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Multiresponse systems optimization using a goal attainment approach

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A goal attainment approach to optimize multiresponse systems is presented. This approach aims to identify the settings of control factors to minimize the overall weighted maximal distance measure with respect to individual response targets. Based on a nonlinear programming technique, a sequential quadratic programming algorithm, the method is proved to be robust and can achieve good performance for multiresponse optimization problems with multiple conflicting goals. Moreover, the optimization formulation may include some prior work as special cases by assigning proper response targets and weights. Fewer assumptions are needed when using the approach as compared to other techniques. Furthermore, the decision-maker's preference and the model's predictive ability can easily be incorporated into the weights' adjustment schemes with explicit physical interpretation. The proposed approach is investigated and compared with other techniques through various classical examples in the literature.

1. Introduction

Response Surface Methodology (RSM) (Box and Draper, 1987; Khuri and Cornell, 1996; Myers and Montgomery, 2002) is increasingly being used in various industries (semiconductor, chemical, food industry, etc.) for quality improvement and process optimization. The general analysis scheme of RSM encompasses the following: (i) a Design of Experiment (DoE) is performed to obtain reliable measurements of the response; (ii) a first- or second-order polynomial model is fitted using least-squares regression; and (iii) the optimal settings of the input parameters are determined.

Most early work in RSM only considers single response variables. There is a growing interest focusing on MultiResponse Systems (MRSs), which is prevalent across various application areas. The Dual Response Surface (DRS) approach, simultaneously modeling variance and mean of the quality feature associated with a process, can be viewed as the simplest form in MRSs. It has been widely explored (for example by the work of Vining and Myers (1990), Del Castillo and Montgomery (1993), Lin and Tu (1995), Copeland and Nelson (1996), Semple (1997), Kim and Lin (1998), Del Castillo *et al.* (1999), and Tang and Xu (2002)). When more responses are to be investigated, however, the existing optimal formulations for DRS might not be appropriate. Although conventional experimental design and model fitting techniques are still useful, the challenge is how to simultaneously determine the optimum factor settings for multiple responses and hence attain the overall desired quality.

One difficulty in MRS optimization lies in the different properties of multiple responses. For example, the various responses may have different types of optimality, such as "Nominal-The-Best" (NTB), "Larger-The-Better" (LTB) or "Smaller-The-Better" (STB), and may be measured in different units with substantially different magnitudes. Moreover, the multiple responses might not increase or decrease simultaneously and hence a complex trade-off or compromise may be necessary. With the increasing demand from customers for overall quality, a systematic and robust strategy to optimize all responses simultaneously is crucial.

This paper is organized as follows. A comprehensive literature review on MRS optimization is given in Section 2. The proposed goal attainment optimization approach is described in Section 3. A modified approach to accommodate the predictive ability of a response model is also included in this section. Three examples in the literature are investigated in Section 4. Conclusions and discussions on the comparisons among various techniques are presented in Section 5.

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2. Literature review

A simple and straightforward approach for MRS optimization is to superimpose the response contour plots and determine an optimal point by visual inspection (Lind *et al.*, 1960). However, this can only be useful when the dimensions of the inputs and response variable are low. The MRS optimization is a typical multiobjective optimization problem. The Multiobjective Optimization (MO) is concerned with the minimization of a vector of objectives $\mathbf{F}(\mathbf{x})$ that may be subject to a series of constraints or bounds:

$$\text{Minimize} \quad \mathbf{F}(\mathbf{x}) = \{f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_n(\mathbf{x})\},$$

subject to

$$g_i(\mathbf{x}) = 0 \quad i = 1, 2, \ldots, m_1,$$
$$h_i(\mathbf{x}) \le 0 \quad i = 1, 2, \ldots, m_2,$$
$$(\mathbf{x}) \in X,$$

where $\mathbf{x} = [x_1, x_2, \ldots, x_a]^T$ is the set of inputs (a denotes the number of control factors) and X is the feasible set. In general, no solution minimizes all of the objectives simultaneously. The concept of a *Pareto*-optimality also called noninferiority, efficient, or compromise etc., solution has been widely used to characterize optimal solutions for the MO problem (Censor, 1977). The definition of noninferior solution is as follows:

> $\mathbf{x}^*$ *is said to be a noninferior solution of the MO problem if there exists no other feasible* $\mathbf{x}$ (*i.e.*, $\mathbf{x} \in X$) *such that* $\mathbf{F}(\mathbf{x}) \le \mathbf{F}(\mathbf{x})^*$, *i.e., no other feasible* $\mathbf{x}$ such that $f_j(\mathbf{x}) \le f_j(\mathbf{x})^*$ *for all* $j = 1, \ldots, n$ *with strict inequality for at least one j.*

Intuitively a noninferior solution is one in which an improvement in one objective function requires a degradation of at least one other objective function. A general solution approach is to change the multiobjective problem with various constraints into a single scalar measure and solve it as a single objective problem:

$$\text{Minimize} \quad p(\mathbf{x}) \quad \mathbf{x} \in X.$$

The single measure $p(\mathbf{x})$ has conventionally been defined as the following: the distance from the ideal design point "ρ" (Khuri and Conlon, 1981; Vining, 1998), a desirability function "D" (Harrington, 1965; Derringer and Suich, 1980; Del Castillo *et al.*, 1996; Kim and Lin, 2000); the weighted sum of response objective functions (Montgomery *et al.*, 1972); a quality loss function (Pignatiello, 1993; Leon, 1996; Ames *et al.*, 1997; Plante, 1999); a standardized performance index (Barton and Tsui, 1991); or a process ability criterion (Plante, 2001). However, it is usually difficult to select the weights that measure the relative importance associated with each objective in the weighted sum method. Moreover, the weighted sum method or quality loss function method may not find *Pareto* optimal points that lie upon a nonconvex boundary of attainable sets (Papalambros and Wilde, 2000).

Other improvements in MRS optimization involve optimizing the multiresponse process via constrained confidence regions (Del Castillo, 1996) and the interactive multicriteria method (Boyle and Shin, 1996). For a review on MRS optimization related problems, see Myers (1999) and the discussion therein. The following subsections briefly review two main approaches in this field, namely the generalized distance approach and the desirability function approach.

2.1. *The generalized distance approach*

The generalized distance approach developed by Khuri and Conlon (1981) (hereafter referred to as the KC approach) can be considered a two-step process. First the individual optima of the estimated responses over the experimental region are obtained. Next, the compromise optimum is obtained by minimizing the distance function ρ, the distance from the ideal optimum. The variances and covariance of the responses are used in determining the weights of a distance function as (Khuri and Conlon, 1981):

$$\rho = [(\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})^T \{\mathrm{var}[\hat{\mathbf{y}}(\mathbf{x})]\}^{-1} (\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})]^{1/2}, \qquad (1)$$

where $\hat{\mathbf{y}}(\mathbf{x})$ is the vector of predicted responses at location $\mathbf{x}$, $\mathrm{var}[\hat{\mathbf{y}}(\mathbf{x})]$ is the variance-covariance matrix for the predicted responses at this location, and $\boldsymbol{\theta}$ is the response targets' vector. The approach considers the deviation from the response targets and accounts for the variances and correlations of the responses. However, the method is limited because it requires that all predicted response functions are identical with respect to the set of input variables and the functional form of these input variables. Moreover, all responses are assumed to be of the same importance and no preference of the Decision-Maker (DM) or economical implications of the process are considered.

Vining (1998) extended the approach of KC and Pignatiello (1993) by taking the expected value of the loss function:

$$\hat{\mathbf{E}} = [(\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})^T \mathbf{C} (\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})] + \mathbf{trace}[\mathbf{C}\{\mathrm{var}[\hat{\mathbf{y}}(\mathbf{x})]\}], \quad (2)$$

where $\mathbf{C}$ is a positive definite matrix of costs or weights, and the other terms have the same definitions as Equation (1). The first term $[(\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})^T \mathbf{C} (\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})]$ represents the penalty imposed for the deviation of any responses from target values, and the second term $\mathbf{trace}[\mathbf{C}\{\mathrm{var}[\hat{\mathbf{y}}(\mathbf{x})]\}]$ represents the penalty imposed by the quality of the prediction. The method considers the correlations among the responses and the process economics. Moreover, it takes into account the effect of predictive ability on the optimal solutions. The method also includes, as a special case, the distance measure of the KC approach by choosing suitable parameters such as $\mathbf{C}$ and $\boldsymbol{\theta}$. The difficulty with this method is that the choice of $\mathbf{C}$ may be subjective and the computation of the variance-covariance matrix is complicated for practitioners when the responses have different model forms. In addition, the penalty for deviation of the responses from targets is given the same importance as the penalty for poor quality of the response predictions. Furthermore, similar to the KC approach, an examination of linear dependence among responses is necessary. Here, a mitigating measure might be used by adding a tuning parameter α $(0 \le \alpha \le 1)$ in the formulation:

$$\hat{\mathbf{E}} = [(\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})^T \mathbf{C}(\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})] + \alpha \mathbf{trace}[\mathbf{C}\{\text{var}[\hat{\mathbf{y}}(\mathbf{x})]\}], \quad (3)$$

Thus, the effect of the predictive term on the optimal solutions would be well investigated.

2.2. *The desirability function approach*

The desirability function approach transforms response i to a scale-free value between zero and one called the desirability d_i. The desirabilities are then combined into a single objective measure to be maximized, using a geometric mean function (Harrington, 1965):

$$D = (d_1 d_2 \ldots d_n)^{1/n}. \quad (4)$$

Derringer (1994) extended the technique to a general form using a weighted geometric mean:

$$D = \left(d_1^{w_1} d_2^{w_2} \ldots d_n^{w_n}\right)^{1/\sum w_j}, \quad (5)$$

where w_j is the relative weights among the n response $(j = 1, 2, \ldots, n)$. The relative weights allow the DM's preferences for the responses to be taken into account. The main idea of the desirability function approach is to find a systematic and interpretable way to transform the responses to a desirability function. Derringer and Suich (1980) (hereafter referred to as DS) choose, for each response, levels $A \le B \le C$ such that if $\hat{y} < A$ or $\hat{y} > C$, the response $\hat{y}$ is unacceptable and otherwise. The two-sided transformation desirability d can be defined as:

$$d = \begin{cases} \left\{\dfrac{(\hat{y} - A)}{(B - A)}\right\}^u & \text{for } A \le \hat{y} \le B, \\ \left\{\dfrac{(\hat{y} - C)}{(B - C)}\right\}^v & \text{for } B \le \hat{y} \le C, \\ 0 & \text{otherwise,} \end{cases} \quad (6)$$

where u and v are parameters that control the shape of the desirability function. The final solution $\mathbf{x}^*$ is the one that maximizes the geometric mean of the individual response desirabilities.

To ensure that the desirability function and its derivative are continuous, Del Castillo *et al.* (1996) presented a modified technique in which different priorities are assigned to the responses so that the importance of different responses can be considered explicitly.

2.3. *The fuzzy approach*

Recently, Kim and Lin (2000) (hereafter referred to as KL) improved the desirability approach by suggesting an alternative scheme. They assumed that the degree of satisfaction with respect to the jth response is equal to one when the response equals its target value T_j and decreases unbounded as the response moves away from its target. Once a response is below the lower target $T_j^{\min}$ or above the upper target $T_j^{\max}$, the desirability value is zero (meaning the DM does not accept such a solution). The general desirability functions they suggested take the form:

$$d(z) = \begin{cases} \dfrac{\exp(t) - \exp(t|z|)}{\exp(t) - 1} & \text{if } t \ne 0, \\ 1 - |z| & \text{if } t = 0, \end{cases} \quad (7)$$

where t is called the exponential constant which is used to adjust the shape of the desirability function, and z is a standardized parameter representing the distance of the estimated response from its target in units of the maximum allowable deviation. Then an optimization scheme is given by:

$$\underset{\mathbf{x}}{\text{Maximize}}\ \lambda,$$

subject to

$$d_j(z) \ge \lambda. \quad (8)$$

This formulation aims at maximizing the minimum degree of satisfaction λ with respect to all the responses, which is equivalent to the following problem:

$$\text{Maximize}(\min[d_1(z), d_2(z), \ldots d_n(z)]). \quad (9)$$

The optimization scheme using the "maximin" is robust to the potential dependencies between responses. It considers multiple conflicting responses as well as the model predictive ability, which is not given in the conventional desirability function approach.

The desirability function approach provides a flexible scheme for the optimization of a MRS. Through the choice of parameters u and v in Equation (6) and t in Equation (7), the DM can express their preference for the different responses. However, a "good" desirability function is rather difficult to define. We have to determine the desirability function shape, which should represent the tendency of desirability as accurately as possible for a real process. The characteristic of the process, however, is usually unknown in advance. Therefore, a reasonable guess is required for the desirability function and a great deal of caution is needed in the application of the desirability function method (Box and Draper, 1987). Comparing KC's distance approach with DS's desirability function approach, we find that the former has a more explicit optimal measure (the distance from response targets), while the latter is more flexible for incorporating the DM's preference (by adjusting the desirability function shape). In this paper, we propose an approach with both desirable characteristics.

3. Goal attainment approach for MRS optimization

3.1. *The optimization scheme*

With the complex conflicts of interest common in today's industry, a well-defined mathematical representation of the DM's preferences to achieve the optimum responses simultaneously is difficult (if at all possible) to build. On the contrary, from a DM's viewpoint, it will be of great value to make the multiple responses attain designated targets as closely as possible. This ideal status cannot be achieved simultaneously in general, because of the conflicting characteristics among responses. Hence, the deviations of variables from their targets are introduced as the objective function in the optimization procedure. This leads to the application of the techniques of goal programming (Steuer, 1986; Schniederjans, 1995; Taha, 1997) in various MO problems.

In this paper, we propose a goal attainment scheme (Gembicki and Haimes, 1975), a variant of goal programming, for MRS in the formulation as:

$$\text{Minimize} \quad \delta,$$

subject to

$$\begin{aligned} &\left|\frac{\hat{y}_j(\mathbf{x}) - T_j^*}{\omega_j}\right| \le \delta & j = 1, 2, \ldots n, \\ &g_i(\mathbf{x}) = 0 & i = 1, 2, \ldots, m_1, \\ &h_i(\mathbf{x}) \le 0 & i = 1, 2, \ldots, m_2, \\ &\mathbf{x} \in X, & \end{aligned} \tag{10}$$

where $\mathbf{T}^* = \{T_1^*, T_2^*, \ldots, T_n^*\}$ are a set of designated targets, which are associated with a set of response function objectives $\hat{\mathbf{Y}}(\mathbf{x}) = \{\hat{y}_1(\mathbf{x}), \hat{y}_2(\mathbf{x}), \ldots, \hat{y}_n(\mathbf{x})\}$, where $\mathbf{x} = [x_1, x_2, \ldots, x_a]^T$ is a set of control factors and δ (called the attainment factor) is an unrestricted scalar variable. Normally, the MRS problems only include bounds of control factors over X such as: $\mathbf{x}_l \le \mathbf{x} \le \mathbf{x}_u$ for a rectangular region or $\mathbf{x}\mathbf{x}^T \le r^2$ for a spherical region (where r is the radius of the zone of interest). The term $\omega_j\delta$ introduces an element of slackness into the problem, which otherwise imposes that the targets T_j be rigidly met and it also enables the DM to express a measure of the relative trade-offs between the objectives. The relative degree of under- or over-achievement of the targets is controlled by a vector of weighting coefficients $\omega = \{\omega_1, \omega_2, \ldots, \omega_n\} (\ge 0)$. Note that if some $\omega_j = 0$, it means that the maximum limits for the objectives $\hat{y}_j(\mathbf{x})$ are T_j^*.

In addition, according to the scheme for minimax optimization presented in Brayton *et al.* (1979), there exists the following equivalent scheme:

$$\text{Minimize } \delta \text{ such that } f_j(\mathbf{x}) \le \delta \equiv \min_x \max_j \{f_j(\mathbf{x})\}. \tag{11}$$

In the proposed approach, we take:

$$f_j(\mathbf{x}) = \left|\frac{\hat{y}_j(\mathbf{x}) - T_j^*}{\omega_j}\right|, \quad j = 1, \ldots, n \quad (\omega_j > 0).$$

It should be noted that in Equation (10), a non-smooth objective constraint:

$$\left|\frac{\hat{y}_j(\mathbf{x}) - T_j^*}{\omega_j}\right| \le \delta,$$

can be simply replaced by the following two equivalent smooth constraints:

$$\text{Minimize } \delta$$

subject to

$$\begin{aligned} &\frac{\hat{y}_j(\mathbf{x}) - T_j^*}{\omega_j} \le \delta, \\ &-\left(\frac{\hat{y}_j(\mathbf{x}) - T_j^*}{\omega_j}\right) \le \delta \quad j = 1, 2, \ldots n. \end{aligned} \tag{12}$$

The mechanism of the goal attainment approach is illustrated for a dual response system in Fig. 1. In the objective function space, the lower bound between A and B describes the noninferior solutions set. Given vector $\mathbf{T}^*$ and ω, the direction of the vector $\mathbf{T}^* + \delta\omega$ can be determined and Equation (10) can be transformed into (here we assumed that $\mathbf{T}^* \le \hat{\mathbf{Y}}$):

$$\text{Minimize } \delta$$

subject to

$$\mathbf{T}^* + \delta\omega - \hat{\mathbf{Y}} \ge 0.$$

Therefore, the problem is equivalent to finding a feasible point on this vector in objective space which is closest to the origin. It is obvious that the optimal solution will be the first point at which $\mathbf{T}^* + \delta\omega$ intersects the feasible region in the objective space. Should this point of intersection exist, it would clearly be a noninferior solution. As it can be shown, the approach may find noninferior optimal points that lie upon a nonconvex boundary of attainable sets. It

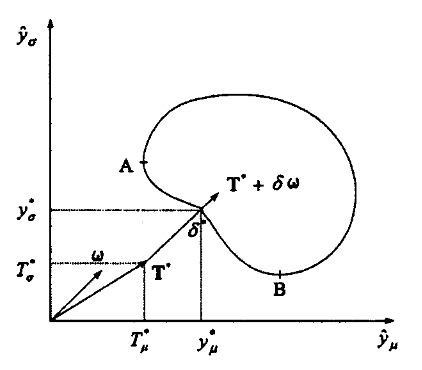

Fig. 1. The mechanism of the goal attainment approach for a dual response system.

also should be noted that $\delta > 0$, $\delta = 0$ and $\delta < 0$ represent respectively that the goals are unattainable, attainable and over-attainable which implies an improved solution will be obtained.

Equation (10) can be posed as a NonLinear Programming (NLP) problem and solved in Sequential Quadratic Programming (SQP) (see the Appendix), a popular algorithm for NLP. The SQP algorithm is one of feasible direction methods. Namely, the primal feasibility is maintained during this optimization (search through feasible region), hence the method is often referred to as a *primal* method (Bazaraa *et al.*, 1993). Moreover, the method can obtain a quadratic or superlinear convergence behavior for even nonconvex solutions. Therefore, the SQP method represents the state-of-the-art in NLP methods. Many different SQP software programs are available. The routines of SQP for goal attainment are available in the Matlab™ optimization toolbox. Our modifications of the code and related considerations for the MRS problems will be discussed in the following section.

3.2. *Relationships and comparison of optimization formulations*

There are several approaches in the literature that have a close relationship with the proposed scheme. The standardized performance approach by Barton and Tsui (1991) attempted to maximize the minimum weighted deviation from tolerance limits. Their formulation is:

$$SP = \underset{\mathbf{x}}{\text{maximize}}\left\{\underset{y}{\text{minimum}}\left[\text{minimum}\left(\left(\frac{\mu_j - LS_j}{\sigma_j}\right), \left(\frac{US_j - \mu_j}{\sigma_j}\right)\right)\right]\right\},$$

where μ_j is the expected value of the performance measure, LS_j and US_j respectively represent the lower and the upper tolerance limits, and σ_j is the standard deviation of the jth error term. Plante (2001) proposed the following model as a special case of their process capability approach:

$$\underset{\mathbf{x}}{\text{Maximize}}\ C$$

subject to

$$\frac{\mu_j - LS_j}{\sigma_j} \geq C, \quad \frac{US_j - \mu_j}{\sigma_j} \geq C,$$
$$C > 0, \quad j = 1, \ldots, m.$$

It is interesting to note that several approaches (Khuri and Conlon, 1981; Barton and Tsui, 1991; Kim and Lin, 2000; Plante, 2001) and the proposed goal attainment approach can all be incorporated into the general frame of Equation (11) with different $f_j(\mathbf{x})$ as shown in Table 1. Also note that maximum C = minimum (-C).

From Table 1, it is clear that the weights of Barton and Tsui (1991) and Plante (2001) are the inverse of the standard deviation for each response. The weights of the KC

Table 1. Comparison of $f_j(\mathbf{x})$ within different approaches

Approach	$f_j(\mathbf{x})$
Khuri and Conlon (1981)	$\rho = [(\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})^T\{\text{var}[\hat{\mathbf{y}}(\mathbf{x})]\}^{-1} \times(\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta})]^{1/2}$
Barton and Tsui (1991)	$\text{Maximum}((\frac{LS_j-\mu_j}{\sigma_j}), (\frac{\mu_j-US_j}{\sigma_j}))$
Kim and Lin (2000)	$-d_j(z)$ (Equation (7))
Special cases of Plante (2001)	$(\frac{LS_j-\mu_j}{\sigma_j})$ and $(\frac{\mu_j-US_j}{\sigma_j})$
Currently proposed approach	$\lvert\frac{\hat{y}_j(\mathbf{x})-T_j^*}{\omega_j}\rvert$

approach are the inverse of the variance-covariance matrices among responses. For these approaches, the weights are all fixed in the entire optimization stage. In addition, we shall show that our approach includes the approach of KL by choosing suitable targets T_j^* and weights ω_j in the NTB, LTB or STB cases.

For a NTB type response with a symmetric desirability function and $t = 0$ (Kim and Lin, 2000):

$$-d(z) = |z| - 1$$
$$= \begin{cases} \dfrac{\hat{y}_j(\mathbf{x}) - T_j^{\max}}{T_j^{\max} - T_j^*} = \dfrac{\hat{y}_j(\mathbf{x}) - 2T_j^* + T_j^{\min}}{T_j - T_j^{\min}} & T_j^{\min} \leq T_j^* \leq \hat{y}_j(\mathbf{x}) \leq T_j^{\max}, \\[2ex] \dfrac{\hat{y}_j(\mathbf{x}) - T_j^{\min}}{T_j^{\min} - T_j^*} = \dfrac{\hat{y}_j(\mathbf{x}) - 2T_j^* + T_j^{\max}}{T_j - T_j^{\max}} & T_j^{\min} \leq \hat{y}_j(\mathbf{x}) \leq T_j^* \leq T_j^{\max}. \end{cases} \quad (13)$$

Therefore, the proposed formulation can repeat the KL formulation by letting:

$$T_j^{1^*} = (2T_j^* - T_j^{\min}) = T_j^{\max}, \omega_j^1 = (T_j - T_j^{\min}) = (T_j^{\max} - T_j^*),$$

and

$$T_j^{2^*} = (2T_j^* - T_j^{\max}) = T_j^{\min}, \omega_j^2 = (T_j^{\max} - T_j) = (T_j^* - T_j^{\min}),$$

respectively. Note that

$$f_j(\mathbf{x}) = \frac{\hat{y}_j(\mathbf{x}) - T_j^{\min}}{T_j^{\min} - T_j^*} = \frac{y_j(\mathbf{x}) - 2T_j^* + T_j^{\max}}{T_j - T_j^{\max}} < 0,$$

and ω will always be positive.

Accordingly, for the STB and LTB type responses:

$$-d(z) = |z| - 1$$
$$= \begin{cases} \dfrac{\hat{y}_j(\mathbf{x}) - T_j^{\min}}{T_j^{\max} - T_j^{\min}} & T_j^{\min} \leq \hat{y}_j(\mathbf{x}) \leq T_j^{\max} \quad \text{STB type}, \\[2ex] \dfrac{T_j^{\max} - \hat{y}_j(\mathbf{x})}{T_j^{\max} - T_j^{\min}} & T_j^{\min} \leq \hat{y}_j(\mathbf{x}) \leq T_j^{\max} \quad \text{LTB type}. \end{cases} \quad (14)$$

These two cases can be repeated by letting $T_j^{3*} = T_j^{min}$, $\omega_j^3 = (T_j^{max} - T_j^{min})$ and $T_j^{4*} = T_j^{max}$, $\omega_j^4 = (T_j^{max} - T_j^{min})$, respectively, in the proposed approach. When $t \neq 0$, KL gave a mechanism to tune the shape of the desirability function (see Equation (7)) to incorporate the DM's preference. In the proposed scheme, the DM's preference will be realized by the tuning weights.

Similarly, we also can repeat the approaches of Barton and Tsui (1991) and the special cases of Plante (2001) by defining $\omega_j^5 = 1/\sigma_j$ and

$$T_j^{5*} = \begin{cases} LS_j \\ US_j \end{cases}.$$

In summary, the proposed approach and several other approaches can all be included in a general optimization frame. The proposed approach, however, provides more flexible means to consider different targets and weights according to the DM's preference. Furthermore, it includes some of the prior formulations as special cases by choosing suitable targets and weights.

3.3. *Consideration of model predictive capability*

It should be noted that the KC approach considered the predictive ability of the estimated response models by incorporating the variance of responses while the KL approach did this by tuning the shape of desirability functions. However, both the DS and the proposed approaches implicitly assume that the goodness of fit for all responses is the same. Consequently, the results can be misleading when some responses have a substantially better fit than others. In principle, an estimated response with a lower predictive ability (worse model fitting) should have a smaller effect in the optimization. If the weight of one response is relatively large, it should have more effect in the final optimization results. In order to determine the weight for a given magnitude of predictive ability, we need to find a relationship between the weights and a predictive ability index. The model's predictive ability can be measured by many criteria such as R^2, adjusted R^2 or Mean-Square-Error (MSE) etc. For simplicity of presentation, we use the well-known R^2. Other criteria can be used in a similar manner. The larger R^2 is, the better the predictive capability, and the response is allowed to have a larger impact on the optimal results (closer to the response targets), thus a smaller weight in the optimization scheme. (Note that in Equation (10), a relatively smaller weight parameter implies that the final response is closer to the ideal goal.) A natural assignment is thus:

$$\omega_j' = \left(\frac{1}{R^2}\right)\omega_j \quad \text{for } 0 < R^2 \leq 1,$$

where, ω_j is the weight without considering the predictive capability.

3.4. *The implementation steps and considerations*

The following steps and considerations are recommended to implement the proposed scheme.

Step 1. Develop the experimental design, conduct the experiments and collect the data.

Step 2. Fit the response surface for multiple responses, usually a polynomial regression model is used. The predictive capability of the model is a very important consideration and should be justified by meaningful criteria, such as R^2 or adjusted R^2 value.

Step 3. Determine the targets T_j^* (ideal responses) and bounds of targets T_j^{min} and T_j^{max} as well as constraints of control factors.

Basically, there are two ways to determine the response targets: the natural one is from practical industry requirements and experience; the other one is by optimizing each individual response (the first step of the KC approach). The proposed algorithm guarantees the final optimal solution will lie within the goal bounds. The constraints on control factors $\mathbf{x}$ indicate the region of interest of a design point. The common regions are: $\mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$ for rectangular region or $\mathbf{x}\mathbf{x}^T \leq r^2$ for a spherical region (where r is the radius of the zone of interest).

Step 4. Determine the weight ω_j for each response.

The weights will determine the relative compromise of different responses and hence the DM's preference on multiple objectives. There are several approaches to choose weights. The DM can change the weights based on preference and requirements for different targets. We have shown in the above section how to repeat other formulations by choosing suitable targets and weights. Two popular weight assignments are given below:

- Setting the $\omega_j = 1$, for every response. The proposed scheme will lead to the maximum distance measure (denoted by DIS), i.e., the deviation from an individual ideal goal is minimized. This measure is suitable for cases when all responses are close in magnitude.
- Setting the $\omega_j = |T_j^*|$, that is the weights are equal to their response targets respectively. It indicates that the same percentage (denoted by PER_G) under- or over-attainment of the targets is achieved. This measure can be used in the cases when the magnitudes of all responses are very different.

As mentioned earlier, we can consider the model predictive capability by further adjusting the weights, i.e. using $\omega_j' = (1/R^2)\omega_j$.

In this paper, we will employ the absolute distance (DIS), percentage of deviation (PER_G) and MSE to compare the optimization performance of various approaches. The first two measurements allow explicit physical interpretations, while DIS and MSE are suitable for the cases where all responses are close in the magnitude. Specifically, the measurements are defined as follows:

$$DIS_j = |\hat{y}_j - T_j^*|,$$

$$PER_G = \sum_{j=1}^{n} (|\hat{y}_j - T_j^*|/T_j^*)/n,$$

$$PER_{G\max} = \max(|\hat{y}_j - T_j^*|/T_j^*, j = 1, \ldots, n)), \text{ and}$$

$$MSE = \sum_{j=1}^{n} (\hat{y}_j - T_j^*)^2/n,$$

where, $\hat{y}_j$ is the jth predicted response, T_j^* is the jth ideal response point and n is the number of responses.

Step 5. Optimization: formulation and computation.

Once the modeling components are determined, the optimization problem can be formulated, as proposed. Note that a set of starting points $\mathbf{x}_0$ are needed to initiate the procedure. It should also be noted that a gradient-based optimization method may fail to reach to the optimal point in the case of non-differentiable points or may not satisfy the global optimization conditions. Therefore, it is recommended that the optimization program be iterated using all experimental design points as the starting points of the optimization. The best solution is chosen as the result. Although the scheme may not principally guarantee the global optimum, it is straightforward and from our experience, it does provide a global optimal solution in many cases.

Step 6. Recommend the suggested solutions.

The best response may require that control factors attain a level with high cost. In many circumstances, the DM may only need some solutions that satisfy predefined targets with a suitable cost. Therefore, the recommendation of different combinations within the bound of targets will be valuable for manufacturing organizations.

4. Examples and comparisons

In this section, three published examples will be investigated and compared. We shall focus on the optimization aspect and compare several approaches against the proposed approach.

Table 2. The setting targets and constraints parameters of the tire tread compound

Responses	*Target lower bound*	*Target (T^*)*	*Target upper bound*
y_1	120	130	
y_2	1000	1300	
y_3	400	500	600
y_4	60	67.5	75

$|x_i| \le \sqrt{3}, i = 1, 2, 3,\ \omega_j = 1$ or $\omega_j = T^*, j = 1, 2, 3, 4.$

4.1. *Example 1: Tire treads compound study*

Derringer and Suich (1980) used the desirability approach to optimize the four quality indices of a tire tread associated with three control factors. The four responses are y_1: PICO abrasion index (LTB type of response); y_2: 200% modulus (LTB type of response); y_3: elongation at break (NTB type of response); and y_4: hardness (NTB type of response). The parameters for the proposed approach are given in Table 2. Three control factors are x_1 which is the hydrated silica level; x_2 which is the silane coupling agent level; and x_3 the sulfur concentration. A three-variable rotatable central composite design with six center points was employed to generate the data which was then fitted to the full second-order model as follows:

$$y_1 = 139.12 + 16.49x_1 + 17.88x_2 + 10.91x_3 - 4.01x_1^2 - 3.45x_2^2 - 1.57x_3^2 + 5.13x_1x_2 + 7.13x_1x_3 + 7.88x_2x_3,$$

$$y_2 = 1261.11 + 268.15x_1 + 246.5x_2 + 139.48x_3 - 83.55x_1^2 - 124.79x_2^2 + 199.17x_3^2 + 69.38x_1x_2 + 94.13x_1x_3 + 104.38x_2x_3,$$

$$y_3 = 400.38 - 99.67x_1 - 31.4x_2 - 73.9x_3 + 7.93x_1^2 + 17.3x_2^2 + 0.43x_3^2 + 8.75x_1x_2 + 6.25x_1x_3 + 1.25x_2x_3,$$

$$y_4 = 68.91 - 1.41x_1 + 4.32x_2 + 1.63x_3 + 1.56x_1^2 + 0.06x_2^2 - 0.32x_3^2 - 1.63x_1x_2 + 0.13x_1x_3 - 0.25x_2x_3.$$

The results of the proposed approach are summarized and compared with the DS approach in Table 3. Note that in the DS results, y_3 has been "sacrificed", thus it has a significant departure from its ideal goal which led to a large DIS (34.3), $PER_{G\max}$ (6.86%) and overall MSE (294.12). It is also clear in the proposed approach with $\omega_j = 1$ makes the overall distance measure deviating from individual response targets optimal ($DIS_j = \delta = 3.497$) and the MSE is very low (12.23, as mentioned before, the index is comparable when all responses are similar in magnitude), while $\omega_j = T^*$ makes the overall percentage under- or over-attainment of the ideal goal optimal. Here the attainment factor $\delta = 2.216\%$ in the optimization scheme, i.e., every predictive response has a low percentage of PER_G (2.216 %), a more balanced performance compared with the DS approach (for which $PER_{G\max} = 6.86\%$).

Table 3. Comparison of results: DS approach versus the proposed approach

Parameters	*DS approach*	*Proposed approach* ($\omega_j = 1$)	*Proposed approach* ($\omega_j = T^*$)
Optimal setting			
$\mathbf{x}^*$	(−0.05, 0.145, −0.868)	(−0.309, 0.69, −1.06)	(−0.268, 0.264, −0.912)
Predicted response			
$\hat{\mathbf{Y}}(\mathbf{x}^*)$	(129.5, 1300, 465.7, 68)	(126.5, 1296.5, 496.5, 70.996)	(127.12, 1271.19, 488.92, 68.996)
Attainment factor			
δ		3.497	2.216%
DIS_j	(0.5, 0, 34.3, 0.5)	(3.497, 3.497, 3.497, 3.497)	(2.88, 28.8, 11.08, 1.49)
$\mathrm{PER_G}$ ($\mathrm{PER_{Gmax}}$) (%)	1. 9 96 (6.860)	2. 2097 (5.181)	2. 2160 (2.216)
MSE	294.12	12.23	425.87
Degree of desirability	(0.189, 1, 0.656, 0.932)	(0.13, 0.99, 0.96, 0.534)	(0.14, 0.9, 0.89, 0.8)

The values of the degree of desirability are also listed in Table 3 for comparison. Note that desirability of y_3 has been significantly improved. We also observed that when $\omega_i = 1$, the degree of desirability of y_4 is reduced significantly (from 0.932 to 0.534) although the value (70.996) still is within the acceptable scope. This is because that level of desirability in a triangle desirability function in the DS approach (a linearly increasing function from 60 to 67.5 and then a linearly decreasing function from 67.5 to 75) is very sensitive to any deviation from the response targets especially when the range of the acceptable bounds of the response is small (from 60 to 75). This implies that the desirability function approach, in some cases, might be too subjective to represent real cases. Hence, the balanced performance should be measured by various measures (MSE, DIS, $\mathrm{PER_G}$) to avoid a misleading conclusion. It also should be noted that the magnitude of all responses should be investigated when using these measures for a reasonable comparison.

Furthermore, in MRS, there must be some trade-offs among different responses. In our approach, the trade-off between responses can be controlled according to the preference of the DM through weight adjustment. For example, Table 4 gives the results based on different preferences for the responses. The boldface values are the ones close to the results of the DS approach in Table 2 (129.5, 1300, 465.7, 68). Note that DS only represents one specific set of preferences, while the proposed approach provide a flexible framework to assess different cases and hence is a robust approach.

4.2. *Example 2: The foaming properties of whey protein*

This example was investigated by Khuri and Conlon (1981) through a generalized distance approach. It investigated the effects of heating temperature (x_1), PH level (x_2), redox potential (x_3), sodium oxalate concentration (x_4), and sodium lauryl sulfate concentration (x_5) on the foaming properties of whey protein concentrates. The four response variables are the maximum overrun (y_1), the time at first drop (y_2), the undenatured protein (y_3), and soluble protein (y_4) and all are LTB type of responses. A central composite design with six center points was employed in the study and a full second-order regression model for each of the four responses with their R^2 values are as follows:

$$\begin{aligned}
y_1 = {} & 1176.98 - 176.08x_1 - 18.17x_2 + 57.58x_3 + 21.84x_4 \\
& + 19.08x_5 - 56.97x_1^2 - 23.84x_2^2 - 44.84x_3^2 - 34.09x_4^2 \\
& - 9.22x_5^2 - 25x_1x_2 - 48.88x_1x_3 - 12.25x_1x_4 \\
& - 36.75x_1x_5 - 2.88x_2x_3 + 16.75x_2x_4 + 11.0x_2x_5 \\
& - 4.38x_3x_4 + 2.38x_3x_5 - 1.0x_4x_5 \quad (R^2 = 0.94), \\
y_2 = {} & 9.44 + 1.08x_1 + 3.69x_2 + 1.60x_3 - 0.21x_4 - 1.5x_5 \\
& + 0.56x_1^2 - 0.13x_2^2 + 0.24x_3^2 + 0.37x_4^2 \\
& 1.06x_5^2 + 2.15x_1x_2 - 0.46x_1x_3 - 2.75x_1x_4 \\
& -2.13x_1x_5 + 0.19x_2x_3 - 0.85x_2x_4 - 2.35x_2x_5 \\
& -0.96x_3x_4 - 1.21x_3x_5 + 0.63x_4x_5 \quad (R^2 = 0.84), \\
y_3 = {} & 77.79 - 10.12x_1 - 8.68x_2 - 0.10x_3 - 0.71x_4 \\
& + 1.37x_5 - 4.16x_1^2 - 4.77x_2^2 - 2.36x_3^2 - 0.34x_4^2 \\
& - 0.33x_5^2 - 6.21x_1x_2 + 2.77x_1x_3 + 1.77x_1x_4
\end{aligned}$$

Table 4. Partial results of the responses and control factors considering preference sets

ω_1	ω_2	ω_3	ω_4	y_1	y_2	y_3	y_4	x_1	x_2	x_3
130	1300	470	67.5	129.1753	1291.753	467.0183	67.928 23	−0.063 32	0.117 604	−0.856 37
130	1300	470	70	130.4006	1304.006	471.4485	69.784 27	−0.158 19	0.477 927	−0.89479
130	1300	470	69	129.9815	1299.815	469.9332	69.009 81	−0.129 89	0.323 331	−0.87282
129.5	**1300**	**465.7**	**68**	**129.4685**	**1299.684**	**465.5868**	**68.016 53**	**−0.050 58**	**0.146 299**	**−0.865 97**
157.5	1300	450	67.5	145.5645	1318.876	415.8987	72.6152	0.011695	1	−0.42168
157.5	1300	450	71.25	146.0803	1274.73	417.3722	73.897 58	−0.23163	1	−0.12956

Table 5. The setting targets and constraints parameters of the foaming properties of WPC

Responses	*Target lower bound*	*Target(T^*)*	*Target upper bound*
y_1	1271.12	1496.77	1722.42
y_2	24.20	34.97	45.74
y_3	77.21	90.17	103.13
y_4	102.92	123.45	143.98

A nonlinear constraint is needed: $\sum_{i=1}^{5} x_i^2 \le 5$ as in KC. $\omega_j = 1$.

$$+0.71x_1x_5 - 1.68x_2x_3 - 0.26x_2x_4 + 0.48x_2x_5 + 0.04x_3x_4 + 1.51x_3x_5 + 0.03x_4x_5 \quad (R^2 = 0.96),$$

$$y_4 = 103.81 - 8.25x_1 + 7.51x_2 + 2.38x_3 + 1.13x_4 + 1.66x_5 - 7.37x_1^2 - 4.66x_2^2 - 2.58x_3^2 - 2.01x_4^2$$
$$1.07x_5^2 - 0.11x_1x_2 + 0.47x_1x_3 + 2.09x_1x_4 + 0.77x_1x_5 - 0.78x_2x_3 + 0.29x_2x_4 - 0.16x_2x_5 + 1.44x_3x_4$$
$$4.09x_3x_5 + 0.29x_4x_5 \quad (R^2 = 0.91).$$

It is straightforward to obtain the individual optimum response using a common single objective optimization procedure, for example, ridge analysis for second-order polynomial models (Draper, 1963). According to the first step of KC, the individual maxima and their 95% confidence intervals for the example are regarded as the response targets and bounds as shown in Table 5.

Table 6 displays the results of the proposed approach and the KC approach. The results indicate ($\omega_j = 1$), that although the y_2, y_3 and y_4 responses of the proposed approach deteriorate slightly compared to the KC approach, the y_1 response was significantly improved (from 1434 to 1478.43) and led to a lower overall MSE (from 1155.3 to 287.81). Therefore, a better balance among targets is attained on the MSE and DIS measure. However, the KC approach is slightly better on the measure of average percentage of deviation ($\mathrm{PER_G}$ = 19.7%). Hence, the preference of the DM will be an important consideration in the choice of optimal solutions. The optimization results of example 2 taking into account model predictive ability were shown in the last column of Table 6. The y_2 response has the lowest R^2 (=0.84, as compared with other R^2 = 0.94, 0.96, 0.91) and thus has decreased from 16.63 to 16.36. The responses y_1, y_3, and y_4 are all improved (from 1478.43 to 1480.14; from 78.23 to 78.40; from 105.11 to 106.27) and lead to lower MSE (from 287.81 to 264.07) and $\mathrm{PER_G}$ (from 20.44 to 20.32%).

4.3. *Example 3: Mechanical properties of JS-SS400 steel*

This real example taken from Kim and Lin (2000) investigated the effects of steel composition as well as rolling and cooling conditions with six input variables: (i) the percentage of carbon x_1; (ii) the percentage of manganese x_2; (iii) the percentage of silicon x_3; (iv) the thickness of the strips or plates x_4; (v) the milling temperature x_5; and (vi) the coiling temperature x_6 on the mechanical properties of JS-SS400-type steel. The mechanical properties were measured by three responses: (i) the tensile strength y_1 (NTB type); (ii) the yield strength y_2 (LTB type); and (iii) the elongation y_3 (LTB type). A second-order polynomial model based on a coded data set with their R^2 value proposed by Kim and Lin (2000) is:

$$y_1 = -101.0145 + 1.8625x_2 + 2.4005x_6 - 0.0101x_2^2 - 0.2030x_4^2 - 0.0088x_5^2 + 0.2127x_1x_4 + 0.0777x_1x_5 - 0.1393x_1x_6 \quad (R^2 = 0.98),$$

$$y_2 = 22.5934 + 2.5767x_3 + 0.4271x_5 - 0.004x_2^2 - 0.0159x_4^2 - 0.0326x_2x_3 + 0.0219x_2x_6 - 0.0198x_5x_6 \quad (R^2 = 0.94),$$

$$y_3 = -1160.1051 + 18.7135x_1 + 10.8304x_2 + 13.5285x_5 - 0.5210x_1^2 + 0.0209x_2^2 - 0.0322x_3^2 + 0.0054x_5^2 + 0.0483x_2x_3 - 0.0251x_3x_5 - 0.1741x_2x_5 \quad (R^2 = 0.80).$$

The response models have different sets of input variables. This is not allowed in the KC approach. The ideal targets and bounds (Kim and Lin, 2000) are listed in Table 7.

The allowable ranges of x_1 to x_6 (x_i^{min}, x_i^{max}) are as follows: $x_1 = (16, 20)$ and $x_2 = (70, 90)$ if $7.00 \le x_4 < 10.00$; $x_1 = (18, 22)$ and $x_2 = (18, 22)$ if $10.00 < x_4 \le 12.7$; $x_3 = (0, 30)$; $x_4 = (7.00, 12.70)$; $x_5 = (85, 89)$; $x_6 = (60, 64)$.

Table 6. Comparison of results: KC approach versus the approach proposed

Parameters	*KC approach*	*Proposed approach ($\omega_j = 1$) (without R^2 consideration)*	*Proposed approach ($\omega_j = 1$) (with R^2 consideration)*
Optimal setting			
$\mathbf{x}^*$	(−1.31, −0.16, 0.30, 0.46, 1.72)	(−1.503, 0.019, 0.764, 0.638, 1.324)	(−1.457, 0.037, 0.768, 0.624, 1.377)
Predicted response			
$\hat{\mathbf{Y}}(\mathbf{x}^*)$	(1434.0, 16.98, 81.61,106.59)	(1478.43, 16.63, 78.23, 105.11)	(1480.141, 16.36, 78.4, 106.27)
Attainment factor			
δ		18.34	15.63
DIS_j	(62.77, 17.99, 8.56, 16.86)	(18.34, 18.34, 11.93, 18.34)	(16.63, 18.61, 11.76, 17.18)
$\mathrm{PER_G}$ ($\mathrm{PER_{G\,max}}$) (%)	19.7 (51.44)	20. 44 (52.44)	20. 32 (53.21)
MSE	1155.3	287.81	264.07

Table 7. Ideal targets and bounds of mechanical properties of JS-SS400 steel

Responses	*Target lower bound*	*Target (T^*)*	*Target upper bound*
y_1	43.10	47.55	52.00
y_2	26.30	48.08	48.08
y_3	20.00	43.67	43.67

Table 8 shows the current operating conditions and optimization results by the proposed approach. It is clear that the PER index (from 25.82 to 22.21% and 22.67%) and PER_{Gmax} (from 44.95 to 31.30% and 35.4%) are improved by the proposed approach. The DIS of y_1 and y_2 are improved (from 1.99 and 14.98 to 1.18 and 14.49) while the DIS of y_3 is worse (from 13.67 to 15.46) after considering the predictive ability by R^2.

Table 9 shows a comparison of results obtained using the KL approach versus the proposed approach. The proposed approach produced a competitive result. We improved the PER index (from 8.73 and 8.65% to 5 and 5.15%) and PER_{Gmax} (from 21.18 and 22.01% to 7.255 and 8.08%). The DIS of y_1 and y_2 are improved (from 0.2364 and 3.4883 to 0.2363 and 3.3042) while the DIS of y_3 is lower (from 3.1683 to 3.5263) after considering the predictive ability by R^2.

5. Discussions and conclusions

A goal attainment modeling approach for the optimization of multiple response surfaces is proposed in this paper. The proposed approach has several methodological advantages over existing approaches.

First, the approach combines the advantages of the KC, DS and KL approaches. The optimization measure is the weighted distance departure from response targets that has a direct physical interpretation. It is similar to the KC approach to some extent because the latter is equivalent to employing variances and covariances of responses to determine the weights. The main difference, however, is that the proposed approach allows for more flexibility in choosing weights and can incorporate the DM's preference into the distance measure with weights, making the approach more robust. It also employs the basic idea of the desirability function approach in this respect and can achieve a better balance among all the responses depending on the magnitude of responses. Moreover, it has been shown that the proposed optimization formulation may fully or partly include some prior work such as the KL approach as special cases by assigning proper response targets and weights.

Second, similar to the KL approach, the proposed approach allows for a more flexible form of the fitted response functions, i.e., different functional forms and different sets of input variables. This is not the case in the KC approach. Furthermore, the proposed approach does not require the assumption of a transformation scheme of the objective functions, which, however, is the basic requirement in the DS and KL approaches.

Third, the new approach is robust to dependencies among responses. Moreover, the predictive ability of the fitted model can be taken into account in the weights adjustment using R^2. In this aspect, the KL approach incorporated models' predictive ability through the adjustment of desirability function shape using R^2 or adjusted R^2. On the contrary, the KC approach must remove the dependence between responses in advance and the predictive ability of the models has not been discussed in the DS approach. Table 10 organizes the KC, DS and KL approaches with the proposed scheme in terms of the optimization measure, model assumption and characteristics etc.

It should also be noted that minimax (or maximin) to optimization has some drawbacks as well. In particular, the proposed approach only considers the response with maximum weighted distance or percentage of deviation from the target, and thus useful information associated with other responses could be missed, which may lead to an unreasonable decision in some cases. For example, if we have two candidate solutions, which are the same in one objective function value, but different in the other, they may still have the same goal-attainment value for their two objectives, a misleading solution thus may be generated. As another extreme case, the approach may prefer an operating set-up with

Table 8. Comparison of results: current operation condition versus the proposed approach

Parameters	*Current operation condition*	*Proposed approach ($\omega_j = T$) (without R^2 consideration)*	*Proposed approach ($\omega_j = T$) (with R^2 consideration)*
Optimal settings	(17.74, 78.08, 15.42, 9.55, 6.75, 63.24)	(17.96, 70.00, 20.76, 7.00, 89, 60.0)	(17.93, 71.43, 18.89, 7, 87.89, 60)
Predicted response $\hat{Y}(x^*)$	(48.88, 33.79, 24.04)	(45.56, 33.10, 30)	(46.37, 33.59, 28.21)
Attainment factor			
δ		0. 3116	0.2832
DIS_j	(1.33, 14.29, 19.63)	(1.99, 14.98, 13.67)	(1.18, 14.49, 15.46)
PER_G (PER_{Gmax}) (%)	25.82 (44.95)	22.21 (31.30)	22. 67 (35.4)
MSE	197.10	138.41	150.12

Table 9. Comparison of results: KL approach versus the proposed approach

Parameters	*KL (Without R^2 consideration $(t_1, t_2, t_3) = (-3.0, 0.0, 3.0)$)*	*KL (Without R^2 consideration: $(t'_1, t'_2, t'_3) = (-2.7, 0.6, 4.4)$)*	*Proposed approach ($\omega_j = T$) (without R^2 consideration)*	*Proposed approach ($\omega_j = T$) (with R^2 consideration)*
Optimal settings	(18.02, 109.67, 9.57, 12.01, 85.00, 64.00)	(18.00, 110.00, 9.23, 11.97, 85.00, 64.00)	(17.96, 110.00, 12.398, 7.00, 85.00, 64.00)	(17.9603, 110.00, 12.215, 7.00, 85.00, 64.00)
Predicted response				
$\hat{Y}(x^*)$	(47.72, 45.85, 34.42)	(47.65, 46.28, 34.06)	(47.7864, 44.5917, 40.5017)	(47.7863, 44.7758, 40.1437)
Attainment factor				
δ			0.07255	0.0646
DIS_j	(0.17, 2.23, 9.52)	(0.1, 1.8, 9.61)	(0.2364, 3.4883, 3.1683)	(0.2363, 3.3042, 3.5263)
PER_G ($PER_{G\max}$) (%)	8.73 (21.18)	8.65 (22.01)	5 (7.255)	5.15 (8.08)
MSE	31.88	31.87	7.42	7.80

$(PER_{G1}, PER_{G2}, PER_{G3}, PER_{G4}) = (0.49, 0.49, 0.49, 0.49)$ to that with $(PER_{G1}, PER_{G2}, PER_{G3}, PER_{G4}) = (0.1, 0.1, 0.1, 0.5)$. It is thus recommended that several approaches be adopted to validate the final solution when necessary.

The requirement of the approach is that the response functions are a continuously twice differentiable function. This is a common condition for the gradient-based optimization methods. Another requirement is that the response targets are available in advance. This can be easily obtained through practical experience or single objective optimization method. This is because the experiments are normally conducted in some operating window, i.e., the control factor vector **x** subject to some bound. In this case, the proposed approach could still be useful through a reasonable choice of the response targets within the region of interest even if the responses themselves are unbounded (LTB, STB types). In addition, considering all experimental points as the starting points in the optimization procedure

Table 10. A comparison of the three existing approaches and the proposed approach

	DS approach	*KC approach*	*KL approach*	*Proposed approach*
Optimization measure	Maximize the overall degree of satisfaction of all responses	Minimize the distance from response targets (variances and covariances of responses are incorporated into a distance function)	Maximize the minimal desirability of all responses	Minimize the maximal weighted distance from response targets
Modeling assumption	Assumption of a transformation scheme for the desirability function	Each response function should be of the same functional form and use the same design variables	No assumptions on the response function form; assumption of a transformation scheme for the desirability function	No assumptions on the response function form (the response targets should be available in advance)
Dependence between responses	No effect on the solution procedure and affects the final results	Dependence must be removed in advance	No effect on the solution procedure, and method is robust to dependencies	No effect on the solution procedure, and method is robust to dependencies.
Fitted surface model predictive ability	Assumes same predictive ability for all individual responses	Takes into account predictive ability through the prediction variances of responses	Takes into account predictive ability through the adjustment of the desirability function shape	Different predictive abilities can be incorporated into the weights adjustment
DM's preference	The preference can be incorporated into the shape adjustment of the desirability function	Doesn't take into account.	The preference can be incorporated into the shape adjustment of the desirability function	The preference can be incorporated into the weights adjustment

within the region of interest can significantly reduce the potential problems with local optimum.

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References

Ames, A.E., Mattucci, N., MacDonald, S., Szonyi, G. and Hawkins, D.M. (1997) Quality loss functions for optimization across multiple response surfaces. *Journal of Quality Technology*, **29**, 339–346.

Barton, R.R. and Tsui, K.L. (1991) Multivariate yield maximization using CAD/CAE models: efficient approximations based on mean and variance. *Design Theory and Methodology*, **31**, 31–35.

Bazaraa, M.S., Sherali, H.D. and Shetty, C.M. (1993) *Nonlinear Programming: Theory and Algorithms*, 2nd edn., Wiley, New York, NY.

Biggs, M.C. (1975) Constrained minimization using recursive quadratic programming: some alternative subproblem formulations, in *Towards Global Optimization*, Dixon, L.C.W. and Szego, G.P. (eds.), pp. 341–349, North Holland, Amsterdam.

Box, G.E.P. and Draper, N.R. (1987) *Empirical Model Building and Response Surfaces*, Wiley, New York, NY.

Boyle, C.R. and Shin, W.S. (1996) An interactive multiple-response simulation optimization method. *IIE Transactions*, **28**, 453–462.

Brayton, R.K., Director, S.W., Hachtel, G.D. and Vidigal, L. (1979) A new algorithm for statistical circuit design based on quasi-Newton methods and function splitting. *IEEE Transactions on Circuits and Systems*, **26**, 784–794.

Censor, Y. (1977) Pareto optimality in multiobjective problems. *Applied Mathematics and Optimization*, **4**, 41–59.

Copeland, K.A.F. and Nelson, P.R. (1996) Dual response optimization via direct function minimization. *Journal of Quality Technology*, **28**, 331–336.

Del Castillo, E. (1996) Multiresponse process optimization via constrained confidence regions. *Journal of Quality Technology*, **28**, 61–70.

Del Castillo, E., Fan, S.K. and Semple, J. (1999) Optimization of dual response systems: a comprehensive procedure for degenerate and nondegenerate problems. *European Journal of Operational Research*, **112**, 174–186.

Del Castillo, E. and Montgomery, D.C. (1993) A nonlinear programming solution to the dual response problem. *Journal of Quality Technology*, **25**, 199–204.

Del Castillo, E., Montgomery, D. and McCarville, D. (1996) Modified desirability functions for multiple response optimization. *Journal of Quality Technology*, **28**, 337–345.

Derringer, G. (1994) A balancing act: optimizing a product's properties. *Quality Progress*, **27**, 51–58.

Derringer, G. and Suich, R. (1980) Simultaneous optimization of several response variables. *Journal of Quality Technology*, **12**, 214–219.

Draper, N.R. (1963) Ridge analysis of response surfaces. *Technometrics*, **5**, 469–479.

Gembicki, F.W. and Haimes, Y.Y. (1975) Approach to performance and sensitivity multiobjective optimization: the goal attainment method. *IEEE Transactions on Automatic Control*, **20**, 769–771.

Han, S.P. (1967) Superlinearly convergent variable metric algorithms for general nonlinearly programming problems. *Mathematical Programming*, **11**, 263–282.

Harrington, E.C. (1965) The desirability function. *Industrial Quality Control*, **21**, 494–498.

Khuri, A. and Conlon, M. (1981) Simultaneous optimization of multiple responses represented by polynomial regression functions. *Technometrics*, **23**, 363–375.

Khuri, A. and Cornell, J. (1996) *Response Surfaces: Designs and Analysis*, Dekker, New York, NY.

Kim, K.J. and Lin, D.K.J. (1998) Dual response surface optimization: a fuzzy modeling approach. *Journal of Quality Technology*, **30**, 1–10.

Kim, K.J. and Lin, D.K.J. (2000) Simultaneous optimizations of mechanical properties of steel by maximizing exponential desirability functions. *Applied Statistics*, **49**, 311–325.

Leon, N.A. (1996) A pragmatic approach to multiple-response problem using loss function. *Quality Engineering*, **9**, 213–220.

Lin, D.K.J. and Tu, W. (1995) Dual response surface optimization. *Journal of Quality Technology*, **27**, 34–39.

Lind, E., Goldin, J. and Hickman, J. (1960) Fitting yield and cost response surfaces. *Chemical Engineering Progress*, **56**, 62–68.

Montgomery, D.C., Talavage, J.J. and Mullen, C.J. (1972) A response surface approach to improving traffic signal settings in a street network. *Transportation Research*, **6**, 69–80.

Myers, R.H. (1999) Response surface methodology—current status and future directions. *Journal of Quality Technology*, **31**, 30–44.

Myers, R.H. and Montgomery, D.C. (2002) *Response Surface Methodology: Process and Product Optimization Using Designed Experiments*, Wiley, New York, NY.

Papalambros, P.Y. and Wilde, D.J. (2000) *Principles of Optimal Design*, Cambridge University Press, Cambridge, UK.

Pignatiello, J.J. (1993) Strategies for robust multiresponse quality engineering. *IIE Transactions*, **25**, 5–15.

Plante, R.D. (1999) Multicriteria models for the allocation of design parameter targets. *European Journal of Operational Research*, **115**, 98–112.

Plante, R.D. (2001) Process capability: a criterion for optimizing multiple response product and process design. *IIE Transactions*, **33**, 497–509.

Powell, M.J.D. (1978) A fast algorithm for nonlinearly constrained optimization calculations, in *Numerical Analysis*, Watson, G.A. (ed.), pp. 144–157, Springer-Verlag, New York, NY.

Schniederjans, M.J. (1995) *Goal Programming: Methodology and Applications*, Kluwer Academic Publishers, Boston, MA.

Semple, J. (1997) Optimality conditions and solution procedures for nondegenerate dual-response systems. *IIE Transcations*, **29**, 743–752.

Steuer, R.E. (1986) *Multiple Criteria Optimization: Theory, Computation and Application*, Wiley, New York, NY.

Taha, H.A. (1997) *Operations Research: An Introduction*, Prentice Hall, Upper Saddle River, NJ.

Tang, L.C. and Xu, K. (2002) A unified approach for dual response surface optimization. *Journal of Quality Technology*, **34**, 437–447.

Vining, G.G. (1998) A compromise approach to multiresponse optimization. *Journal of Quality Technology*, **30**, 309–313.

Vining, G.G. and Myers, R.H. (1990) Combining Taguchi and response surface philosophies: a dual response approach. *Journal of Quality Technology*, **22**, 38–45.

Appendix

The SQP algorithm

Based on the work of Han (1967), Biggs (1975) and Powell (1978), the SQP algorithm closely mimics Newton's method for constrained optimization just as is done for unconstrained optimization, given the general optimization problem stated below:

$$\text{Minimize} \quad f(\mathbf{x}),$$

subject to

$$g_i(\mathbf{x}) = 0 \quad i = 1, \ldots, m_1,$$
$$h_i(\mathbf{x}) \le 0 \quad i = 1, \ldots, m_2.$$

Here $\mathbf{x} \in X$ and all functions are assumed to be continuously twice differentiable. The basic idea of SQP is the formulation of a QP subproblem based on a quadratic approximation of the Lagrangian function $\mathbf{L}(\mathbf{x}_k)$ subject to constraints linearized about the current iterate $(\mathbf{x}_k, \boldsymbol{\lambda}_k, \mathbf{u}_k)$:

$$\text{Minimize} \quad f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^T \mathbf{q} + \frac{1}{2}\mathbf{q}^T \nabla^2 \mathbf{L}(\mathbf{x}_k)\,\mathbf{q},$$

subject to

$$\nabla g_i(\mathbf{x}_k)^T \mathbf{q} + g_i(\mathbf{x}_k) = 0, \quad i = 1, \ldots, m_1,$$
$$\nabla h_i(\mathbf{x}_k)^T \mathbf{q} + h_i(\mathbf{x}_k) \le 0, \quad i = 1, \ldots, m_2,$$

Here

$$\nabla^2 \mathbf{L}(\mathbf{x}_k) = \nabla^2 f(\mathbf{x}_k) + \sum_{i=1}^{m_1} \lambda_{ki} \nabla^2 g_i(\mathbf{x}_k) + \sum_{i=1}^{m_2} u_{ki} \nabla^2 h_i(\mathbf{x}_k),$$

is the Hessian of the Lagrangian at $\mathbf{x}_k$ with the Lagrange multiplier vectors $\boldsymbol{\lambda}_k$ and $\mathbf{u}_k$, and $\mathbf{q} = \mathbf{x} - \mathbf{x}_k$ is the direction of the search. In addition to primal feasibility, the Karush-Kuhn-Tucker (KKT) condition requires that the optimization problem needs to find Lagrange multipliers $\boldsymbol{\lambda}$ and $\mathbf{u}$ such that:

$$\nabla f(\mathbf{x}_k) + \nabla^2 \mathbf{L}(\mathbf{x}_k)\mathbf{q} + \sum_{i=1}^{m_1} \lambda_i \nabla g_i(\mathbf{x}_k) + \sum_{i=1}^{m_2} u_i \nabla h_i(\mathbf{x}_k) = \mathbf{0},$$
$$u_i[h_i(\mathbf{x}_k) + \nabla h_i(\mathbf{x}_k)^T \mathbf{q}] = 0 \quad i = 1, \ldots, m_2,$$
$$\mathbf{u} \ge \mathbf{0}, \quad \boldsymbol{\lambda} \text{ unrestricted}.$$

Hence, if $\mathbf{q}_k$ solves QP $(\mathbf{x}_k, \boldsymbol{\lambda}_k, \mathbf{u}_k)$ with Lagrange multipliers $\boldsymbol{\lambda}_{k+1}$ and $\mathbf{u}_{k+1}$, and if $\mathbf{q}_k = \mathbf{0}$, then $\mathbf{x}_k$ along with $(\boldsymbol{\lambda}_{k+1}, \mathbf{u}_{k+1})$ yields a KKT solution for the original problem. Otherwise, we set $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{q}_k$ as before and form a new iteration. The step length parameter α_k is determined by an appropriate line search procedure so that a sufficient decrease in a merit function $\psi(\mathbf{x})$ is obtained. Here the merit function is defined for guiding and measuring the process of the algorithm. Under appropriate circumstances, it will serve as a descent function for an algorithm, decreasing in value at each step so that it is minimized at a solution to the original problem. In the goal attainment approach, the merit function is defined as (Brayton *et al.*, 1979):

$$\psi(\mathbf{x}) = \sum_{j=1}^{n} \begin{cases} \tau_j \max\{0, y_j(\mathbf{x}) - T_j^* - \omega_j \delta\} & \text{if } \omega_j = 0, \\ \max_j f_j(\mathbf{x}) \quad j = 1, \ldots, n & \text{otherwise,} \end{cases}$$

where τ_j is the penalty parameter.

Corresponding to the varied point, a computation is carried out to set up the model of the QP subproblem to be solved at the next iteration until the optimality conditions are satisfied within a given tolerance.

Biographies

Kai Xu received a Ph.D. degree from Huazhong University of Science and Technology in 2000 in the area of Reliability Engineering. His research interests are in response surface methodology, fuzzy logic and neural networks, data mining and decision support, quality assurance of automobile engine systems. He has published many scholarly articles in several international journals, including *IIE Transactions*, *Journal of Quality Technology*, *Reliability Engineering and System Safety*, *IEEE Transactions on Electronic Packaging Manufacturing*, *SAE Transactions*, and *Applied Soft Computing*. He has been a reviewer for numerous international journals in the areas of quality and reliability, automobile and operations research. He is a member of IIE, ASQ and IEEE.

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