	171.2
Pignatiello	(74.55, 472.90,332.75)_	187.0	176.7	173.8	192.9	174.2	186.2
Del Castillo	(84.16,450.00, 329.87)	186.0	174.5	172.0	192.6	173.0	185.0

5. Conclusions

In this article, the existing issues in MRS are discussed from a different point of view. Furthermore, some of the important aspects in MRS such as correlation structure, process economics, and quality of response models have been discussed. It is obvious that an optimum approach would be the one which simultaneously considers all three aspects. Seemingly unrelated regression is a technique that can be considered to account for the correlation among the responses of interest. To improve the quality of description, future researches could be focused on utilizing efficient methods of model building. Furthermore, application of artificial neural networks could be helpful to estimate the complex relationships among the responses and control factors.

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