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A Multiple Criteria Response Surface Optimization Procedure

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Abstract

This paper deals with the problem of multiple criteria response surface optimization. The method proposed for solving this problem consists of two parts. In the first part the original problem is converted into a constrained problem where all but one response functions are assigned minimum levels which are to be satisfied, while the remaining response function is optimized over this constraint set. The shadow prices of the optimized program are used in the second stage as weights of the multiple criterion objective which then applies the weighted steepest descent method in a search for an improved design point.

I. Introduction

In this paper we deal with the problem

$$\text{minimize} \quad f(x), \ x \in E^n \tag{1}$$

s.t.

$$g_i(x) \leq 0 \qquad i = 1,2,\ldots,m \tag{2}$$

where $f(x)$ is an estimated response surface function which is to be optimized and $g_i(x)$, $i = 1,2,\ldots,m$ are estimated response functions. The difference between problem (1)-(2) and an ordinary nonlinear program is the fact that problem (1)-(2) is not given explicitly. The response functions of (1)-(2) can be approximated by polynomial fitting techniques [1][3] and can be optimized by methods such as Ridge Analysis [2][3], and restricted gradient methods [4],[5],[6],[7] which utliize information on the estimated partial derivatives of the objective function (1). In this paper we propose a procedure which makes use of a design consisting of n points and their associated measured responses in order to construct a polygonal approximation of the constrained surface. This polygonal approximation when optimized yields a new point which may be evaluated in addition to the n existing design points. The new point is then used for updating the polygonal approximation. The process moves to its second stage when either the new generated point is not significantly different from an already existing design point or the response function value at the new point does not show a significant improvement over the best design combination experienced thus far. In the second stage of the analysis, first order partial derivatives of the polynomial response function approximations are used in the construction of a restricted descent method. New design points are evaluated along the dimension of the descent direction to determine a local minimum. The process terminates if no descent direction can be found at a given local minimum point, or if points along the new descent direction do not yield at least one significant better value for $f(x)$.

II. The Polygonal Approximation Method

In the process of optimizing the constrained response surface function we construct a design consisting of points $x_1, x_2, \ldots, x_k$, $x_j \in E^n$ and define the convex hull of these points as

$$x = \sum_{j=1}^{k} \lambda_j x_j \tag{3}$$

$$\sum_{j=1}^{k} \lambda_j = 1 \tag{4}$$

$$\lambda_j \geq 0 \qquad \text{for } j = 1,2,\ldots,k \tag{5}$$

Since $f(x)$ and $g_i(x)$ are not given explicitly a polygonal approximation of problem (1)-(2) yields the following linear program

$$\text{minimize} \sum_{j=1}^{k} \lambda_j f(x_j) \tag{6}$$

s.t.

$$\sum_{j=1}^{k} \lambda_j g_i(x_j) \leq 0 \qquad i = 1,2,\ldots,m \tag{7}$$

$$\sum_{j=1}^{k} \lambda_j = 1 \tag{8}$$

$$\lambda_j \geq 0 \tag{9}$$

where $f(x_j)$ is the actual value of $f(x)$ at the design point x_j, and $g_i(x_j)$ is the actual value of $g_i(x)$ at the point x_j.

The solution to (6)-(9) is obtained by the simplex method and the solution vector is denoted by λ_j^*. The optimum solution λ_j^* is then transformed into the original variable space by letting

$$x^* = \sum_{j=1}^{k} \lambda_j^* f_j(x) \tag{10}$$

Using x^* as the new experimental point does not guarantee that x^* yields an improved value for $f(x)$. This is not surprising because $f(x^*)$ is subjected to experimental error and $\sum_{j=1}^{k} \lambda_j f_j(x)$ which is based on previously evaluated design points, is subjected to experimental errors as well. On the other hand, solving the linear program (6)-(9) does produce a relatively good estimate of the shadow prices associated with each constraint $g_i(x) \leq 0$. These shadow prices can be employed in the process of generating a new point which is not necessarily a convex combination of previously evaluated design points. The generation of the new point can be done by minimizing the unconstrained expression

$$\hat{f}(x) - \sum_{i=1}^{m} \pi_i \hat{g}_i(x) \tag{11}$$

where π_i are the shadow prices obtained as part of the optimal solution of (6)-(9), and $\hat{f}(x)$, $\hat{g}_i(x)$ are polynomial approximations of the true response functions $f(x)$, $g_i(x)$. If

$$\min \{\hat{f}(x) - \sum_{i=1}^{m} \pi_i \hat{g}_i(x)\} - \pi_0 < 0 \tag{12}$$

where π_0 is the shadow price associated with (4) and $\hat{x}$ is the point minimizing (11), then by adding $\hat{\lambda} f(\hat{x})$ to the objective function (6), $\hat{\lambda} g_i(\hat{x})$ to the constraints (7), and $\hat{\lambda}$ to (8) and re-solving (6)-(9), a new point x^* is generated where a new experiment is to be performed.

This procedure works well when the true response functions $f(x)$ and $g_i(x)$ are convex. However, since these response functions are not explicitly given, the convexity assumption may not hold in most cases. It may also be true that (11) is unbounded and therefore $\hat{x}$ may not be generated by solving it. An alternative procedure for generating a new design point is worked out by finding a direction vector $d \in E^n$ which originates at x^*, the optimum of (6)-(9), and leads into an improved design point. This procedure replaces subproblem (11) by the problem

$$\text{minimize} \quad f(x^* + \alpha d) \tag{13}$$

s.t.

$$g_i(x^* + \alpha d) \leq 0 \qquad i = 1,2,\ldots,m \tag{14}$$

Problem (13)-(14) is a one-dimensional program in $\alpha \in E^1$, and is solved by an ordinary search which evaluates several design points along the direction d.

d is constructed by the negative weighted gradient vector

$$d = -\nabla\hat{f}(x^*) + \sum_{i=1}^{m} \pi_i \nabla\hat{g}_i(x^*) \tag{15}$$

where $\nabla\hat{f}(x^*)$, $\nabla\hat{g}_i(x^*)$ are the gradients of the polynomial approximation of the response functions at the point x^*.

If (15) generates improved responses, then program (6)-(9) is updated and the procedure is repeated. If, on the other hand, no improved responses are found along d the process terminates and the best evaluated design point is selected as the optimum of (1)-(2).

The negative weighted gradient of (15) is actually the first direction taken by subproblem (11) where x^* is the initial point of this unconstrained subprogram. Due to the fact that $\hat{f}(x)$ and $\hat{g}_i(x)$ are only approximations of the true response functions, it becomes more important to verify that the progress of the objective function in the direction of the optimum is actually taking place. This verification enables the decision maker to update the polynomial approximations $f(x)$ and $g_i(x)$ and to obtain new shadow prices before any new direction is generated. Another advantage of (15) over (11) is the fact that the new point obtained by (13)-(14) is feasible and does not violate any constraint in (2) while there is no guarantee that the point obtained by (11) is feasible. Also, if $\hat{f}(x)$ and $\hat{g}_i(x)$ are linear approximations, than (13)-(15) is still applicable while (11) is not.

III. Concluding Remarks

The problem of optimizing a response function where the constraints are also a set of response surfaces, arises in a situation where there are several competing objectives each of which is an unknown response function and the overall objective is a sum of the weighted objectives $\sum_{j=1}^{m+1} w_j f_j(x)$. The problem of assigning appropriate weights to different objectives is a difficult task. In this paper we developed a procedure for indirect weight assignment. This procedure seeks a design point which satisfies a minimum level of each objective. By converting m objectives into constraints and letting one objective be determined accordingly, the original problem is transformed into a linear program and the shadow price associated with each constraint at the optimum of this LP is the weight assigned to each objective in the overall criterion $\sum_{j=1}^{m+1} w_j f_j(x)$. where $w_1 = 1$ and $w_j = -\pi_j$, $j \neq 1$. Applying the steepest descent method to this weighted objective, results in expression (15) which is the weighted negative gradient of the multiple response problem.

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