Optimization Criteria Ability to Depict Pareto Frontiers

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***Abstract*- Optimization criteria ability to depict Pareto frontiers is evaluated using two examples from the literature. Results show that criteria built on different approaches perform differently. Performance of a desirability-based method is unsatisfactory whereas the consistent performance of a global criterion gives confidence to use it in real-life problems developed under the Response Surface Methodology.**

***Index Terms*- Bias, Compromise, Desirability, Dual, Pareto, Variance.**

I. Introduction

Typically, multiple response optimization (MO) problems have many Pareto optimal solutions that impact differently on process or product. Some of them may lead to operation conditions more hazardous, more costly or more difficult to implement and control. Therefore, it is of decision-maker (DM) interests to use a method with the ability to capture a set of nondominated solutions evenly distributed along the Pareto frontier. Nondominated solutions are those where any improvement in one response cannot be done without degrading the value of, at least, another response. If the method fails to capture them, the DM may have denied the possibility of finding a more favorable compromise solution.

Methods ability to depict Pareto Frontiers has been rarely evaluated in the Response Surface Methodology (RSM) framework, which difficult the practitioners task of choosing an effective criterion to solve MO problems. This article compares the working abilities of two easy-to-use optimization criteria and helps practitioners in making more informed decisions when they need to select an optimization criterion for solving real-life problems developed under the RSM, which is comprehensively exposed in [1]. The remainder of the article is organized as follows: Next section provides a literature overview; then selected optimization criteria are reviewed; Sections IV and V include the examples and results discussion, respectively; Conclusions are presented in Section VI.

Manuscript received February 11, 2014.

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II. Literature Overview

Most real-life problems involve multiple and conflicting objectives so their analysis has been a widely research subject. As a result, a great quantity and variety of criteria to generate solutions for multiresponse problems are available in the literature. The two most popular criteria in the RSM framework are built on desirability and loss function approaches.

An extensive review on desirability-based criteria is presented in [2]. From the popular desirability criterion proposed by Derringer and Suich [3], later modified by Derringer [4], to less known proposal of Das and Sengupta [5], twelve methods were reviewed. Reference [6] provides an extensive review on loss function-based criteria and summarizes the relative merits of twelve multivariate loss and desirability criteria. Reference [7] combines the strengths of two popular loss function-based criteria, namely the Pignatiello's and Vining's criteria [8]-[9].

Other contributions introduced in the last decade are the mean squared error [10], weighted signal-to-noise ratio [11], PCA-based grey relational analysis [12], weighted principal component [13], capability index [14], patient rule induction [15], design envelopment analysis [16], compromise programming [17], goal programming [18], physical programming [19]-[20], bayesian probability [21], weighted Tchebycheff formulations [22], modified ε-constraint method [23]-[25]. This list is not exhaustive. Many other researchers have contributed to the growing wealth of knowledge in the field. However, little attention is paid to methods ability to depict Pareto frontiers. Exceptions are the works by Costa et al. [26] and Köksoy and Doganaksoy [27], though these studies only evaluated a very small number of criteria and case studies.

III. Optimization Criteria

In the next subsections two criteria built on different approaches are reviewed, namely a desirability-based criterion (DAM criterion) and a global criterion-based criterion (GC criterion).

A. DAM criterion

Ch'ng et al. [28] proposed to minimize an arithmetic mean of individual desirability functions defined as

$$\left(\sum_{i=1}^{n} \omega_i \left| d_i - d_i(T_i) \right| \right) \Big/ n \qquad (1)$$

ISBN: 978-988-19253-5-0
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

where $d_i(T_i)$ is the value of the i-th individual desirability function for $\hat{y}_i$ at target value T_i, ω_i represents the priority (weight or importance) assigned to $\hat{y}_i$, n is the number of responses, and $\sum_{i=1}^{n}\omega_i = 1$. The individual desirability functions are defined as

$$d = \frac{2\hat{y} - (U + L)}{U - L} + 1 = \frac{2}{U - L}\hat{y} + \frac{-2L}{U - L} = m\hat{y} + c \qquad (2)$$

where $0 \le d \le 2$ and U and L are upper and lower bounds of estimated responses that are usually available for product or process quality control.

B. GC criterion

Costa and Pereira [29] proposed to minimize an arithmetic function defined as

$$\sum_{i=1}^{n}\left(\frac{|\hat{y}_i - T_i|}{U_i - L_i}\right)^{p_i} \qquad (3)$$

where p_i are user-specified parameters (shape or power factors, $p_i > 0$). In this criterion, like for the previous one, for Smaller-The-Best (STB) response type (the estimated response value is expected to be smaller than the upper bound U; $\hat{y} < U$) the target value T=L, and for Larger-The-Best (LTB) response type (the estimated response value is expected to be larger than a lower bound L; $\hat{y} > L$) the target value T=U.

IV. EXAMPLES

To better understand the working abilities of the criteria (1) and (3), namely its ability to depict Pareto frontiers, two examples were selected from the literature. Examples only deal with the optimization of two responses so as to display the Pareto frontier graphically. The first example has appeared repeatedly in the literature and its objective is to maximize the conversion of a polymer and minimize the thermal activity. The second one deals with the optimization of metal removal rate for a cutting machine.

Example 1- A central composite design with four center points was run to determine the settings for reaction time (x_1), reaction temperature (x_2), and amount of catalyst (x_3) to maximize the conversion (y_1) of a polymer and achieve a target value for the thermal activity (y_2). Estimated response models are

$$\hat{y}_1 = 81{,}0943 + 1{,}0290\ x_1 + 4{,}0426\ x_2 + 6{,}2060\ x_3 - 1{,}8377\ x_1^2 + 2{,}9455\ x_2^2 - 5{,}2036\ x_3^2 + 2{,}1250\ x_1 x_2 + 11{,}3750\ x_1 x_3 - 3{,}8750\ x_2 x_3$$

$$\hat{y}_2 = 59{,}8505 + 3{,}5855\, x_1 + 0{,}2547\, x_2 + 2{,}2312\, x_3 + 0{,}8360\, x_1^2 + 0{,}0742\, x_2^2 + 0{,}0565\, x_3^2 - 0{,}3875\, x_1 x_2 - 0{,}0375\, x_1 x_3 + 0{,}3125\ x_2 x_3$$

The ranges for y_1 and y_2 are [80, 100] and [55, 60], respectively. Assuming that y_1 is a LTB-type response, its target value is set equal to 100; y_2 is a NTB-type response and its target value is 57.5. The constraints for the input variables are $-1.682 \le x_i \le 1.682$ $(i = 1, 2, 3)$.

DAM criterion can't yield a satisfactory representation of Pareto frontier. This criterion only generated three alternative solutions (see Table I for details) whereas GC criterion generated a larger set of alternative solutions. Figure 1 shows that GC criterion yielded a satisfactory representation of the Pareto frontier for this problem, generating solutions with low bias values for $\hat{y}_2$, including solutions with $\hat{y}_2$ on target value, and solutions with $\hat{y}_1$ value close to the target ($\hat{y}_1 = 98$). This means that GC criterion can satisfy decision-makers with different sensitivities to conversion and thermal activity responses, which are in conflict.

TABLE I
DAM Solutions

(ω_1, ω_2)	(x_1, x_2, x_3)	$(\hat{y}_1, \hat{y}_2)$	D
(0.22, 0.78)	(−0.5434, 1.682, −0.5984)	(95.21, 57.50)	0.053
(0.89, 0.11)	(0.0221, 1.682, −0.2019)	(96.13, 60.00)	0.227
(0.86, 0.14)	(−1.682, 1.682, −1.058)	(98.03, 55.00)	0.155

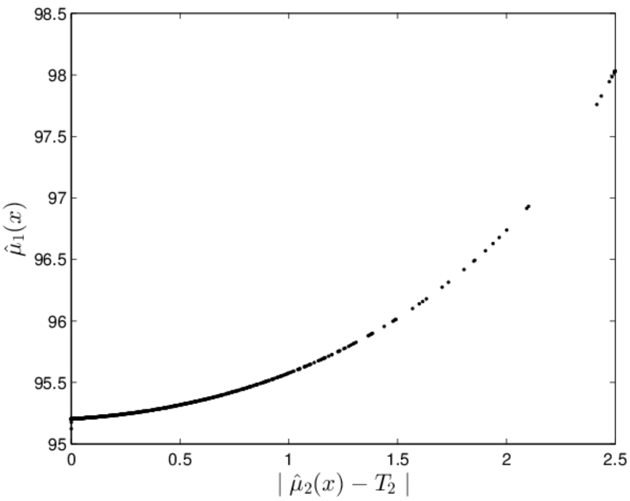

Fig. 1 – GC Solutions

Example 2- Metal removal rate for a cutting machine was evaluated using a central composite design with three replicates. Design variables are cutting speed (x_1), cutting depth (x_2), and cutting feed (x_3). The models fitted to mean ($\hat{\mu}$) and standard deviation ($\hat{\sigma}$) responses are as follows:

$$\hat{\mu} = 79.89 + 1.25\, x_1 - 0.15\, x_2 + 0.08\, x_3 - 1.47\, x_1 x_2 + 0.75\, x_1 x_3 + 0.87\, x_2 x_3 - 2.07\, x_1^2 - 0.22\, x_2^2 - 0.49\, x_3^2$$

ISBN: 978-988-19253-5-0
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

$$\hat{\sigma} = 1.79 + 0.11\,x_1 + 0.35\,x_2 - 0.15\,x_3 + 0.64\,x_1x_2 - 0.18\,x_1x_3 + 0.97\,x_2x_3 - 0.26\,x_1^2 - 0.09\,x_2^2 + 0.04\,x_3^2$$

The mean response is of NTB-type ($69 < \hat{\mu} < 83$) with target value equal to 71 and $\hat{\sigma}$ is of STB-type ($\hat{\sigma}<1.95$) with target value equal to zero. The constraints for the input variables are $-\sqrt{3} \le x_i \le \sqrt{3}$ (i = 1, 2, 3).

In this example both criteria performed satisfactorily, generating a large set of alternative solutions evenly distributed along the Pareto frontier, such as Figures 2-3 show.

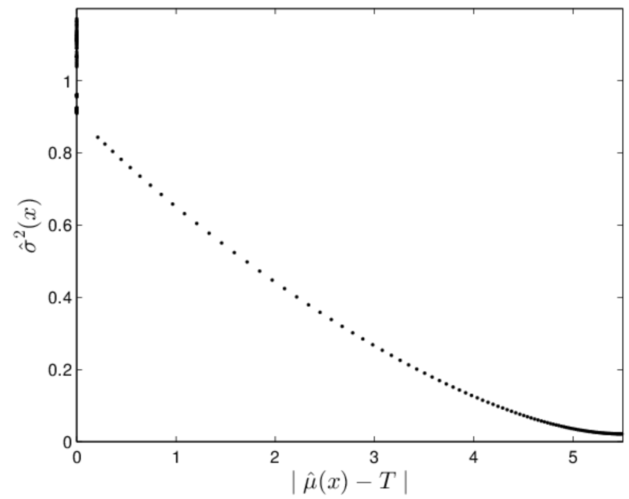

Fig. 2 – DAM Solutions

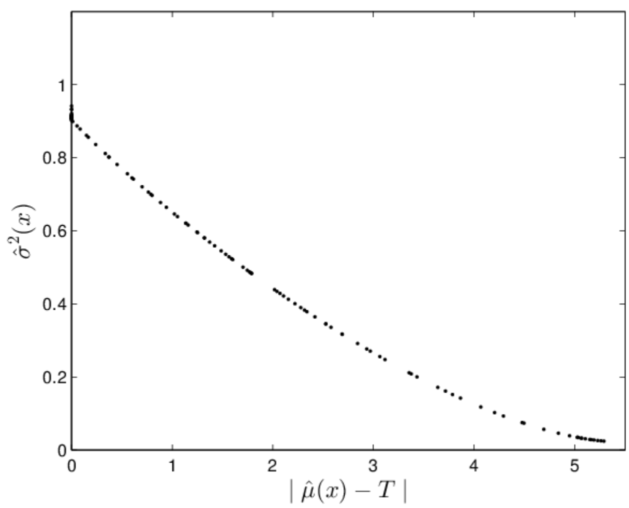

Fig. 3 – GC Solutions

V. DISCUSSION

The lack of a generally agreed upon examples that must be used to evaluate optimization criteria performance does not contribute to a clear understanding of their working abilities. Results of some examples can make a criterion look effective when, in fact, it has serious limitations. In addition, criteria ability to depict Pareto frontiers has been rarely illustrated in the literature.

Effective optimization criteria can explore all Pareto frontier and yield, at least, a discrete representation of that frontier. However, presented examples show that desirability-based (DAM) criterion do not perform always as desired. Example 2 shows the DAM criterion ability to depict Pareto frontiers, and that it can perform similarly to the GC criterion, whereas Example 1 shows DAM criterion limitations. In fact, results yielded by DAM criterion do not give confidence to use it in real-life problems. DAM criterion is similar to weighted sum criteria $\left(\sum \omega \mathrm{F}_{(x)}\right)$, which limitations to depict Pareto frontiers in highly convex and nonconvex surfaces are well illustrated in the literature [30]-[31], so its poor performance was expected.

GC criterion is a weighted exponential sum function and presented examples show that it can yield discrete representations of Pareto frontiers. Costa et al. [26] argued that shape factors $0.25 \le p_i \le 3$ are, in general, appropriate to GC criterion depict a representative set of optimal solutions for problems developed in the RSM framework. This is a relevant advantage over the other criteria available in the literature and gives confidence to use GC criterion in real-life problems. Nevertheless, higher p_i values may be necessary to obtain complete representations of some Pareto frontiers, namely for those where exist highly convex and nonconvex regions [32]-[33]. In these cases, such as Marler and Arora [34] noted, to use higher p_i values enables to better capture all Pareto optimal points, but non-Pareto optimal points may be also captured.

VI. CONCLUSIONS

Determining the optimal factor settings that optimize multiple objectives or responses is critical for producing high quality products and high capability processes, and can have tremendous impact on reducing waste and costs. However, conflicting responses are usual in real-life problems and optimal factor settings for one or more responses may lead to degradation of, at least, another one. This is illustrated in Example 1, where the two mean responses are in conflict, and in Example 2, where the conflicting responses are the mean and standard deviation of the metal removal rate for a cutting machine.

A large variety of alternative solutions can be found for multiple response problems, and different impacts on process or product can also be expected. Some optimal solutions lead to operation conditions more hazardous, more costly or more difficult to implement and control. Therefore, to satisfy decision-makers with different sensitivity to optimization objectives, a criterion that can capture solutions evenly distributed along the Pareto frontier have to be used.

This article successfully demonstrates the working ability of a global criterion-based criterion to generate solutions along the Pareto frontier in problems with conflicting objectives, and results show the superiority of GC criterion over a desirability-based criterion. GC criterion is relatively easy to understand and apply, which are appealing advantages over other existing criteria, and a stimulus to apply it in real-life problems.

Results presented here are novel because optimization criteria ability to generate evenly distributed solutions along

Pareto frontier has been rarely evaluated in the literature. Nevertheless, further research is needed to better understand GC criterion working ability and define the range values for shape or power factors when the number of responses is large (four or more) and responses surfaces are nonconvex. The comparison with other effective approaches must also be considered, namely with the most popular desirability-based criterion introduced by Derringer and Suich [3] or any variant of it.

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