Mean and Standard Deviation Optimization of Multiple Responses

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Abstract — Small bias and high robustness at optimal variable settings are desirable properties to all the responses involved in a multiresponse optimization problem. An approach that considers those properties and can be easily used by practitioners is presented. Its feasibility is illustrated through two examples from the literature and the results compared with those of other popular and effective methods.

Index Terms — Compromise programming, Loss function, Robustness, RSM, Variance.

I. INTRODUCTION

OPTIMIZATION of systems (processes and products) often involves incommensurate and conflicting quality characteristics (responses). Those responses must in some sense be optimized simultaneously because a separate analysis of them may result in incompatible solutions. For example, it is of common knowledge that as the dose of a drug increases, so do its efficacy and toxic side effects. However, in problems where both efficacy and toxicity responses are measured at each dose, the efficacy response is optimized at a higher dose level, whereas the toxicity response is minimized at a lower dose level. This makes difficult to identify the dose level of the drug that are optimal for both responses, because the objective must be to find the dose level that simultaneously maximize efficacy while minimizing toxicity [1].

Besides the optimization of multiple mean responses, the dual and multiple dual response problems, where the objective is to optimize the mean and variance of single and multiple responses, respectively, are also common in practice. Systems variability cannot be ignored, because it results in non-conforming product or poor process performance. Such as Kim and Lin [2] showed, unacceptable compromise solutions are achieved if the analyst focuses on mean and ignores the responses variability.

Various approaches that consider the responses variance level and exploit the responses correlation information in addition to process economics (feasibility of assigning priorities to individual responses based on either technical and economic considerations or decision-maker’s preferences) have been used in the Response Surface Methodology (RSM) framework. The Capability Index [3], Goal Programming [4], Physical Programming [5], Neural Networks [6], Probability-based [7] are examples of those approaches. All of them have their own merits. However, the lack of recommendations for proper use, unavailability of the algorithms employed, and inherent (mathematical/statistical) complexity of some existing approaches and methods are major reasons by which they are of little practical use or appealing to non-statistician practitioners.

This article aims at achieving desirable response properties at variable settings, namely low bias and variance, using a compromise programming-based criterion along with optimization performance measures as alternative to other methods mathematically sound but less appealing to practitioners, namely to those who have limited mathematical or statistical background. The feasibility and effectiveness of the suggested approach is illustrated through examples from the literature and its results compared with those of several methods.

The remainder of the article is organized as follows: Section II provides a review on the literature; the optimization criterion and measures suggested for evaluating the compromise solutions are introduced in Section III; Section IV includes the examples; results discussion is presented in Section V and conclusions in Section VI.

II. LITERATURE REVIEW

A strategy often used in the RSM framework for optimizing multiple responses consists of converting them into a single response by combining the individual responses into a composite function followed by its optimization. While desirability function and loss function approaches are the most popular among practitioners to determine the composite function, the desirability-based methods are, in general, easier to use and understand. Derringer and Suich’s method [8], or modifications of it [9], is the most popular desirability-based method and is available in many data analysis software packages. However, to use this method the analyst needs to specify values to four types of shape parameters when responses are of different types. This is not a simple task and it impacts on the optimal variable settings. Some authors, including Chiao and Hamada [10], criticize the method arguing that the composite function does not allow a clear interpretation except the principle that a higher value is preferred.

In contrast to desirability-based methods, there are loss function-based methods that consider the responses variance level and exploit the responses correlation information, leading to solutions that, theoretically, are more realistic when the responses have significantly different variance levels or are highly correlated. The next sub-sections include a brief review on two methods that will be used for comparative purposes in this article: a multivariate loss
function and a “maximin” desirability function.

A. Multivariate loss function

Arguing that little attention had been focused on multiple correlated responses with asymmetric loss function, Wu and Chyu [11] introduced a multivariate loss function-based method that considers responses bias (deviation from target) and robustness (sensitivity to uncontrollable factors). They proposed to minimize an expected loss function defined as

$$E[L(y(x))] = \sum_{i=1}^{r} \left( \hat{y}_i - \theta \right)^{2} + \sum_{i=2}^{r} \sum_{j=1}^{r} \left[ \hat{\sigma}_{ij} + (\hat{y}_i - \theta)(\hat{y}_j - \theta) \right]$$

where \( \hat{y}_i \) represents the estimated mean responses, \( \hat{\sigma}_{ij} \) and \( \hat{\sigma}_{yi} \) are estimated variance and covariance of the responses, and \( c_i \) and \( c_{ij} \) are loss coefficients.

The minimization of expected loss functions is an appealing approach often used in practice to find the best design variables setting in multiresponse problems. The results are expressed in monetary units rather than in process or product-specific units, which facilitates its interpretation, namely by engineering and management communities. Wu and Chyu (2004) provided formulae to calculate the loss coefficients based on the amount of quality loss but these values may be difficult to determine and correlate with different scales, relative variabilities, and relative costs for multiple responses. Moreover, loss functions do not allow weighting the mean and variance of each response separately, their power is limited to a quadratic value, and assume that potential dependencies among responses. Their proposal is appealing approach often used in practice to find the best compromises solutions of interest [12]-[13].

B. “Maximin” desirability function

Kim and Lin [2] proposed a “maximin” formulation that considers the model’s predictive ability and is robust to the potential dependencies among responses. Their proposal is

$$\text{Maximin} \left( d_{\mu}(\hat{y}_\mu(x)), ..., d_{\sigma_i}(\hat{y}_{\sigma_i}(x)), ..., d_{\sigma_{ij}}(\hat{y}_{\sigma_{ij}}(x)) \right)$$

where \( d_{\mu_i} \) and \( d_{\sigma_i} \) \( i = 1, ..., r \) are exponential desirability functions of the mean and standard deviation responses defined as

$$d = \begin{cases} \frac{e^{t} - e^{\frac{|z|}{t}}}{e^{t+1} - 1} & , \ t \neq 0 \\ 1 - |z| & , \ t = 0 \end{cases}$$

where \( t \) is a shape factor \((-\infty < t < \infty)\), and \( z \) is a standardized parameter representing the distance of the estimated response from its target in units of the maximum allowable deviation (see Kim and Lin article for details).

This formulation only considers the response with maximum weighted distance or percentage of deviation from the target, which may lead to an unreasonable decision in some cases [2]. To accommodate specific needs of a given problem, these authors extended the above formulation to cope with the following situations: responses are alternatives rather than all being essential; models have significant differences in the level of predictive capability; assignment of different weights on mean and standard deviation; compensation of the “maximin” criterion.

III. ALTERNATIVE APPROACH

An objective function built on the Compromise Programming technique along with optimization performance measures that allows evaluating the desired response’s properties at optimal variable settings is proposed in this article.

Compromise Programming is a mathematical programming technique that has proven to be extremely powerful in incorporating and resolving conflicting objectives concurrently by locating efficient solutions in convex and non-convex response surfaces [14]. It can be generalized into the metric

$$\text{Min } L_p = \text{Min} \left( \sum_{i=1}^{r} \left( \frac{u_i - f_i(x)}{u_i} \right)^p \right)^{1/p}$$

where \( u \) is the utopia (ideal) point, \( p \) is the parameter that defines the type of metric, and \( \lambda_i \) represents priorities or the relative worth of the \( i \)-th response. As the root \( 1/p \) does not impact on the solutions, Costa and Pereira [15] proposed the criterion defined by (5) to optimize multiple mean responses. Here, we use the same criterion to optimize the mean and standard deviation of multiple responses, that is,

$$\text{Minimize} \sum_{i=1}^{r} \left( \frac{\hat{y}_i - \theta_i}{U_i - L_i} \right)^{p_i}$$

where \( \theta_i \) \((\theta_{\mu_i}, \theta_{\sigma_i})\) corresponds to the target value of the \( i \)-th estimated response \( \hat{y}_i(\hat{\mu}, \hat{\sigma}) \), \( p_i \) are user-specified parameters (response priorities, \( p_i > 0 \)), and \( U_i \) and \( L_i \) are specification limits assigned to responses (mean and standard deviation) that are available for process or product quality control. Note that \( \theta_{\mu_i} \) is the target value of the mean response \( \hat{\mu}_i \) and \( \theta_{\sigma_i} \) is the target value of the standard deviation \( \hat{\sigma}_i \).

As regards the weighting scheme, by setting \( \lambda_i = 1/\left(U_i - L_i\right) \) less (subjective) information is required from the analysts. This is important, because simple and effective procedures for guiding the analyst in assigning values to \( \lambda_i \) are not known to the best of our knowledge. Moreover, it makes possible the combination of responses which by nature have different measuring units, considers the existing differences in response properties, such as the scale and allowable range, and provides flexibility for testing different specification limits, if appropriate.

According to Messac et al. [14] the presence of parameters that the analyst can use to manipulate the objective function’s curvature is vital to capture points on the Pareto frontier. In particular, these authors have proved that using exponents to assign priorities to responses is an effective practice to capture points in convex and non-convex part of response
surfaces. Thus, changing the parameter \( p_i \) in (5) will provide the required flexibility to explore trade-offs among responses and obtain a solution of interest in terms of bias and robustness.

The modulus set in the numerator is another distinctive aspect of this criterion. It simplifies the mathematical formulation of the objective function designed to accommodate Nominal-The-Best (NTB - the value of the estimated response is expected to achieve a particular target value), Smaller-The-Better (STB - the value of the estimated response is expected to be smaller than an upper bound) and Larger-The-Better (LTB - the value of the estimated response is expected to be larger than a lower bound) response types and makes it appealing for practitioners who have to choose an approach or criterion for multiresponse optimization. As Izarbe et al. [16] noted, practitioners prefer techniques that are easy to understand and use.

In (5) the target value for standard deviation is not, necessarily, set equal to zero, as it is typically considered in other methods. A target value for standard deviation up to a certain level is acceptable as it may be useful to explore trade-offs among responses.

An ideal compromise solution in multiresponse problems is the one where all the responses are on-target and, simultaneously, have minimal variance. This is very difficult, if at all possible, to achieve in practice. The alternative is to identify the best compromise solution among the multiple responses. For this purpose we suggest the measures proposed by Costa et al. [17].

A. Optimization Measures

An endless number of solutions may exist for a multiresponse problem, and how good a solution is depends on either technical and economical issues or analyst's preferences.

In the RSM framework few authors have explicitly addressed the evaluation of response’s properties separately. In general they focus on the output value of the objective function. Costa et al. [17] and Ko et al. [18] are exceptions. Here the optimization measures proposed in [17] are used, because they do not depend on the weights assigned to responses.

To assess compromise solutions in terms of bias, they suggested an optimization measure that considers the response types, response specification limits and response deviations from target. This measure, named cumulative bias \( B_{cum} \), is defined as

\[
B_{cum} = \sum_{i=1}^{q} W_i \left| y_i^* - \theta_i \right|
\]

where \( y_i^* \) represents the estimated response value at “optimal” variable settings, \( \theta_i \) is the target value and \( W_i \) is a parameter that takes into account the specification limits and response type of the \( i \)-th response. This parameter is defined as follows: \( W = 1/(U - L) \) for STB and LTB-type responses; \( W = 2/(U - L) \) for NTB-type response. The cumulative bias gives an overall result of the optimization process instead of focusing on the value of a single response, which is reasonable in multiresponse problems. Nevertheless, the bias of each response can be easily obtained from (6).

To assess the robustness, Costa et al. [17] proposed the following measure:

\[
Rob = trace \left[ \phi \sum_{y} \sigma^2(x) \right]
\]

where \( \sum_{y} \sigma^2(x) \) represents the variance-covariance matrix of the responses at “optimal” variable settings and \( \phi \) is a matrix whose diagonal and non-diagonal elements are \( \phi_{ii} = 1/(U_i - L_i)^2 \) and \( \phi_{ij} = 1/(U_i - L_j)(U_j - L_i), i \neq j \), respectively. Note that replications of the experimental runs are required for assessing the robustness and \( U \) and \( L \) represent the specification limits of the variance models. Although the replicates increase the time and cost of experimentation, they are expected to provide significant improvements in robustness that overbalance or at least compensate the time spent and the additional cost.

As highlighted in [17], using \( B_{cum} \) and \( Rob \) do not exclude other measures from being also used. As concerns the results of \( B_{cum} \) and \( Rob \), the lower their values are, the better the compromise solution is. In practice, \( B_{cum} \) and \( Rob \) take values greater than or equal to zero, but zero is the most favourable.

IV. EXAMPLES

Two examples from the literature are used to validate the feasibility of the suggested approach and evaluate the compromise solutions achieved from different approaches in terms of bias and robustness. The examples were selected in order to consider problems where different response-types, feasible regions, number of responses and variables exist.

A. Example 1

Kim and Lin [2] considered an example from the chemical engineering literature where the objective was to determine the effects of concentration of surfactant (\( x_1 \)), concentration of salt (\( x_2 \)), and time of stirring (\( x_3 \)) on the properties of the colloidal gas aphrons (micro bubbles of 10-100 µm in diameter), which are measured by three responses: the stability (\( y_1 \)), volumetric ratio (\( y_2 \)), and temperature (\( y_3 \)). The response models are as follows:

\[
\hat{\mu}_1 = 4.95 + 0.82 x_1 - 0.45 x_2 + 0.00 x_3 - 0.16 x_1^2 + 0.27 x_2^2 + 0.00 x_3^2 - 1.11 x_1 x_2 + 0.07 x_1 x_3 + 0.00 x_2 x_3 + 0.00 x_1 x_2 x_3
\]

\[
\hat{\mu}_2 = 0.46 + 0.13 x_1 - 0.06 x_2 + 0.05 x_3 - 0.06 x_1^2 + 0.27 x_2^2 + 0.10 x_3^2 + 0.00 x_1 x_2 + 0.05 x_1 x_3 + 0.00 x_2 x_3 + 0.00 x_1 x_2 x_3
\]

\[
\hat{\mu}_3 = 28.75 - 1.48 x_1 + 0.00 x_2 + 2.33 x_3 - 0.78 x_1^2 + 1.18 x_2^2 + 0.00 x_3^2 + 0.00 x_1 x_2 + 0.02 x_1 x_3 + 0.00 x_2 x_3 + 0.00 x_1 x_2 x_3
\]

\[
\hat{\sigma}_1 = 0.06 + 0.00 x_1 + 0.11 x_2 + 0.06 x_3 + 0.12 x_1^2 + 0.00 x_2^2 + 0.10 x_3^2 + 0.00 x_1 x_2 + 0.05 x_1 x_3 + 0.00 x_2 x_3 + 0.00 x_1 x_2 x_3
\]

\[
\hat{\sigma}_2 = 0.02 - 0.01 x_1 + 0.01 x_2 - 0.01 x_3 + 0.00 x_1^2 + 0.00 x_2^2 + 0.00 x_1 x_2 + 0.02 x_1 x_3 + 0.00 x_2 x_3 + 0.00 x_1 x_2 x_3
\]

\[
\hat{\sigma}_3 = 6.08 - 1.53 x_1 + 0.49 x_2 + 4.85 x_3 + 0.00 x_1^2 + 2.26 x_2^2 + 0.00 x_3^2 + 0.00 x_1 x_2 - 0.65 x_1 x_3 + 0.00 x_2 x_3 - 0.67 x_1 x_2 x_3
\]
The estimated mean responses, $\hat{\mu}_1$, $\hat{\mu}_2$ and $\hat{\mu}_3$, are of LTB-, STB-, and NTB-type, respectively: $\hat{\sigma}_i$ ($i=1,2,3$) are of STB-type. The constraints for the input variables are $-1 \leq x_i \leq 1$ ($i=1,2,3$). Table I shows the response specifications according to [2].

As regards the results displayed in Table II, the solution achieved from criterion (5), denoted by NC, is better than the solution KL1, which corresponds to the solution of the “maximin” criterion in the case of ($i=0$) linear desirability functions are used and standard deviation models are not considered in (3). Even when standard deviation models are considered, NC is slightly better in terms of $B_{cum}$ and $Rob$ than the solution yielded by “maximin” criterion, which is denoted by KL2. In fact, using the models above presented, the $B_{cum}$ and $Rob$ values are lower in the NC and KL2 solutions than in KL1 due to the smaller value of $\hat{\sigma}_3$, which is outside of the specifications in KL1. As Kim and Lin (2006) point out, the existing methods may produce unacceptable solution since they just focus on the mean of the responses, and the variability of the responses is simply ignored. Moreover, note that $\hat{\sigma}_3$ value is lower in NC than in KL2 and NC solution displayed in Table II is obtained keeping responses priorities unchanged, that is, with $p_i$ values equal to one to all responses. This solution is also, at least, in close agreement with those presented in [2] when variations of the integrated modelling approach to simultaneously optimize the location and dispersion effects of multiple responses are used.

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B. Example 2

A plasma enhanced chemical vapour deposition process study was reported in [19] and revisited in [11]. Eight parameters ($x_1$,...,$x_8$) were considered to optimize the mean and variance of two quality characteristics, namely, the deposition thickness ($y_1$) and a refractive index ($y_2$). The responses models presented in [11] are as follows:

$$
\hat{\mu}_1 = 2.83 - 0.007 x_1 + 0.010 x_2 - 0.129 x_3 - 0.000 x_4 + 0.209 x_5
+ 0.083 x_6 + 0.009 x_7 - 0.210 x_8 - 0.021 x_3 x_4 - 0.076 x_3 x_5 + 0.156 x_3 x_8
- 0.019 x_4 x_5 + 0.006 x_4 x_5 - 0.035 x_4 x_8
$$

The estimated mean responses, $\hat{\mu}_1$, $\hat{\mu}_2$, and $\hat{\mu}_3$, are of LTB-, STB-, and NTB-type, respectively; $\hat{\sigma}_i$ ($i=1,2,3$) are of STB-type. The constraints for the input variables are $-1 \leq x_i \leq 1$ ($i=1,2,3$). Table I shows the response specifications according to [2].

As regards the results displayed in Table II, the solution achieved from criterion (5), denoted by NC, is better than the solution KL1, which corresponds to the solution of the “maximin” criterion in the case of ($i=0$) linear desirability functions are used and standard deviation models are not considered in (3). Even when standard deviation models are considered, NC is slightly better in terms of $B_{cum}$ and $Rob$ than the solution yielded by “maximin” criterion, which is denoted by KL2. In fact, using the models above presented, the $B_{cum}$ and $Rob$ values are lower in the NC and KL2 solutions than in KL1 due to the smaller value of $\hat{\sigma}_3$, which is outside of the specifications in KL1. As Kim and Lin (2006) point out, the existing methods may produce unacceptable solution since they just focus on the mean of the responses, and the variability of the responses is simply ignored. Moreover, note that $\hat{\sigma}_3$ value is lower in NC than in KL2 and NC solution displayed in Table II is obtained keeping responses priorities unchanged, that is, with $p_i$ values equal to one to all responses. This solution is also, at least, in close agreement with those presented in [2] when variations of the integrated modelling approach to simultaneously optimize the location and dispersion effects of multiple responses are used.

The estimated mean responses, $\hat{\mu}_1$ and $\hat{\mu}_2$, are of NTB-type; $\hat{\sigma}_i$ ($i=1,2$) is of STB-type. The responses specifications are presented in Table III where we assume that the upper bounds for $\hat{\sigma}_i$ correspond to the higher values obtained from the experimental runs.

Considering that the region of control factors is measurable, with $x_i=(1,2)$, $x_3=(1,2,3)$, and $x_4 \in [1,3]$ for $i=2,4, \ldots, 8$, the criterion proposed by Costa and Pereira [15] yielded a solution with marginal differences to that of Wu and Chyu [11] displayed in Table IV, setting the weights to $p_i$ values higher than those obtained in the continuous region, which seems indicate that considering continuous regions may lead to better compromise solutions in terms of bias and variance.

If the region is discrete, with $x_1 = 1$ or $x_1 = 3$, keeping the responses weights ($p_i$ values) equal to one, Costa and Pereira criterion yielded a solution equal to that reported by Wu and Chyu [11]. It is important to point out that compromise solutions for the discrete region produced $B_{cum}$ and $Rob$ values higher than those obtained in the continuous region, which seems indicate that considering continuous regions may lead to better compromise solutions in terms of bias and variance.

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These results are very interesting as Wu and Chyu [11] showed that their method outperforms others that have been used in practice.

V. DISCUSSION

Previous examples show that there are not significant differences among the results obtained from methods that differ in terms of their theoretical basis (optimization scheme) and statistical properties. This may help to understand why there is no widely-accepted method for optimizing multiple responses in spite of some methods are more appealing than others, in particular for users who have limited mathematical or statistical background.

Ease of understanding and use are relevant aspects for practitioners when they choose a specific approach or criterion for multiresponse optimization, but the type and amount of information required from them is critical for achieving an effective compromise solution. To date, there is no procedure to guide the analyst in the selection of appropriate parameters/weights and starting points to the optimization routine. These tasks terminate, in general, by virtue of time constraints or satisfaction of the decision-maker with the solution(s). Moreover, the objective function results can vary significantly as the weighting coefficients change and very little is usually known about how to choose these coefficients. In practice, it is difficult, if at all possible, to determine beforehand the variations required in the weights so as to produce a solution of preference, that is, so as to know which response(s) will change and which is the direction and magnitude of that change.

As Messac and Ismail-Yahaya [20] showed, aggregate objective functions must provide the flexibility of changing their curvature in order to be effective in practice. Nevertheless, this is not a simple task and becomes harder when the number of user-specified parameters, input variables and responses increase. In Costa and Pereira criterion the curvature of response surfaces can be manipulated easily and in some cases, like the examples show, minimum or no cognitive effort is required from the analyst. In particular, the solutions for examples 1 and 2 (for the discrete region) were obtained keeping the responses priorities unchanged (equal to one). In example 2, for the measurable region, the curvature of the objective function was adjusted to capture solution(s) of preference, keeping priority values assigned to responses are less than or equal to three \( p_i \leq 3 \). This fact is relevant, because this guideline may facilitate the analyst task of identifying a solution of preference. This does not mean that using natural numbers \( p_i = 1, 2, 3 \), such as it was made in both examples, is always the best choice to achieve satisfactory solutions for problems similar to those revisited here. For example, to change the weights in steps of 0.5 units, or even in steps of 0.25 units, can provide improvements in responses values or in their properties.

VI. CONCLUSIONS

In this article the authors present an approach for simultaneous optimization of multiple responses in the RSM framework as alternative to methods statistically sound and often used in practice. The approach is easy to understand, easy to use, and can be employed in situations where it is critically important to obtain an effective compromise solution between mean and variance of multiple responses.

The objective function is a variant of the compromise programming technique, and from a methodological viewpoint its relevant features are the following:

- It allows accommodation of different response types and explicitly considers the response specifications;
- It requires a number of weights just equal to the number of responses and the curvature of the aggregate function can be easily manipulated.

Its effectiveness was illustrated through two examples from the literature and their results compared with those of other approaches, which help practitioners in evaluating their performance and making a better-informed choice among them. The selected examples do not cover all possible scenarios with respect to the number of responses and input variables, model’s form and response types. Nevertheless, the results provide evidence that the approach justifies its use in practice.

To assess the properties of a compromise solution at variable settings, namely the response’s bias and robustness, optimization measures were used. They can be employed along with any method of practitioner’s interest, and are particularly useful if an optimization routine is used to generate a large number of compromise solutions, because they may serve to discard those ones with \( B_{cum} \) and \( R_{ob} \) values less favourable. In fact, whereas a large number of solutions may provide insights into the trade-offs among the responses, some of them may have a small chance of being chosen as a solution of preference. Thus, they may be promptly identified and discarded. Considering that practitioners are increasingly taking advantage of multiresponse optimization methods, investigation on this topic is of interest and will be considered in future research. Another issue that remains an open research field is the intricate task of assigning priorities to responses. To specify limits for the weights range and effective steps to their change are issues that must be explored further. This information will be a useful guideline for the analyst, because it can reduce the number of weights values combination and by consequence the time for testing them.

REFERENCES