

Optimization of Triple Response Systems by Using the Dual Response Approach and the Hooke-Jeeves Search Method

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Abstract. This paper presents an extended computing procedure for the global optimization of the triple response system (TRS) where the response functions are nonconvex (nonconcave) quadratics and the input factors satisfy a radial region of interest. The TRS arising from response surface modeling can be approximated using a nonlinear mathematical program involving one primary (objective) function and two secondary (constraints) functions. An optimization algorithm named triple response surface algorithm (TRSALG) is proposed to determine the global optimum for the nondegenerate TRS. In TRSALG, the Lagrange multipliers of target (secondary) functions are computed by using the Hooke-Jeeves search method, and the Lagrange multiplier of the radial constraint is located by using the trust region (TR) method at the same time. To ensure global optimality that can be attained by TRSALG, included is the means for detecting the degenerate case. In the field of numerical optimization, as the family of TR approach always exhibits excellent mathematical properties during optimization steps, thus the proposed algorithm can guarantee the global optimal solution where the optimality conditions are satisfied for the nondegenerate TRS. The computing procedure is illustrated in terms of examples found in the quality literature where the comparison results with a gradient-based method are used to calibrate TRSALG.

Keywords: Triple Response System (TRS), Global Optimization, Nonlinear Programming (NLP), Trust Region (TR); Hooke-Jeeves' Search Method

1. INTRODUCTION

The advent of the dual response approach proposed by Myers and Carter (1973) has sparked tremendous in-

terest in the application and analysis of multiple response optimization problems. In their approach, the objective is to optimize a “primary” second-order polynomial response function subject to some equality con-

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straint on a quadratic “secondary” response function. Many results using the dual response approach have been reported over the last three decades, inspiring researchers to exploit its applicability in different fields. A common instance of a dual response system is in the area of robust parameter design. Genichi Taguchi (Taguchi and Wu, 1980; Taguchi, 1986, 1987) introduced his approach for reducing variation and improving product (or process) quality characteristics simultaneously. After the concept has been pointed out by applying the optimization approach to quality control (QC), Vining and Myers (1990) integrate the Taguchi and response surface methods into the dual response approach for achieving some of the goals of Taguchi’s philosophy. From that time on, the dual response system (DRS) has been suggested as one of the primary means for allowing the adoption of Taguchi’s philosophy while providing a more rigorous approach to the analysis. Furthermore, some modifications based on the dual response approach utilize the generalized nonlinear programming algorithms for the purpose of improving the optimization performance (see Del Castillo and Montgomery, 1993; Lin and Tu, 1995). However, these methods may settle on local optima and thus the global optimum can only be achieved by conducting some ad hoc analyses.

To achieve global optimality that the above-mentioned methods can not achieve, Semple (1997) proposed an optimization algorithm of DRS for the nondegenerate case, thus termed DRSALG. The algorithm guarantees the global optimal solution by using the trust-region-based approach. For the degenerate problem in DRS, Del Castillo, Fan, and Semple (1999) designed a modified trust-region algorithm that is an extension of Semple’s algorithm for the generalized DRS. The new algorithm dubbed DR2 can either solve the degenerate or nondegenerate problems for DRS. To date, it has become manifest that the development of the optimization methods and practical applications for DRS has been widely recognized. However, the DRS represents merely one of the practical instances that could realistically occur in practice. Surprisingly few studies have been devoted to the case dealing with more than two responses within the context of the dual response approach. To further enhance the dual response approach’s practicality, a triple response system (TRS) subject to the radial inequality constraint is studied in this paper. Thus, the algorithm to be presented in this paper is termed the triple response surface algorithm (TRSALG), where the Hooke–Jeeves (HJ) search method (1961) is used to locate suitable Lagrange multipliers. The formal definition of TRS will be given in the next section.

2. TRIPLE RESPONSE SYSTEM

The objective of this paper is to develop an algorithm based on DRSALG to solve TRS inside the search

of a radial bound. TRS arises in a variety of modeling situations where three competing objectives must be managed at the same time. All the objectives can be approximated by using second-order polynomials called quadratic functions. The goal of TRS is to minimize one of the functions (the *primary* response) while maintaining two desirable conditions on the remaining target functions (the *secondary* responses), as defined by

$$\begin{aligned} \text{Min } f(\mathbf{x}) &= b_0 + \mathbf{x}^T \mathbf{B} \mathbf{x} + \mathbf{b}^T \mathbf{x} \\ \text{s.t } g_1(\mathbf{x}) &= d_0^1 + \mathbf{x}^T \mathbf{C}_1 \mathbf{x} + \mathbf{d}_1^T \mathbf{x} = T_1 \\ g_2(\mathbf{x}) &= d_0^2 + \mathbf{x}^T \mathbf{C}_2 \mathbf{x} + \mathbf{d}_2^T \mathbf{x} = T_2 \\ \mathbf{x}^T \mathbf{x} &\leq r^2 \end{aligned} \quad (1)$$

where \mathbf{B} , \mathbf{C}_1 and $\mathbf{C}_2 \in \mathbf{R}^{k \times k}$ are symmetric matrices that contain the parameters of the quadratic terms, i.e.,

$$\mathbf{B} = \begin{bmatrix} b_{11} & b_{12}/2 & \cdots & b_{1k}/2 \\ \vdots & b_{22} & \cdots & b_{2k}/2 \\ \vdots & & \ddots & \vdots \\ b_{k1}/2 & \cdots & \cdots & b_{kk} \end{bmatrix},$$

$$\mathbf{C}_i = \begin{bmatrix} c_{11}^i & c_{12}^i/2 & \cdots & c_{1k}^i/2 \\ \vdots & c_{22}^i & \cdots & c_{2k}^i/2 \\ \vdots & & \ddots & \vdots \\ c_{k1}^i/2 & \cdots & \cdots & c_{kk}^i \end{bmatrix},$$

where $i=1, 2$. The vectors \mathbf{b} , \mathbf{d}_1 and \mathbf{d}_2 contain the parameter estimates of linear terms, and b_0 , d_0^1 and d_0^2 are the scalars which estimate the intercepts. The vector $\mathbf{x} \in \mathbf{R}^{k \times 1}$ represents a set of factors which are under the control of the process engineer, and T_1 , T_2 (the *target* values) and $r > 0$ (the *radius* of the norm constraint) are given constants. In problem (1), the inequality constraint confines the search for the optimal operating conditions where the designed experiment takes place. Hence, there have several logical selections for r if a composite design (CCD) is chosen to fit TRS.

In DRS, Myers and Carter (1973) have shown that, if the matrix $(\mathbf{B} - \mu \mathbf{C} + \theta \mathbf{I})$ is positive definite (p.d.), then the stationary point \mathbf{x} is given by

$$(\mathbf{B} - \mu \mathbf{C} + \theta \mathbf{I}) \mathbf{x} = \frac{1}{2} (\mu \mathbf{d} - \mathbf{b}),$$

where the Lagrange multipliers μ , θ additionally satisfy $\theta \geq 0$ and $\theta = 0$ whenever $\mathbf{x}^T \mathbf{x} \leq r^2$. However, in this paper DRS is extended to TRS by considering the following two equality constraints:

$$\begin{aligned} g_1(\mathbf{x}) &= \mathbf{x}^T \mathbf{C}_1 \mathbf{x} + \mathbf{d}_1^T \mathbf{x} = T_1 \\ g_2(\mathbf{x}) &= \mathbf{x}^T \mathbf{C}_2 \mathbf{x} + \mathbf{d}_2^T \mathbf{x} = T_2. \end{aligned}$$

From the mathematical program in (1), the *parametric trust region* problem is constructed that formalizes the parametric optimization to make TRS similar to a trust region problem $(D(\mu_1, \mu_2))$ as expressed by

$$\begin{aligned} \text{Min } d(\mathbf{x}) &= \mathbf{x}^T \mathbf{B} \mathbf{x} + \mathbf{b}^T \mathbf{x} - \sum_{i=1}^2 \mu_i (\mathbf{x}^T \mathbf{C}_i \mathbf{x} + \mathbf{d}_i^T \mathbf{x} - T_i) \\ \text{s.t } \mathbf{x}^T \mathbf{x} &\leq r^2, \end{aligned}$$

where $i=1, 2$ and then the stationary point \mathbf{x} of TRS is generated via

$$(\mathbf{B} - \mu_1 \mathbf{C}_1 - \mu_2 \mathbf{C}_2 + \theta \mathbf{I}) \mathbf{x} = \frac{1}{2} (\mu_1 \mathbf{d}_1 + \mu_2 \mathbf{d}_2 - \mathbf{b}) \quad (2)$$

It is noteworthy that both the stationary point \mathbf{x} and its associated response values of g_1 and g_2 are viewed as functions of μ_1 and μ_2 . Thus, there are three unknown parameters to solve, the Lagrange multiplier, μ_1 , μ_2 and θ , for determining the stationary point \mathbf{x} . The following section presents the computation of the Lagrange multipliers in the nondegenerate case of TRS.

2.1 Nondegenerate TRS

Problem (1) is now reduced to the search that will be conducted within the three-dimensional parameter space (μ_1, μ_2, θ) . It can be considered an extension of DRS suggested by Myers and Carte (1973) and therefore the parameter space is defined by:

$$\Gamma = \{(\mu_1, \mu_2, \theta) : (\mathbf{B} - \mu_1 \mathbf{C}_1 - \mu_2 \mathbf{C}_2 + \theta \mathbf{I}) \text{ is p.d., } \theta \geq 0\}$$

Note that a parameter search performed in this manner is only successful if the global optimum is a stationary solution achieved for some $(\mu_1, \mu_2, \theta) \in \Gamma$. Theorem 2.1 that follows shows the global optimality for the multiple response system (MRS). In instances where this is not the case, the search will get stuck (at what is called a “gateway” point on the boundary of Γ). That is, the search cannot find a suitable $(\mu_1, \mu_2, \theta) \in \Gamma$ to make the Hessian matrix $(\mathbf{B} - \mu_1 \mathbf{C}_1 - \mu_2 \mathbf{C}_2 + \theta \mathbf{I})$ p.d. When this situation occurs, it is said to be a degenerate case. To discuss the nondegeneracy of TRS, consider the matrix $(\mathbf{B} - \mu_1 \mathbf{C}_1 - \mu_2 \mathbf{C}_2 + \theta \mathbf{I})$ for fixed values of μ_1 and μ_2 , and consider its ordered eigenvalues $\{\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n\}$. It is reasonable to treat μ_1 and μ_2 (associated with both secondary responses) as constants. The reason is that the target values (T_1, T_2) of constraint responses are given constants by the process engineer in advance. If there exists a global solution to TRS, then (T_1, T_2) is mapped to a unique set (μ_1, μ_2) . For μ_1 and μ_2 , let the eigenspace corresponding to the smallest eigenvalue be denoted by $\mathbf{E}_{\lambda_1}^{(\mu_1, \mu_2)}$. The non-degeneracy can be defined through $\mathbf{E}_{\lambda_1}^{(\mu_1, \mu_2)} = \{\mathbf{q} : (\mathbf{B} - \mu_1 \mathbf{C}_1 - \mu_2 \mathbf{C}_2) \mathbf{q} = \lambda_1 \mathbf{q}\}$. See Definition 2.1. To illustrate, the degenerate situation will be pictorially shown in the following section.

Theorem 2.1 Let \mathbf{B}, \mathbf{C}_i be symmetric matrices, possibly indefinite. Let \mathbf{x}_1 be a solution to multiple response system (MRS) with $(\mathbf{B} - \sum_i \mu_i \mathbf{C}_i + \theta \mathbf{I})$ p.d. and $\theta \geq 0$. Then, for MRS, with $r^2 = \mathbf{x}_1^T \mathbf{x}_1$ and $T_i = \mathbf{x}_1^T \mathbf{C}_i \mathbf{x}_1 + \mathbf{d}_i^T \mathbf{x}_1$

$T_i = \mathbf{x}_1^T \mathbf{C}_i \mathbf{x}_1 + \mathbf{d}_i^T \mathbf{x}_1$, \mathbf{x}_1 is the unique global minimum. For any other feasible point \mathbf{x}_2 , the inequality holds:

$$f(\mathbf{x}_1) - f(\mathbf{x}_2) \leq -(\mathbf{x}_1 - \mathbf{x}_2)^T (\mathbf{B} - \sum_i \mu_i \mathbf{C}_i + \theta \mathbf{I}) (\mathbf{x}_1 - \mathbf{x}_2).$$

If $\theta = 0$, \mathbf{x}_1 then is the unique global minimum to the MRS inside the radial bound.

Definition 2.1 Problem (1) is said to be *locally nondegenerate* on $(\mu_1, \mu_2) \in R$ provided that for μ_1 and μ_2 the vector $(\mu_1 \mathbf{d}_1 + \mu_2 \mathbf{d}_2 - \mathbf{b})$ is not perpendicular to $\mathbf{E}_{\lambda_1}^{(\mu_1, \mu_2)}$. Problem (1) is said to be *degenerate* on $(\mu_1, \mu_2) \in R$ otherwise.

3. SOLUTION PROCEDURE OF NON-DEGENERATE TRS

To solve the nondegenerate case of TRS, an extended dual response approach is proposed in this paper. Semple’s DRSALG (1997) is a two-stage algorithm for optimizing the nondegenerate DRS. First, the root-finding method such as regula falsi (RF) or modified regula falsi (MRF) is used to determine the Lagrange multiplier of the equality constraint, and then a trust region method is used to locate the Lagrange multiplier of the radial constraint. Following DRSALG, TRSALG is developed for TRS. In particular, a multidimensional search method without using derivatives, the Hooke-Jeeves method is used to simultaneously seek μ_1 and μ_2 that could satisfy both secondary response constraints. Afterwards, the trust region method is used to calculate the optimal θ at fixed μ_1 and μ_2 . If the solution is found with $(\mu_1, \mu_2, \theta) \in \Gamma$, then it can be guaranteed a unique global solution to TRS.

The Hooke-Jeeves’ algorithm (1961) is a well-known pattern search procedure that is widely used to optimize nonlinear functions without using derivatives. The algorithm performs repeatedly two types of search routines: an exploratory cyclic search and a pattern search. The Hooke-Jeeves’ algorithm requires deterministic evaluation of the function being optimized. If the minimum of the objective along any line is unique and the convergence sequence is contained in a compact set, then the pattern search direction is descent iteration from iteration, thus converging to a stationary point (zero gradient). This method is extremely effective at solving the minimization problem that has only one minimizer along the each coordinate axis instead of solving the problem with multiple optimal solutions. Therefore, the Hooke and Jeeves’ method can solve effectively the unique solution of the error sums-of-squares function transformed from the TRS problem, as will be shown shortly. The details regarding the proposed algorithm TRSALG are described in the next two subsections: locating Lagrange multiplier θ and computation for μ_1 and μ_2 .

3.1 Locating θ

For the aforementioned parametric trust region problem $D(\mu_1, \mu_2)$ of TRS, the key process is to compute the Lagrange multiplier θ at fixed μ_1 and μ_2 such that the resulting Hessian matrix is p.d. The main idea of the trust region method is to update the interval $[\theta^l, \theta^u]$ of θ which contains the desired solution θ^* at fixed μ_1 and μ_2 , and locate the solution iff $(\mathbf{B} - \mu_1 \mathbf{C}_1 - \mu_2 \mathbf{C}_2 + \theta \mathbf{I})$ is p.d. on the sphere of radial r or $\theta = 0$ inside the radial bound. The following mathematical formulation is referred to Semple's DRS approach. The technique for solving the parametric trust region problem in the region $(-\lambda_1, \infty) \cap [0, \infty)$ had been investigated extensively in abundant trust region literatures. Note that a solution is required for $(-\lambda_1, \infty) \cap [0, \infty)$ and the Newton's method may diverge, so the safeguarding scheme is necessary when the iteration falls outside the interval $(-\lambda_1, \infty)$.

What follows is primarily concerned with the solution to the parametric secular equation (if exists):

$$\phi_\mu(\theta) = \frac{1}{4} \nabla D(\mu_1, \mu_2, \theta)^T H(\mu_1, \mu_2, \theta)^{-2} \nabla D(\mu_1, \mu_2, \theta) = r^2 \quad (3)$$

where

$$\begin{aligned} \nabla D(\mu_1, \mu_2) &= (\mu_1 \mathbf{d}_1 + \mu_2 \mathbf{d}_2 - \mathbf{b}), \\ H(\mu_1, \mu_2, \theta) &= \mathbf{B} - \mu_1 \mathbf{C}_1 - \mu_2 \mathbf{C}_2 + \theta \mathbf{I}, \end{aligned}$$

$(\mu_1, \mu_2, \theta) \in \Gamma$ and μ_1, μ_2 is considered fixed parameters. Then, applying the Schur decomposition to equation (3) yields the rational form

$$\phi_\mu(\theta) = \sum_{i=1}^n \frac{\gamma_i^2}{(\theta + \lambda_i)^2}, \quad (4)$$

where γ_i is the i -th projection component of γ . See the details of the above transformation in Semple (1997). In the nondegenerate case ($\gamma_i \neq 0$), the problem (3) has a unique solution for $r > 0$ that can be found by either solving

$$r^2 = \phi_\mu(\theta) = \sum_{i=1}^n \frac{\gamma_i^2}{(\theta + \lambda_i)^2} \quad \text{on } (-\lambda_1, \infty) \cap [0, \infty),$$

or setting $\theta = 0$ on the case where $\phi_\mu(\theta) < r^2$ on $(-\lambda_1, \infty) \cap [0, \infty)$. By contrast, differentiating the secular function as it appears in (3) with respect to θ yields $\phi'_\mu(\theta) = \|\mathbf{z}\|^2$, $\phi'_\mu(\theta) = -2\mathbf{w}^T \mathbf{z}$, and $\phi'_\mu(\theta) = 6\|\mathbf{w}\|^2$ (Semple, 1997 and Fan, 2003).

$\|\mathbf{x}^T \mathbf{x}\|$ in equation (3) is monotone decreasing and convex on $\theta \in (-\lambda_1, \infty)$ (Fan, 2003). Newton's iteration to the reciprocal transformation of equation (3), termed Reinsch's equation, can be formed:

$$\theta_{k+1} = \theta_k - (r^2 \|\mathbf{z}\|^2 - \|\mathbf{z}\|^4) / 2r^2 \mathbf{z}^T.$$

According to the safeguard mechanism in the trust region method, the lower bound for $-\lambda_1$ is thus com-

puted as $\theta_k - (\mathbf{w}^T \mathbf{z} / \mathbf{w}^T \mathbf{w})$. Note that when θ_k is less than the lower bound for $-\lambda_1$, then the θ_k is safeguarded by the lower bound of θ to avoid the current solution overshooting the working interval (Fan, 2003). For the detail of the solution procedure of the trust region method, see Semple (1997) and Fan (2003).

3.2 Construction of the initial intervals of (μ_1, μ_2)

The results of section 3.1 can now be utilized to construct the initial intervals for μ_1 and μ_2 . Following Semple's DRSALG (1997), the initial intervals are established by means of solving the following five trust region subproblems:

- (i) Min $f(\mathbf{x}) = \mathbf{x}^T \mathbf{B} \mathbf{x} + \mathbf{b}^T \mathbf{x}$
s.t. $\mathbf{x}^T \mathbf{x} \leq r^2$;
- (ii) Min $g_1(\mathbf{x}) = \mathbf{x}^T \mathbf{C}_1 \mathbf{x} + \mathbf{d}_1^T \mathbf{x}$
s.t. $\mathbf{x}^T \mathbf{x} \leq r^2$;
- (iii) Max $g_1(\mathbf{x}) = \mathbf{x}^T \mathbf{C}_1 \mathbf{x} + \mathbf{d}_1^T \mathbf{x}$
s.t. $\mathbf{x}^T \mathbf{x} \leq r^2$;
- (iv) Min $g_2(\mathbf{x}) = \mathbf{x}^T \mathbf{C}_2 \mathbf{x} + \mathbf{d}_2^T \mathbf{x}$
s.t. $\mathbf{x}^T \mathbf{x} \leq r^2$;
- (v) Max $g_2(\mathbf{x}) = \mathbf{x}^T \mathbf{C}_2 \mathbf{x} + \mathbf{d}_2^T \mathbf{x}$
s.t. $\mathbf{x}^T \mathbf{x} \leq r^2$.

Let the optimal solutions to (i-v) be denoted by \mathbf{x}_{\min}^f , $\mathbf{x}_{\min}^{g_1}$, $\mathbf{x}_{\max}^{g_1}$, $\mathbf{x}_{\min}^{g_2}$ and $\mathbf{x}_{\max}^{g_2}$, respectively. In TRS, the parametric trust region problem is defined as follows:

$$\begin{aligned} D(\mu_1, \mu_2) \quad & \text{Min } f(\mathbf{x}) - \mu_1 g_1(\mathbf{x}) - \mu_2 g_2(\mathbf{x}) \\ & \text{s.t. } \mathbf{x}^T \mathbf{x} \leq r^2. \end{aligned}$$

The first step is to solve the three trust region problems (i-iii) when setting $\mu_2 = 0$. Then, the parametric trust region problem is reduced to

$$\begin{aligned} D(\mu_1, \mu_2) \quad & \text{Min } f(\mathbf{x}) - \mu_1 g_1(\mathbf{x}) \\ & \text{s.t. } \mathbf{x}^T \mathbf{x} \leq r^2. \end{aligned}$$

Note that (i) is $D(\mu_1, \mu_2)$ with $\mu_1 = \mu_2 = 0$; (ii) is $D(\mu_1, \mu_2)$ with $\mu_1 = -\infty$ at $\mu_2 = 0$; (iii) is $D(\mu_1, \mu_2)$ with $\mu_1 = \infty$ at $\mu_2 = 0$. In DRSALG (1997), an assumption that T_1 satisfies $g_1(\mathbf{x}_{\min}^{g_1}) < T_1 < g_1(\mathbf{x}_{\max}^{g_1})$ is used. If T_1 equals $g_1(\mathbf{x}_{\min}^{g_1})$ or $g_1(\mathbf{x}_{\max}^{g_1})$, the problem is solved by (ii) or (iii), respectively. If T_1 is outside this range, the problem is infeasible. After computing the constant $g_1(\mathbf{x}_{\min}^f)$, one of three cases occurs: (a) $g_1(\mathbf{x}_{\min}^f) = T_1$; (b) $g_1(\mathbf{x}_{\min}^f) < T_1$; (c) $g_1(\mathbf{x}_{\min}^f) > T_1$.

Case (a): $g_1(\mathbf{x}_{\min}^f) = T_1$

In this case, the solution \mathbf{x}_{\min}^f is just the feasible solution of TRS. Furthermore, the solution is the absolute optimal solution for TRS when $g_2(\mathbf{x}_{\min}^f)$ also equals to T_2 .

Case (b): $g_1(\mathbf{x}_{\min}^f) < T_1$

In this case, the initial interval for μ_1 is constructed by

$$\mu_1^l = 0 \leq \mu_1^* \leq f(\mathbf{x}_{\max}^{g_1}) - f(\mathbf{x}_{\min}^f) / (g_1(\mathbf{x}_{\max}^{g_1}) - T_1) \equiv \mu_1^U$$

Case (c): $g_1(\mathbf{x}_{\min}^f) > T_1$

In this case, the initial interval for μ_1 is constructed by

$$\mu_1^l \equiv f(\mathbf{x}_{\min}^f) - f(\mathbf{x}_{\min}^{g_1}) / (T_1 - g_1(\mathbf{x}_{\min}^{g_1})) \leq \mu_1^* \leq 0 = \mu_1^U$$

For cases (b-c), see the proof in Semple (1997).

After computing the interval of μ_1 , the second step is to construct the initial interval for μ_2 in the feasible interval of μ_1 . The intermediate μ_1' chosen within the interval of μ_1 is used to check if the interval of μ_2 contains T_2 . The problem is infeasible if the constructed interval of μ_2 does not contain T_2 . Based on a suitable μ_1' in the interval of μ_1 , the trust region problem in the following is solved

$$\begin{aligned} D(\mu_1, \mu_2) \quad & \text{Min } f(\mathbf{x}) - \mu_1' g_1(\mathbf{x}) - \mu_2 g_2(\mathbf{x}) \\ \text{s.t. } & \mathbf{x}^T \mathbf{x} \leq r^2. \end{aligned}$$

In a similar manner, the trust region problems (iv-v) are solved to construct the initial interval of μ_2 for a suitable μ_1' . In the corresponding three cases, μ_1 is replaced by μ_2 , \mathbf{x}_{\min}^f is replaced by $\mathbf{x}_{\min}^{g_2}$, and $\mathbf{x}_{\max}^{g_1}$ is replaced by $\mathbf{x}_{\max}^{g_2}$. Upon completing the construction of the initial intervals of μ_1 and μ_2 , the optimal Lagrange multipliers (μ_1^* , μ_2^*) are bracketed. However, the order of constructing bounds for μ_1 or μ_2 is exchangeable if the infeasibility occurs in any order. If it is the case, then the step one is to construct the initial interval of μ_2 at $\mu_1 = 0$ instead to solve the trust region problems of (i), (iv) and (v). Then, the same procedure is followed by a reverse order.

3.3 Update of μ_1 and μ_2

The HJ search method (1961) is used to find the suitable value of μ_1 and μ_2 for which the equality constraints in (1) are satisfied. The HJ algorithm starts with an exploratory move to determine an appropriate direction of search (pattern) by considering one variable at a time along the individual coordinate directions. Following the exploratory search, a series of pattern moves are made to accelerate the search in the direction determined in the exploratory search. Exploratory searches and pattern moves are repeated until a termination criterion is met. For more details on HJ algorithm, see Bazaraa, Sherali, and Shetty (1993). Due to nice convergence properties of Hooke and Jeeves' search method (see Bazaraa *et al.*, 1993), the search method can guarantee that the found solutions of μ_1 and μ_2 are optimal if the generated sequence is closed and bounded. Denote that the two variables to be sought be a vector $\boldsymbol{\mu} = (\mu_1,$

$\mu_2)$ in two-dimensional parameter space, $(\mu_1, \mu_2) \in \mathbf{R}^2$. The objective function in updating (μ_1, μ_2) is defined as

$$\text{Minimize } h(\boldsymbol{\mu}_k) = \sum_{i=1}^2 |g_i(\mathbf{x}_k(\mu_{1k}, \mu_{2k})) - T_i|^2,$$

where g_i is the secondary response in (1) for $i=1, 2$, and \mathbf{x}_k is the stationary point at the fixed values of μ_{1k} and μ_{2k} at the k -th iteration. The objective is to minimize the squared error between secondary responses and their targets. This type of search is halted if a solution $(\mu_1, \mu_2) \in \mathbf{R}^2$ is found with $h(\boldsymbol{\mu}_k) < \varepsilon = 10^{-6}$ (where ε = tolerance for convergence). The unique, absolute minimum of $h(\boldsymbol{\mu}_k)$ is zero and the search space is also bounded by the constructed initial intervals. Hence, the global convergence property of HJ search in such a circumstance can be guaranteed if TRS is nondegenerate.

3.4 TRSALG

The TRSALG is performed by two steps, which computes the optimal solution for TRS that is locally nondegenerate in (T_1, T_2) . The main idea behind TRSALG have been introduced in Sections 3.2-3.3: first, fix μ_1 and μ_2 at suitable values and compute the value of θ at the same time such that the resulting stationary point makes the Hessian matrix p.d. The Figure 1 shows the formal solution procedure of the two-stage parametric approach for optimizing TRS.

4. AN EXAMPLE TAKEN FROM RESPONSE SURFACE METHODOLOGY LITERATURE

Two examples taken from the literature will be presented in this section to illustrate TRSALG. The generalized reduced gradient (GRG) results are also listed for the calibration purpose. The GRG algorithm has been proved one of the most robust and efficient NLP methods available to solve small to moderate size problems (Lasdon *et al.*, 1978). Many GRG codes are available. The optimizer termed "SOLVER" embedded into the Microsoft EXCEL is the GRG2 code from Lasdon *et al.* (1974) and Lasdon *et al.* (1978), and it is used to calibrate the TRSALG results in this paper.

4.1 Example 1

This example is from Shah, Montgomery and Carlyle (2004). It is original from Tseo *et al.* (1983). It investigated the effects of washing temperature (x_1), washing time (x_2), and washing ratio (x_3) on the springiness (y_1), thiobarbituric acid number (y_2), percent cooking loss (y_3), and whiteness index (y_4) for minced mullet flesh. The experimental design is a central composite design (CCD) in $k=3$ design variables and the experimenter observed 4 responses. For the pur-

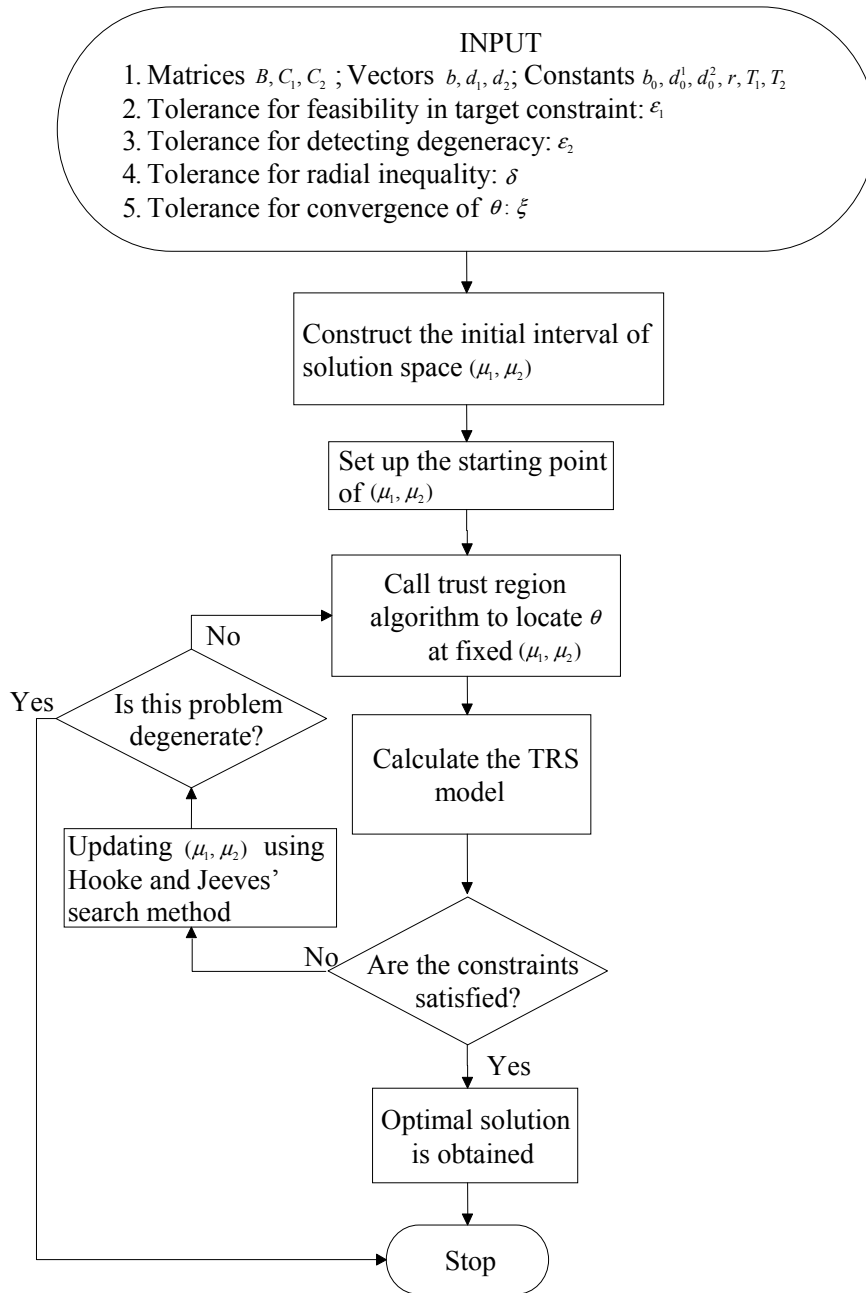


Figure 1. The Formal Procedure of TRSALG.

pose of the illustration of TRS, the thiobarbituric acid number (y_2) will be minimized that is called the primary response, and the percent cooking loss (y_3) and whiteness index (y_4) will be wished to be on target that are called the secondary responses.

Assume that the target value of y_4 is on $T_1 = 40$ and the target value of y_3 is on $T_2 = 25$. Since a CCD is used in the designed experiment, the radius of the inequality constraint is set to $r = \sqrt{3}$. The required matrices, vectors and constants, taken directly from the regression analysis, are

$$\begin{aligned}
 B &= \begin{bmatrix} 8.1529 & 1.29 & -0.29 \\ & 0.426 & 0.2062 \\ \text{sym.} & & 0.9793 \end{bmatrix}, \\
 C_1 &= \begin{bmatrix} -3.1519 & 0.0444 & 0.2381 \\ & 0.6435 & -0.1132 \\ \text{sym.} & & 0.5728 \end{bmatrix}, \\
 C_2 &= \begin{bmatrix} 3.4525 & 0.9 & 1.05 \\ & 0.8008 & -0.2875 \\ \text{sym.} & & 1.5786 \end{bmatrix},
 \end{aligned}$$

$$b = \begin{bmatrix} 5.6151 \\ -0.218 \\ -1.1808 \end{bmatrix}, d_1 = \begin{bmatrix} 2.4364 \\ 0.6307 \\ 0.2692 \end{bmatrix}, d_2 = \begin{bmatrix} 0.7442 \\ -0.012 \\ 1.0711 \end{bmatrix},$$

$$b_0 = 21.2616, d_0^1 = 50.7102, d_0^2 = 17.9326.$$

By solving five trust region problems as mentioned in Section 3.2, the initial intervals of Lagrange multipliers are found $\mu_1 \in [-2.59727, 0]$ and $\mu_2 \in [0, 5.87565]$. In order to clearly pinpoint the target location on the secondary response surface, the optimal response surface is plotted over infinitesimal grid points inside $\mu_1 \in [-5, 0]$ and $\mu_2 \in [0, 5]$. The three-dimensional plots of y_3 and y_4 are shown in Figures 2~3, respectively. Table 1 shows the computation results for the Lagrange multipliers and optimal solutions for the TRS problem by using GRG2 and TRSALG. Note that the sign of the Lagrange multiplier θ in GRG2 is opposite from TRS ALG since the Hessian matrix in GRG2 is $(B - \mu_1 C_1 - \mu_2 C_2 - \theta I)$. Table 2 shows the squared errors by using GRG2 and TRSALG. From a practical point of view, both algorithms reach the same optimal solution.

Figure 4 exhibits the contour plot of $h(\mu)$ in the search space by solving the trust region problems. The HJ search needs five complete iterations for convergence. As can be seen from the figure, every search direction is descent since the minimum of the objective along any line is unique, leading to the ultimate convergence to the minimum point with zero objective value. The summary of the computation results is given in Table 3.

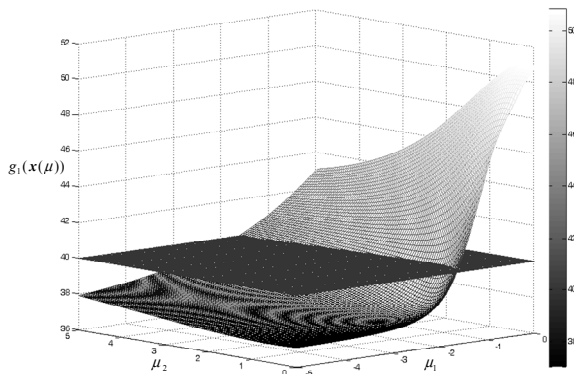


Figure 2. Plot of y_3 and Target ($T_1 = 40$) Response with respect to (μ_1, μ_2) in Example 1.

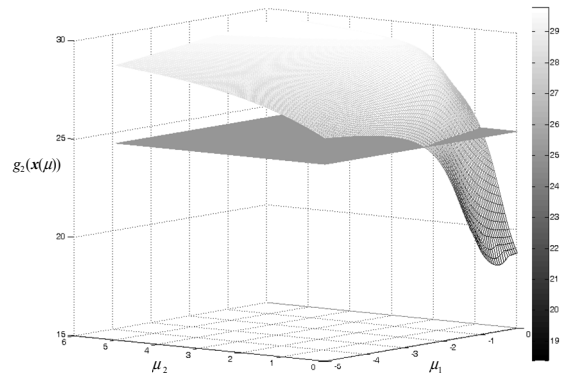


Figure 3. Plot of y_4 and Target ($T_1 = 25$) Response w.r.t (μ_1, μ_2) in Example 1.

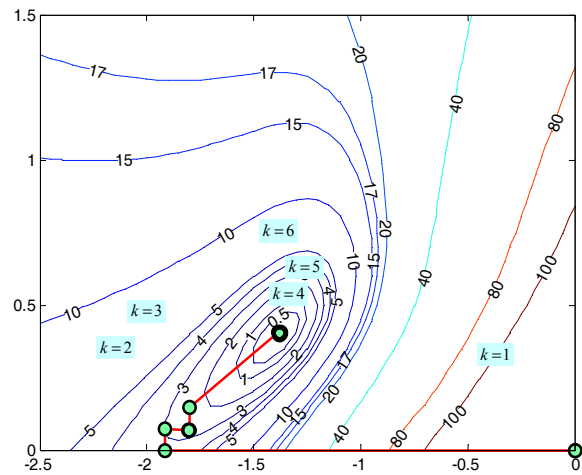


Figure 4. The Search Route by Using Hooke and Jeeves' Method for Example 1.

4.2 Example 2

This example is from Fan (1996). It is original from Vining and Myers (1990). The purpose of the experiment was to analyze the effect of the speed (x_1), pressure (x_2), and distance (x_3) factors upon a printing machine's ability to apply coloring inks onto package labels. In Fan (1996) the primary response of this example is to be minimized subject to two linear target functions as follows:

Table 1. Solution of GRG2 and TRSALG.

Algorithm	$\mu^* = (\mu_1, \mu_2)$	$\theta(\mu^*)$	Solution x^*
GRG2	(-1.38169, 3.96207e-001)	-8.42257e-001	(-1.56711, 6.91265e-001, -2.57538e-001)
TRSALG	(-1.38169, 3.96207e-001)	8.42258e-001	(-1.56711, 6.91265e-001, -2.57537e-001)

Table 2. Squared Errors returned by Using GRG2 and TRSALG.

Algorithm	$h(\mu^*)$	$f(x^*)$
GRG2	6.17389e-014	2.98038e+001
TRSALG	2.32356e-012	2.98038e+001

Table 3. Summary of Computation Results of TRSALG for Example 1.

Iteration k	μ_k $h(\mu_k)$	$\theta(\mu) = \theta(\mu_1, \mu_2)$	Iteration of TR	Solution x_k
1	(0.00000, 0.00000) 1.54363e+002	8.42258e-001	5	(-1.56711, 6.91266e-001, -2.57537e-001)
2	(-1.91448, 7.40264e-002) 2.97599e+000	1.64734	5	(-1.65022, 5.12205e-001, 1.20031e-001)
3	(-1.80068, 1.44772e-001) 2.40709e+000	1.43995	5	(-1.64377, 5.41440e-001, 6.97651e-002)
4	(-1.37520, 3.99839e-001) 1.77073e-003	8.36147e-001	5	(-1.56472, 6.93931e-001, -2.64759e-001)
5	(-1.38189, 3.96094e-001) 1.69826e-006	8.42451e-001	5	(-1.56718, 6.91182e-001, -2.57313e-001)
6	(-1.38169, 3.96207e-001) 2.32356e-012	8.42258e-001	5	(-1.56711, 6.91266e-001, -2.57537e-001)

Min. $34.9 + 11.5x_1 + 15.3x_2 + 29.2x_3 + 4.2x_1^2 - 1.3x_2^2 + 16.8x_3^2 + 7.7x_1x_2 + 5.1x_1x_3 + 14.1x_2x_3$
 s.t. $3x_1 - 5x_2 - 4x_3 = 1, 2x_1 + x_2 + x_3 = 2, x_1^2 + x_2^2 + x_3^2 \leq r^2.$

To lend itself to TRS, the linear constraints are squared to quadratic constraints as

$g_1(x) = (3x_1 - 5x_2 - 4x_3)^2 = 1^2,$
 $g_2(x) = (2x_1 + x_2 + x_3)^2 = 2^2.$

The resulting parameters are

$B = \begin{bmatrix} 4.2 & 3.85 & 2.55 \\ & -1.3 & 7.05 \\ sym. & & 16.8 \end{bmatrix}, C_1 = \begin{bmatrix} 9 & -15 & -12 \\ & 25 & 20 \\ sym. & & 16 \end{bmatrix},$
 $C_2 = \begin{bmatrix} 4 & 2 & 2 \\ & 1 & 1 \\ sym. & & 1 \end{bmatrix}, b = \begin{bmatrix} 11.5 \\ 15.3 \\ 29.3 \end{bmatrix}, d_1 = \begin{bmatrix} -6 \\ 10 \\ 8 \end{bmatrix}, d_2 = \begin{bmatrix} -8 \\ -4 \\ -4 \end{bmatrix},$

with $b_0 = 34.9, d_0^1 = 0, d_0^2 = 0.$ Note that the linear constraints are transformed into quadratic function, which is intentionally created for the evaluation purpose. The results from TRSALG and the GRG2 for this example are shown in Table 4. The Lagrange multipliers obtained

by using both algorithms are shown in Table 5. Here, the different radial bounds are tried by 1.0, 2.0 and 3.0. When $r^2 = 1.0$ is solved, GRG2 finds the result of $\Gamma = (\mu_1, \mu_2, \theta)$ that dose not make the Hessian matrix $(B - \mu_1 C_1 - \mu_2 C_2 - \theta I)$ p.d. Notice that the Lagrange multiplier θ is negative in the GRG2 results. This is called the degenerate case where TRSALG cannot find the unique global solution. In the mean time, TRSALG can detect the situation of degeneracy (or called gateway point) at $\Gamma = (-1.73124e-001, -6.34584e-001, 2.15876)$, which makes the vector $(\mu_1 d_1 + \mu_2 d_2 - b)$ is orthogonal to $E_{\lambda_1}^{(\mu_1, \mu_2)}$. Degeneracy can be pictured from Figures 5~6. Observe that the surface is plotted in condition that the Hessian matrix $(B - \mu_1 C_1 - \mu_2 C_2 + \theta I)$ is p.d. at each grid but is not continuous at some target levels of the secondary responses. As $r^2 = 2.0, 3.0,$ TRSALG can find a global optimal solution that makes the Hessian matrix $(B - \mu_1 C_1 - \mu_2 C_2 + \theta I)$ is p.d. (where the Lagrange multiplier θ is positive). The GRG2 results are now confirmed as the global optimal solutions as well. Figures 7~8 shows the response surface plot of the secondary responses and Figure 9 shows the search contour plot of $h(\mu)$ while solving the TRS problem with radial bound $r^2 = 3.0.$ The HJ search needs 4 iterations for convergence and each pattern search is in a descent direction toward the zero-gradient stationary point.

Table 4. Computation Results of TRSALG and GRG2 for Example 2.

r^2	TRSALG		GRG2	
	Solution x^*	$f(x^*)$	Solution x^*	$f(x^*)$
1.0	-	-	(-2.89742e-001, 5.40759e-001, -7.89702e-001)	2.11709e+001
2.0	(-2.64256e-001, 8.20939e-001, -1.12082e-000)	1.90818e+001	(-2.64272e-001, 8.20933e-001, -1.12082)	1.90817e+001
3.0	(-2.45136e-001, 1.03148e-000, -1.36965e-000)	1.80992e+001	(-2.45131e-001, 1.03149e-000, -1.36965e-000)	1.80992e+001

Table 5. The Lagrange Multipliers returned by Using TRSALG and GRG2 for Example 2.

r^2	TRSALG	GRG2
	$\Gamma = (\mu_1, \mu_2, \theta)$	$\Gamma = (\mu_1, \mu_2, \theta)$
1.0	-	(1.16024e-002, -6.61993e-001, -3.12585e-000)
2.0	(-3.79730e-001, -5.24403e-001, 1.38195e-000)	(-3.79729e-001, -5.24374e-001, -1.38194e-000)
3.0	(-6.66710e-001, -3.90434e-001, 6.59930e-001)	(-6.66709e-001, -3.90444e-001, -6.59942e-001)

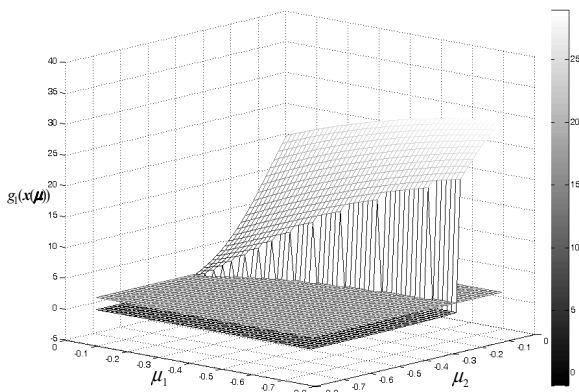


Figure 5. Plot of $g_1(x(\mu))$ and Target ($T_1 = 1$) with $r^2 = 1.0$ for Example 2.

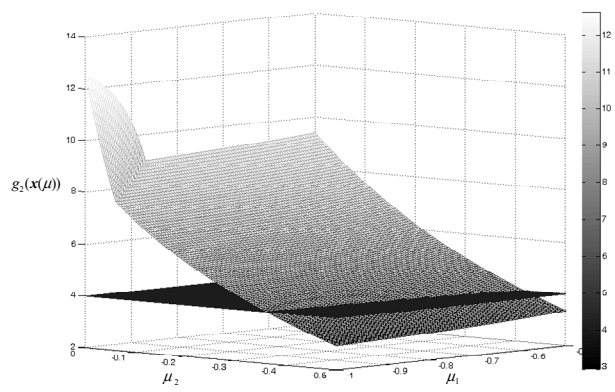


Figure 8. Plot of $g_2(x(\mu))$ and Target ($T_2 = 4$) with $r^2 = 3.0$ for Example 2.

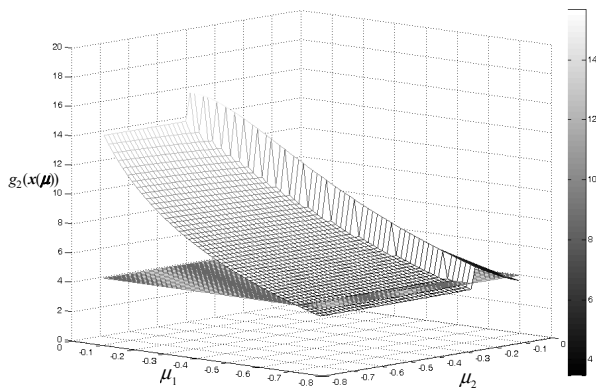


Figure 6. Plot of $g_2(x(\mu))$ and Target ($T_2 = 4$) with $r^2 = 1.0$ for Example 2.

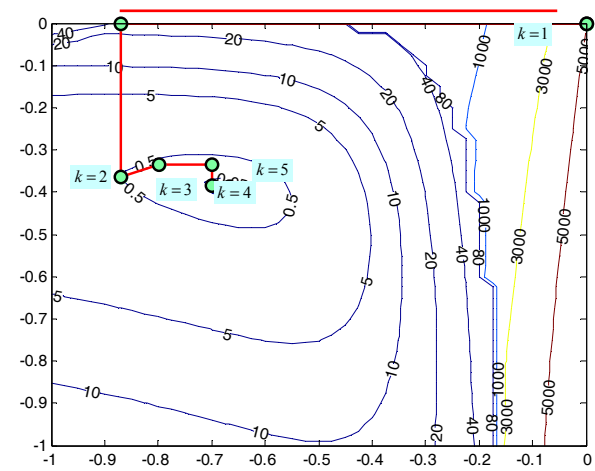


Figure 9. The Search Route by Using Hooke and Jeeves' method for Example 2.

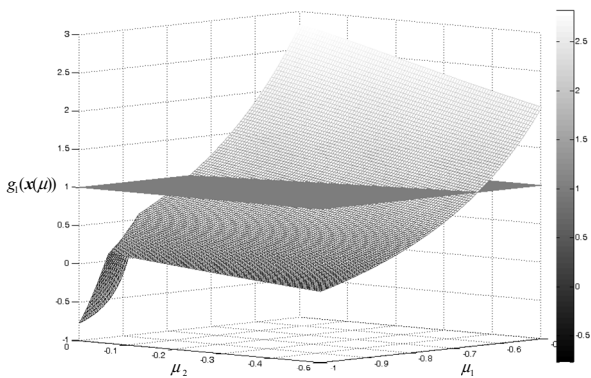


Figure 7. Plot of $g_1(x(\mu))$ and Target ($T_1 = 1$) Response with $r^2 = 3.0$ for Example 2.

5. CONCLUSIONS

This paper discusses the TRS problem that is extended from DRS. A new computing algorithm, termed TRSALG, for achieving the global optimal solution to the nondegenerate TRS is proposed. TRSALG is developed based on two types of nonlinear programming (NLP) methods, the trust region and Hooke-Jeeves' pattern search methods. TRS is shown to be solvable in terms of the second-order conditions for global optimality in Theorem 3.1, under the nondegeneracy assumption.

tion defined in Definition 3.1. Therefore, TRSALG is only successful if the second-order KKT conditions hold. The first step of TRSALG is to use the HJ search for searching appropriate Lagrange multipliers of the equality constraints and then use the trust region method to locate the Lagrange multiplier of the radial inequality constraint. As long as TRSALG converges, the solution returned must be a global optimum; otherwise, TRS is detected as a degenerate case. The proposed algorithm is illustrated in terms of examples found in the quality literature where the comparison results with a gradient-based method are used to calibrate TRSALG.

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