A Generalized Global Optimization Algorithm for Dual Response Systems

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During exploration of an industrial process, the engineer/experimenter must take into account both the mean and variance of the system in order to seek the appropriate parameter settings for better production outputs. This situation leads to the problem of determining optimal operating conditions for one response function while keeping a desirable target on the other response, the so-called dual response (DR) system. The purpose of this paper is to present an ANSI FORTRAN implementation of a comprehensive algorithm for the global (or near-global) optimization of DR systems within a radial region of experimentation. The algorithm, DR2, is a new computational procedure that guarantees a global optimal solution for nondegenerate problems and returns a near-global one for degenerate problems. Three degenerate problems published in the response surface methodology literature are provided which compare the performance of DR2 with that of other algorithms. In one of these examples, the Taguchi's "target is best" case is used to illustrate an important application of DR2. In the final parts of the paper, DR2 is tested against an implementation of sequential quadratic programming (SQP)-MINOS. Computational results based on large simulations show that DR2 is more effective at locating optimal operating conditions (near global optima) even if the DR system is degenerate.

Introduction

Myers and Carter (1973) developed a contour-based approach for the dual response (DR) system by plotting various Lagrange multipliers versus the primary and secondary response values and then confining the search point inside the spherical experimental region to visualize its optimum. Whenever this method successfully locates the optimal solution, it must be a *global* one as well (Semple (1997)). However, it is occurring quite often in practice that the optimal solutions do not satisfy the global optimality conditions, a situation that is called *degeneracy* (explained in more detail below). In the degenerate case, the contour method fails to find the optimal solution, and the general gradient search methods may only attain a local optimal solution.

Recently, Del Castillo, Fan, and Semple (1997) presented an ANSI FORTRAN implementation of an algorithm DRSALG that guarantees global optimal solutions to *nondegenerate* DR systems within a spherical experimental region. The relevance of DRSALG was shown by providing global optimal solutions for problems from the literature which, in some cases, were substantially better than the best solutions reported. The majority of DR problems are nondegenerate, but degenerate problems can occur and cannot be solved by DRSALG. Del Castillo, Fan, and Semple (1999) show that degenerate problems

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occur around 30% of the time with three control factors, 27% of the time with four control factors, and 22% of the time with five control factors. For more details, see Appendix F in Fan (1996).

In response surface methodology (RSM), the number of process factors included in the empirical model is rarely larger than 5 or 6. Typically, a "screening experiment" is conducted in an earlier phase to eliminate the less significant variables. Thus the remaining number of significant variables is small. It can be seen from the earlier simulations (see Fan (1996)) that the likelihood of degeneracy in the DR system is averaged approximately 25% to 40% if the problem size is smaller than 5. Obviously, degeneracy may happen quite often in practice.

Furthermore, RSM is performed in a sequential manner. When the design center (i.e., current operating conditions) is far from the optimum, curvature is often small and the first-order model will be appropriate. When the experimental block is moved along the path of *steepest descent (ascent)* (see, e.g., Myers and Montgomery (1995)) to the vicinity of the optimum, a second-order model may be necessary due to significant curvature. A dual response analysis can thus be utilized to locate the optimal operating conditions. From the same simulations reported by Fan, it is also shown that degeneracy tends to be *aggravated* as curvature increases. Pertaining to the considerations of problem sizes and curvature, degeneracy in the DR problem has to be solved if the experimenter wishes to seek the global optimal operating conditions without undue difficulty.

Del Castillo, Fan and Semple (1999) devised a generalized algorithm, called DR2, that computes global optimal solutions for nondegenerate problems and approximate global optimal solutions for degenerate problems. In particular, DR2 always provides better solutions than two general purpose nonlinear optimization procedures that have been used frequently in dual response applications. This paper presents an ANSI FORTRAN implementation of DR2, partly motivated by Myers, Khuri, and Carter (1989, p. 150) who pointed out that there is a lack of software for industrial use in finding optimal conditions. Thus, the main focus of this article is on providing the RSM practitioners with a useful optimization tool in a portable code to deal with some day-to-day routine work and, of course, help attain better performance of the process under investigation. It is important to note that DR2 could also be an additional "add-on" to the methods and/or models proposed by several RSM researchers (Del Castillo and Montgomery (1993), Lin and Tu (1995), Copeland and Nelson (1996), Kim and Lin (1998), and Vining and Bohn (1998)).

In order to make our presentation clear, this article is organized as follows. In the next section, the rationale behind the algorithm is briefly discussed; subsequently, the computer program is tested and illustrated by means of several degenerate problems appearing in the literature. The comparison against the GINO (Lasdon and Waren (1990)) nonlinear solver is exhibited as well. In the final section, numerical evidence is presented to demonstrate DR2's effectiveness in comparison to a general purpose nonlinear programming solver, MINOS (Brooke, Kendrick, and Meeraus (1996)), in the cases of degenerate and generalized DR systems. DR2's solution times, based on several simulated DR systems, are displayed in the final section.

A Description of the Algorithm for DR Systems

The DR2 algorithm solves the constrained quadratic program of the form

$$\begin{aligned} \text{Min. } \widehat{Y}_p(\mathbf{x}) &= b_0 + \mathbf{b}'\mathbf{x} + \mathbf{x}'\mathbf{B}\mathbf{x} \\ \text{s. t. } \widehat{Y}_s(\mathbf{x}) &= c_0 + \mathbf{c}'\mathbf{x} + \mathbf{x}'\mathbf{C}\mathbf{x} = T \\ \mathbf{x}'\mathbf{x} &\le \rho^2, \end{aligned} \tag{1}$$

where $\mathbf{x}' = [x_1, x_2, \ldots, x_k]$ is a set of control factors which are known to significantly influence the process. Both $\widehat{Y}_p$ (the primary response) and $\widehat{Y}_s$ (the secondary response) are supposed to have adequate quadratic fit. There is no specialized structure such as convexity or concavity assumed on the two responses. Therefore Equation (1) presents a nonlinear (and typically non-convex) quadratic programming problem involving two quadratic constraints. We note that the program also works in cases where either one or both of the responses are fit using a linear model. The required adjustment is to square the corresponding linear response functions. Their regression coefficients are included in the matrices $\mathbf{B}$, $\mathbf{C}$; the vectors $\mathbf{b}$, $\mathbf{c}$; and the intercepts b_0, c_0. The positive value of ρ defines a radial bound that ensures the solution inside the assumed spherical region where the designed experiment was performed. Thus, for example, $\rho = \alpha = \sqrt[4]{F}$, where F is the number of factorial runs, is a logical selection for a rotatable central composite design (CCD); see, for example, Khuri and Cornell (1996). We demonstrate a case of this sort later (see Example 3). Another choice is to use $\rho = \alpha = \sqrt{k}$ recommended by Myers et al. (1992) where the CCD forms a perfect spherical region and has excellent variance properties when there are sufficient center replicates. The radial constraint, $\mathbf{x}'\mathbf{x} \le \rho^2$, can also be used even when the geometry of designs is cuboidal (e.g., as in a "face centered" CCD with a $\alpha = 1$ or 3^k design), provided that the solution found is not far outside the experimental region. Example 2 illustrates this situation.

Taguchi (1986) has advocated the necessity of considering both the mean and the variance of the quality characteristics simultaneously. However, robust parameter design has received considerable criticism from various statisticians (see Nair et al. (1992)). In particular, Taguchi's so-called signal-to-noise (SN) ratios have been shown to be inefficient under certain conditions (see, e.g., Box (1988)). Response surface alternatives for parameter design problems may provide a more rigorous statistical approach than the use of SN ratios. Vining and Myers (1990) applied the dual response approach to achieve some of the goals of Taguchi's philosophy without recourse to SN ratios (an example of this is given later). The mean and variance responses (modeled separately by second-order polynomials) are treated as primary and secondary responses in the three different cases considered by Taguchi:

Case 1 "Target is best," which means keeping the mean response $\widehat{Y}_\mu$ at a specified value, μ_0, while minimizing the variance response, $\widehat{Y}_\sigma$:

$$\begin{aligned} &\text{Min. } \widehat{Y}_\sigma \\ &\text{s. t. } \widehat{Y}_\mu = \mu_0 \,. \end{aligned}$$

Case 2 "The larger the better," which means making the mean response, $\widehat{Y}_\mu$, as large as possible, while controlling the variance response, $\widehat{Y}_\sigma$:

$$\begin{aligned} &\text{Max. } \widehat{Y}_\mu \\ &\text{s. t. } \widehat{Y}_\sigma = \sigma_0 \,. \end{aligned}$$

Case 3 "The smaller the better," which means making the mean response $\widehat{Y}_\mu$ as small as possible, while controlling the variance response $\widehat{Y}_\sigma$:

$$\begin{aligned} &\text{Min. } \widehat{Y}_\mu \\ &\text{s. t. } \widehat{Y}_\sigma = \sigma_0 \,. \end{aligned}$$

In each of the three cases, a spherical constraint may be added as in Equation (1). What follows will analyze the special solution structure of DR systems.

If a feasible point $\mathbf{x}^*$ in Equation (1) satisfies the first-order necessary conditions for local optimality which are

$$\begin{aligned} (\mathbf{B} - \mu\mathbf{C} + \theta\mathbf{I})\,\mathbf{x} &= \frac{1}{2}(\mu\mathbf{c} - \mathbf{b}) \qquad (2) \\ \text{and } \ (\mathbf{x}'\mathbf{x} - \rho^2) &= 0 \quad \text{for } \theta \ge 0, \end{aligned}$$

where μ and θ are the Lagrange multipliers associated with $\widehat{Y}_p$ and $\widehat{Y}_s$, respectively, and $\mathbf{x}^*$ also satisfies the following second-order necessary condition

$$\Gamma = \{(\mu, \theta) : (\mathbf{B} - \mu\mathbf{C} + \theta\mathbf{I}) \text{ is positive definite}\}\,, \qquad (3)$$

then it can be shown that $\mathbf{x}^*$ is a unique global optimal solution to Equation (1) (Semple (1997)). The type of DR problems whose global optima reside in Γ are classified as nondegenerate and can be readily solved by DRSALG. However, DRSALG will fail and stall at a "gateway" point on the boundary of Γ if the problem is degenerate. Other than the degenerate local minimum described by Fletcher (1971), which can be approximately solved by adding an arbitrarily small perturbation, degeneracy makes the problem difficult to solve. In order to define degeneracy, suppose the value of μ is fixed. Then, the problem in Equation (1) is related to the so-called *parametric trust region* problem (see, e.g., Sorensen (1982)):

$$\begin{aligned} &\text{Min. } \widehat{Y}_p(\mathbf{x}) - \mu(\widehat{Y}_s(\mathbf{x}) - T) \\ &\text{s. t. } \mathbf{x}'\mathbf{x} \le \rho^2, \end{aligned} \qquad (4)$$

which has a stationary equation identical to Equation (2). If $(\mathbf{B} - \mu\mathbf{C} + \theta\mathbf{I})$ is positive definite, then the solution $\mathbf{x}^*(\mu)$ of the problem in Equation (4) satisfying the first-order necessary conditions is the unique global optimum. However, $\mathbf{x}^*(\mu)$ will not always be feasible because $\widehat{Y}_s(\mathbf{x}^*(\mu)) \ne T$. If μ is determined such that $\widehat{Y}_s(\mathbf{x}^*(\mu)) = T$, then $\mathbf{x}^*(\mu)$ also solves the problem in Equation (1).

Calculating μ to meet the secondary-response constraint (i.e., $\widehat{Y}_s(\mathbf{x}^*(\mu)) - T = 0$) can be achieved whenever the function is continuous on some local interval $[a, b]$ where the optimal value of μ is enclosed, implying $\widehat{Y}_s(\mathbf{x}^*(a)) < T < \widehat{Y}_s(\mathbf{x}^*(b))$. Degeneracy is related to the continuity of the $\widehat{Y}_s(\mathbf{x}^*(\mu))$ function. The local nondegenerate definition that follows will help explain why continuity on $\widehat{Y}_s(\mathbf{x}^*(\mu))$ depends on the eigenstructure of the matrix $(\mathbf{B} - \mu\mathbf{C})$. If the eigenvalues of this matrix are ranked $\lambda_1 \le \lambda_2 \le$

$\ldots \leq \lambda_k$ (when the value of μ has been fixed), then it can be shown that $\widehat{Y}_s(\mathbf{x}^*(\mu))$ is continuous on $[a,b]$ provided that $(\mu\mathbf{c}-\mathbf{b})$ is not perpendicular to the first eigenspace

$$\mathbf{E}_1^{\mu} = \{\mathbf{q} : (\mathbf{B}-\mu\mathbf{C})\mathbf{q} = \lambda_1\mathbf{q}\} \tag{5}$$

on this interval (see Semple (1997, Lemma 2.1 and Theorem 2.2)). This leads to the following nondegeneracy definition from Semple (1997).

Definition 1. The problem in Equation (1) is said to be *nondegenerate* on $\mu \in [a,b]$ provided that for each $\mu \in [a,b]$ the vector $(\mu\mathbf{c}-\mathbf{b})$ is not orthogonal to $\mathbf{E}_1^{\mu}$. The problem in Equation (1) is said to be degenerate on $[a,b]$ otherwise.

The degenerate situation is illustrated in Figure 1. From Figure 1, it is clear that degeneracy is related to the continuity of the $\widehat{Y}_s(\mathbf{x}^*(\mu))$ function. At the gateway point μ_d the vector $(\mu\mathbf{c}-\mathbf{b})$ is orthogonal to $\mathbf{E}_1^{\mu_d}$ when degeneracy occurs. There is generally a discontinuous gap on $\widehat{Y}_s(\mathbf{x}^*(\mu))$, and thus some target value (e.g., T_0 in Figure 1) cannot be attained by searching the global optimal solution only throughout the two-parameter space Γ. Computational difficulties due to discontinuity arise as a result of degeneracy, referred to as the "hard case" in Moré and Sorensen (1983), when $(\mu\mathbf{c}-\mathbf{b}) \perp \mathbf{E}_1^{\mu}$ and $\widehat{Y}_s(\mathbf{x}^*(\mu)) \neq T$ on Γ. Therefore, the continuity of the function $\widehat{Y}_s(\mathbf{x}^*(\mu))$ depends on the eigenstructure of the matrix $(\mathbf{B}-\mu\mathbf{C})$, of which the eigenvector associated with the smallest eigenvalue spans the first eigenspace $\mathbf{E}_1^{\mu}$.

DRSALG has been augmented with a check for the discontinuity of $\widehat{Y}_s(\mathbf{x}^*(\mu))$ using the *modified regula falsi* method (see, e.g., Conte and de Boor (1980), pp. 77–78). Let's consider Figure 1 as an example. Suppose that T_0 is desired for the equality constraint and the initial working interval $[a,b]$ is constructed (for details, see Semple (1997)). For the end points in the initial working interval, first it needs to solve two ordinary trust region (TR) problems, compute the values, $\widehat{Y}_s(\mathbf{x}^*(\mu_a))$ and $\widehat{Y}_s(\mathbf{x}^*(\mu_b))$, and find an initial estimate μ_1 based on these two function values compared to T_0. Subsequently, every step of modified regula falsi will produce an improved estimate for μ; by solving Equation (4) using the TR method, it will evaluate the value of the secondary response on the incumbent optimum $\mathbf{x}_k^*$, will reduce the working interval by updating the upper or lower bound, and then will repeat the bracketing process iteratively. After a finite number of modified regula falsi steps, the working interval becomes too narrow without

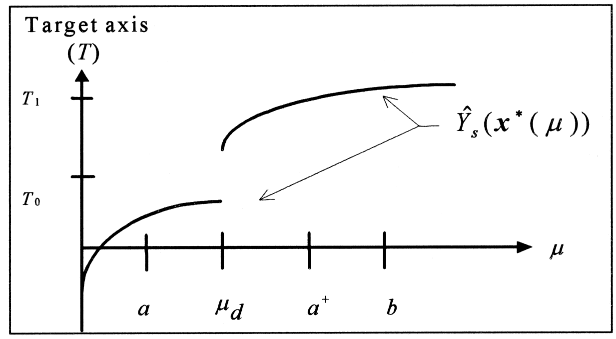

FIGURE 1. Local Degeneracy in $[a,b]$.

$\widehat{Y}_s(\mathbf{x}^*(\mu_k)) \rightarrow T$, and the problem is then considered numerically degenerate (see Figure 1). When a problem is degenerate, then, in general, discontinuity is detected in less than 30 modified regula falsi iterations. Once degeneracy is detected, a procedure described in Del Castillo, Fan, and Semple (1999) is performed by DR2 to find the approximate global optima. This procedure that follows consists of a rotation of the problem in the direction where degeneracy occurs, followed by a 2-step axis search procedure.

Since degeneracy indicates $(\mu\mathbf{c}-\mathbf{b}) \perp \mathbf{E}_1^{\mu_d}$, the original axes, say, $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$, are rotated so that the eigenvector $\mathbf{q}_1$ associated with the smallest eigenvalue λ_1 of $(\mathbf{B}-\mu_d\mathbf{C})$ becomes the first axis $\mathbf{z}_1$ in the new coordinate system based on the orthonormal basis $\mathbf{Q} = [\mathbf{q}_1 \mid \mathbf{q}_2 \mid \cdots \mid \mathbf{q}_k]$. Herein, $\mathbf{q}_1$ can be quickly computed via a few steps of inverse iteration (see, e.g., Golub and van Loan (1984)). Then $\mathbf{Q}$ can be formed by utilizing the Gram-Schmidt orthogonalization procedure (see, e.g., Golub and van Loan (1984)). By the rotational transformation via $\mathbf{x} = \mathbf{Q}\mathbf{z}$ illustrated in Figure 2, Equation (1) becomes

$$\begin{aligned} \text{Min. } & \widehat{Y}_p(\mathbf{z}) = b_0 + \widetilde{\mathbf{b}}'\mathbf{z} + \mathbf{z}'\widetilde{\mathbf{B}}\mathbf{z} \\ \text{s. t. } & \widehat{Y}_s(\mathbf{z}) = c_0 + \widetilde{\mathbf{c}}'\mathbf{z} + \mathbf{z}'\widetilde{\mathbf{C}}\mathbf{z} \\ & \mathbf{z}'\mathbf{z} \leq \rho^2, \end{aligned} \tag{6}$$

where $\widetilde{\mathbf{b}}' = \mathbf{b}'\mathbf{Q}$, $\widetilde{\mathbf{B}} = \mathbf{Q}'\mathbf{B}\mathbf{Q}$, and so on. The radial constraint does not change in the new $\mathbf{z}$-coordinates because $\mathbf{Q}$ is orthonormal ($\mathbf{Q}'\mathbf{Q} = \mathbf{I}$).

Degeneracy results from orthogonality on the direction of $\mathbf{q}_1$, so removing z_1's effect from Equation (6) can effectively rectify this computational difficulty around μ_d. Consequently, z_1 is selected as the grid variable; namely, z_1 satisfies $-\rho \leq z_1 \leq \rho$ and

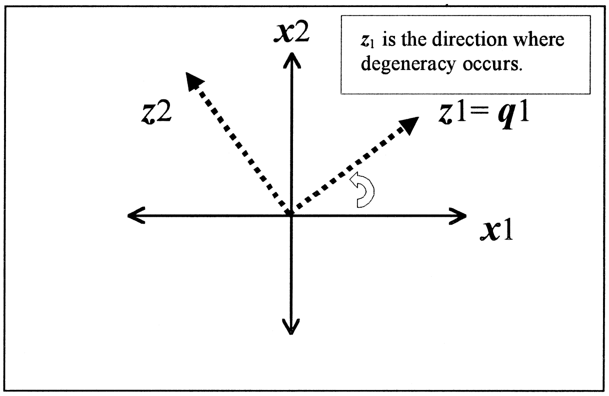

FIGURE 2. The Rotation Procedure.

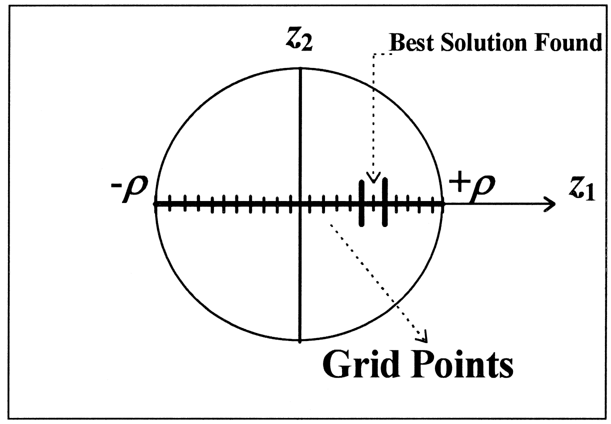

FIGURE 3. Grid Point Search in the Direction z_1.

this interval can be equally divided into many subintervals by many grid points (illustrated in Figure 3). If z_1 is, in turn, fixed at each grid point, then Equation (6) is decomposed into a series of DR subproblems having $(k-1)$ control factors. New matrices, vectors, intercepts, and radii need adjustments to account for the fixed grid variable. Each subproblem with lower dimensions is created and swiftly solved by DRSALG, and the best solution found among the subproblems is earmarked. In order to increase accuracy, a new working interval for z_1 is constructed by two grid points adjacent to the best solution obtained in the first pass of grid search. Then the best solution found in the second pass (local refinement) can be transformed back to the original variables through $\mathbf{x} = \mathbf{Qz}$.

DR2 will find global optimal solutions of the nondegenerate DR problems by calling DRSALG as a subroutine and will use the procedures aforementioned to return an approximate global optimal solution (due to the computational accuracy dictated by the mesh used in the grid search) in degenerate cases.

Program Operation

The computer program simply prompts the user to enter the names of an input file, an output file, and a file for diagnostic information. The input file should be an ASCII (text) file that contains the values of k, ρ, the coefficients of the fitted quadratic responses and T. The output file generated by DR2 contains the optimal operating condition and the optimal value of $\widehat{Y}_p$. The diagnostic file generated by DR2 contains qualitative and quantitative information about how the problem was solved. DR2 will ask the user to input the numbers of subintervals required in the axis search procedure if the problem is found to be degenerate and if its size (k) is greater than two. The default values for the axis search are $40\sqrt{k}$ for the first pass and 20 for the second pass. These default settings are recommended from practical experience although the user can freely enter other values if desired.

The input file must conform to the following format (all entries on the same row must be separated by spaces):

Row 1: Number of controllable factors (k) ρ

Row 2 to $k+1$: $\mathbf{B}$ matrix coefficients (row by row)

Row $k+2$: $\mathbf{b}'$ vector coefficients

Row $k+3$: b_0 constant

Row $k+4$ to $2k+3$: $\mathbf{C}$ matrix coefficients (row by row)

Row $2k+4$: $\mathbf{c}'$ vector coefficients

Row $2k+5$: c_0 constant

Row $2k+6$: T (target value)

We note this is the same input file format required by the DRSALG program (Del Castillo, Fan, and Semple (1997)).

Examples

Example 1

Consider a two-dimensional problem discussed in Myers and Carter's (1973). The fitted primary and secondary response functions are

$$\widehat{Y}_p = 53.69 + 7.26x_1 - 10.33x_2$$

$$+ 7.22x_1^2 + 6.43x_2^2 + 11.36x_1x_2$$

and

$$\widehat{Y}_s = 82.17 - 1.01x_1 - 8.61x_2 + 1.40x_1^2 - 8.76x_2^2 - 7.20x_1x_2.$$

It is of interest to find optimal operating conditions which maximize $\widehat{Y}_p$ subject to $\mathbf{x}'\mathbf{x} \leq 1.0$ and $84 < \widehat{Y}_s < 88$. Because this response is maximized, we minimize $-\widehat{Y}_p$. The matrix $\mathbf{B}$, vector $\mathbf{b}$ and intercept b_0 have all been multiplied by -1. Here, the matrices, vectors and intercepts in Equation (1) are

$$\mathbf{B} = \begin{pmatrix} -7.22 & -5.68 \\ -5.68 & -6.43 \end{pmatrix} \quad \mathbf{C} = \begin{pmatrix} 1.40 & -3.6 \\ -3.6 & -8.76 \end{pmatrix}$$

$$\mathbf{b} = \begin{pmatrix} -7.26 \\ 10.33 \end{pmatrix} \qquad \mathbf{c} = \begin{pmatrix} -1.01 \\ -8.61 \end{pmatrix}$$

$$b_0 = -53.69 \qquad c_0 = 82.17\,.$$

The value $\rho = 1.0$ in the radial constraint is specified along with three different target values: $T = 85$, 86, and 87. The input for the case of $T = 85$ is shown in Input Listing 1. The output and diagnostic files for this case are shown in Output Listing 1. Degeneracy was detected after 26 steps of the modified regula falsi method (as shown in the diagnostic file). The global optimal solution cannot be found on Γ because the target value (85) falls in the discontinuity gap at $\mu_d = 0.579986$. DR2 also returned a value $\theta = 9.5965 \cong -\lambda_1$, which makes $(\mathbf{B} - \mu_d\mathbf{C} + \theta\mathbf{I})$ positive semi-definite.

INPUT LISTING 1. Input File for Example 1

```
2  1
-7.22 -5.68
-5.68 -6.43
-7.26 10.33
-53.69
1.40 -3.6
-3.6 -8.76
-1.01 -8.61
82.17
85
```

OUTPUT LISTING 1. Output and Diagnostic Files for Example 1

```
(output file)

*******************************
 * DR2 RETURNS AN APPROXIMATE  *
 *      GLOBAL OPTIMUM         *
 *******************************
 *    RESULTS SEQUENTIALLY     *
 *    OBTAINED FROM:           *
 *******************************
 * 1.DRSALG                    *
 * 2.AXIS-SEARCH PROCEDURE     *
 * 3.SPECIALIZED 1-DIMENSIONAL *
 *   PROBLEM SOLVER            *
 *******************************
 PROBLEM SIZE:   2
 TARGET VALUE ON THE SECONDARY
 RESPONSE:    85.000000
 OPTIMAL VALUE ON THE PRIMARY
 RESPONSE:   -68.511370


 *******************************
 *  OPTIMUM SOLUTION IN THE    *
 *  ORIGINAL COORDINATES       *
 *******************************
 X 1 =      .380000
 X 2 =     -.922548

(diagnostic file)

 **************************
 * DIAGNOSTICS FOR        *
 * DETECTION OF DEGENERACY*
 * IN THE MODIFIED DRSALG *
 * ALGORITHM              *
 **************************
 * CAN NOT CONVERGE IN
 * 26  STEPS OF MRF
 *------------------------
 * DISCONTINUITY OCCURS AT:
 * (i.e.,THE GATEWAY POINT)
 * MU(d)=       .579986
 * THETA(d)=     9.596500
```

For the three target values, DR2 detected degeneracy and quickly computed their answers. The results are given in Table 1. The GRG2 results are those found by using GINO (Lasdon and Waren (1990)). We also employed the dual quasi-Newton (QN) optimization algorithm embedded in SAS/IML (SAS

TABLE 1. Optimal Solutions Returned by DR2 and GRG2 for Example 1

T	$\mathbf{x}^*$ (DR2)	$-\widehat{Y}_p(\mathbf{x}^*)$ (DR2)	$\mathbf{x}^*$ (GRG2)	$-\widehat{Y}_p(\mathbf{x}^*)$ (GRG2)
85	(0.38,−0.922548)	−68.51137	(0.984739,−0.17403)	−67.886173
86	(0.964,−0.26471)	−67.68432	(0.964356,−0.264592)	−67.690455
87	(0.92,−0.385896)	−67.390967	(0.923231,−0.384245)	−67.435342

TABLE 2. Optimal Solutions Returned by QN in SAS/IML for Example 1

T	$\mathbf{x}^*$ (QN in IML)	$-\widehat{Y}_p(\mathbf{x}^*)$ (QN in IML)
85	(0.98474, −0.17403)	−67.886205
86	(0.964361, −0.264591)	−67.690546
87	(0.923231, −0.384245)	−67.435344

Institute (1998)) to the problem (see Table 2). The default settings in the grid search procedure were employed whenever degeneracy was detected.

For this problem, the DR2 results are at least as good as those obtained by GINO and QN. The solution found by DR2 is $\mathbf{x}' = (0.38, -0.9225)$ with $\widehat{Y}_p = 68.5113$ when the target value is 85. (Recall that we are maximizing $\widehat{Y}_p$ so this solution is slightly better than the ones reported by GINO and QN). These optimal operating conditions are quite different from $\mathbf{x}' = (0.9847, -0.174)$, which was obtained by the other two algorithms, and from $\mathbf{x}' = (0.85, -0.6)$, which was recommended by Myers and Carter (1973), even though the $\widehat{Y}_p$ values of these solutions are only slightly worse.

Example 2

In order to illustrate how effectively DR2 repairs degeneracy, consider the printing machine problem analyzed in Vining and Myers (1990) where the response surfaces were fit using data from a replicated 3^3 full factorial experiment. The three variables are coded between −1 and 1. The purpose is to minimize the standard-deviation response while keeping the mean response at $T = 26$, 30, 34, and $\mathbf{x}'\mathbf{x} \leq 3$. The resulting quadratic programming problem utilizes

$$\mathbf{B} = \begin{pmatrix} 4.2 & 3.85 & 2.55 \\ 3.85 & -1.3 & 7.05 \\ 2.55 & 7.05 & 16.8 \end{pmatrix}$$

$$\mathbf{C} = \begin{pmatrix} 32 & 33 & 37.75 \\ 33 & -22.4 & 21.8 \\ 37.75 & 21.8 & -29.1 \end{pmatrix}$$

$$\mathbf{b} = \begin{pmatrix} 11.5 \\ 15.3 \\ 29.2 \end{pmatrix} \qquad \mathbf{c} = \begin{pmatrix} 177 \\ 109.4 \\ 131.5 \end{pmatrix}$$

$$b_0 = 34.9 \qquad c_0 = 327.6\,.$$

The global optima for these three target values fell outside Γ since DR2 detects degeneracy after 21 iterations of the modified regula falsi method (see the diagnostic file). The corresponding eigenvector $\mathbf{q}_1$, $\mathbf{Q}$ basis and some computational results from the rotation and axis search procedures are listed in the diagnostic file. The solutions computed via DR2 and GRG2 are shown in Table 3 below. Listing 2 displays the input, output and diagnostic files for $T = 34$.

INPUT LISTING 2. Input File for Example 2

```
3   1.73205
4.2   3.85   2.55
3.85  -1.3   7.05
2.55  7.05   16.8
11.5  15.3   29.2
34.9
32.0  33.0   37.75
33.0  -22.4  21.8
37.75  21.8  -29.1
177.0  109.4  131.5
327.6
34
```

OUTPUT LISTING 2. Output and Diagnostic Files for Example 2

(output file)

```
*******************************
 * DR2 RETURNS AN APPROXIMATE  *
 *      GLOBAL OPTIMUM         *
 *******************************
 *    RESULTS SEQUENTIALLY     *
 *    OBTAINED FROM:           *
 *******************************
 * 1.DRSALG                    *
 * 2.AXIS-SEARCH PROCEDURE     *
 *******************************
 PROBLEM SIZE:   3
 TARGET VALUE ON THE SECONDARY
 RESPONSE:    34.000000
 OPTIMAL VALUE ON THE PRIMARY
 RESPONSE:    14.645083

 *******************************
 *  OPTIMUM SOLUTION IN THE    *
 *  ORIGINAL COORDINATES       *
 *******************************
 X 1 =     -.007597
 X 2 =    -1.500964
 X 3 =     -.864322
```

(diagnostic file)

```
 *************************
 * DIAGNOSTICS FOR        *
 * DETECTION OF DEGENERACY*
 * IN THE MODIFIED DRSALG *
 * ALGORITHM              *
 *************************
 * CAN NOT CONVERGE IN
 * 21  STEPS OF MRF
 *------------------------
 * DISCONTINUITY OCCURS AT:
```

```
* (i.e.,THE GATEWAY POINT)
* MU(d)=      -.701155
* THETA(d)=    34.290370
********************************
* DIAGNOSTICS IN THE ROTATION  *
*        PROCEDURE             *
********************************
*TOTAL INVERSE ITERATION STEPS: 3
*-------------------------------
* THE EIGENVECTOR X1 =      .150980
* THE EIGENVECTOR X2 =     -.861710
* THE EIGENVECTOR X3 =      .484418
*-------------------------------
*GRAM-SCHMIDT ORTHOGONALIZATION
*----------- QBASIS ------------
QBASIS X   1   1 =      .150980
QBASIS X   2   1 =     -.861710
QBASIS X   3   1 =      .484418
-----------------------------
QBASIS X   1   2 =      .510179
QBASIS X   2   2 =      .487654
QBASIS X   3   2 =      .708457
-----------------------------
QBASIS X   1   3 =      .846713
QBASIS X   2   3 =     -.140177
QBASIS X   3   3 =     -.513252
-----------------------------


**********************************
* DIAGNOSTICS IN DRSALG & AXIS   *
* SEARCH PROCEDURE               *
**********************************
* 1ST PASS OF AXIS-SEARCH:
* TOTAL SUBPROBLEMS:          68
* TOTAL INFEASIBLE SUBPROBLEMS:          23
* INFEASIBLE PCT:      33.823530%
* PSEUDO-FEASIBLE SUBPROBLEMS:          0
* TOTAL DEGENERATE SUBPROBLEMS:          0
* DEGENERACY PCT:   0.000000E+00%
*--------------------------------
* 2ND PASS OF AXIS-SEARCH:
* TOTAL SUBPROBLEMS:          21
* TOTAL INFEASIBLE SUBPROBLEMS:          1
* INFEASIBLE PCT:       4.761905%
* PSEUDO-FEASIBLE SUBPROBLEMS:          0
* TOTAL DEGENERATE SUBPROBLEMS:          0
* DEGENERACY PCT:   0.000000E+00%
*--------------------------------
* MESH IN THE 1ST PASS:          40
* MESH IN THE 2ND PASS:          20


**********************************
*  OPTIMUM OPERATING CONDITIONS  *
*             IN QBASIS          *
**********************************
Z  1 =      .873556
Z  2 =    -1.348161
Z  3 =      .647584
RHO (EXCLUSIVE OF Z1):          1.495626
FINAL VALUE OF MU:    -.103157
FINAL RADIAL LAGRANGE
MULTIPLIER:      .831623
ERROR IN YHAT (TARGET):     .000707
```

In comparison with GRG2, the DR2 results for this problem present a substantial reduction in the standard-deviation response as well as dramatically different operating conditions. This might provide better knowledge to tell a process engineer where to run the process for quality improvement. The QN algorithm—an implementation of sequential quadratic programming (SQP)—obtained equally good answers (see Table 4). Furthermore, it is worth noting that the solution to every subproblem created in the axis search procedure satisfies the sufficient conditions for global optimality in the reduced subspace (as shown in the diagnostic file). The optimal solutions found by DR2 for this example are expected to be close to global optima within the numerical tolerances specified by the mesh since the subproblems were all nondegenerate.

Example 3

Lin and Tu (1995) and Copeland and Nelson (1996) argued that relaxing the equality constraint on the secondary response and then using an inequality instead is more appropriate for dual response analysis. A similar approach can be achieved with DR2 by trying different target values. For illustration, consider the following example taken from Derringer and Suich (1980). Suppose the PICO Abrasion Index (Y_1) is considered as the primary response $\widehat{Y}_p$ and the Elongation at Break (Y_3) is taken as the secondary response $\widehat{Y}_s$. Here, a 3-factor CCD with 6 center replicates was run to fit both responses. Initially, let us assume an experimenter tries to seek the (x_1, x_2, x_3) that would maximize $\widehat{Y}_p$ subject to $\widehat{Y}_s = 500$ and $\mathbf{x}'\mathbf{x} \leq 3$. This radius, ($\sqrt{3}$), is a reasonable choice since the axial points are at a distance of 1.633 from the design center. By multiplying $\widehat{Y}_p$ by -1, the problem described above becomes one of

TABLE 3. Optimal Solutions Generated via DR2 and GRG2 for Example 2

T	$\mathbf{x}^*$ (DR2)	$\widehat{Y}_p(\mathbf{x}^*)$ (DR2)	$\mathbf{x}^*$ (GRG2)	$\widehat{Y}_p(\mathbf{x}^*)$ (GRG2)
26	(0.0026,−1.3496,−1.0855)	20.627023	(−0.6087,0.5021,−1.5418)	23.242914
30	(0.0107,−1.4284,−0.9794)	17.58829	(−0.6557,0.5642,−1.5005)	21.62719
34	(−0.0075,−1.5009,−0.8643)	14.645083	(−0.6998,0.6196,−1.4581)	20.157075

TABLE 4. Optimal Solutions Generated via QN in SAS/IML for Example 2

T	$\mathbf{x}^*$ (QN in IML)	$\widehat{Y}_p(\mathbf{x}^*)$ (QN in IML)
26	$(-0.0018,-1.3502,-1.0847)$	20.62498
30	$(-0.0178,-1.4328,-0.9729)$	17.5404
34	$(-0.0391,-1.5051,-0.8561)$	14.5913

minimization with

$$\mathbf{B} = \begin{pmatrix} 4.01 & -2.565 & -3.565 \\ -2.565 & 3.45 & -3.94 \\ -3.565 & -3.94 & 1.57 \end{pmatrix}$$

$$\mathbf{C} = \begin{pmatrix} 7.93 & 4.375 & 3.125 \\ 4.375 & 17.31 & 0.625 \\ 3.125 & 0.625 & 0.43 \end{pmatrix}$$

$$\mathbf{b} = \begin{pmatrix} -16.49 \\ -17.88 \\ -10.91 \end{pmatrix} \qquad \mathbf{c} = \begin{pmatrix} -99.67 \\ -31.40 \\ -73.92 \end{pmatrix}$$

$$b_0 = -139.12 \qquad c_0 = 400.38\,.$$

We can try various target values such as $T = 495$, 500, and 505. The solutions generated via DR2 and GRG2 are exhibited in Table 5. Listing 3 includes the corresponding input, output, and diagnostic files for the case $T = 500$.

INPUT LISTING 3. Input File for Example 3

```
3  1.73205
4.01 -2.565 -3.565
-2.565 3.45 -3.94
-3.565 -3.94 1.57
-16.49 -17.88 -10.91
-139.12
7.93 4.375 3.125
4.375 17.31 0.625
3.125 0.625 0.43
-99.67 -31.40 -73.92
400.38
500
```

OUTPUT LISTING 3. Output and Diagnostic Files for Example 3

```
(output file)

******************************
 * DR2 RETURNS AN APPROXIMATE  *
 *     GLOBAL OPTIMUM          *
 ******************************
 *   RESULTS SEQUENTIALLY      *
 *   OBTAINED FROM:            *
 ******************************
 * 1.DRSALG                    *
 * 2.AXIS-SEARCH PROCEDURE     *
 ******************************
 PROBLEM SIZE:   3
 TARGET VALUE ON THE SECONDARY
 RESPONSE:   500.000000
 OPTIMAL VALUE ON THE PRIMARY
 RESPONSE:  -128.695926

 ******************************
 *  OPTIMUM SOLUTION IN THE    *
 *  ORIGINAL COORDINATES       *
 ******************************
 X 1 =     -.680006
 X 2 =     1.477715
 X 3 =     -.594935

(diagnostic file)

 *************************
 * DIAGNOSTICS FOR        *
 * DETECTION OF DEGENERACY*
 * IN THE MODIFIED DRSALG *
 * ALGORITHM              *
 *************************
 * CAN NOT CONVERGE IN
 * 21  STEPS OF MRF
 *------------------------
 * DISCONTINUITY OCCURS AT:
 * (i.e.,THE GATEWAY POINT)
 * MU(d)=       .230642
 * THETA(d)=     7.019864

 ********************************
 * DIAGNOSTICS IN THE ROTATION  *
 *       PROCEDURE              *
 ********************************
 *TOTAL INVERSE ITERATION STEPS:          3
 *-------------------------------
 * THE EIGENVECTOR X1 =      .514246
 * THE EIGENVECTOR X2 =      .642178
 * THE EIGENVECTOR X3 =      .568470
 *-------------------------------
 *GRAM-SCHMIDT ORTHOGONALIZATION
 *----------- QBASIS ------------
 QBASIS X   1   1 =      .514246
 QBASIS X   2   1 =      .642178
 QBASIS X   3   1 =      .568470
 -----------------------------
 QBASIS X   1   2 =      .816706
 QBASIS X   2   2 =     -.164339
 QBASIS X   3   2 =     -.553158
 -----------------------------
 QBASIS X   1   3 =      .261804
 QBASIS X   2   3 =     -.748732
 QBASIS X   3   3 =      .608981
 -----------------------------

 **********************************
 * DIAGNOSTICS IN DRSALG & AXIS   *
 * SEARCH PROCEDURE               *
 **********************************
 * 1ST PASS OF AXIS-SEARCH:
 * TOTAL SUBPROBLEMS:          68
 * TOTAL INFEASIBLE SUBPROBLEMS:         38
 * INFEASIBLE PCT:      55.882350%
 * PSEUDO-FEASIBLE SUBPROBLEMS:         0
 * TOTAL DEGENERATE SUBPROBLEMS:         0
 * DEGENERACY PCT:   0.000000E+00%
 *--------------------------------
 * 2ND PASS OF AXIS-SEARCH:
 * TOTAL SUBPROBLEMS:          21
 * TOTAL INFEASIBLE SUBPROBLEMS:          8
 * INFEASIBLE PCT:      38.095240%
 * PSEUDO-FEASIBLE SUBPROBLEMS:         0
 * TOTAL DEGENERATE SUBPROBLEMS:         0
 * DEGENERACY PCT:   0.000000E+00%
```

```
*---------------------------------
* MESH IN THE 1ST PASS:         40
* MESH IN THE 2ND PASS:         20

**********************************
*  OPTIMUM OPERATING CONDITIONS  *
*            IN QBASIS           *
**********************************
Z  1 =      .261063
Z  2 =     -.469118
Z  3 =    -1.646746
RHO (EXCLUSIVE OF Z1):          1.712263
FINAL VALUE OF MU:     .241921
FINAL RADIAL LAGRANGE
MULTIPLIER:     .361398
ERROR IN YHAT (TARGET):     .011426
```

In this example, the DR2 results are almost identical to those returned by GRG2 and QN (see also Table 6). However, although the solutions obtained from DR2 do not satisfy the sufficient conditions for global optimality, we are confident that they must be very close to global optima because the subproblems were all nondegenerate (see the associated diagnostic file).

From the computational results based on the three examples previously discussed, we have found that the QN algorithm seems to soundly compete with DR2 in locating better optimal operating conditions. Thus, several computational experiments of DR2 against another SQP implementation are conducted via simulations in the next section.

Computational Tests and Solution Times

In fact, it is impossible to claim that DR2 will produce a global optimal solution for degenerate DR problems. However, because the grid search procedure in DR2 explores nearly all of the feasible region on the rotated axis, it is reasonable to expect a very close approximation to the global optimum from an aspect of the objective function value.

To lend substance to this claim, we compared DR2 against MINOS (Brooke, Kendrick, and Meeraus (1996)), an implementation of sequential quadratic programming using the direction of negative curvature embedded in GAMS 2.50 (GAMS Development Corp. (1998)). MINOS employs a projected Lagrangian algorithm to solve general nonlinear programs by performing a gradient search on the objective function subject to satisfying iterative linearized versions of the nonlinear constraints (see Murtagh and Saunders (1982, 1983)). One thousand feasible DR problems were randomly generated for each of three sizes, n = 3, 4, and 5, where coefficients in both responses and the target value were from a $U[-10, 10]$ distribution and $\rho = \sqrt{n}$ was used. The degenerate cases were first screened out via modified regula falsi among these 1,000 problems. Each degenerate problem was solved using (i) DR2 and (ii) MINOS. We followed all the default settings recommended by GAMS/MINOS and used default settings in the grid search procedure (first mesh = $40\sqrt{n}$ and the second mesh = 20).

A procedure was declared to have found an improved solution whenever two conditions were satisfied: (i) the objective function value was smaller and (ii) the Euclidean distance between solutions was greater than 1. The results are summarized in Table 7 and suggest that DR2 is an attractive alternative to MINOS for degenerate problems. There was an instance of the size $n = 3$, where MINOS had problems maintaining feasibility during optimization. Moreover, in all 16 instances where MINOS determined a better solution, DR2 found the same solution when a finer mesh was used.

An analysis of DR2 on general (nondegenerate and degenerate) DR problems was conducted on a smaller set of problems so that our solutions were compared with those obtained using MINOS for the entire population. One hundred problems of sizes n = 3, 4, and 5 were generated from a $U[-10, 10]$ distribution using a different random seed. Both procedures were run under their default settings as before. The results are given in Table 8.

TABLE 5. Optimal Solutions Returned by DR2 and GRG2 for Example 3

T	$\mathbf{x}^*$ (DR2)	$-\widehat{Y}_p(\mathbf{x}^*)$ (DR2)	$\mathbf{x}^*$ (GRG2)	$-\widehat{Y}_p(\mathbf{x}^*)$ (GRG2)
495	(−0.6554,1.5031,−0.5575)	−130.04592	(−0.6734,1.5037,−0.534)	−130.05026
500	(−0.68,1.4777,−0.5949)	−128.69592	(−0.6993,1.4787,−0.5694)	−128.69984
505	(−0.7246,1.4521,−0.6051)	−127.38125	(−0.7242,1.4521,−0.6056)	−127.38047

TABLE 6. Optimal Solutions Returned by QN in SAS/IML for Example 3

T	$\mathbf{x}^*$ (QN in IML)	$-\widehat{Y}_p(\mathbf{x}^*)$ (QN in IML)
495	(−0.6734,1.5037,−0.5340)	−130.0502
500	(−0.6993,1.4787,−0.5694)	−128.6998
505	(−0.7242,1.4521,−0.6056)	−127.3804

In contrast to the percentages in Table 7, the percentages in Table 8 are more indicative of actual performance in the context of general DR problems that might occur in practice. Moreover, it seems that MINOS has trouble dealing with degenerate cases. For the record, there were 30 degenerate problems for $n = 3$, 23 for $n = 4$, and 21 for $n = 5$. MINOS did not return any better solution than DR2 for these 300 general DR problems. For the nondegenerate problems (70 for $n = 3$, 79 for $n = 4$, and 79 for $n = 5$), MINOS, designed to search local solutions, produced, at best, the same solution as DR2. These results do not diminish MINOS in any way; instead, they underscore the advantages of using more specialized algorithms to solve more specialized problems.

In order to gain a better understanding about how efficiently DR2 works, the solution times of DR2 under the default settings were recorded (see Table 9) based on larger simulations used in Table 7. All problems were run on the same Pentium II, 233 MHz personal computer. The excellent performance of DR2 can be attributed to its superior speed on nondegenerate problems. With regard to degenerate problems, the solution times of DR2 seem to increase as the problem size increases. Thus, MINOS may have a potential advantage on speed of solving large-size degenerate problems over DR2.

TABLE 7. Degeneracy: DR2 and MINOS (Brooke, Kendrick, and Meeraus (1996))

Improvement in objective value (Δf^*)	$k = 3$ (302 cases)		$k = 4$ (263 cases)		$k = 5$ (216 cases)	
	DR2	MINOS	DR2	MINOS	DR2	MINOS
$0 < \Delta f^* \leq 1$	13	3	15	1	18	0
	(4.3%)	(1%)	(5.7%)	(0.38%)	(8.3%)	(0%)
$1 < \Delta f^* \leq 5$	48	6	44	1	38	0
	(15.9%)	(2%)	(16.7%)	(0.38%)	(17.6%)	(0%)
$5 < \Delta f^* \leq 10$	26	3	21	1	27	0
	(8.6%)	(1%)	(8%)	(0.38%)	(12.5%)	(0%)
$10 < \Delta f^*$ 40	1	32	0	27	0	
	(13.2%)	(0.3%)	(12.2%)	(0%)	(12.5%)	(0%)
Totals	127	13	112	3	110	0
	(42.05%)	(4.3%)	(42.6%)	(1.14%)	(50.96%)	(0%)

TABLE 8. General Problems: DR2 and MINOS (Brooke, Kendrick, and Meeraus (1996))

Improvement in objective value (Δf^*)	$k = 3$ (100 cases)		$k = 4$ (100 cases)		$k = 5$ (100 cases)	
	DR2	MINOS	DR2	MINOS	DR2	MINOS
$0 < \Delta f^* \leq 1$	0	0	1	0	0	0
$1 < \Delta f^* \leq 5$	5	0	1	0	0	0
$5 < \Delta f^* \leq 10$	10	0	4	0	7	0
$10 < \Delta f^*$	11	0	16	0	10	0
Totals	26%	0%	22%	0%	20%	0%

TABLE 9. Solution Times of DR2 for 1,000 Simulations

Problem Size	Nondegenerate Problems (sec per problem)	Degenerate Problems (sec per problem)	1,000 Combined (sec per problem)
$k = 3$	0.0059 (302 cases)	0.4009 (698 cases)	0.1252
$k = 4$	0.0079 (263 cases)	0.8773 (737 cases)	0.2365
$k = 5$	0.0114 (216 cases)	1.5335 (784 cases)	0.3402

The results of the comparisons of DR2 to MINOS are probably self-evident. On average, for degenerate cases, DR2 attained better solutions about 44% of the time. MINOS attained better solutions only in about 2% of the cases. For all the cases where DR2 found inferior solutions, at least as good a solution was confirmed using a finer mesh. Hence, the foregoing computational tests provide some evidence to suggest that DR2's objective function solution to the degenerate DR system is near global. Note that, in order to maintain good speed, we do not recommend solving too many subproblems in DR2. A FORTRAN implementation of DR2 is available from the author upon request.

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Key Words: *Dual Responses, Optimization, Quality Control, Response Surface Methodology*.

FORTRAN Program Listing

Editor's Note: A copy of the FORTRAN program listing can be obtained electronically through StatLib. Sending the e-mail message SEND INDEX FOR JQT to statlib@lib.stat.cmu.edu will produce a listing of archived *JQT* algorithms and provide further information. Alternatively, the web site for the StatLib Index, http://www.stat.cmu.edu/, lists the available archive of *JQT* computer programs and also gives instructions on how to obtain the programs.