쌍대반응표면 최적화에서 편차와 분산의 가중치 결정에 관한 연구
Determining the Relative Weights of Bias and Variance in Dual Response Surface Optimization

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ABSTRACT

Mean squared error (MSE) is an effective criterion to combine the mean and the standard deviation responses in dual response surface optimization. The bias and variance components of MSE need to be weighted properly in the given problem situation. This paper proposes a systematic method to determine the relative weights of bias and variance in accordance with a decision maker's prior and posterior preference structure.

1. INTRODUCTION

Response surface methodology consists of a group of techniques used in the empirical study between a 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 (Box and Draper, 1987; Khuri and Cornell, 1996; Myers and Montgomery, 1995). The conventional response surface methodology focused on the mean of the response, assuming the variance of the response is constant. However, the equal variance assumption may not be valid in practice.

The dual response surface approach, introduced by Myers and Carter (1973) and popularized by Vining and Myers (1990), has received a great deal of attention for its attempt to tackle a non-equal variance problem. Suppose that there is a response y which is determined by a set of k input variables, coded x_1, x_2, …, x_k. The dual response surface approach first fits models for the mean ($\hat{\omega}_\mu$) and the standard deviation ($\hat{\omega}_\sigma$) as separate responses. A quadratic (second-order) polynomial form is widely used for the model building:

$$\hat{\omega}_\mu = \hat{\beta}_0 + \sum_{i=1}^{k}\hat{\beta}_i x_i + \sum_{i=1}^{k}\hat{\beta}_{ii} x_i^2 + \sum\sum_{i<j}^{k}\hat{\beta}_{ij} x_i x_j \,, \quad (1)$$

$$\hat{\omega}_\sigma = \hat{\gamma}_0 + \sum_{i=1}^{k}\hat{\gamma}_i x_i + \sum_{i=1}^{k}\hat{\gamma}_{ii} x_i^2 + \sum\sum_{i<j}^{k}\hat{\gamma}_{ij} x_i x_j \,. \quad (2)$$

Various methods have been proposed for the optimization of dual response surfaces. Tang and Xu (2002) provides a good review of the existing methods. Lin and Tu (1995) proposed a simple, yet effective approach based on mean squared error (MSE) minimization:

$$\text{Minimize} \quad \text{MSE} = (\hat{\omega}_\mu - T)^2 + \hat{\omega}_\sigma^2 \,, \quad (3)$$

where T is the target value for the mean. MSE consists of two terms: the bias ($(\hat{\omega}_\mu - T)^2$) and the variance ($\hat{\omega}_\sigma^2$). As noted in Lin and Tu (1995), a natural extension of MSE, called a weighted MSE (WMSE), is formed by imposing the relative weights on the bias and variance terms:

$$\text{WMSE} = \lambda(\hat{\omega}_\mu - T)^2 + (1-\lambda)\hat{\omega}_\sigma^2 \,, \quad (4)$$

where λ is the weighting factor which has a value between 0 and 1.

To date, there has been lack of systematic methods for determining λ in WMSE. Recently, Ding et al. (2004) proposed a data-driven approach to determine λ. But, this data-driven approach has a major shortcoming in that it utilizes no input from the decision maker (DM). In essence, the value of λ should be determined in accordance with the DM's preference information or judgments, which involves tradeoffs on various factors in quality and costs. The purpose of this paper is to develop a systematic method to determine λ in WMSE in such a way that the obtained λ faithfully reflects the DM's preference structure.

In the proposed method, the bias and variance values resulting from a process setting of the input variables are considered to form a vector. The DM expresses his/her preference structure by providing the ranking of such alternative vectors. Then, the proposed procedure finds the λ value congruent with the given ranking of the vectors. The pairwise ranking scheme, which compares only a pair of vectors at a time, is employed so that the preference articulation process does not impose a heavy burden on the DM.

Section 2 presents the basic idea and the details of the proposed method. Section 3 illustrates the proposed procedure through an example problem, and conclusions are made in Section 4.

2. PROPOSED METHOD

2.1. Basic Idea

Consider an experiment where m experimental conditions are tested with n replicates at each condition. Let $y_1^i, y_2^i, ..., y_n^i$ denote the n replicates obtained at condition i (i = 1, 2, …, m). The bias (z_1^i) and variance (z_2^i) at condition i are obtained as:

$$z_1^i = (\bar{y}^i - T)^2 \quad \text{and} \quad z_2^i = \frac{1}{n-1}\sum_{r=1}^{n}(y_r^i - \bar{y}^i)^2, \quad (5)$$

where $\bar{y}^i$ is the mean of $y_1^i, y_2^i, ..., y_n^i$. Let $\mathbf{z}^i$ be the vector consisting of z_1^i and z_2^i, i.e., $\mathbf{z}^i = (z_1^i, z_2^i)^{\mathrm{T}}$. Then, the WMSE value associated with condition i is simply expressed as:

$$\mathrm{WMSE}^i = \boldsymbol{\lambda}\mathbf{z}^i, \quad (6)$$

where $\boldsymbol{\lambda} = (\lambda, 1-\lambda)$. In effect, WMSE is regarded as a biattribute value function evaluated through the bias and variance (Keeney and Raiffa, 1976).

The basic premise of the proposed idea is that the λ value should be congruent with the DM's preference structure. More specifically, the ranking of $\mathbf{z}^i$'s given by the DM should be consistent with the ordering of the corresponding WMSE values. For example, if the DM prefers $\mathbf{z}^i$ to $\mathbf{z}^j$ (denoted as $\mathbf{z}^i \succ \mathbf{z}^j$), $\boldsymbol{\lambda}\mathbf{z}^i$ should be less than $\boldsymbol{\lambda}\mathbf{z}^j$ ($\boldsymbol{\lambda}\mathbf{z}^i < \boldsymbol{\lambda}\mathbf{z}^j$). Suppose, in general, the ranking of $\mathbf{z}^i$'s given by the DM is $\mathbf{z}^1 \succ \mathbf{z}^2 \succ \cdots \succ \mathbf{z}^m$. This implies $\boldsymbol{\lambda}\mathbf{z}^1 < \boldsymbol{\lambda}\mathbf{z}^2 < \cdots < \boldsymbol{\lambda}\mathbf{z}^m$. Then, the appropriate choice of λ, called the "optimal" λ and denoted by λ^*, can be made by finding $\lambda \in [0, 1]$ which satisfies $\boldsymbol{\lambda}\mathbf{z}^1 < \boldsymbol{\lambda}\mathbf{z}^2 < \cdots < \boldsymbol{\lambda}\mathbf{z}^m$. If m is a large number, it may become quite difficult for the DM to articulate the ranking of all $\mathbf{z}^i$'s. In order to facilitate the preference articulation process, we employ the pairwise ranking scheme which compares only a pair of vectors at a time.

2.2. Proposed Procedure

In this section, a systematic procedure for determining λ in WMSE is proposed. The overall procedure is given in Fig. 1. The proposed procedure consists of two major phases: weight calculation phase and infeasibility resolution phase. The weight calculation phase (Step 1) computes λ based on the given pairwise rankings. If infeasibility should happen in weight calculation, the infeasibility resolution phase (Steps 2 and 3) removes or minimizes the inconsistency contained in the pairwise rankings. The details of the proposed procedure are presented below.

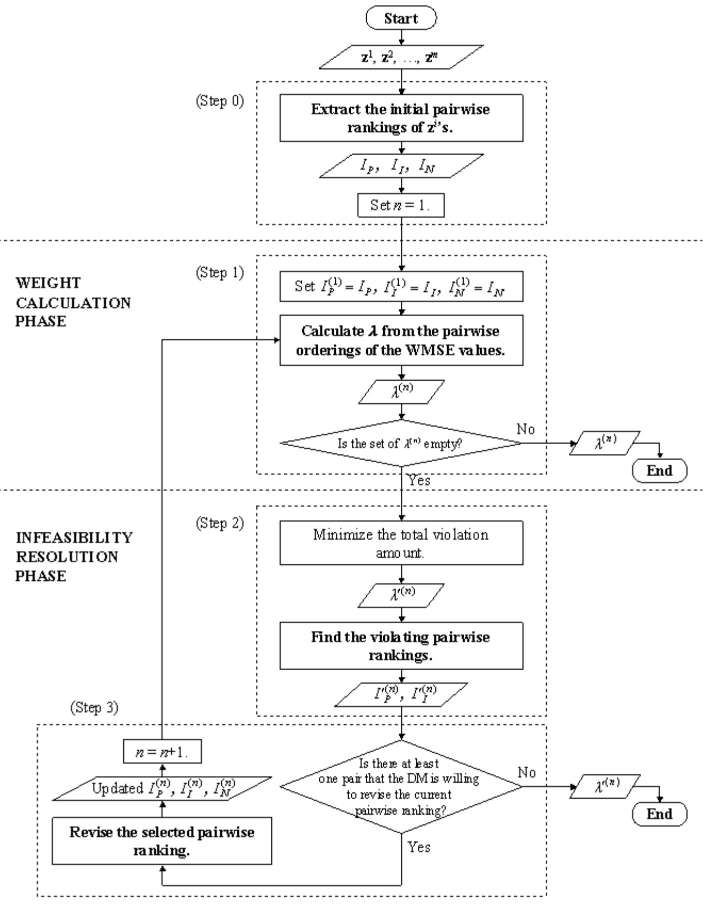

Fig. 1. The Proposed Procedure.

<u>Step 0. Extract the initial pairwise rankings of $\mathbf{z}^i$'s.</u>

The DM pairwise ranks $\mathbf{z}^1$, $\mathbf{z}^2$, …, $\mathbf{z}^m$ in the following manner (Ben Khélifa and Martel, 2001):

(i) $\mathbf{z}^i$ is preferred to $\mathbf{z}^j$ ($\mathbf{z}^i \succ \mathbf{z}^j$);
(ii) $\mathbf{z}^i$ is less preferred to $\mathbf{z}^j$ ($\mathbf{z}^i \prec \mathbf{z}^j$);
(iii) $\mathbf{z}^i$ is indifferent to $\mathbf{z}^j$ ($\mathbf{z}^i \sim \mathbf{z}^j$);
(iv) The comparison is to be held back ($\mathbf{z}^i \,?\, \mathbf{z}^j$).

If the DM does not feel comfortable with the comparison due to, for example, lack of confidence, he/she is allowed to choose no pairwise ranking in (iv). After completing the pairwise rankings, the following three index sets of ordered pairs are constructed:

$$I_P = \{(i, j) \mid \mathbf{z}^i \succ \mathbf{z}^j\},$$
$$I_I = \{(i, j) \mid \mathbf{z}^i \sim \mathbf{z}^j\}, \text{ and}$$
$$I_N = \{(i, j) \mid \mathbf{z}^i \,?\, \mathbf{z}^j\},$$

where the subscripts P, I, and N denote *Preferred*, *Indifferent*, and *Not compared*, respectively. The set I_P is associated with (i) and (ii), I_I (iii), and I_N (iv). Note that (ii) can be easily transformed to (i) by changing the position of $\mathbf{z}^i$ and $\mathbf{z}^j$. The iteration counter (n) is set at 1.

<u>Step 1. Calculate λ from the pairwise orderings of the WMSE values.</u>

The pairwise orderings of the WMSE values

$\boldsymbol{\lambda}\mathbf{z}^1$, $\boldsymbol{\lambda}\mathbf{z}^2$, …, $\boldsymbol{\lambda}\mathbf{z}^m$ are constructed based on the three index sets given in the current n-th iteration, i.e., $I_P^{(n)}$, $I_I^{(n)}$, and $I_N^{(n)}$, which were made in Step 3 of the previous iteration. The initial index sets I_P, I_I, and I_N from Step 0 serve as $I_P^{(1)}$, $I_I^{(1)}$, and $I_N^{(1)}$. The pairwise orderings in the n-th iteration are given as:

$$\boldsymbol{\lambda}\mathbf{z}^i < \boldsymbol{\lambda}\mathbf{z}^j,\ \forall(i, j) \in I_P^{(n)}, \quad (7)$$

$$\boldsymbol{\lambda}\mathbf{z}^i = \boldsymbol{\lambda}\mathbf{z}^j,\ \forall(i, j) \in I_I^{(n)}. \quad (8)$$

It should be noted that the pairwise orderings of the WMSE values for $\forall(i, j) \in I_N^{(n)}$ are not made. By solving each inequality or equality in (7)-(8) for $\lambda \in [0, 1]$, the individual set of λ for the (i, j) pair ($\lambda_{(i,j)}^{(n)}$) is obtained as an interval or a single value. The set of λ satisfying all the inequalities and equalities ($\lambda^{(n)}$) is obtained by intersecting $\lambda_{(i,j)}^{(n)}$'s, $\forall(i, j)$. If $\lambda^{(n)} \neq \varnothing$, the algorithm successfully ends, and the current solution $\lambda^{(n)}$ is the final set of λ. $\lambda^{(n)}$ is the set of λ values which are congruent with all the current pairwise rankings. Otherwise, go to Step 2.

Step 2. Find the violating pairwise rankings.

In Step 1, the feasible set of λ is null when there is an inconsistency among the pairwise rankings. To resolve the inconsistency, the conflicting pairwise rankings should be changed or deleted. The purpose of Step 2 is to find such pairwise rankings.

For $(i, j) \in I_P^{(n)}$, $\boldsymbol{\lambda}\mathbf{z}^i$ should be less than $\boldsymbol{\lambda}\mathbf{z}^j$ to satisfy the condition in (7). If not, $\boldsymbol{\lambda}\mathbf{z}^i - \boldsymbol{\lambda}\mathbf{z}^j$ denotes how much the inequality is violated. Similarly, if $\boldsymbol{\lambda}\mathbf{z}^i \neq \boldsymbol{\lambda}\mathbf{z}^j$ for $(i, j) \in I_I^{(n)}$ in (8), the violation amount is $|\boldsymbol{\lambda}\mathbf{z}^i - \boldsymbol{\lambda}\mathbf{z}^j|$. The total violation amount in the n-th iteration ($V^{(n)}$) is obtained by summing up each violation amount for $\forall(i, j) \in I_P^{(n)}$ and $\forall(i, j) \in I_I^{(n)}$:

$$V^{(n)} = \sum_{(i,j)\in I_P^{(n)}} \max\{0, \boldsymbol{\lambda}\mathbf{z}^i - \boldsymbol{\lambda}\mathbf{z}^j\} + \sum_{(i,j)\in I_I^{(n)}} |\boldsymbol{\lambda}\mathbf{z}^i - \boldsymbol{\lambda}\mathbf{z}^j|. \quad (9)$$

The total violation amount is employed as a measure of the inconsistency existing in the pairwise rankings. Then, an optimization model to minimize $V^{(n)}$ is formulated and solved:

$$\begin{aligned} &\underset{\lambda}{\text{minimize}} \quad V^{(n)} \\ &\text{subject to} \quad 0 \le \lambda \le 1. \end{aligned} \quad (10)$$

The above formulation aims to identify the λ value, denoted as $\lambda'^{(n)}$, which minimizes the total violation amount with respect to all the pairwise rankings given in the n-th iteration.

Based on $\lambda'^{(n)}$, the violating pairwise rankings are specified. The index sets of violating pairs are constructed as:

$$I'^{(n)}_P = \{(i, j) \,|\, \boldsymbol{\lambda}'^{(n)}\mathbf{z}^i - \boldsymbol{\lambda}'^{(n)}\mathbf{z}^j \ge 0, (i, j) \in I_P^{(n)}\},$$

$$I'^{(n)}_I = \{(i, j) \,|\, \boldsymbol{\lambda}'^{(n)}\mathbf{z}^i - \boldsymbol{\lambda}'^{(n)}\mathbf{z}^j \neq 0, (i, j) \in I_I^{(n)}\},$$

where $\boldsymbol{\lambda}'^{(n)} = (\lambda'^{(n)}, 1 - \lambda'^{(n)})$.

Step 3. Revise the selected pairwise ranking.

In order to resolve the inconsistency, (some of) the pairwise rankings in violation should be revised. Revising a pairwise ranking involves changing (e.g., $\mathbf{z}^i \succ \mathbf{z}^j$ to $\mathbf{z}^i \prec \mathbf{z}^j$ or $\mathbf{z}^i \sim \mathbf{z}^j$) or deleting the ranking judgment, and thus requires the DM's agreement.

The DM examines the pairwise rankings for $\forall(i, j) \in I'^{(n)}_P$ and $\forall(i, j) \in I'^{(n)}_I$, and decides whether there is at least one pair for which he/she is willing to revise the current pairwise ranking. If there is no such pair, the algorithm stops with $\lambda'^{(n)}$, which was obtained in Step 2. Otherwise, the DM selects one of pairs to be revised. Among the candidate pairs, only one pair is selected at one time because revising one pairwise ranking may resolve all the inconsistency in the next iteration. After the revision, the index sets $I_P^{(n)}$, $I_I^{(n)}$, and $I_N^{(n)}$ are updated accordingly. The algorithm then goes back to Step 1. The value of n is increased by 1.

3. ILLUSTRATIVE EXAMPLE

The "printing process" problem, which was originally discussed in Box and Draper (1987), is used with some embellishments to illustrate the proposed method. The purpose of the problem is to improve the quality of a printing process (Y) by controlling speed (x_1) and pressure (x_2). The experiment was conducted in a 32 factorial design with 9 replicates. The nine alternative vectors are obtained as: $\mathbf{z}^1$ = (200256.25, 1037.10)^T, $\mathbf{z}^2$ = (151321.00, 257.60)^T, $\mathbf{z}^3$ = (46081.78, 7330.27)^T, $\mathbf{z}^4$ = (137888.44, 2279.47)^T, $\mathbf{z}^5$ = (60352.11, 19200.67)^T, $\mathbf{z}^6$ = (6214.69, 11303.37)^T, $\mathbf{z}^7$ = (97240.03, 8817.77)^T, $\mathbf{z}^8$ = (25069.44, 11887.07)^T, $\mathbf{z}^9$ = (1.36, 63605.37)^T.

3.1. Step-by-step illustration of the proposed procedure

Step 0. Extract the initial pairwise rankings of $\mathbf{z}^i$'s.

The DM pairwise ranks $\mathbf{z}^1$, $\mathbf{z}^2$, …, $\mathbf{z}^9$: I_P = {(2, 1), (2, 4), (2, 5), (2, 7), (2, 9), (3, 1), (3, 4), (3, 5), (3, 7), (3, 9), (4, 1), (4, 5), (4, 7), (4, 9), (6, 1), (6, 2), (6, 3), (6, 4), (6, 5), (6, 7), (6, 8), (6, 9), (8, 1), (8, 4), (8, 5), (8, 7), (8, 9), (9, 1)}, I_I = {(3, 8)}, I_N = {(1, 5), (1, 7), (2, 3), (2, 8), (5, 7), (5, 9), (7, 9)}. Set $n = 1$.

<Iteration I>

Step 1. Calculate λ from the pairwise orderings of the WMSE values.

Set $I_P^{(1)} = I_P$, $I_I^{(1)} = I_I$, and $I_N^{(1)} = I_N$. Based on $I_P^{(1)}$, $I_I^{(1)}$, and $I_N^{(1)}$, the pairwise orderings of $\boldsymbol{\lambda}\mathbf{z}^1$, $\boldsymbol{\lambda}\mathbf{z}^2$, …, $\boldsymbol{\lambda}\mathbf{z}^9$ are constructed as in (7)-(8). The inequalities and equalities in the orderings are solved for $\lambda \in [0, 1]$, then $\lambda_{(i,j)}^{(1)}$'s are obtained. The intersection of $\lambda_{(i,j)}^{(1)}$'s is null ($\lambda^{(1)} = \varnothing$). Therefore, the algorithm goes to Step 2.

Step 2. Find the violating pairwise rankings.

The optimization model in (10) is solved with $V^{(n)}$ replaced by $V^{(1)}$. The optimal solution to the model is $\lambda'^{(1)} = 0.179$ and the corresponding total violation amount is $V^{(1)} = 21579.07$. Then, $I'^{(1)}_P$ and $I'^{(1)}_I$ are constructed as: $I'^{(1)}_P = \{(2, 4), (2, 5), (2, 7), (4, 7), (9, 1)\}$, $I'^{(1)}_I = \{(3, 8)\}$.

Step 3. Revise the selected pairwise ranking.

The DM selects $(9,1) \in I'^{(1)}_P$ for revision and chooses to delete the current pairwise ranking $\mathbf{z}^9 \phi\, \mathbf{z}^1$. Then, $I_P^{(1)}$ is updated with (9, 1) deleted, and $I_N^{(1)}$ with (9, 1) added. $I_I^{(1)}$ is kept as it is. Let $n = 2$.

<Iteration II>

Step 1. Calculate λ from the pairwise orderings of the WMSE values.

The pairwise orderings of $\boldsymbol{\lambda}\mathbf{z}^1$, $\boldsymbol{\lambda}\mathbf{z}^2$, …, $\boldsymbol{\lambda}\mathbf{z}^9$ are constructed again based on $I_P^{(2)}$, $I_I^{(2)}$, and $I_N^{(2)}$. The orderings remain the same as in Iteration I except $\boldsymbol{\lambda}\mathbf{z}^9 < \boldsymbol{\lambda}\mathbf{z}^1$ which was deleted in Step 3 of Iteration I. Since the intersection of $\lambda_{(i,j)}^{(2)}$'s is still null ($\lambda^{(2)} = \varnothing$), the algorithm goes to Step 2 again.

Step 2. Find the violating pairwise rankings.

The optimization model in (10) is solved again with $V^{(n)}$ replaced by $V^{(2)}$. The resulting solution $\lambda'^{(2)}$ is 0.137. The corresponding total violation amount $V^{(2)}$ is 1152.71. Then, $I'^{(2)}_P$ and $I'^{(2)}_I$ are constructed as: $I'^{(2)}_P = \{(2, 4)\}$ and $I'^{(2)}_I = \{(3, 8)\}$. The violation amounts for pairs (2, 4) and (3, 8) are 90.04 and 1062.67, respectively.

Step 3. Revise the selected pairwise ranking.

The DM selects $(3,8) \in I'^{(2)}_I$ and chooses to change the current pairwise ranking $\mathbf{z}^3 \sim \mathbf{z}^8$ into $\mathbf{z}^3 \phi\, \mathbf{z}^8$. Then, $I_I^{(2)}$ is updated with (3, 8) deleted, and $I_P^{(2)}$ with (3, 8) added. $I_N^{(2)}$ is kept as it is. Let $n = 3$.

<Iteration III>

Step 1. Calculate λ from the pairwise orderings of the WMSE values.

The pairwise orderings of $\boldsymbol{\lambda}\mathbf{z}^1$, $\boldsymbol{\lambda}\mathbf{z}^2$, …, $\boldsymbol{\lambda}\mathbf{z}^9$ are constructed again based on $I_P^{(3)}$, $I_I^{(3)}$, and $I_N^{(3)}$. The orderings remain the same as in Iteration II except $\boldsymbol{\lambda}\mathbf{z}^3 = \boldsymbol{\lambda}\mathbf{z}^8$ which is now changed to $\boldsymbol{\lambda}\mathbf{z}^3 < \boldsymbol{\lambda}\mathbf{z}^8$. Now, the intersection of $\lambda_{(i,j)}^{(3)}$'s is not null ($\lambda^{(3)} = \{\lambda \mid 0.091 \le \lambda < 0.131\}$). Therefore, the algorithm successfully ends with $\lambda^{(3)}$ as the final set of λ.

3.2. Summary of results

The proposed method has found a feasible set of λ by deleting $\mathbf{z}^9 \phi\, \mathbf{z}^1$ and changing $\mathbf{z}^3 \sim \mathbf{z}^8$ into $\mathbf{z}^3 \phi\, \mathbf{z}^8$ in Iteration I and II, respectively. The number of pairwise rankings in violation decreased from 6, 2, to 0, and the total violation amount also dropped from 21579.07, 1152.71, to 0 in Iterations I, II and III, respectively. The final set of λ is obtained as $\{\lambda \mid 0.091 < \lambda < 0.131\}$. Any λ value between 0.091 and 0.131 is congruent with the DM's preference structure.

4. CONCLUSION

This paper proposed a systematic method to determine λ in WMSE based on a DM's preference structure. The proposed procedure extracts the pairwise rankings of the alternative vectors, which consist of the bias and variance elements, from a DM. Then, it finds the λ value congruent with the given rankings. The proposed procedure was illustrated through an example problem.

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