OPTIMIZATION OF DESIRABILITY FUNCTIONS AS A DNLP MODEL BY GAMS/BARON

Basak Akteke Ozturk*, Gulser Koksal** and Gerhard Wilhelm Weber*

* Institute of Applied Mathematics, Middle East Technical University, Ankara - Turkey
** Department of Industrial Engineering, Middle East Technical University, Ankara - Turkey

e-mails: bozturk@metu.edu.tr, koksal@ie.metu.edu.tr, gweber@metu.edu.tr

Abstract
Desirability functions of Derringer and Suich, one of the widely used approaches in multiresponse optimization, have nondifferentiable points in their formulations as a drawback. To solve the optimization problem of the overall desirability function, one way is to modify the individual desirability functions by approximation approaches and then to use the gradient based methods. Another way is to use the optimization techniques that do not employ the derivative information. In this study, we propose a new approach which is easy to implement and does not need assumptions like convexity and smoothness. Our approach is based on writing the optimization problem of the overall desirability function as a mixed-integer nonlinear problem, and then putting a constraint on the integer variable to obtain a continuous formulation. The resulting problem is solved as a nonlinear model with discontinuous first order derivatives (DNLP) with Branch And Reduce Optimization Navigator (BARON), a new solver of the General Algebraic Modeling System (GAMS) for nonconvex optimization problems. The solutions obtained for two example problems are better than those of the others.

Keywords: desirability functions, multiresponse optimization, multiobjective optimization, nonlinear mixed-integer programming, nonsmooth function, quality engineering, GAMS/BARON

1. Introduction

Most industrial processes and products have more than one response or quality characteristic affected by several factors or variables. To find the best levels of these variables during product or process design, it is necessary to take into account all these quality characteristics simultaneously, which is known as multiresponse or multiobjective optimization. A wide range of multiresponse optimization and multicriteria decision making (MCDM) approaches available in the literature can be used for these problems. The most commonly used approaches are multivariate analysis of variance (MANOVA), response surface methodology (RSM), Taguchi method, loss functions, Mahalanobis distance and desirability functions. Each of these methods has its own strengths and limitations.

Desirability functions approach is based on the idea that when one of the quality characteristics of an industrial process or product with many characteristics is not in the desired limits, then the overall quality of the industrial process or the product is not desirable. By this approach the process (and/or product) variables $x$ which yield the most desirable responses are found. The desirability function approach for the optimization of the multiresponse problems was originally introduced by Harrington [5]. Then another version was developed by Derringer and Suich [4] which has been the one widely used in the literature. In their study, the overall desirability function, delivered as the geometric mean of linear individual desirability functions, is optimized by a univariate search technique which does not use any derivative information of the function. Castillo et al. [3] demonstrated a modified version of the Derringer and Suich's desirability functions for the linear case based on polynomial approximations of the individual desirability functions at their nondifferentiable points. Then, the optimization problem of the overall desirability function obtained from the geometric mean of the smoothed functions is solved by a generalized reduced gradient method. Ch'ng et al. [1] proposed a new formula to compute the overall desirability function other than the geometric mean together with a change of variables in the individual desirabilities in such a way that no nondifferentiable points occur in the functions. There are many other studies with desirability functions focusing on other drawbacks than nondifferentiability such as those in the studies of Khuri and Conlon [7], Kim and Lin [8] and Jeong and Kim [6].

The desirability functions continue to be a commonly preferred method because it easily converts a multiresponse problem into a single response one. The desirability functions considered in this study are of Derringer and Suich’s type. They can be linear or nonlinear; usually piecewise smooth including a finite number of nondifferentiable points at their target value, where the maximum desirability occurs.
In section 2, we present the individual and overall desirability functions and the optimization problem of the overall desirability functions of Derringer and Suich’s [4]. In section 3, we summarize the current approaches to solve the maximization problem of these functions. We propose a new approach based on reformulating two-sided individual desirability functions and write the optimization problem of the overall desirability functions in section 4. We use our approach on two examples and present the results obtained from BARON solver of GAMS.

2. Desirability Functions

In a multiresponse optimization problem each response can be expressed as $Y_j(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ ($j = 1,2,\ldots,m$), where $x \in \mathbb{R}^n$ ($\mathbb{R}$ denoting the real numbers) are the decision variables or controllable factors. An individual desirability function $d_j(Y_j(\cdot)) : \mathbb{R} \rightarrow \mathbb{R}$ assigns a number between 0 and 1; 0 being a completely undesirable and 1 being a completely desirable or ideal response value. The individual desirabilities are then combined into an overall desirability $D(x)$, using the weighted geometric mean:

$$D(x) = \left( \prod_{j=1}^{m} w_j d_j(Y_j(x)) \right)^{1/m} \sum_{j=1}^{m} w_j$$  \hspace{1cm} (1)

Here, $m$ is the number of responses and $w_j \geq 0$ are the weights. Formulations of one-sided and two-sided individual desirability functions, defining responses as $y_j = Y_j(x)$, $y_j \in \mathbb{R}$ ($j = 1,2,\ldots,m$), are as follows:

**One-sided desirability:**

$$d_j(y_j) = \begin{cases} 0, & y_j \leq l_j, \\ \frac{y_j - l_j}{u_j - l_j}, & l_j < y_j < u_j, \\ 1, & y_j \geq u_j. \end{cases}$$  \hspace{1cm} (2)

**Two-sided desirability:**

$$d_j(y_j) = \begin{cases} 0, & y_j \leq l_j, \\ \frac{y_j - l_j}{t_j - l_j}, & l_j < y_j \leq t_j, \\ \frac{y_j - t_j}{u_j - t_j}, & t_j < y_j < u_j, \\ 0, & u_j \geq y_j. \end{cases}$$  \hspace{1cm} (3)

Here, $l_j$ is the minimum and $u_j$ is the maximum acceptable value of $y_j$, and $t_j$ is the most desirable value of $y_j$ and could be selected anywhere between $l_j$ and $u_j$ ($j = 1,2,\ldots,m$). The value of $r$ used in Equation (2) should be specified by the user. Larger the $r$, more desirable the $y_j$ values closer to $u_j$, and vice versa. $s$ and $t$ in Equation (3) have a similar meaning.

The problem is to maximize the overall desirability function given in (1):

$$\text{maximize } D(x)$$

subject to

i. bounds of the factors $x$,
ii. bounds of the responses $y_j$,  \hspace{1cm} (4)
iii. the nonzero condition of the individual desirability functions, $d_j(y_j) \geq 0$.

The desirability function approach requires that for each response $y_j$, an empirical model (typically a polynomial) is built for the relation between the response and the factors using the response surface methodology. These models are used in the individual desirability functions (2) and (3), which in turn are substituted in the overall desirability function (1). Then a single objective optimization method is used to solve the optimization problem given in (4), i.e., we want $D(x)$ as close to unity as possible. In this formulation of desirability functions, possible correlations between the responses are not taken into account.

3. Optimization of Desirability Functions

The optimization of overall desirability functions becomes a complicated task when there are two-sided individual desirability functions in the problem. In the two-sided desirability functions formulation (3), the target value is a nondifferentiable point and hence the function is not smooth at this point. To optimize the overall desirability function given in (1) involving two-sided desirabilities, one way is to use the optimization techniques that do not employ the derivative information to find the optimum. Another way is to modify the individual desirability functions by approximation approaches to smooth it and then use the gradient based methods.

3.1 Direct Search Optimization Methods

These methods do not use the derivative information of the function in the optimization process. The
estimated responses \( \hat{Y}_j(x) \) \((j = 1, 2, \ldots, m)\) are continuous functions of the factors \( x \), the individual desirabilities \( d_j(\hat{Y}_j(x)) \) of the estimated responses are also continuous functions of the factors \( x \), and hence, the overall desirability function \( D(x) \) is a continuous function of the factors \( x \). Therefore, the direct search methods can be used to optimize the overall desirability over the domain of the factors. In the study of Derringer and Suich [4], firstly second degree polynomials are fit by regression to some data collected through experimentation to model the relations between the responses and the factors. Then, the individual desirabilities of these responses are calculated and used to calculate the overall desirability. Hence, for each set of factor levels, an overall desirability value is obtained. Then, all factor levels are searched to find the optimal \( D \) by a direct search method similar to that of Hooke and Jeeves [11].

3.2 Modified Desirability Functions Approach

The idea in the modification approach is to smooth the two-sided desirability functions by a local polynomial approximation at their nondifferentiable points and being able to use the gradient based methods, which are widely available and more popular. Castillo et al. [3] proposed a smoothing technique for the linear case \((s=t=1)\) of the two sided individual desirability functions to get rid of the nondifferentiable points. Then the overall desirability function is optimized with a gradient based method, generalized reduced gradient (GRG). This approach is referred to as GRG, in short, in this paper.

The nondifferentiable point of a two-sided desirability function is at \( t_j \) \((j = 1, 2, \ldots, m)\) where the optimal value of the function occurs. The approximation function has to be a polynomial of degree 4 for each \( j = 1, \ldots, m \):

\[
    f_j(y_j) = A_j + B_j y_j + C_j y_j^2 + D_j y_j^3 + E_j y_j^4
\]

with five unknowns \( A_j, B_j, C_j, D_j \) and \( E_j \), since it has to satisfy the following conditions for each \( j \):

1. the desirability value of the approximating function at \( t_j \) must be equal to the value of the nondifferentiable desirability function at \( t_j \);
2. the desirability value of the approximating function at \( t_j - \delta_j \) must be equal to the value of the nondifferentiable desirability function at \( t_j - \delta_j \), where \( \delta_j \) is the half size of a small neighborhood around \( t_j \);
3. the desirability value of the approximating function at \( t_j + \delta_j \) must be equal to the value of the nondifferentiable desirability function at \( t_j + \delta_j \);
4. the derivative of the approximating function at \( t_j - \delta_j \) must be equal to the derivative of the nondifferentiable desirability function at \( t_j - \delta_j \);
5. the derivative of the approximating function at \( t_j + \delta_j \) must be equal to the derivative of the nondifferentiable desirability function at \( t_j + \delta_j \).

These five conditions are expressed as a system of five linearly independent equations with the five unknowns, \( A_j, B_j, C_j, D_j \) and \( E_j \), for each \( j = 1, \ldots, m \). Therefore, generically, we have a unique solution on this system.

Herewith, the approximated individual desirability function \( \overline{d}_j(y_j) \) becomes

\[
    \overline{d}_j(y_j) = \begin{cases} 
    a_j + b_j y_j, & l_j \leq y_j \leq t_j - \delta_j y_j, \\
    f_j(y_j), & t_j - \delta_j y_j \leq y_j \leq t_j + \delta_j y_j, \\
    c_j + d_j y_j, & t_j + \delta_j y_j \leq y_j \leq u_j, \\
    0, & \text{otherwise},
    \end{cases}
\]

with coefficients \( a_j \) and \( b_j \) for the function on \( [l_j, t_j - \delta_j y_j] \) and \( c_j \) and \( d_j \) are coefficients of the function on \( [t_j + \delta_j y_j, u_j] \) for the case of a single nondifferentiable point at \( t_j \). After modifying all individual desirability functions as given in equation (5), the overall desirability function is computed with these modified and, hence, smoothed functions. Castillo et al. [3] used GRG2 method provided by Microsoft® Excel, as well as many others, to optimize the overall desirability function.

Although modifying desirability functions helps us to get rid of the nondifferentiable points, this method may lead to inaccurate results for some inexperienced users because it needs numerous calculations. Here, the smoothing technique means an approximation of the model; hence, it can lead to sub-optimal solutions.

4. Proposed Approach: DNLP Model of Desirability Functions solved by GAMS/BARON

An overall desirability function which involves only one-sided desirability functions does not contain any nondifferentiable point. Hence, it is a smooth
function and its optimization problem can be solved by a gradient based method. We treat the optimization problem of the overall desirability functions involving at least a two-sided desirability function. These kinds of overall desirability functions are nonsmooth functions; hence its maximization is a nonsmooth optimization problem. For details of nonsmooth optimization, we refer to the book of Clarke [2].

For a two-sided individual desirability function, we introduce a mixed-integer formulation with \( z_k (k = 1, 2, \ldots, p) \) being a binary coefficient and \( p \) being the number of the responses having two-sided desirabilities:

\[
d_k(x, z_k) = z_k d_k(Y_k(x)) + (1 - z_k) d_k(Y_k(x)).
\]

Here, \( z_k = 1 \), i.e., \( d_k(x, z_k) = d_k(Y_k(x)) \), if the value of the response is in \([ l_k, t_k] \); and \( z_k = 0 \), i.e., \( d_k(x, z_k) = d_k(Y_k(x)) \), if the value of the response is in \([ t_k, u_k] \), where \( l_k < t_k < u_k \).

The overall desirability function \( D(x, z) \) with \( m \)-\( p \) being the number of one-sided desirabilities, becomes:

\[
D(x, z) = \prod_{j=1}^{m-p} w_j d_j(x) \cdot \prod_{k=1}^{p} w_k d_k(x, z_k),
\]

for \( x := (x_1, x_2, \ldots, x_n)^T \) and \( z := (z_1, z_2, \ldots, z_p)^T \).

The optimization problem can be stated as follows:

maximize \( D(x, z) \)

such that \( x \in [ l, u ] \),

\[
y_j \in [ l_j, u_j ] \quad \forall j,
\]

\( d(x) \geq 0, \)

\( d(x, z) \geq 0, \)

\( h(z) = 0.\)

Here, \( x \) is the vector of the factors with the constraint set (a “box”) \([ l, u ] := [ l_1, u_1 ] \times [ l_2, u_2 ] \times \cdots \times [ l_n, u_n ] \),

\( l_i \) the lower limit and \( u_i \) the upper limit of \( x_i \) \((i = 1, 2, \ldots, n)\), \( y_j \) \((j = 1, 2, \ldots, m)\) are the responses with lower bounds \( l_j \) and upper bounds \( u_j \). \( d(x) := (d_1(x), d_2(x), \ldots, d_{m-p}(x))^T \) are the one-sided desirability functions given explicitly in (2), two-sided desirability functions, \( d(x, z) := (d_1(x, z_1), d_2(x, z_2), \ldots, d_p(x, z_p))^T \) are given in equations (3) and (6), and \( h(z) := (h(z_1), h(z_2), \ldots, h(z_p))^T \) with

\[
h(z_k) := z_k^2 - z_k.
\]

We show our approach on the wire bonding optimization problem given with full detail in Castillo et al. [3] and the tire tread compound problem given in Derringer and Suich [4]. We formulate the optimization problems of these two problems as in (7) and solve them as a nonlinear model with discontinuous first order derivatives (DNLP) through Branch And Reduce Optimization Navigator (BARON) [10], which is a new solver of the General Algebraic Modeling System (GAMS) [9].

BARON is developed for the global solution of nonlinear and mixed-integer nonlinear programs without any convexity assumption. BARON implements algorithms of the branch-and-bound type enhanced with a variety of constraint propagation and duality techniques for reducing ranges of variables in the course of the algorithm.

4.1 Example: Wire Bonding Process Optimization

The wire bonding system has three control factors: the flow rate \( x_1 \), the flow temperature \( x_2 \), and the block temperature \( x_3 \). The levels of these factors are all between -1 and 1. There are six responses to measure two different locations’ maximum, beginning and finishing bonding temperatures. All of these responses are of the target-is-the-best type. The models for the responses are used as given in Castillo et al. [3]. Their upper, lower and target values are given in Table 1.

<table>
<thead>
<tr>
<th>Response</th>
<th>( l_j )</th>
<th>( t_j )</th>
<th>( u_j )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y_1 )</td>
<td>185</td>
<td>190</td>
<td>195</td>
</tr>
<tr>
<td>( y_2 )</td>
<td>170</td>
<td>185</td>
<td>195</td>
</tr>
<tr>
<td>( y_3 )</td>
<td>170</td>
<td>185</td>
<td>195</td>
</tr>
<tr>
<td>( y_4 )</td>
<td>185</td>
<td>190</td>
<td>195</td>
</tr>
<tr>
<td>( y_5 )</td>
<td>170</td>
<td>185</td>
<td>195</td>
</tr>
<tr>
<td>( y_6 )</td>
<td>170</td>
<td>185</td>
<td>195</td>
</tr>
</tbody>
</table>

The optimization problem (7) of the wire bonding process is solved as a DNLP model with BARON. The results are presented in Table 2 in comparison with the results given in Castillo et al.’s work, i.e., GRG and H&J which refers to direct search method of Hooke-Jeeves [3,11].
In Table 4, BARON results are presented in comparison with the results given in Derringer and Suich’s work (D&S) [4] and Jeong and Kim’s (J&K) [6] work.

Discussion and Further Studies

In maximization of overall desirability functions the current approaches have difficulties with the two-sided desirability functions because of the nondifferentiable points in their formulations. Using direct search methods to find the optimum requires a long computational time as the number of responses increases. Nondifferentiable points, on the other hand, might be smoothened to use the gradient based methods. However, modifying desirability functions like this has been criticized to produce inaccurate results for some inexperienced users due to the numerous calculations.

Our approach based on reformulation of two-sided desirability functions makes the overall desirability function maximization a continuous nonlinear optimization problem. BARON of GAMS provides an appropriate solution algorithm for the new problem. Our experience with the two numerical example problems shows that the proposed method is superior to the formerly suggested methods in terms of reasonably small computational time and effort. As a future study, nondifferentiable cases with different shapes and combinations of desirability functions and response functions can be studied with the proposed approach, and further benefits or weaknesses, if any, can be discovered.

5. Conclusion

Desirability maximization is a widely used approach in solving multi-response optimization problems. We have presented an approach based on mathematical reformulations of the overall desirability function and its optimization problem. This approach is shown to be successful on the two example problems. Moreover, this approach is easy to implement on the problems including a large number of responses with different types.

6. Acknowledgment

This work is supported by The Scientific and Technological Research Council of Turkey (TUBITAK) under the Research Project 105M138.

7. References


Table 2: The results of wire bonding optimization problem.

<table>
<thead>
<tr>
<th></th>
<th>GRG</th>
<th>H&amp;J</th>
<th>BARON</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1$</td>
<td>0.1039</td>
<td>0.1078</td>
<td>0.105</td>
</tr>
<tr>
<td>$x_2$</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>$x_3$</td>
<td>0.7987</td>
<td>0.7973</td>
<td>0.798</td>
</tr>
<tr>
<td>$y_1$</td>
<td>186.0</td>
<td>186.1</td>
<td>186.0368</td>
</tr>
<tr>
<td>$y_2$</td>
<td>174.5</td>
<td>174.5</td>
<td>174.5178</td>
</tr>
<tr>
<td>$y_3$</td>
<td>172.0</td>
<td>172.1</td>
<td>172.0518</td>
</tr>
<tr>
<td>$y_4$</td>
<td>192.6</td>
<td>192.6</td>
<td>192.6509</td>
</tr>
<tr>
<td>$y_5$</td>
<td>173.0</td>
<td>173.1</td>
<td>173.0732</td>
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<tr>
<td>$y_6$</td>
<td>185.0</td>
<td>185.0</td>
<td>184.9922</td>
</tr>
<tr>
<td>$D$</td>
<td>0.3061</td>
<td>0.3076</td>
<td>0.3061</td>
</tr>
</tbody>
</table>

4.2 Example: Tire Tread Compound Problem

The factors of the problem are hydrated silica level $x_1$, silane coupling level $x_2$, and sulfur level $x_3$. The levels of the factors are all between -1 and 1. There are 4 responses: PICO Abrasion Index $y_1$, 200 percent modulus $y_2$, elongation at break $y_3$, and hardness $y_4$. Two of the responses, namely, $y_3$ and $y_4$, are of the target-is-the-best type, whereas the remaining ones, i.e., $y_1$ and $y_2$, are of the maximum-is-the-best type. Their lower, upper and target values are given in Table 3:

Table 3: Desirability parameters of the responses for the tire tread compound example.

<table>
<thead>
<tr>
<th></th>
<th>$l_j$</th>
<th>$t_j$</th>
<th>$u_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y_1$</td>
<td>120</td>
<td>-</td>
<td>170</td>
</tr>
<tr>
<td>$y_2$</td>
<td>1000</td>
<td>-</td>
<td>1300</td>
</tr>
<tr>
<td>$y_3$</td>
<td>400</td>
<td>500</td>
<td>600</td>
</tr>
<tr>
<td>$y_4$</td>
<td>60</td>
<td>67.5</td>
<td>75</td>
</tr>
</tbody>
</table>

The optimization problem (7) of the tire tread compound example is solved as a DNLP model with BARON.

Table 4: The results of tire tread compound problem.

<table>
<thead>
<tr>
<th></th>
<th>D&amp;S</th>
<th>J&amp;K</th>
<th>BARON</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1$</td>
<td>-0.050</td>
<td>-0.157</td>
<td>-0.052</td>
</tr>
<tr>
<td>$x_2$</td>
<td>0.145</td>
<td>1.219</td>
<td>0.148</td>
</tr>
<tr>
<td>$x_3$</td>
<td>-0.868</td>
<td>-0.604</td>
<td>-0.869</td>
</tr>
<tr>
<td>$y_1$</td>
<td>129.5</td>
<td>139.82</td>
<td>129.4252</td>
</tr>
<tr>
<td>$y_2$</td>
<td>1300</td>
<td>1239.10</td>
<td>1300.0000</td>
</tr>
<tr>
<td>$y_3$</td>
<td>465.7</td>
<td>446.51</td>
<td>465.9318</td>
</tr>
<tr>
<td>$y_4$</td>
<td>68.0</td>
<td>73.93</td>
<td>68.0207</td>
</tr>
<tr>
<td>$D$</td>
<td>0.5832</td>
<td>0.3803</td>
<td>0.5832</td>
</tr>
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</table>


