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Optimization of multiple responses considering both location and dispersion effects

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Abstract

An integrated modeling approach to simultaneously optimizing both the location and dispersion effects of multiple responses is proposed. The proposed approach aims to identify the setting of input variables to maximize the overall minimal satisfaction level with respect to both location and dispersion of all the responses. The proposed approach overcomes the common limitation of the existing multiresponse approaches, which typically ignore the dispersion effect of the responses. Several possible variations of the proposed model are also discussed. Properties of the proposed approach are revealed via examples.

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1. Introduction

Response surface methodology (RSM) consists of a group of techniques used in the empirical study of the relationship between the response and a number of input variables. Consequently, the experimenter attempts to find the optimal setting for the input variables that maximizes (or minimizes) the response. For detailed descriptions on various response surface techniques, see Box and Draper (1987) and Khuri and Cornell (1996).

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Most of the work in RSM has been focused on the case where there is only one response of interest. In product or process development, however, it is quite common that several response variables are of interest. In this case, determination of optimum conditions on the input variables would require simultaneous consideration of all the responses. This is called a multiresponse problem (Khuri, 1996).

The multiresponse problem consists of three stages: data collection (design of experiments), model building, and optimization. Although there are challenging problems associated with data collection and statistical model building, we will assume that the data have been collected and the response models have already been fitted reasonably well. In this work, we will focus on the optimization scheme perspective, that is, how we can find an optimal setting of the input variables to "optimize" all the responses simultaneously.

A simple and intuitive approach to a multiresponse problem is to superimpose the response contour plots and determine an "optimal" solution by a visual inspection (Lind et al., 1960). The usefulness of such a method is severely limited by the number of input variables and/or responses.

One of the popular approaches reduces multiple responses to one with a single aggregated measure and solves it as a single objective optimization problem. The aggregated measure has often been defined as a desirability function (Harrington, 1965; Derringer and Suich, 1980; Kim and Lin, 2000), an estimated distance from the ideal design point (Khuri and Conlon, 1981), or a squared error loss function (Pignatiello, 1993; Vining, 1998). Xu et al. (2004) propose a multiresponse optimization method using a goal attainment approach.

The major focus of the aforementioned existing approaches to multiresponse optimization is on the location effect only, ignoring the dispersion effect of the responses. As a result, all observations are assumed to have equal variation. Evidence from real examples, however, indicates that the equal variation assumption may not be valid in practice. In such a case, the existing multiresponse optimization approaches can be misleading.

Recently, the simultaneous optimization of both the location and dispersion effects, called a dual response approach, has received a great deal of attention for its attempt to tackle a non-equal variance problem. Several approaches have been proposed, including a priority-based approach (Myers and Carter, 1973; Vining and Myers, 1990; Copeland and Nelson, 1996), a mean squared error-based approach (Lin and Tu, 1995), and a desirability function-based approach (Derringer and Suich, 1980; Kim and Lin, 1998). Tang and Xu (2002) provide a good review of the existing methods, and propose a goal programming approach for dual response optimization. However, the dual response approach is also limited in that it considers only one response variable.

This paper proposes an integrated approach to simultaneously optimizing both the location and dispersion effects of multiple responses. The topics to be discussed in this paper are developed in the following order. First, the pitfall of the existing multiresponse optimization approaches is demonstrated using a case example. Next, the framework of the proposed modeling approach is introduced, and several possible variations of the proposed approach are discussed. Then, another example is presented. Finally, discussions and concluding remarks are given.

2. Example 1: Colloidal gas aphrons (CGA) study

A real problem with multiple responses reported in the chemical engineering literature (Jauregui et al., 1997) is employed to demonstrate the use of the existing multiresponse optimization approaches. The same example will be used later to illustrate the proposed approach. When surfactant solutions are mixed at high speeds, micro bubbles (10–100 μm in diameter) are formed. It is postulated that these bubbles, called colloidal gas aphrons (CGAs), are composed of a gaseous inner core surrounded by a thin soapy film. The properties of the CGAs are measured by three different responses—stability ($y_1$), volumetric ratio ($y_2$), and temperature ($y_3$). The responses, $y_1$, $y_2$ and $y_3$ are larger-the-better (LTB), smaller-the-better (STB),
and nominal-the-best (NTB)-type responses, respectively. The purpose of the experiment was to determine the effects of concentration of surfactant ($x_1$), concentration of salt ($x_2$), and time of stirring ($x_3$) on the CGA properties.

The experiment was conducted in a central composite design with eight factorial points, six axial points, and a center point. The center point was replicated six times and the other design points were replicated twice. Owing to this replication, response surface models not only for the mean but also for the standard deviation of each response can be fitted. The dataset is displayed in Table 1.

A second-order polynomial model was fitted to each of the mean of the three responses, and then reduced to the best subset model. The best subset models and their $R^2$ values are given below.

$$\hat{y}_{\mu_1}(x) = 4.95 + 0.82x_1 - 0.45x_2 - 0.15x_1^2 + 0.28x_2^2 - 0.11x_1x_2 + 0.07x_1x_3 \ (R^2 = 0.91), \quad (1)$$

| $u$ | $x_1$ | $x_2$ | $x_3$ | Replication | $y_{u1}$ | $y_{u2}$ | $y_{u3}$ | $\bar{y}_{u1}$ | $\bar{y}_{u2}$ | $\bar{y}_{u3}$ | $s_{u1}$ | $s_{u2}$ | $s_{u3}$ |
|-----|------|------|------|-------------|--------|--------|--------|-------------|--------|--------|--------|--------|--------|--------|
| 1   | -1   | -1   | -1   | 1           | 4.50   | 0.17   | 29.0   | 4.50        | 0.22   | 26.00  | 0.00   | 0.06   | 4.24   |
| 2   | 1    | -1   | -1   | 1           | 6.04   | 0.50   | 23.0   | 6.04        | 0.50   | 23.0   | 0.00   | 0.06   | 2.70   |
| 3   | -1   | -1   | -1   | 2           | 6.39   | 0.53   | 25.4   | 6.39        | 0.53   | 25.4   | 0.25   | 0.02   | 1.70   |
| 4   | 1    | -1   | -1   | 1           | 3.81   | 0.17   | 22.0   | 3.81        | 0.17   | 22.0   | 0.25   | 0.02   | 1.70   |
| 5   | -1   | -1   | -1   | 1           | 4.09   | 0.20   | 27.0   | 4.09        | 0.20   | 27.0   | 0.20   | 0.02   | 3.54   |
| 6   | 1    | -1   | -1   | 2           | 5.67   | 0.44   | 25.5   | 5.67        | 0.44   | 25.5   | 0.34   | 0.03   | 3.18   |
| 7   | -1   | -1   | -1   | 1           | 5.19   | 0.40   | 21.0   | 5.19        | 0.40   | 21.0   | 0.34   | 0.03   | 3.18   |
| 8   | 1    | -1   | -1   | 1           | 4.67   | 0.32   | 20.0   | 4.67        | 0.32   | 20.0   | 0.00   | 0.14   | 4.85   |
| 9   | -1   | 0    | 0    | 1           | 4.22   | 0.32   | 41.0   | 4.22        | 0.32   | 41.0   | 0.00   | 0.20   | 4.85   |
| 10  | 1    | 0    | 0    | 1           | 6.73   | 0.57   | 35.5   | 6.73        | 0.57   | 35.5   | 0.00   | 0.20   | 6.73   |
| 11  | 0    | -1   | 0    | 2           | 6.57   | 0.57   | 18.0   | 6.57        | 0.57   | 18.0   | 0.00   | 0.20   | 18.0   |
| 12  | 1    | -1   | 0    | 1           | 3.40   | 0.12   | 43.0   | 3.40        | 0.12   | 43.0   | 0.00   | 0.14   | 4.30   |
| 13  | 0    | 0    | -1   | 1           | 4.32   | 0.28   | 20.0   | 4.32        | 0.28   | 20.0   | 0.00   | 0.14   | 4.30   |
| 14  | 0    | 0    | -1   | 2           | 5.72   | 0.46   | 19.0   | 5.72        | 0.46   | 19.0   | 0.00   | 0.14   | 4.30   |
| 15  | 0    | 0    | -1   | 0           | 5.09   | 0.50   | 34.0   | 5.09        | 0.50   | 34.0   | 0.00   | 0.14   | 4.30   |

Notes: $x_1$, $x_2$, and $x_3$ are coded values.
Measurement units for $y$ are as follows: $y_1 = \log(\text{seconds})$, $y_2 = \text{none (ratio)}$, $y_3 = ^\circ\text{C}$.
$y_{u1}$ is the response data of $y_1$ at the $u$th design point, $j = 1, 2, 3; u = 1, \ldots, 15$.
$y_{u1}/s_{u1}$ denotes the sample mean (sample standard deviation) of $y_{u1}$. 

Table 1
The CGA study data
\[ \hat{y}_{p_2}(x) = 0.46 + 0.13x_1 - 0.06x_2 + 0.05x_3 - 0.07x_1^2 - 0.04x_3^2 \quad (R^2 = 0.87), \]

\[ \hat{y}_{p_3}(x) = 28.36 - 1.48x_1 + 2.33x_3 - 0.15x_1^2 - 1.42x_3^2 - 0.71x_1x_3 \quad (R^2 = 0.12). \]

In the above equations, \( \hat{y}_{p_j}(x) \) denotes the fitted response surface of the mean of the \( j \)th response, \( j = 1, 2, 3 \). Note that \( \hat{y}_{p_2}(x) \) has a significantly lower \( R^2 \) value than other fitted responses. Such a non-equivalent predictive capability issue will be discussed later in Section 5.

The minimum, maximum, and target value of each response were determined based on the problem context. These values are given in Table 2, and were used as the bounds on each response in optimization. In Table 2, \( y_{p_j}^{\text{min}}, y_{p_j}^{\text{max}} \), and \( T_{p_j} \), respectively, represent the lower bound, upper bound, and target value on the \( j \)th mean response. Also, \( d_{p_j}(\hat{y}_{p_j}) \) denotes the desirability value associated with \( \hat{y}_{p_j} \). These values can be determined using Eqs. (1)-(3), as shown in Kim and Lin (2000).

The above problem was solved using the conventional desirability function method (Derringer and Suich, 1980; Derringer, 1994), which will be referred to as the DS method, and the maximin desirability function method (Kim and Lin, 2000), which will be referred to as the KL method. To be brief, the DS method aims to find \( x^* \) to maximize \( \sqrt{d_{p_1}(\hat{y}_{p_1})d_{p_2}(\hat{y}_{p_2})d_{p_3}(\hat{y}_{p_3})} \), while the KL method seeks to find \( x^* \) to maximize the minimum of \( d_{p_1}(\hat{y}_{p_1}), d_{p_2}(\hat{y}_{p_2}), \) and \( d_{p_3}(\hat{y}_{p_3}) \).

In both methods, a linear desirability function is employed for simplicity. Here, we just chose the DS and KL methods to demonstrate the common limitation of the existing approaches. Table 2 shows the optimization results, based on a cuboidal region \(-1 \leq x_i \leq 1 \) \((i = 1, 2, 3)\). Both methods yield acceptable results with respect to \( \hat{y}_{p_j}(x^*) \). The \( y_{p_j}(x^*) \) values from both methods are well within the given bounds, as manifested by the relatively high \( d_{p_j}(\hat{y}_{p_j}(x^*)) \) values (0.41, 0.72, 0.69 in DS and 0.52, 0.52, 0.67 in KL for \( j = 1, 2, 3 \), respectively). Such approaches assume that the variability for all responses is identical.

Suppose the experimenter (or decision maker, DM) chooses to use \( x_{DS} \) for his/her process operation. Assuming the response models given in (1)-(3) are still valid, the process performance on the mean, \( y_{p_j}(x_{DS}) \), would be acceptable as discussed above. The process performance on the standard deviation,
\( y_{e_j}(x_{DS}) \), was not considered in the optimization, but can be estimated \textit{a posteriori} by plugging \( x_{DS}^* \) into the standard deviation response models. There is no guarantee that the resulting \( \hat{y}_{e_j}(x_{DS}^*) \) would be acceptable. In this example, the best subset models for the dispersion effect are:

\[
\hat{y}_{e_1}(x) = 0.06 + 0.11x_2 + 0.06x_3 + 0.12x_1^2 + 0.11x_3^2 - 0.10x_1x_3 + 0.05x_2x_3 \quad (R^2 = 0.84),
\]

\[
\hat{y}_{e_2}(x) = 0.02 - 0.01x_1 + 0.01x_2 - 0.01x_3 + 0.02x_1^2 - 0.01x_1x_3 + 0.02x_2x_3 \quad (R^2 = 0.83),
\]

\[
\hat{y}_{e_3}(x) = 6.08 - 1.53x_1 + 0.50x_2 + 4.85x_3 + 2.26x_2^2 - 0.65x_1x_3 - 0.67x_1x_2x_3 \quad (R^2 = 0.95).
\]

The values of \( y_{e_j}^{\text{min}}, y_{e_j}^{\text{max}}, T_{e_j} \), and \( d_{e_j}(\hat{y}_{e_j}) \) are also shown in Table 2. It turned out that \( \hat{y}_{e_3}(x_{DS}^*) \) is 4.54, far exceeding its upper limit (which is 2.00), and its degree of satisfaction, \( d_{e_3}(\hat{y}_{e_3}(x_{DS}^*)) \), is zero as shown in Table 2. Therefore, \( x_{DS}^* \) is deemed an unacceptable solution if the DM is concerned with the process performance on the standard deviation as well as that on the mean. The KL method has the same kind of problem with \( \hat{y}_{e_3}(x_{KL}^*) \). It is evident that 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.

3. Proposed optimization scheme for multiple responses

We propose an alternative optimization scheme to the multiresponse problem, building on our recent work. The proposed approach combines the idea of maximizing desirability functions for the mean of multiple responses (Kim and Lin, 2000) and for the mean and standard deviation of a single response (Kim and Lin, 1998). Suppose there are \( r \) responses \( y = (y_1, y_2, \ldots, y_r) \) which are determined by a set of input variables \( x = (x_1, x_2, \ldots, x_p) \). A general multiresponse problem can be defined as

\[
y_j = f_j(x_1, x_2, \ldots, x_p) + e_j(x_1, x_2, \ldots, x_p), \quad j = 1, 2, \ldots, r,
\]

where \( f_j \) denotes the response function between the \( j \)th response and the input variables, and \( e_j \) is a random error such that \( \text{E}(e_j) = 0 \) and \( \text{Var}(e_j) = \sigma_j^2 \). Note that \( \sigma_j \) is also a function of \( (x_1, x_2, \ldots, x_p) \).

Following the notion of the conventional desirability function approach, it is assumed that the degree of satisfaction of the DM with respect to the mean of the \( j \)th response variable is maximized when \( \hat{y}_{\mu_j}(x) \) equals its target value \( T_{\mu_j} \) and decreases as \( \hat{y}_{\mu_j}(x) \) moves away from \( T_{\mu_j} \). The DM does not accept a solution \( x \) for which \( \hat{y}_{\mu_j}(x) \leq y_{\mu_j}^{\text{min}} \), nor \( \hat{y}_{\mu_j}(x) \geq y_{\mu_j}^{\text{max}} \). Thus the degree of satisfaction with respect to the mean of the response can be modeled by a function which decreases monotonically from 1 at \( \hat{y}_{\mu_j}(x) = T_{\mu_j} \) to 0 at \( \hat{y}_{\mu_j}(x) \leq y_{\mu_j}^{\text{min}} \) or \( \hat{y}_{\mu_j}(x) \geq y_{\mu_j}^{\text{max}} \). A similar argument can be made for the standard deviation of the \( j \)th response variable.

3.1. Formulation

A multiresponse problem requires an overall optimization, that is, a simultaneous satisfaction of all the responses with respect to both the location and dispersion effects. If a "minimum" \( \sigma \) operator is employed for aggregating all the responses on both effects, a multiresponse optimization problem can be stated as:

Maximize \( \lambda \)

subject to \( d_{e_j}(\hat{y}_{\mu_j}(x)) \geq \lambda, \quad j = 1, 2, \ldots, r, \)

\( d_{e_j}(\hat{y}_{\sigma_j}(x)) \geq \lambda, \quad j = 1, 2, \ldots, r, \)

\( x \in \Omega. \)
Model (7) aims to identify \( x^* \) which maximizes the overall minimal degree of satisfaction (\( \lambda \)) with respect to the mean and the standard deviation of all the responses within the experimental region, i.e.,

\[
\text{Maximize } \{ \min_{x \in \Omega} [d_{p_1}(\bar{y}_{p_1}(x)), \ldots, d_{p_r}(\bar{y}_{p_r}(x)), d_{p_1}(\bar{y}_{p_1}(x)), \ldots, d_{p_r}(\bar{y}_{p_r}(x))] \}.
\]

Additional constraints may be added to the above formulation as appropriate.

### 3.2. General properties

The optimization scheme proposed above (which will be referred to as model (7)) has several methodological advantages over the existing methods. First of all, the proposed approach considers the dispersion effect as well as the location effect of the multiple responses. More specifically, the proposed approach explicitly takes into account practically allowable ranges on the mean and standard deviation of each response and then maximizes the overall satisfaction level which is defined within the specified ranges. Therefore, the optimal setting obtained from the proposed approach would achieve a good balance in the sense that the contributions of both the location and dispersion effects associated with all the responses are properly reflected in the optimization process. This point will be demonstrated using the CGA example in Section 4.

Secondly, the proposed "maximin" approach is robust to the potential dependencies among responses. Such dependency is very difficult to detect or model in reality. Dependency can appear in various forms, while a pairwise linear relationship is probably the only case that can be possibly detected. When the assumption of independency is violated, both the conventional desirability function approach (using the geometric mean or weighted geometric mean to aggregate the individual desirability values) and the generalized distance approach can be very misleading, as noted by Khuri and Conlon (1981). The proposed procedure, on the other hand, focuses on the response which has the lowest degree of satisfaction, and thus the inequalities in model (7) corresponding to other responses are essentially redundant constraints from the optimization viewpoint. Therefore, the existence of dependency among responses does not affect the proposed procedure.

Thirdly, the objective function value (\( \lambda \)) allows a good physical interpretation. The \( \lambda \) value denotes the overall degree of satisfaction (0 \( \leq \lambda \leq 1 \)) based on the specified ranges of mean and standard deviation of all the responses. It can be used as a basis for a meaningful comparison among different design points. A design point \( x_1 \) is preferred to another design point \( x_2 \) if \( \lambda(x_1) > \lambda(x_2) \). Moreover, \( (\lambda(x_1) - \lambda(x_2)) \) represents how much \( x_1 \) is preferred to \( x_2 \) in terms of the overall degree of satisfaction. Such an intuitive interpretation is not available with the aggregated desirability value in the conventional desirability function approach or the expected loss in the loss function approach, as noted by Pignatiello (1993). Finally, the proposed approach can be easily understood and implemented by those with little mathematical or statistical knowledge, possibly with the aid of a software system.

It should also be noted that the proposed approach has possible disadvantages as well. In particular, the proposed optimization scheme is only concerned with the lowest degree of satisfaction, and thus the degree of satisfaction associated with all others are, in effect, ignored. This may lead to an unreasonable solution in some cases. As an extreme example when there are two responses, model (7) would prefer an operating setup with \( d_1 = (d_{p_1}, d_{p_2}, d_{e_1}, d_{e_2}) = (0.5,0.5,0.5) \) to the one with \( d_2 = (d_{p_1}, d_{p_2}, d_{e_1}, d_{e_2}) = (0.99,0.99,0.99,0.49) \). Moreover, model (7) does not differentiate \( d_1 \) from \( d_3 = (0.99,0.99,0.99,0.5) \). In fact, \( d_1 \) and \( d_3 \) are alternative optima in model (7), and thus they are considered equally good. However, such unreasonable outcomes can be avoided by slightly modifying model (7). To this end, some variations of model (7) will be discussed later in Section 5.

Another disadvantage of the proposed approach is that replicates are required to estimate the response models for standard deviation. However, we believe that the advantage of explicitly considering the dispersion effect in the optimization generally outweighs the disadvantage due to the higher costs in terms of the validity and practicality of the resulting solution.
4. Example 1: CGA study—revisited

Now, we return to the CGA study example discussed earlier. The same example is solved using the proposed approach in model (7). The optimal solution (denoted as $x^*_p$) and the resulting $\hat{y}_{\mu_j}(x^*_p)$ and $\hat{y}_{\sigma_j}(x^*_p)$ values are given in Table 2.

Compared with the DS and KL methods, the proposed approach yields quite comparable results in terms of the mean of the responses. While $\hat{y}_{\mu_j}(x^*_p)$ is worse than $\hat{y}_{\mu_j}(x^*_DS)$ and $\hat{y}_{\mu_j}(x^*_KL)$, $\hat{y}_{\mu_j}(x^*_p)$ is better than $\hat{y}_{\mu_j}(x^*_DS)$ and a little worse than $\hat{y}_{\mu_j}(x^*_KL)$, and $\hat{y}_{\mu_j}(x^*_p)$ is better than both $\hat{y}_{\mu_j}(x^*_DS)$ and $\hat{y}_{\mu_j}(x^*_KL)$. Thus, no one approach dominates the others in optimizing the mean responses. However, in terms of the standard deviation, the result from the proposed approach is clearly better than those of the DS and KL methods. The estimated standard deviation for $y_{j1}, y_{j3}(x^*)$, was unacceptable at $x^*_DS$ and $x^*_KL$. It is notable that $\hat{y}_{j3}(x^*_p)$ is 1.64, which is well within the acceptable range [1.00, 2.00] of $y_{j3}$ and its degree of satisfaction is 0.36. In this respect, the proposed approach produces a more balanced and realistic solution.

5. Some variations of the proposed approach

Model (7) is a basic template based on which some modifications can be made to accommodate the specific needs of the given problem situation. This section suggests four possible variations of model (7), which will be referred to as V1, V2, V3, and V4, where V1 is modified for alternative responses; V2 for predictive capability; V3 for weights assignment; and V4 for the maximin criterion. The CGA study example is solved again using models V1 through V4 (to be discussed below), and the results are summarized in Table 3. For an easy comparison with model (7), the result from model (7) is also reproduced in Table 3.

5.1. V1: Consideration of alternative responses

Model (7) can be extended to cope with the situation where the responses were alternatives rather than all being essential. This could be done by employing a “maximum” operator (i.e., taking the maximum of the individual degrees of satisfaction) instead of the “minimum” operator as in model (7).

Suppose all the responses ($y_{ji}$, $j = 1, \ldots, r$) are alternatives, namely, the DM is interested in the response whichever achieves the highest degree of satisfaction. Here, the degree of satisfaction of a response (say, $y_{ji}$) is defined as usual—the minimum of $d_{\mu_i}(\hat{y}_{\mu_j}(x))$ and $d_{\sigma_j}(\hat{y}_{\sigma_j}(x))$. Then, model (7) can be modified to:

$$(V1) \quad \text{Maximize} \quad \max(\lambda_1, \lambda_2, \ldots, \lambda_r)$$

subject to

$$d_{\mu_i}(\hat{y}_{\mu_j}(x)) \geq \lambda_j, \quad j = 1, 2, \ldots, r,$$

$$d_{\sigma_j}(\hat{y}_{\sigma_j}(x)) \geq \lambda_j, \quad j = 1, 2, \ldots, r,$$

$$x \in \Omega.$$  \hspace{1cm} (8)

From the optimization perspective, solving model (8) would be cumbersome. However, model (8) can be separated into r individual response optimization problems like the following:

$$(V1(j)) \quad \text{Maximize} \quad \lambda_j$$

subject to

$$d_{\mu_i}(\hat{y}_{\mu_j}(x)) \geq \lambda_j,$$

$$d_{\sigma_j}(\hat{y}_{\sigma_j}(x)) \geq \lambda_j,$$

$$x \in \Omega.$$
Table 3
Comparison of results for models V1–V4

<table>
<thead>
<tr>
<th>Model (7)</th>
<th>V1</th>
<th>V2</th>
<th>V3</th>
<th>V4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(x^*)</td>
<td>(x^*)</td>
<td>(x = 0.1)</td>
<td>(x = 0.5)</td>
</tr>
<tr>
<td></td>
<td>((-0.21))</td>
<td>((-0.03))</td>
<td>((-0.17))</td>
<td>((-0.22))</td>
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<td>((-0.04))</td>
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<td>((-0.39))</td>
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<td></td>
<td>((-1.00))</td>
<td>((-1.00))</td>
<td>((-0.99))</td>
<td>((-1.00))</td>
</tr>
<tr>
<td>(\hat{y}<em>{a1}(d</em>{a1}))</td>
<td>5.00 (0.50)</td>
<td>4.94 (0.48)</td>
<td>5.00 (0.61)</td>
<td>4.98 (0.49)</td>
</tr>
<tr>
<td>(\hat{y}<em>{a2}(d</em>{a2}))</td>
<td>0.37 (0.45)</td>
<td>0.38 (0.44)</td>
<td>0.38 (0.60)</td>
<td>0.37 (0.46)</td>
</tr>
<tr>
<td>(\hat{y}<em>{a3}(d</em>{a3}))</td>
<td>25.96 (0.73)</td>
<td>26.06 (0.74)</td>
<td>26.00 (1.00)</td>
<td>25.98 (0.73)</td>
</tr>
<tr>
<td>(\hat{y}<em>{a1}(d</em>{a1}))</td>
<td>0.06 (0.36)</td>
<td>0.10 (0.00)</td>
<td>0.07 (0.50)</td>
<td>0.06 (0.36)</td>
</tr>
<tr>
<td>(\hat{y}<em>{a2}(d</em>{a2}))</td>
<td>0.05 (0.50)</td>
<td>0.04 (0.57)</td>
<td>0.05 (0.72)</td>
<td>0.05 (0.50)</td>
</tr>
<tr>
<td>(\hat{y}<em>{a3}(d</em>{a3}))</td>
<td>1.64 (0.36)</td>
<td>1.26 (0.74)</td>
<td>1.56 (0.50)</td>
<td>1.64 (0.36)</td>
</tr>
</tbody>
</table>

V1\((j)\) just focuses on maximizing the degree of satisfaction of the \(j\)th response. Let \(x^*_k\) and \(x^*_j\) denote the optimal solution and the optimal objective function value of V1\((j)\), respectively. Once V1\((j)\) is solved for all \(j (1 \leq j \leq r)\), the optimal solution \(x^*\) of model (8) is determined simply by selecting \(x^*_k\) \((1 \leq k \leq r)\) such that \(x^* = \max \{x^*_1, \ldots, x^*_r\}\). Thus, model (8) can be efficiently solved by solving V1\((j)\) for \(j = 1, \ldots, r\). In fact, V1\((j)\) is equivalent to the “dual” response optimization model (corresponding to the \(j\)th response) proposed in Kim and Lin (1998).

For the CGA example, the optimization result of V1 (given in Table 3) implies that \(y_{a1}\) was the response which could achieve the highest degree of satisfaction. Both \(d_{a1}\) and \(d_{a2}\) are 0.74, thereby yielding the objective function value of 0.74. While the DM may be pleased with such an exceptional level of achievement on \(y_{a1}\), the \(\hat{y}_{a1}\) value turns out to be unacceptable. This would, however, not be a concern if all \(y_{a1}, y_{a2}\) and \(y_{a3}\) were alternatives.

5.2. V2: Consideration of predictive capability

As discussed in Kim and Lin (2000), if there is a significant difference in the levels of predictive capability (goodness of fit) of the estimated response models, it should be considered in the optimization. The proposed model can be modified to incorporate the levels of predictive capability when this is a concern by adjusting the desirability function shape.

To incorporate the predictive capability of a response, Kim and Lin (2000) propose to use

\[
d'(z) = \begin{cases} 
    \frac{d'_{\text{ref}}}{z^t} & \text{if } t' \neq 0, \\
    1 - |z| & \text{if } t' = 0, 
\end{cases}
\]

where \(t' = t + (1 - R^2)(t'_{\text{max}} - t)\). Here, \(t\) is the exponential constant \((-\infty < t < \infty)\) which determines the desirability function shape without considering the predictive capability, and \(t'_{\text{max}}\) is a sufficiently large value of \(t\) such that \(d'(z)\) with \(t'_{\text{max}}\) is extremely concave and thus has practically no effect in the optimization. For simplicity of notation, \(z\) is employed to denote a standardized parameter \((-1 \leq z \leq 1)\) representing the distance of the estimated response from its target in units of the maximum allowable deviation. When \(R^2 = 0, t' = t'_{\text{max}}\) and the corresponding response model would have virtually no effect. In general, when \(0 < R^2 < 1, t < t' < t'_{\text{max}}\) and the impact of the corresponding response model in the optimization is adjusted (i.e., weakened compared to the case of using \(t\)) accordingly. As mentioned in Kirkwood (1996), the realistic values of \(t\) will generally have a magnitude between -10 and 10. We thus suggest \(t'_{\text{max}} = 10\) for practical use.
Following the rationale discussed above, model (7) can be modified to:

(V2) \[
\begin{align*}
\max_x & \quad \lambda \\
\text{subject to} & \quad d_{y_j}(\hat{y}_{y_j}(x)) \geq \lambda, \quad j = 1, 2, \ldots, r, \\
& \quad d_{\sigma_j}(\hat{y}_{\sigma_j}(x)) \geq \lambda, \quad j = 1, 2, \ldots, r, \\
& \quad x \in \Omega,
\end{align*}
\]

where \(d_{y_j}(\hat{y}_{y_j}(x))\) and \(d_{\sigma_j}(\hat{y}_{\sigma_j}(x))\) are the modified desirability functions to incorporate the predictive capability of the mean and standard deviation responses, respectively, as described in (9).

In the CGA example, \(\hat{y}_{\sigma_3}\) model has the highest predictive capability (\(R^2 = 0.95\)) and should receive the highest priority in the optimization process of V2. As can be seen in the V2 column of Table 3, \(\hat{y}_{\sigma_3}\) has improved from 1.64 (in model (7)) to 1.56 (i.e., moved closer to the target value by 0.08), as expected. Other responses improved or deteriorated to accommodate the change in \(\hat{y}_{\sigma_3}\) and subsequent tradeoffs.

5.3. V3: Assignment of different weights on mean and standard deviation

If the DM decides to assign different weights on the degrees of satisfaction for the location and dispersion effects, model (7) can be modified to:

(V3) \[
\begin{align*}
\max_x & \quad \alpha \lambda_\mu + (1 - \alpha) \lambda_\sigma \\
\text{subject to} & \quad d_{\mu_j}(\hat{y}_{\mu_j}(x)) \geq \lambda_\mu, \quad j = 1, 2, \ldots, r, \\
& \quad d_{\sigma_j}(\hat{y}_{\sigma_j}(x)) \geq \lambda_\sigma, \quad j = 1, 2, \ldots, r, \\
& \quad x \in \Omega,
\end{align*}
\]

where \(\alpha\) is a constant between 0 and 1, representing the relative importance between the degree of satisfaction on the mean (\(\lambda_\mu\)) and the degree of satisfaction on the standard deviation (\(\lambda_\sigma\)). As a special case, if \(\alpha = 1\), model (11) reduces to the model given in Kim and Lin (2000).

The CGA example under model (7), where \(\hat{y}_{\tau_1}\) and \(\hat{y}_{\tau_3}\) turned out to have the lowest degree of satisfaction (i.e., \(d_{\tau_1} = d_{\tau_3} = 0.36\)), was essentially driven by the maximization of \(d_{\tau_1}\) and \(d_{\tau_3}\). When \(\alpha\) is set to a small value (such as 0.1) in V3, a much higher weight is placed on maximizing \(\lambda_\sigma\). This would make V3 behave practically in the same manner as in model (7). Consequently, as it can be seen in Table 3, the result of V3 with \(\alpha = 0.1\) is essentially the same as that of model (7).

On the other hand, as \(\alpha\) increases, V3 places more weight on maximizing \(\lambda_\mu\), which is determined as the minimum of \(d_{\mu_1}, d_{\mu_3}\), and \(d_{\mu_5}\). The \(\lambda_\mu\) value of 0.48 (minimum (0.48, 0.48, 0.74)) at \(\alpha = 0.9\) is higher than \(\lambda_\mu\) (0.46) at \(\alpha = 0.1\) or \(\lambda_\mu\) (0.45) of model (7). The result of V3 with \(\alpha = 0.5\) shows a similar pattern with the case of \(\alpha = 0.9\).

5.4. V4: Compensation of the “maximin” criterion

As discussed earlier, model (7) would prefer \(d_1\) to \(d_2\) and may choose \(d_1\) over \(d_3\). Again, this is due to the fact that model (7) is concerned only with the minimum degree of satisfaction of the mean and standard deviation of all the responses. Such a situation can be avoided by modifying model (7) into the following:
\[(V4)\] Maximize \[
\lambda + \beta \sum_{j=1}^{r} (g_{\mu_j} + g_{\sigma_j})
\]
subject to
\[
d_{\mu_j}(\hat{y}_{\mu_j}(x)) \geq \lambda, \; j = 1, 2, \ldots, r, \quad (12.1)
\]
\[
d_{\sigma_j}(\hat{y}_{\sigma_j}(x)) \geq \lambda, \; j = 1, 2, \ldots, r, \quad (12.2)
\]
\[
d_{\mu_j}(\hat{y}_{\mu_j}(x)) - g_{\mu_j} = \lambda, \; j = 1, 2, \ldots, r, \quad (12.3)
\]
\[
d_{\sigma_j}(\hat{y}_{\sigma_j}(x)) - g_{\sigma_j} = \lambda, \; j = 1, 2, \ldots, r, \quad (12.4)
\]
\[x \in \Omega,
\]
where \(g_{\mu_j}\) and \(g_{\sigma_j}\) represent positive slacks associated with the two sets of original constraints given in (12.1) and (12.2), respectively, and \(\beta\) is a positive scaling constant. Due to the second component of the objective function, \(\beta \sum_{j=1}^{r} (g_{\mu_j} + g_{\sigma_j})\), model (12) would definitely choose \(d_3\) over \(d_1\) and likely prefer \(d_2\) to \(d_1\) with a proper selection of \(\beta\).

As a special case, if \(\beta = 0\), model (12) reduces to model (7). As the value of \(\beta\) increases, V4 places more weight on the sum of the slacks, and therefore tends to maximize the total sum of individual degrees of satisfaction as opposed to the "maximin" strategy in model (7). There is no hard and fast rule to determine the optimal value of \(\beta\). As a rough guide, \(\beta\) should not be large enough for \(\beta \sum_{j=1}^{r} (g_{\mu_j} + g_{\sigma_j})\) to mask the effect of \(\lambda\) if the balance among the responses is desired. It would be a good practice to gradually increase \(\beta\) and see the pattern in the resulting solutions to choose the \(\beta\) value to be used.

The CGA example was solved at three different \(\beta\) values; \(\beta = 0.4, 0.7,\) and \(1.0\). The result of V4 with \(\beta = 0.4\) is essentially identical to that of model (7). However, for \(\beta = 1.0\), V4 yields a quite different result. Compared with model (7), \(d_2\) has significantly improved (i.e., \(\Delta d_3 = 0.85 - 0.36 = 0.49\)) by sacrificing \(d_{\sigma_3}\) (i.e., \(\Delta d_{\sigma_3} = 0.00 - 0.36 = -0.36\)). The total sum of the individual degrees of satisfaction at \(\beta = 1.0\) is 3.06. This value is, as expected, higher than that of model (7) or V4 with \(\beta = 0.4\), both of which are 2.90. The result of V4 with \(\beta = 0.7\) shows a similar pattern with that of the case of \(\beta = 0.4\).

6. Discussion

As one of the referees noted, the problem of subset selection discussed in the simulation modeling and analysis literature is similar to the multiresponse optimization problem presented in this paper. The goal of a subset selection problem is to select a subset of the given alternative systems (e.g., alternative inventory policies) so that this selected subset contains the best system, with a specified probability of correct selection (Law and Kelton, 2000). The subset selection models implicitly consider the dispersion effects via the probability of correct selection. Although the subset selection models are typically discussed in a single response context, multiple responses can be considered through the use of a multiattribute value function as a performance measure (Evans et al., 1991; Morrice et al., 1998).

There is, however, a major distinction between the subset selection problem and the multiresponse optimization problem. The subset selection problem assumes that there are a finite number of predefined alternatives. On the other hand, the multiresponse optimization problem searches for the best alternative in the feasible region (denoted as \(\Omega\) in (7)), which contains an infinite number of feasible alternatives. In this view, they represent two different facets of problem solving—subset selection problem is for selection (or evaluation) while multiresponse optimization is for design. (This issue is illustrated in the example problem given in Section 7.)
It is also worth noting the similarities and differences between the desirability function and the multiattribute value (MAV) function. A MAV function \( v \) is one that associates a real number to each point in the outcome space (i.e., \( v : (y_1, y_2, \ldots, y_p) \rightarrow \mathbb{R} \)). Usually, \( v \) is scaled so that its range is \([0, 1]\) (Keeney and Raiffa, 1976). Although two functions have been developed in different fields, they have some common characteristics: they are scale-free, they are between 0 and 1 (0 being the worst and 1 the best), and they are flexible in shape. Conceptually, the two functions are identical in the sense that both functions aim to systematically structure the value tradeoffs associated with multiple conflicting attributes or responses.

With respect to the aggregation scheme of the individual value or desirability functions, the two functions show some difference. In the MAV literature, the most popular form has been an additive function due to its simplicity. An additive value function aggregates individual value functions in a linear, additive manner, and is known to exist under certain assumptions—more specifically, under the condition that the multiple attributes are mutually preferentially independent (Keeney and Raiffa, 1976). In contrast, the desirability function has typically been defined in a nonlinear and/or noncompensatory functional form—geometric mean (Derringer and Suich, 1980) or maximizing function (Kim and Lin, 2000).

7. Example 2: Wheel cover component experiment

We use an experiment conducted in Harper et al. (1987) with some embellishments to further demonstrate the applicability of the proposed method. The purpose of the experiment was to determine the effects of seven injection molding parameters (denoted as \( x_1, x_2, \ldots, x_7 \)) on the quality characteristics of a plastic wheel cover component. The quality characteristics are measured by the total weight \( y_1 \) (in grams) and the balance \( y_2 \) (in inch-ounces). Both \( y_1 \) and \( y_2 \) are NTB-type responses with \((710, 715)\) and \((0.3, 0.4)\) as the specification region, respectively.

The experiment was conducted in a \( 2^7-4 \) fractional factorial design with five replications in each run. The two levels of each \( x_i \) \((i = 1, \ldots, 7)\) are coded as \(-1\) and \(+1\). The response models were fitted as follows (Chiao and Hamada, 2001):

\[
\hat{y}_{ip} (x) = 720.763 + 1.873x_1 + 5.318x_5 - 3.408x_7, \\
\hat{y}_{ip} (x) = 0.967 + 0.113x_1 + 0.328x_5 - 0.174x_7, \\
\log \hat{y}_{a_1} (x) = 0.944 - 0.509x_2 + 1.189x_4 + 1.196x_5 - 0.487x_7, \\
\log \hat{y}_{a_2} (x) = -4.797 - 0.692x_2. \tag{16}
\]

Note that the log-linear model for dispersion effects in (15) and (16) ensures positive values for the variances. Chiao and Hamada (2001) sought to identify the experimental condition at which the probability that all responses simultaneously meet their respective specifications is maximized. Their optimal solution, \( x^{*}_{CH} \), is \((-1, +1, -1, -1, -1, -1, +1)\), where an insignificant factor is denoted by \(-1\). At \( x^{*}_{CH} \), \((\hat{y}_{ip}, \hat{y}_{ip}, \hat{y}_{a_1}, \hat{y}_{a_2})\) is obtained as \((710.16, 0.35, 0.30, 0.06)\).

We now solve this problem using the proposed model in (7). For an illustrative purpose, \((y^{\min}_{aj}, y^{\max}_{aj})\) are set at \((0, 0.5)\) and \((0, 0.2)\) for \( j = 1, 2 \), respectively. A linear membership function is employed for simplicity. The problem is solved with two different feasible region conditions: (a) \( x_i = -1 \) or \(+1\), and (b) \( x_i \in [-1, +1] \), \( i = 1, \ldots, 7 \). Case (a) represents the same feasible region as in Chiao and Hamada (2001), whereas case (b) represents a cuboidal, continuous feasible region. Cases (a) and (b) are differentiated in terms of the number of feasible solutions—finite in case (a) and infinite in case (b). That is, case (a) is a selection problem and case (b) is a design problem.
In case (a), the optimal solution of the proposed approach \((x^*_p)\) turns out to be identical to \(x^*_{CH}\). At \(x^*_p, \lambda = \min(d_{\mu_1}, d_{\mu_2}, d_{\sigma_1}, d_{\sigma_2}) = (0.07, 0.96, 0.41, 0.68) = 0.07\). In case (b), \(x^*_p\) is \((-0.99, +1, -1, -1, +1, 0.82)\) with \(\lambda = \min(0.32, 0.32, 0.38, 0.68) = 0.32\). Case (b) yields a better solution in the sense of a better balance among all the responses as well as a better balance between the location and the dispersion effects. In general, the proposed approach is more effective for a design problem than a selection problem because a good balance among \(\hat{y}_{\mu_j}\) and \(\hat{y}_{\sigma_j} (j = 1, \ldots, r)\) is not likely to be achieved in a given, limited number of experimental points.

8. Concluding remarks

An integrated modeling approach to simultaneously optimizing both the location and dispersion effects of multiple responses has been proposed. Assuming suitable response models have been fitted, the proposed approach focuses on the optimization aspect of the multiple responses. More specifically, the proposed approach aims to identify the setting of input variables to maximize the overall minimal satisfaction level with respect to the mean and standard deviation of all the responses.

The proposed approach overcomes the common limitation of the existing multiresponse approaches, which typically ignore the dispersion effect of the responses. The optimal setting obtained from the proposed approach would achieve a good balance in the sense that the contributions of both the location and dispersion effects associated with all the responses are properly reflected in the optimization process. The basic template of the proposed approach, model (7), can be modified to accommodate the specific needs of the given problem situation. Several possible variations of the proposed model have also been discussed.

There are several issues that should be noted. The response models were fitted by the ordinary least squares method, which assumes a constant variance in error terms. On the other hand, our basic premise is that the error variance is not constant, as manifested by (4)-(6). However, this issue was not pursued in this work for a simpler presentation of the main idea. A generalized linear model with, for example, gamma error could have been used to fit the dispersion effect models. More details on model fitting issues, see Hamada and Nelder (1997), Chiao and Hamada (2001), and Lee and Nelder (2003).

Another issue is concerned with the stochastic aspects in optimization results. In the proposed framework, the fitted response models are essentially treated as deterministic at the optimization stage. However, they actually have uncertainty associated with them. To compensate for such an uncertainty problem, it would be useful to study how sensitive the optimization results are to small changes in the input parameters. A measure of uncertainty could be attached to the obtained \(x^*\).

Finally, the costs associated with the replication, which is required to estimate the dispersion effect response models, could be of practical concern. In the CGA study example, the experiment had only two replicates, except for the center point. This could give an inaccurate representation of the standard deviation. How to ensure an accurate and reliable model for the dispersion effect with only a small number of replicates is an interesting issue for future research.

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