

Multiresponse Surfaces Optimization Based on Evidential Reasoning Theory

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Abstract

During process design or process optimization, it is quite common for experimenters to find optimum operating conditions for several responses simultaneously. The traditional multiresponse surfaces optimization methods do not consider the uncertain relationship among these responses sufficiently. For this reason, the authors propose an optimization method based on evidential reasoning theory by Dempster and Shafer. By maximizing the basic probability assignment function, which indicates the degree of belief that certain operating condition is the solution of this multiresponse surfaces optimization problem, the desirable operating condition can be found.

Key Words: Multiresponse surfaces optimization, Evidential reasoning theory, Design of experiment

1. Introduction

With the keen competition in 21st century, manufacturers must pay more attention to quality of their products. Thus, engineers have to find the best operation conditions by design of experiment (DOE), especially response surface methodology (RSM) in order that they can improve quality characteristics of products. And this problem becomes augmented when it is required to simultaneously optimize more than one quality characteristic. It is so-called multiresponse surfaces optimization. This problem is more complex to deal with than single response surface optimization. Rarely is the resulting "optimum" truly optimal for all of the individual responses taken independently. Instead the optimum represents some explicit compromise among them.

Since the problem of multiresponse surfaces optimization was brought forward, many statisticians and quality engineers have already gone deeply into it. Their research can be classified into three categories: desirability function approach advocated by Derringer and Suich (1980); Mahalanobis distance function approach by Khuri and Conlon (1981); quality

loss function approach by Ames, Szonyi and Hawkins (1997). All these methods are based on a kind of evaluation function, $h(Y(X))$, which is a transformation of multiple responses into a single response based on a certain algorithm. However, practitioners are not sure about the relationships (including correlation, relative importance etc.) among these responses during the process of multi-objectives transformation into a single one. In this case, it isn't ideal to subjectively integrate the objectives in terms of some definite relationships. Considering this uncertainty and regarding multiresponse surfaces optimization as a sequential decision-making process, this paper presents an optimization method based on evidential reasoning theory, which is proposed for solving the problems involving certain degree of uncertainty.

2. Brief Review of Evidential Reasoning Theory

The evidential reasoning theory was developed by Shafer (1976) on a basis of the study of Dempster, and extended by Yager (1987). This theory generalizes Bayesian probability theory by assigning upper and lower bounds for probabilities, as opposed to point values, to both the elements and the subsets of the state space. Thus, it can deal with uncertainty existing in the knowledge about an object. The evidential reasoning theory makes full use of all the available incomplete information obtained from every independent knowledge source, and finally gets the degree of belief of the problem to be solved by evidence accumulation. It allows for dividing the whole problem (evidence) into several sub-problems (sub-evidences). After they are dealt with and then integrated by the rules of combination, the whole problem is solved. There are two important concepts that constitute the framework of evidential reasoning theory as follows:

(1) Basic Probability Assignment and Belief Structure

For a given state space, Ω , denotes all the possible states of the problem of our interest, which is called "frame of discernment" in evidential reasoning theory (Ni Ming, ect.,1996). Elements of Ω are called elementary propositions, each of which may be true or false and is mutually exclusive. The notation 2^{Ω} is used to indicate the power set of Ω . Sure enough, the proposition, $\Omega \in 2^{\Omega}$, is always true, but it doesn't illustrate any useful information. On the contrary, it reflects a state of uncertainty. In order to express degree of belief of certain proposition numerically, function $m: 2^{\Omega} \rightarrow [0,1]$ is defined. Thus, we can use $m(A)$ to denote a measure of the proportion of total belief assigned to the subset A of Ω . We refer $m(A)$ as

basic probability assignment function (BPA) defined in the power set, 2^{Ω} . It subjects to the following conditions:

$$\begin{aligned} 0 \leq m(A) \leq 1 \quad \forall A \in 2^{\Omega} \\ m(\phi) = 0 \\ \sum_{A \in 2^{\Omega}} m(A) = 1 \end{aligned}$$

It is necessary to point out that although BPA looks like probability of Bayesian probability theory, there are some differences between them. Firstly, BPA of a proposition can never be further broken down on its subset. Secondly, additivity and monotonicity is not satisfied. In evidential reasoning theory, we refer $\{m(A): A \in 2^{\Omega}\}$ as belief structure. Specially, if belief structure satisfies the following equation:

$$m(A) + m(\Omega) = 1 \tag{1}$$

it is called a simple support function of proposition A . It conveys that the proposition A is true with a numeric degree of support $m(A)$, and any other distinct propositions may be true or not true with numeric degree of support $m(\Omega)$, called degree of uncertainty.

As mentioned above, an interval, $[BEL(A), PL(A)]$, is used to denote probability of a proposition, in which $BEL(A)$ and $PL(A)$ is called belief function and plausibility function, respectively. They have the following relationships:

$$BEL(A) = \sum_{B \subset A} m(B) \tag{2}$$

$$PL(A) = \sum_{B \cap A \neq \phi} m(B) \tag{3}$$

$$BEL(\neg A) + PL(A) = 1 \tag{4}$$

where $\neg A$ denotes the negative proposition of A .

(2) Rules of Combination

In the evidential reasoning theory, sub-evidences, which are based on the same frames of discernment and from different knowledge sources, are integrated by rules of combination. Then the problem of our interest will be solved. There are two famous rules of combinations: Dempster's rule and Yager's rule (1987). The former is used when there aren't conflicts among these knowledge sources. The latter is used when some conflicts may exist. Let two different belief structures based on the same frames of discernment be: $\{m_1(A): A \in 2^{\Omega}\}$ and $\{m_2(B): B \in 2^{\Omega}\}$, respectively, in which C is the new proposition after A and B are integrated. The two rules are as follows:

$$m(C) = m_1 \oplus m_2(C) = \begin{cases} \frac{\sum_{A \cap B = C} m_1(A)m_2(B)}{1 - \sum_{A \cap B = \phi} m_1(A)m_2(B)} & C \neq \phi \\ 0 & \text{Others} \end{cases} \quad (5)$$

$$m(C) = m_1 \oplus m_2(C) = \begin{cases} \sum_{A \cap B = C} m_1(A)m_2(B) & C \neq \phi, \Omega \\ \sum_{A \cap B = \phi} m_1(\phi)m_2(\phi) + \sum_{A \cap B = \Omega} m_1(\Omega)m_2(\Omega) & \text{Others} \end{cases} \quad (6)$$

3. Apply Evidential Reasoning Theory to MultiResponse Surfaces Optimization

Because multiresponse surfaces optimization based on evidential reasoning theory is executed through evidence accumulation, the difficulties mentioned in introduction can be easily eliminated. First, we regard each response as a knowledge source and acquire expressions of BPA of each response concerning the operation conditions. Then we merge them into the expression of BPA of multiresponse problem, $m_i(T)$, by Yager's rule. At last, we optimize this expression to get the final solution.

The mathematical model of multiresponse surfaces optimization can be written as:

$$\begin{aligned} \max Y(X) &= (Y_1(X), Y_2(X), \dots, Y_m(X))^T \\ \text{s.t. } g_j(X) &\leq 0 \quad j=1,2,\dots,l \end{aligned}$$

where $X=(x_1, x_2, \dots, x_n)^T$ denotes operation conditions. When applying evidential reasoning theory to multiresponse surfaces optimization, the frames of discernment are defined as: $\Omega = \{T, F : \forall X \in g_j(X) \quad j=1,2,\dots,l\}$, where T represents that the selected X is the optimum solution, F indicates that the selected X isn't the optimum solution, and $\Omega=(T, F)$ illustrates that the selected X can't be determined whether it is the desired solution. Thus the power set, $2^{\Omega} = \{\phi, T, F, (T,F)\}$, denotes all the possible cases. During searching optimum process, we don't know whether certain X is the desired optimum solution. So the belief structure, $\{m(T), m(F), m(T,F)\}$, can be used to indicate this uncertainty. In terms of evidential reasoning theory, we have the following equation:

$$m(T) + m(F) + m(T,F) = 1 \quad (7)$$

For the sake of obtaining the BPA of multiresponse surfaces, the BPA of individual response must be acquired first. Since BPA doesn't possess additivity ($m(T) + m(F) \neq 1$), we can't deduce $m(F)$ from $m(T)$. It is impossible to define $m(T)$ directly. Thus, we attempt to define it from two sides (two sub-evidences) and then apply Dempster's rule to merge them

into one. By this means, we can get $m(T)$, $m(F)$ and $m(T,F)$ indirectly. Considering the simple relationship of simple support function, we define two belief structures: $\{m_i^{(1)}(F)$, $m_i^{(1)}(T,F)\}$ and $\{m_i^{(2)}(T)$, $m_i^{(2)}(T,F)\}$, $i=1,2,\dots,m$. For each response, here $m_i^{(1)}(F)$ represents the elementary proposition "the operation conditions, X, isn't the optimum solution of the ith response"; $m_i^{(2)}(T)$ denotes the elementary proposition "X is the optimum solution of the ith response"; $m_i^{(1)}(T,F)$ and $m_i^{(2)}(T,F)$ indicates the degree of uncertainty that X is neither clearly accepted nor positively rejected as the optimum solution. They satisfy the relationship denoted by equation (1). Now we need to define $m_i^{(1)}(F)$ and $m_i^{(2)}(T)$. Because the optimum solutions and range of individual responses can be provided as evidences to computing process, and we don't have other additional knowledge about these responses, the following expressions of $m_i^{(1)}(F)$ and $m_i^{(2)}(T)$ are calculated as:

$$m_i^{(1)}(F) = \begin{cases} 0 & Y_i(X) \geq Y_{\max i} \\ \frac{Y_{\max i} - Y_i(X)}{Y_{\max i} - Y_{\min i}} & Y_{\min i} \leq Y_i(X) < Y_{\max i} \\ 1 & Y_i(X) < Y_{\min i} \end{cases} \tag{8}$$

$$m_i^{(2)}(T) = \begin{cases} 0 & Y_i(X) < Y'_{\min i} \\ \frac{Y_i(X) - Y'_{\min i}}{Y_{\max i} - Y'_{\min i}} & Y'_{\min i} \leq Y_i(X) < Y_{\max i} \\ 1 & Y_i(X) \geq Y_{\max i} \end{cases} \tag{9}$$

Where $Y_{\max i}$ and $Y_{\min i}$ indicate the minimum and maximum of the ith response taken independently, and $Y'_{\min i} = \min_j \{Y_i(X_j^*)\}$, X_j^* denotes the optimum solution of the jth response. According to the equation (1), we can get the expressions of $m_i^{(1)}(T,F)$ and $m_i^{(2)}(T,F)$.

After the BPAs of the two sub-evidences concerning each response are obtained, Dempster's rule is adopted to integrate them. In this way, $m_i^{(T)}$, $m_i^{(F)}$ and $m_i(T,F)$ are gained by

$$m_i(T) = \frac{m_i^{(1)}(T,F) \cdot m_i^{(2)}(T)}{1 - m_i^{(1)}(F) \cdot m_i^{(2)}(T)} \tag{10}$$

$$m_i(F) = \frac{m_i^{(2)}(T,F) \cdot m_i^{(1)}(F)}{1 - m_i^{(1)}(F) \cdot m_i^{(2)}(T)} \tag{11}$$

$$m_i(T,F) = \frac{m_i^{(1)}(T,F) \cdot m_i^{(2)}(T,F)}{1 - m_i^{(1)}(F) \cdot m_i^{(2)}(T)} \tag{12}$$

Up to now, we have already got the BPAs of individual response with regard to operation conditions, X . In order to solve the multiresponse surfaces optimization problem, we need to integrate these sub-evidences and get the BPA of the multiresponse problem. There may exist conflicts among these responses, so Yager's rule is adopted. It should be pointed out that this integrating process is sensitive to the order of combination because Yager's function isn't homogeneous. So we need to rank the responses in descending order of importance before we begin to integrate them. The integrating process can be realized by the recursive equations:

$$D_{i+1}(T) = D_i(T)m_{i+1}(T) + D_i(T)m_{i+1}(T, F) + D_i(T, F)m_{i+1}(T) \quad (13)$$

$$D_{i+1}(F) = D_i(F)m_{i+1}(F) + D_i(F)m_{i+1}(T, F) + D_i(T, F)m_{i+1}(F) \quad (14)$$

$$D_{i+1}(T, F) = D_i(T, F)m_{i+1}(T, F) + D_i(F)m_{i+1}(T) + D_i(T)m_{i+1}(F) \quad (15)$$

Where $D_1(T) = m_1(T)$, $D_1(F) = m_1(F)$, $D_1(T, F) = m_1(T, F)$, $i = 1, 2, \dots, m-1$.

It is obvious that $D_m^{(T)} = m_f^{(T)}$ denotes the degree of belief of the proposition, " the selected operation condition, X , is the optimum solution of multiresponse surfaces optimization problem". Maximizing $m_f^{(T)}$, we'll get the solution of optimization, X^* . In this way, a complex multiresponse surfaces optimization problem is transformed into a single objective optimization problem, which can be solved by any classical method:

$$\begin{aligned} \max \quad & m_f(T) \\ \text{s.t.} \quad & g_j(X) \leq 0 \quad j=1, 2, \dots, k \end{aligned}$$

4. Application Example

In order to illustrate the approach of applying evidential reasoning theory to multiresponse surfaces optimization explicitly, we present an multiresponse experiment, which is outlined by Khuri and Cornell (1987) and originally done by Schmidt et al. They investigated the effects of cysteine (x_1) and calcium chloride (x_2) combinations on the textural and water-holding characteristics of dialyzed whey protein concentrates gel systems. These characteristics are measured by cohesiveness (Y_1) and compressible water (Y_2). We shall consider a simultaneous optimization of these two responses. A central composite design with five center point replications was used. Table 1 indicates the experimental data:

Table 1. Experimental Data and Response Values

x_1 (mM)-original	x_2 (mM)-original	x_1 -coded	x_2 -coded	Y_1 (mm)	Y_2 (g)
8.0	6.5	-1	-1	1.95	0.22
34.0	6.5	1	-1	1.37	0.67
8.0	25.9	-1	1	1.74	0.57
34.0	25.9	1	1	1.20	0.69
2.6	16.2	-1.414	0	1.75	0.33
39.4	16.2	1.414	0	1.13	0.67
21.0	2.5	0	-1.414	1.68	0.42
21.0	29.9	0	1.414	1.51	0.57
21.0	16.2	0	0	1.80	0.44
21.0	16.2	0	0	1.79	0.50
21.0	16.2	0	0	1.79	0.50
21.0	16.2	0	0	1.77	0.43
21.0	16.2	0	0	1.73	0.47

Using JMP4.0 to fit the models for the two responses, we get two response surfaces as follows:

$$\hat{Y}_1 = 1.776 - 0.250x_1 - 0.078x_2 - 0.156x_1^2 - 0.079x_2^2 + 0.010x_1x_2$$

$$\hat{Y}_2 = 0.468 + 0.131x_1 + 0.073x_2 + 0.026x_1^2 + 0.024x_2^2 - 0.083x_1x_2 \quad (x_1^2 + x_2^2 \leq 2)$$

Maximizing the two response surfaces dependently, we get the operation conditions, $X_1=(-0.819,-0.546)^T$ and $X_2=(1.373,-0.041)^T$, correspondingly $Y_{\max 1}=1.900(\text{mm})$ and $Y_{\max 2}=0.714(\text{mm})$. It is obvious that there is a conflict with regard to cysteine (x_1) between the two responses. This also illustrates that we can't optimize individual response surfaces independently., we can get $Y'_{\min 1}=1.141(\text{mm})$ and $Y'_{\min 2}=0.234(\text{g})$ in terms of the above X_1 and X_2 . In the same way $Y_{\min 1}=1.104(\text{mm})$ and $Y_{\min 2}=0.228(\text{g})$ can be obtained by minimizing the two response surfaces.

Then, two belief structures, $\{m_i^{(1)}(F), m_i^{(1)}(T,F)\}$, $i=1,2$, are defined for the two responses. The above results and the two response surfaces substitute the corresponding symbols in equations of (8) and (9). Using Dempster's rule (equations (10)-(12)) ,we'll get the BPAs of the two responses. At last, $m_f(T)$ is obtained through Yager's rule (equations (13)-(15)). Now, the only thing we need to do is maximizing $m_f(T)$. The final result is included in table 2:

Table 2. The Optimum Solution of $mf(T)$ through Lingo 4.0

Variable	Value	Reduced Cost
X1	-0.7384774	0.1995856E-08
X2	1.206089	0.0000000
Objective value(MT)	0.7357987	
MT1	0.6049038	
MT2	0.6585281	

From this result, we can see that the total BPA, $m_i(T)$, amounts to maximum, 0.7357987, when the setting of operation condition is $X=(-0.7384774, 1.206089)^T$. This means that the solution of this multiresponse surfaces optimization problem is $X=(-0.7384774, 1.206089)^T$, correspondingly cohesiveness, $Y_1=1.658$ (mm), and compressible water $Y_2=0.582$ (g). Of course, the three methods mentioned in introduction can also be used to solve this example. However, with the increase of the number of responses and uncertainty, our proposed method will show more advantages

5. Conclusions

In this research, we present a new method to solve the problem of multiresponse surfaces optimization. This method considers the essence of the optimization and the uncertainty among the responses. Through the process of evidence accumulation, subjectivity can be reduced at some degree. In addition, what is necessary to point out is that although we only discuss the larger-the-best case in our paper, this method can also be used in the cases of smaller-the-best and nominal-the-best (Vining and Myers, 1990) by defining corresponding belief functions.

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