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SENSITIVITY ANALYSIS FOR PARAMETRIC NONLINEAR
PROGRAMMING USING PENALTY METHODS

by

Robert L. Armacost
Anthony V. Fiacco

Serial T-340
30 July 1976

The George Washington University
School of Engineering and Applied Science
Institute for Management Science and Engineering

(Program in Logistics)

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Recently, it has been shown that a class of penalty function algorithms can readily be adapted to generate sensitivity analysis information for a large class of parametric nonlinear programming problems. In particular, estimates of the partial derivatives (with respect to the problem parameters) of the components of a solution vector and the optimal value function have been successfully calculated for a number of nontrivial examples. The approach has been implemented using the well known Sequential Unconstrained Minimization Technique (SUMT) computer program. This paper, a continuation and amplification of a recent paper by Armacost, gives a detailed summary of the significant underlying theoretical results, reviews recent additions to the computer program that include Lagrange multiplier sensitivity calculations, and elaborates on the kind of information that can be generated by further analyzing and interpreting results obtained in applying the technique to a well known inventory model.

*U.S. Coast Guard Headquarters, Washington, D.C. 20590.

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1. Introduction

Initial numerical results resulting from the implementation of a penalty function technique for obtaining sensitivity information in parametric nonlinear programming were given by Armacost and Fiacco (1974). The work is based on the theory developed by Fiacco and McCormick (1968) and extended by Fiacco (1973). This paper reports on refinements and extensions of the computational procedures implemented by Armacost and Mylander (1973) and Armacost (1976), using the SUMT-Version 4 computer code with the logarithmic-quadratic loss penalty function to estimate the partial derivatives of the solution point and the objective function optimal value, the derivatives here being taken with respect to the specified problem parameters.

Fiacco (1973) developed the necessary general formulas for the partial derivatives of the "optimal value function," the components of a local solution point and its associated optimal Lagrange multipliers, for a large class of parametric nonlinear programming problems composed of twice differentiable functions. He also obtained approximation formulas

in terms of the well known logarithmic-quadratic penalty function. Recently, Armacost and Fiacco (1975) particularized and simplified these formulas for various problem structures and developed formulas for the first and second derivatives of the optimal value function of the given problem. Additionally, Armacost and Fiacco (1976) have applied the general theory to easily prove the well known result that, when the parameters are the right-hand side components of the constraints, the optimal Lagrange multipliers give the gradient of the optimal value function (with respect to the parameters). Further, it was shown that the first derivatives of the Lagrange multipliers give the components of the Hessian of the optimal value function, and explicit formulas were developed for the Hessian in terms of the problem functions.

In their first report on computational experience, Armacost and Fiacco (1974) concentrated primarily on presenting computational experience associated with the calculation of the first derivatives of a local solution point. The practical implementability of the approach was demonstrated.

In a subsequent paper, Armacost (1976) reported on additional computational experience, focusing on the calculation of the derivatives of the optimal value function and the Lagrange multipliers, also implementing a potentially valuable refinement that allows for computerized screening for "key" parameters. This paper may be regarded as a continuation and amplification of the Armacost paper.

For problems involving a large number of parameters, a very large number of partial derivatives may be calculated if one proceeds indiscriminately. This is not only time-consuming, but may also be quite burdensome to a user who must evaluate the overall significance of the results. One

measure of the latter is the effect of a perturbation on the solution value. It is quite possible and often observed in practice that the optimal objective function value is much more sensitive to a few of the many parameters present. With this in mind, the method developed by Armacost and Fiacco (1975) to estimate the first order sensitivity of the optimal value function was incorporated in the computer program to provide an option for preliminary screening of the parameters to eliminate further calculations involving perturbations of parameters having "little" effect on the optimal value function. (A user can easily introduce his own criteria of significance in this determination.) Using the formulas developed by Fiacco (1973), a second option is included which permits the calculation of the sensitivity estimates for the Lagrange multipliers. The computer code and options used to accomplish these and other calculations are discussed in Section 3.

In Section 4, a sensitivity analysis is conducted for a multi-item inventory model developed by Schrady and Choe (1971) for the U.S. Navy. The example analyzed is the same small one treated by Schrady and Choe, though readily extended to a large-scale model. The results illustrate the potential value of a detailed automated post-optimality sensitivity analysis in practical situations, and hopefully dramatize the numerous rich interpretations and insights that can be derived from this information, as well as indicating the caution that must be taken in making valid inferences.

The recently obtained basic theoretical results validating the computational algorithm are summarized rather completely in the next section so that the paper might be self contained.

2. Supporting Theory

The parametric mathematical programming problems considered here are of the form

$$\begin{aligned} & \text{minimize } f(x, \epsilon) \\ & x \in E^n \\ & \text{subject to } g_i(x, \epsilon) \geq 0, \quad i=1, \dots, m, \\ & h_j(x, \epsilon) = 0, \quad j=1, \dots, p, \end{aligned} \quad P(\epsilon)$$

where x is the usual vector of variables and ϵ is a k -component vector of numbers called "parameters." It is desired ultimately to develop a complete characterization of a solution $x(\epsilon)$ of Problem $P(\epsilon)$ as a function of ϵ . In our current work, we have concentrated on certain recently computationally tractable measures of change in a solution as ϵ is perturbed from a specified value. (Without loss of generality, we assume that the specified value is $\epsilon=0$.)

When certain assumptions are satisfied, Fiacco (1973) and Armacost and Fiacco (1975) have characterized the "first order sensitivity" of a "Kuhn-Tucker Triple" and the first and second order sensitivity of the optimal value function of Problem $P(\epsilon)$. (These quantities are defined as the theory is presented.) Additionally, they have developed formulas for efficiently estimating this sensitivity when the logarithmic-quadratic loss penalty function algorithm is used to solve Problem $P(\epsilon)$. The main theoretical results are summarized here.

The Lagrangian for Problem $P(\epsilon)$ is defined as

$$L(x, u, w, \epsilon) \equiv f(x, \epsilon) - \sum_{i=1}^m u_i g_i(x, \epsilon) + \sum_{j=1}^p w_j h_j(x, \epsilon),$$

where u_i , $i=1, \dots, m$ and w_j , $j=1, \dots, p$ are "Lagrange multipliers" associated with the inequality and equality constraints, respectively. Any vector $(\bar{x}, \bar{u}, \bar{w})$ satisfying the usual (first order) Kuhn-Tucker conditions (Fiacco and McCormick, 1968) of Problem $P(\bar{\epsilon})$ is called a Kuhn-Tucker triple.

The following four assumptions are sufficient to establish the results and are assumed to hold throughout the paper:

- A1 -- The functions defining Problem $P(\epsilon)$ are twice continuously differentiable in (x, ϵ) in a neighborhood of $(x^*, 0)$.
- A2 -- The second order sufficient conditions for a local minimum of Problem $P(0)$ hold at x^* with associated Lagrange multipliers u^* and w^* .
- A3 -- The gradients $\nabla_x g_i(x^*, 0)$ (i.e., $(\partial g_i(x^*, 0)/\partial x_1, \dots, \partial g_i(x^*, 0)/\partial x_n)^T$, the superscript T denoting transposition) for all i such that $g_i(x^*, 0) = 0$, and $\nabla_x h_j(x^*, 0)$, $j=1, \dots, p$ are linearly independent.
- A4 -- Strict complementary slackness holds at $(x^*, 0)$ (i.e., $u_i^* > 0$ for all i such that $g_i(x^*, 0) = 0$).

Theorem 1: (Local characterization of a Kuhn-Tucker triple (Fiacco, 1973) of Problem $P(\epsilon)$.) If assumptions A1, A2, A3 and A4 hold for Problem $P(\epsilon)$ at $(x^*, 0)$, then

- (a) x^* is a local isolated minimizing point of Problem $P(0)$ and the associated Lagrange multipliers u^* and w^* are unique;
- (b) for ϵ in a neighborhood of 0, there exists a unique, once continuously differentiable vector function $y(\epsilon) =$

$(x(\epsilon), u(\epsilon), w(\epsilon))^T$ satisfying the second order sufficient conditions for a local minimum of Problem $P(\epsilon)$ such that $y(0) = (x^*, u^*, w^*)^T = y^*$ and hence, $x(\epsilon)$ is a locally unique, local minimum of Problem $P(\epsilon)$ with associated unique Lagrange multipliers $u(\epsilon)$ and $w(\epsilon)$; and

- (c) for ϵ near 0, the set of binding inequalities is unchanged, strict complementary slackness holds for $u_i(\epsilon)$ for i such that $g_i(x(\epsilon), \epsilon) = 0$, and the binding constraint gradients are linearly independent at $x(\epsilon)$.

This result provides a characterization of a local solution of Problem $P(\epsilon)$ and its associated optimal Lagrange multipliers near $\epsilon=0$. It generalizes a theorem first presented by Fiacco and McCormick (1968, Theorem 6) and is closely related to a generalization of the same theorem provided independently by Robinson (1974). It shows that the Kuhn-Tucker triple $y(\epsilon)$ is unique and well behaved, under the given conditions. Since $y(\epsilon)$ is once differentiable, the partial derivatives of the components of $y(\epsilon)$ are well defined. This fact and Assumption A1 also mean that the functions defining Problem $P(\epsilon)$ are once continuously differentiable functions of ϵ along the "solution trajectory" $x(\epsilon)$ near $\epsilon=0$, and the Lagrangian is a once continuously differentiable function of ϵ along the "Kuhn-Tucker point trajectory."

We are thus motivated to determine a means to calculate the various partial derivatives, since this yields a first order estimate of the locally optimal Kuhn-Tucker triple and the problem functions near $\epsilon=0$.

Denote by $\nabla_{\epsilon} x(\epsilon) \equiv (\partial x_i(\epsilon) / \partial \epsilon_j)$, $i=1, \dots, n$, $j=1, \dots, k$, the $n \times k$ matrix of partial derivatives of $x(\epsilon)$ with respect to ϵ , and define $\nabla_{\epsilon} u(\epsilon)$ and $\nabla_{\epsilon} w(\epsilon)$ in a similar fashion. We then define

$\nabla_{\epsilon} y(\epsilon) \equiv (\nabla_{\epsilon}^T x(\epsilon), \nabla_{\epsilon}^T u(\epsilon), \nabla_{\epsilon}^T w(\epsilon))^T$, an $(n+m+p) \times k$ matrix.

When $y(\epsilon)$ is available, $\nabla_{\epsilon} y(\epsilon)$ can be calculated by noting that Conclusion (b) of the theorem implies the satisfaction of the Kuhn-Tucker conditions for $P(\epsilon)$ at $y(\epsilon)$ near $\epsilon=0$, i.e.,

$$\begin{aligned} \nabla_x L[x(\epsilon), u(\epsilon), w(\epsilon), \epsilon] &= 0, \\ u_i(\epsilon) g_i[x(\epsilon), \epsilon] &= 0, \quad i=1, \dots, m, \\ h_j[x(\epsilon), \epsilon] &= 0, \quad j=1, \dots, p. \end{aligned} \quad (1)$$

Since the Jacobian $M(\epsilon)$ of this system with respect to (x, u, w) (i.e., the matrix obtained by differentiating the left side of (1) with respect to the components of (x, u, w)) is nonsingular under the given assumptions, the total derivative of the system with respect to ϵ is well defined and must equal zero. This yields

$$M(\epsilon) \nabla_{\epsilon} y(\epsilon) = N(\epsilon),$$

where $N(\epsilon)$ is the negative of the Jacobian of the Kuhn-Tucker system with respect to ϵ , and hence

$$\nabla_{\epsilon} y(\epsilon) = M(\epsilon)^{-1} N(\epsilon).$$

The class of algorithms based on twice continuously differentiable penalty functions can be used without additional assumptions and without requiring $y(\epsilon)$ to provide an estimate of $\nabla_{\epsilon} y(\epsilon)$. Furthermore, most of the information required to make the estimate is already available in the typical implementations of these algorithms. Here, we use the logarithmic-quadratic penalty function for Problem $P(\epsilon)$ (Fiacco and McCormick, 1968) defined as

$$W(x, \epsilon, r) \equiv f(x, \epsilon) - r \sum_{i=1}^m \ln g_i(x, \epsilon) + (1/2r) \sum_{j=1}^p h_j^2(x, \epsilon) . \quad (2)$$

Under the given assumptions, the following facts are known for Problem P(0) from penalty function theory (Fiacco and McCormick, 1968, Theorems 10 and 17):

- (1) For $r > 0$ and small, there exists a unique once continuously differentiable vector function $x(0, r)$ such that $x(0, r)$ is a locally unique minimizing point of $W(x, 0, r)$ in $R^{\#}(0) \equiv \{x: g_i(x, 0) > 0, i=1, \dots, m, \text{ and } h_j(x, 0) = 0, j=1, \dots, p\}$ and such that $x(0, r) \rightarrow x(0, 0) = x^*$;
- (2) $\lim_{r \rightarrow 0} r \sum_{i=1}^m \ln g_i[x(0, r)] = 0$;
- (3) $\lim_{r \rightarrow 0} (1/2r) \sum_{j=1}^p h_j^2[x(0, r), 0] = 0$; and
- (4) $\lim_{r \rightarrow 0} W[x(0, r), 0, r] = f(x^*, 0)$.

The following theorem extends these results for Problem P(ϵ), where ϵ is allowed to vary in a neighborhood of 0, and provides a basis for approximating the sensitivity information associated with Problem P(ϵ). The notation $\nabla_x^2 W$ denotes the matrix of second partial derivatives of W with respect to x .

Theorem 2: (Relationship of solutions of Problem P(ϵ) and minima of $W(x, \epsilon, r)$, (Fiacco 1973).) If Assumptions A1 - A4 hold, then in a neighborhood about $(\epsilon, r) = (0, 0)$ there exists a unique once continuously differentiable vector function $y(\epsilon, r) = [x(\epsilon, r), u(\epsilon, r), w(\epsilon, r)]^T$ satisfying

$$\begin{aligned}\nabla_x L(x, u, w, \epsilon) &= 0, \\ u_i g_i(x, \epsilon) &= r, \quad i=1, \dots, m, \\ h_j(x, \epsilon) &= w_j r, \quad j=1, \dots, p,\end{aligned}$$

with $y(0,0) = (x^*, u^*, w^*)$ and such that, for any (ϵ, r) near $(0,0)$ and $r > 0$, $x(\epsilon, r)$ is a locally unique unconstrained local minimizing point of $W(x, \epsilon, r)$, $g_i[x(\epsilon, r), \epsilon] > 0$, $i=1, \dots, m$, and $\nabla_x^2 W[x(\epsilon, r), \epsilon, r]$ is positive definite.

Corollary 2.1: (Convergence of estimates using $W(x, \epsilon, r)$, (Fiacco, 1973).) If Assumptions A1, A2, A3 and A4 hold for Problem $P(\epsilon)$, then for any ϵ near 0,

- (a) $\lim_{r \rightarrow 0^+} y(\epsilon, r) = y(\epsilon, 0) = y(\epsilon)$, the Kuhn-Tucker triple characterized in Theorem 1; and
- (b) $\lim_{r \rightarrow 0^+} \nabla_\epsilon y(\epsilon, r) = \nabla_\epsilon y(\epsilon, 0) = \nabla_\epsilon y(\epsilon)$.

This result motivates use of $\nabla_\epsilon y(\epsilon, r)$ to estimate $\nabla_\epsilon y(\epsilon)$, when ϵ is near 0 and r is near 0, once $y(\epsilon, r)$ is available. Theorem 2 provides the basis for an efficient calculation of $\nabla_\epsilon y(\epsilon, r)$. Since, at a local solution point $x(\epsilon, r)$ of $W(x, \epsilon, r)$, it follows that

$$\nabla_x W[x(\epsilon, r), \epsilon, r] = 0, \quad (3)$$

we can differentiate (3) with respect to ϵ to obtain

$$\nabla_x^2 W[x(\epsilon, r), \epsilon, r] \nabla_\epsilon x(\epsilon, r) + \nabla_\epsilon (\nabla_x W[x(\epsilon, r), \epsilon, r]) = 0. \quad (4)$$

By Theorem 2, $\nabla_x^2 W$ is positive definite for (ϵ, r) near $(0,0)$ and $r > 0$, so $\nabla_x^2 W$ has an inverse and $\nabla_\epsilon x(\epsilon, r) = -\nabla_x^2 W[x(\epsilon, r), \epsilon, r]^{-1} \cdot \nabla_{\epsilon x}^2 W[x(\epsilon, r), \epsilon, r]$.

Also, since

$$u_i(\epsilon, r) = r/g_i(x(\epsilon, r), \epsilon), \quad i=1, \dots, m, \quad (5)$$

and

$$w_j(\epsilon, r) = h_j(x(\epsilon, r), \epsilon)/r, \quad j=1, \dots, p, \quad (6)$$

for (ϵ, r) near $(0, 0)$ and $r > 0$, these equations can be differentiated with respect to ϵ to obtain

$$\nabla_{\epsilon} u_i(\epsilon, r) = -(r/g_i^2) [\nabla_x g_i(x(\epsilon, r), \epsilon) \cdot \nabla_{\epsilon} x(\epsilon, r) + \partial g_i(x(\epsilon, r), \epsilon)/\partial \epsilon], \quad (7)$$

$$\nabla_{\epsilon} w_j(\epsilon, r) = (1/r) [\nabla_x h_j(x(\epsilon, r), \epsilon) \cdot \nabla_{\epsilon} x(\epsilon, r) + \partial h_j(x(\epsilon, r), \epsilon)/\partial \epsilon]. \quad (8)$$

Solving (4) and calculating (7) and (8) then yields the components of $\nabla_{\epsilon} y(\epsilon, r)$, which can be used to estimate $\nabla_{\epsilon} y(\epsilon)$ for (ϵ, r) near $(0, 0)$.

The next results extend this theory to an analysis of the optimal value function of Problem $P(\epsilon)$ along the Kuhn-Tucker point trajectory $[x(\epsilon), u(\epsilon), w(\epsilon)]^T$.

The optimal value function is defined as:

$$f^*(\epsilon) \equiv f[x(\epsilon), \epsilon], \quad (9)$$

and the "optimal value Lagrangian" is defined as:

$$L^*(\epsilon) = L[x(\epsilon), u(\epsilon), w(\epsilon), \epsilon]. \quad (10)$$

Theorem 3: (First and second order changes in the optimal value function, Armacost and Fiacco (1975).) If assumptions A1 - A4 hold for Problem $P(\epsilon)$, then for ϵ near 0, $f^*(\epsilon)$ is a twice continuously differentiable function of ϵ , and

$$(a) \quad f^*(\varepsilon) = L^*(\varepsilon) ;$$

$$(b) \quad \nabla_{\varepsilon} f^*(\varepsilon) = \nabla_{\varepsilon} L(x, u, w, \varepsilon) \Big|_{(x, u, w) = (x(\varepsilon), u(\varepsilon), w(\varepsilon))}$$

$$= \nabla_{\varepsilon} f(x, \varepsilon) - \sum_{i=1}^m u_i \nabla_{\varepsilon} g_i(x, \varepsilon)$$

$$+ \sum_{j=1}^p w_j \nabla_{\varepsilon} h_j(x, \varepsilon) \Big|_{(x, u, w) = (x(\varepsilon), u(\varepsilon), w(\varepsilon))} ;$$

$$(c) \quad \nabla_{\varepsilon}^2 f^*(\varepsilon) = \nabla_{\varepsilon} (\nabla_{\varepsilon} L(x(\varepsilon), u(\varepsilon), w(\varepsilon), \varepsilon))^T .$$

The logarithmic-quadratic loss penalty function (2) can also be used to provide estimates of the first and second order sensitivity of the optimal value function. Let the optimal value penalty function be defined as $W^*(\varepsilon, r) \equiv W(x(\varepsilon, r), \varepsilon, r)$.

Theorem 4: (First and second order sensitivity of $W^*(\varepsilon, r)$ and estimates for $f^*(\varepsilon)$, Armacost and Fiacco (1975).) If Assumptions A1 - A4 hold for Problem P(ε), then for (ε, r) near $(0, 0)$ and $r > 0$, $W^*(\varepsilon, r)$ is a twice continuously differentiable function of ε and

$$(a) \quad \lim_{r \rightarrow 0^+} W^*(\varepsilon, r) = L^*(\varepsilon) = f^*(\varepsilon) ;$$

$$(b) \quad \nabla_{\varepsilon} W^*(\varepsilon, r) = \nabla_{\varepsilon} L(x, u, w, \varepsilon) \Big|_{(x, u, w) = (x(\varepsilon, r), u(\varepsilon, r), w(\varepsilon, r))} ;$$

$$(c) \quad \lim_{r \rightarrow 0^+} \nabla_{\varepsilon} W^*(\varepsilon, r) = \nabla_{\varepsilon} L(x(\varepsilon), u(\varepsilon), w(\varepsilon), \varepsilon) = \nabla_{\varepsilon} f^*(\varepsilon) ; \quad (11)$$

$$(d) \quad \nabla_{\varepsilon}^2 W^*(\varepsilon, r) = \nabla_{\varepsilon} (\nabla_{\varepsilon} L(x(\varepsilon, r), u(\varepsilon, r), w(\varepsilon, r), \varepsilon))^T ;$$

$$(e) \quad \lim_{r \rightarrow 0^+} \nabla_{\varepsilon}^2 W^*(\varepsilon, r) = \nabla_{\varepsilon}^2 f^*(\varepsilon) .$$

This result provides a justification for estimating $f^*(\varepsilon)$, $\nabla_{\varepsilon} f^*(\varepsilon)$ and $\nabla_{\varepsilon}^2 f^*(\varepsilon)$ by $W^*(\varepsilon, r)$, $\nabla_{\varepsilon} W^*(\varepsilon, r)$ and $\nabla_{\varepsilon}^2 W^*(\varepsilon, r)$, respectively, when r is positive and small enough.

Since Corollary 2.1 and continuity imply that $\lim_{r \rightarrow 0^+} f(x(\epsilon, r), \epsilon) = f^*(\epsilon)$, another estimate of the optimal value function (9) is provided by $f^\#(\epsilon, r) \equiv f(x(\epsilon, r), \epsilon)$ when $r > 0$ and small. Direct application of the chain rule for differentiation then yields, for $x = x(\epsilon, r)$,

$$\nabla_\epsilon f^\#(\epsilon, r) = \nabla_x f(x, \epsilon) \nabla_\epsilon x(\epsilon, r) + \nabla_\epsilon f(x, \epsilon). \quad (12)$$

Under the given assumptions, continuity also assures that $\nabla_\epsilon f^\#(\epsilon, r) \rightarrow \nabla_\epsilon f^*(\epsilon)$ as $r \rightarrow 0^+$. Thus, both $\nabla_\epsilon f^\#(\epsilon, r)$ and $\nabla_\epsilon W^*(\epsilon, r)$ are estimates of $\nabla_\epsilon f^*(\epsilon)$ for r sufficiently small.

It should be noted that these estimates are functionally related since

$$\begin{aligned} \nabla_\epsilon W^*(\epsilon, r) = \nabla_\epsilon f^\#(\epsilon, r) - \sum_{i=1}^m u_i (\nabla_x g_i \nabla_\epsilon x(\epsilon, r) + \nabla_\epsilon g_i) \\ + \sum_{j=1}^p w_j (\nabla_x h_j \nabla_\epsilon x(\epsilon, r) + \nabla_\epsilon h_j) \Big|_{x=x(\epsilon, r)}. \end{aligned}$$

From this expression, it is clear that $\nabla_\epsilon f^\#(\epsilon, r)$ is the better estimate of $\nabla_\epsilon f^*(\epsilon)$, the remaining terms in $\nabla_\epsilon W^*(\epsilon, r)$ simply constituting "noise" that is eliminated as $r \rightarrow 0^+$. However, by using the expression for $\nabla_\epsilon W^*(\epsilon, r)$ given by (11), $\nabla_\epsilon W^*(\epsilon, r)$ can be evaluated without necessitating the calculation of $\nabla_\epsilon x(\epsilon, r)$, which is required to compute (12). Thus, the cruder but computationally much cheaper estimate of $\nabla_\epsilon f^*(\epsilon)$ given by Equation (11) has now been introduced as an option in the computer program as a preliminary screening device to identify crucial parameters. Restriction of subsequent calculations to these parameters, and other calculations such as the sharper estimate of $f^*(\epsilon)$ given by (12) are provided as additional options.

In summary, the basis for the estimation procedure utilized here for a specific problem, say Problem $P(0)$, is the minimization of the penalty function $W(x, \epsilon, r)$ given by (2). This yields a point $x(\epsilon, r)$ which may be viewed as an estimate of a (local) solution x^* of Problem $P(0)$. The associated optimal Lagrange multipliers u^* and w^* are then estimated by using the relationships given in (5) and (6), respectively. The first partial derivatives of these quantities with respect to ϵ are then obtained by first solving (4) and then applying (7) and (8). The estimate $f(x(\epsilon, r), \epsilon)$ of $f^*(\epsilon)$ is immediately available when $x(\epsilon, r)$ has been determined, and the two estimates of $\nabla_{\epsilon} f^*(\epsilon)$ given by (11) and (12) were already discussed. Various options and computer codes implementing the procedure are discussed in the next section.

3. User Options, Computer Codes and an Example

The basic SUMT-Version 4 computer program and instructions for its use are described in Mylander, Holmes and McCormick (1971). The basic sensitivity analysis subroutines, user instructions, and instructions for integrating the sensitivity package with the SUMT-Version 4 code are described in Armacost and Mylander (1973).

Briefly, the conduct of a sensitivity analysis is controlled by the variable NEXOP3 which is given a value on the "Second Option Card" in the SUMT input data deck. There are four choices: no sensitivity analysis, a sensitivity analysis at the final subproblem, a sensitivity analysis at each subproblem along the penalty function minimizing trajectory, or a sensitivity analysis at the final subproblem for a range of differencing increments. In conjunction with this option, two additional options are added here and come into play whenever a sensitivity analysis is conducted.

The first option (technically Option 4) is controlled by the variable NEXOP4 and determines whether the partial derivatives of the Lagrange multipliers will be calculated. When the calculation is done, the formulas developed by Fiacco (1973) are used.

The second option added here (Option 5) permits a screening of the parameters to reduce the number of partial derivatives which are estimated by limiting further analysis to parameter changes which affect the optimal value of the objective function by an amount exceeding 0.1 percent of its current value. This option is controlled by the variable NEXOP5. The estimate of sensitivity of the optimal value function with respect to a particular parameter under this option is calculated using the Armacost and Fiacco (1975) result which involves the partial derivative of the Lagrangian taken with respect to the parameter under consideration.

Subroutines LMULT and PRESEN and related coding in Subroutine SENS implement Option 4 and Option 5, respectively. Subroutines SENS, LMULT and PRESEN are listed in Appendix A. Specific instructions for using these two options in conjunction with the "Second Option Card" are given below in Table 1. This information should be added to Table 5 in Mylander, Holmes and McCormick (1971).

As an illustration of the kind of information that can be generated, consider the following simple (convex) parametric nonlinear programming problem,

$$\begin{aligned} &\text{minimize } f(x, \epsilon) = x_1 + \epsilon_2 x_2 \\ &\text{subject to } g_1(x, \epsilon) = \epsilon_1^2 - x_1^2 - x_2^2 \geq 0. \end{aligned} \quad A(\epsilon)$$

for $\epsilon_1 > 0$ and ϵ_2 not restricted.

TABLE 1
THE SECOND OPTION CARD

Option	Column	Value	Meaning
4	28	=0	Do not estimate the partial derivatives of the estimates of the Lagrange multipliers.
		=1	Estimate the partial derivatives of the estimates of the Lagrange multipliers whenever a sensitivity analysis of the solution point is conducted.
5	35	=0	Estimate the partial derivatives of the optimal value function and eliminate those parameters which do not affect the optimal value function from subsequent sensitivity calculations.
		=1	Estimate the partial derivatives of the optimal value function with respect to all parameters, but continue all subsequent sensitivity calculations with respect to all parameters.
		=2	Do not estimate the partial derivatives of the optimal value function first. Conduct the sensitivity analysis with respect to all parameters.

To dramatize the complexity of the relationships that can arise even in such trivial problems, we first give the solution in closed form. Application of the Kuhn-Tucker conditions yields the following:

$$x(\epsilon) = \begin{bmatrix} x_1(\epsilon) \\ x_2(\epsilon) \end{bmatrix} = \begin{bmatrix} -\frac{\epsilon_1}{\sqrt{1 + \epsilon_2^2}} \\ -\frac{\epsilon_1 \epsilon_2}{\sqrt{1 + \epsilon_2^2}} \end{bmatrix},$$

$$u(\epsilon) = \sqrt{1 + \epsilon_2^2} / 2\epsilon_1 ,$$

and

$$g_1(x(\epsilon), \epsilon) = 0 .$$

(It may be readily verified that Assumptions A1 - A4 are satisfied.)

From the expression for $x(\epsilon)$, we find that

$$f^*(\epsilon) = -\epsilon_1 \sqrt{1 + \epsilon_2^2} .$$

Taking partial derivatives with respect to ϵ_1 and ϵ_2 , we obtain

$$\nabla_{\epsilon} x(\epsilon) = \frac{1}{\sqrt{1 + \epsilon_2^2}} \begin{bmatrix} -1 & \frac{\epsilon_1 \epsilon_2}{(1 + \epsilon_2^2)} \\ -\epsilon_2 & \frac{-\epsilon_1}{(1 + \epsilon_2^2)} \end{bmatrix} ,$$

$$\nabla_{\epsilon} f^*(\epsilon) = (\partial f^*(\epsilon)/\partial \epsilon_1, \partial f^*(\epsilon)/\partial \epsilon_2)$$

$$= \left(-\sqrt{1 + \epsilon_2^2} , -\epsilon_1 \epsilon_2 / \sqrt{1 + \epsilon_2^2} \right) ,$$

and

$$\nabla_{\epsilon} u^*(\epsilon) = \left(-\sqrt{1 + \epsilon_2^2} / 2\epsilon_1^2 , \epsilon_2 / \left(2\epsilon_1 \sqrt{1 + \epsilon_2^2} \right) \right) .$$

Suppose we are particularly interested in the values $\epsilon_1=2$, $\epsilon_2=1$.

Evaluation of the above expressions yields

$$f^* = -2\sqrt{2} , \quad \nabla_{\epsilon} f^* = (-\sqrt{2}, -\sqrt{2}) ,$$

$$x^* = \begin{bmatrix} -\sqrt{2} \\ -\sqrt{2} \end{bmatrix} , \quad \nabla_{\epsilon} x^* = \begin{bmatrix} -\sqrt{2}/2 & \sqrt{2}/2 \\ -\sqrt{2}/2 & -\sqrt{2}/2 \end{bmatrix} ,$$

$$u^* = \sqrt{2}/4, \quad \nabla_{\epsilon} u^* = (-\sqrt{2}/8, \sqrt{2}/8).$$

The numerical results obtained by the computer program are included in Table 2 for the optimal value function and Lagrange multiplier sensitivity. The values of the first order optimal value function sensitivity computed both by the chain rule (Equation (12)) and by taking partial derivatives of the Lagrangian with respect to the parameters (Equation (11)) are presented for comparison. As indicated previously and expected, the chain rule estimates are sharper. The subproblems correspond to minimizations of the penalty function $W(x, \epsilon, r)$ for several values of $r > 0$, the value of r decreasing as the subproblem index increases. The values of f are given by $f(x(\epsilon, r), \epsilon)$, while the values of u and $\nabla_{\epsilon} u$ were obtained by applying formulas (5) and (7). The components of $x(\epsilon)$ and $\nabla_{\epsilon} x(\epsilon)$ were calculated also but are not portrayed.

TABLE 2
SENSITIVITY ESTIMATES FOR PROBLEM $A(\epsilon)$, WHERE $\epsilon = (2, 1)$

Subproblem	f	Lagrangian		Chain Rule		u	$\partial u / \partial \epsilon_1$	$\partial u / \partial \epsilon_2$
		$\partial f / \partial \epsilon_1$	$\partial f / \partial \epsilon_2$	$\partial f / \partial \epsilon_1$	$\partial f / \partial \epsilon_2$			
1	-1.9999	-1.9999	-.9999	-1.3333	-1.3333	.4999	-.3333	.1666
2	-2.5393	-1.5440	-1.2947	-1.4087	-1.4088	.3860	-.2100	.1761
3	-2.7765	-1.4439	-1.3833	-1.4139	-1.4139	.3609	-.1844	.1767
4	-2.8128	-1.4243	-1.4064	-1.4142	-1.4142	.3560	-.1790	.1768
5	-2.8245	-1.4127	-1.4123	-1.4142	-1.4142	.3531	-.1768	.1768
6	-2.8274	-1.4137	-1.4137	-1.4142	-1.4142	.3532	-.1767	.1768
7	-2.8282	-1.3899	-1.4141	-1.4142	-1.4142	.3475	-.1737	.1768
Analytical	-2.8282	-1.4142	-1.4142	-1.4142	-1.4142	.3537	-.1769	.1768

The results are typical of those that have been obtained to date, convergence of the sensitivity estimates being reliable and stable with less stability noted in the estimates of the optimal Lagrange multipliers. It appears that the sensitivity estimates will converge satisfactorily whenever the SUMT algorithm succeeds in determining a good estimate of a Kuhn-Tucker point.

4. A Large-scale Multi-item Inventory Model

Traditionally, inventory models have been formulated to minimize some function of the ordering, holding and shortage (or backorder) costs subject to various constraints. Schrady and Choe (1971) have formulated an inventory model which appears to have much greater relevance for an inventory system in a noncommercial environment, such as institutional or military. The costs used in the traditional models may be quite artificial and the real objective of the system is often maximization of a measure of readiness or service, here assumed to be equivalent to minimization of stockouts. In addition, the stock points of such supply systems are inevitably constrained by investment and reorder work load limitations.

Schrady and Choe's multi-item inventory system assumes these constraints along with the specific objective of minimizing the total time-weighted shortages. The decision variables are taken to be the "reorder quantities" and the "reorder points," respectively, how much to order and when to order each item in the inventory. A three-item example problem was solved by Schrady and Choe (1971) using the SUMT computer code (Mylander, et al., 1971). Subsequently, McCormick (1972) showed how the special structure of this inventory model can be used to facilitate the use of the SUMT code to solve very large inventory problems. He also

extended the model to include constraints on storage volume and the probability of depletion of critical items.

The model and example presented here are the original ones due to Schrady and Choe. The computer program described in the preceding section was used to solve the example and calculate the partial derivatives of various quantities of interest, with respect to each parameter involved in defining the model. (The analysis can be applied to the extended model without difficulty.)

Detailed development of the model is beyond the scope of this paper. The interested reader is referred to the Schrady-Choe and McCormick papers. Here, we give a summary treatment of the various conditions and relationships upon which the model is based. We then tabulate the results obtained in solving the resulting nonlinear programming problem and applying the sensitivity analysis methodology. A number of observations and interpretations are offered to illustrate the many uses to which the sensitivity information might be applied.

It is assumed that the amount of each item in inventory is always known, that all demand which occurs when the on-hand stock is zero is backordered, and that the demand which occurs during the time between the placement of an order and its receipt by the stock point (i.e., the "lead time demand") is normally distributed with known mean μ_i and variance σ_i^2 .

For the i th item, let

c_i = item unit cost (in dollars),

λ_i = mean demand per unit time (in units),

r_i = reorder point,

Q_i = reorder quantity,

$\phi(x)$ = the Normal (0,1) density function,
 $\phi(z) = \int_z^{\infty} \phi(x)dx$ = the Normal (0,1) complementary cumulative distribution function.

In addition, Let K_1 be the investment limit in dollars, K_2 the number of orders per unit of time that constitutes reorder work load limit, and N the total number of items in the inventory.

It can be shown that the expected time-weighted shortage of item i at any point in time is given by

$$B_i(Q_i, r_i) = \frac{1}{Q_i} [\beta_i(r_i) - \beta_i(Q_i + r_i)]$$

where

$$\beta_i(r_i) = \frac{1}{2} \left[\sigma_i^2 + (r_i - \mu_i)^2 \right] \phi \left(\frac{r_i - \mu_i}{\sigma_i} \right) - \frac{\sigma_i}{2} (r_i - \mu_i) \phi \left(\frac{r_i - \mu_i}{\sigma_i} \right).$$

The expected on-hand inventory of item i is given by $r_i + Q_i/2 - \mu_i + B_i(Q_i, r_i)$ and the expected number of orders placed per unit time for item i is λ_i/Q_i .

Using the above expressions and assumptions, Schrady and Choe (1971) indicate that meaningful approximations of the given quantities are obtained even when the second term is dropped from the expression for the expected shortages, and when the last term is dropped from the expression for expected on-hand inventory. The given assumptions and simplifications then lead readily to the following nonlinear programming problem (which Schrady and Choe (1971) proved convex),

$$\begin{array}{ll} \text{minimize} & Z(Q, r) \equiv \sum_{i=1}^N \beta_i(r_i)/Q_i \\ & Q, r \end{array}$$

$$\text{subject to } g_1(Q, r) \equiv K_1 - \sum_{i=1}^N c_i (r_i + Q_i/2 - \mu_i) \geq 0, \quad (SC)$$

$$g_2(Q, r) \equiv K_2 - \sum_{i=1}^N \lambda_i / Q_i \geq 0,$$

with r_i unrestricted in sign, $Q_i \geq 0$, $i=1, \dots, N$, $Q = (Q_1, \dots, Q_N)^T$, $r = (r_1, \dots, r_N)^T$, and g_1 and g_2 representing the investment and work load constraints, respectively.

The problem data for the Schrady-Choe three-item example and the initial starting point for the SUMT program are shown in Table 3. As indicated in the table, the lead time demands and standard deviations, the item unit costs and mean demands, and the investment and work load limits are all treated as parameters in conducting the sensitivity analysis.

Table 4 gives the computer solution and Table 5 the final estimate of the first partial derivatives of the optimal value function Z^* with respect to the problem parameters. Relative to the criterion used in the computer program, the Table 5 results indicate that the optimal value function is sensitive to parameters K_2 , c_1 , σ_2 , c_2 , σ_3 and c_3 . Many inferences are possible. For example, the fact that the solution is particularly sensitive to the values of the standard deviations of the lead time demand of items 2 and 3 might indicate that, since these parameters were obtained by sampling, additional sampling of these lead time demands may very well be warranted to reduce the associated standard deviations.

Table 5 also suggests that the optimal solution value is very sensitive to all of the item costs. If the structure of Problem (SC) is examined, this result may at first appear contradictory since the c_i appear only

TABLE 3

INVENTORY PROBLEM DATA

QUANTITY	ITEM i		
	1	2	3
μ_i	100	200	300
σ_i	100	100	200
c_i	1	10	20
λ_i	1,000	1,500	2,000
K_1	\$ 8,000		
K_2	15 re-orders/unit time		
Q_i^0	600	270	300
r_i^0	200	250	400

(MEAN OF LEAD-TIME DEMAND)

(S.D. OF LEAD-TIME DEMAND)

(ITEM UNIT COST - DOLLARS)

(MEAN DEMAND/UNIT TIME)

(INVESTMENT LIMIT)

(RE-ORDER WORKLOAD LIMIT)

(AMOUNT ORDERED)

(RE-ORDER LEVEL)

TABLE 4
SOLUTION AND LAGRANGE MULTIPLIERS

	QUANTITY	ITEM i		
		1	2	3
V A R :	Q_i^*	533	246	285
	r_i^*	253	277	437
L M :	u_1^*	.0052		
	u_2^*	.6230		

TABLE 5
OPTIMAL VALUE FUNCTION DERIVATIVES

PARTIALS	ITEM i		
	1	2	3
$\partial Z^*/\partial \mu_i$	-.0000	-.0003	-.0008
$\partial Z^*/\partial \sigma_i$	.0119	.0897 ^a	.1729 ^a
$\partial Z^*/\partial c_i$	2.1713 ^a	1.0345 ^a	1.4452 ^a
$\partial Z^*/\partial \lambda_i$	.0012	.0025	.0022
$\partial Z^*/\partial K_1$		-.0052	
$\partial Z^*/\partial K_2$		-.6230 ^a	

^aDeemed "significant" by criterion, $|\Delta_1 Z^*|/Z^* > .001$ for a unit change in the given parameter, where $\Delta_1 Z^*$ is the estimated first order change in Z^* . This criterion was selected arbitrarily for illustrative purposes. Criteria appropriate to the particular application can be selected by a user.

in the investment constraint and the optimal value function, according to Table 5, is apparently not very sensitive to the investment limit K_1 . The problem is one of precise interpretation. The partial derivatives measure rate of change. But inspection of the investment constraint $g_1(Q, r)$ at (Q^*, r^*) reveals that the change in an item cost c_i by any amount Δc_i has the same effect on the constraint as a change in the investment limit K_1 of $-(r_i^* + Q_i^*/2 - \mu_i)\Delta c_i$. Since the quantity in parentheses may be verified from Tables 3 and 4 to be much greater than one for all i , it follows that the effect of changing any c_i by any increment δ will be much greater on the constraint (and hence, on the optimal value Z^* , since the constraint is binding) than the effect of changing K_1 by the same amount δ . This implies that $|\partial Z^*/\partial c_i| > |\partial Z^*/\partial K_1|$ for each i and, in fact, it can be shown here that $\partial Z^*/\partial c_i = -(r_i^* + Q_i^*/2 - \mu_i)\partial Z^*/\partial K_1$, so that the relationships indicated are indeed precisely verified.

The above observations might also suggest that some care must be taken in interpreting the results. Changes in the parameter associated with the largest (in absolute value) partial derivative will give the greatest local change in the optimal value of the objective function, compared to a change of the same magnitude in any other parameter taken individually. This follows because either the objective function and/or some of the constraints (as above) are most significantly affected by this parameter change at the current solution. General rules have not been given for selection of optimal changes in the parameters, i.e., for determining the optimal magnitude and combination of such changes. It is well beyond the scope of this paper to pursue this "macro-analysis" determination, though it should be noted that the greatest local rate of decrease in the

optimal value function is along the direction of the negative of the gradient of this function in parameter space (i.e., along the vector composed of the negative of the components of the partial derivatives with respect to the various parameters). A user would nonetheless have to determine the feasibility of this direction of change and, if feasible, the optimal move along this vector, taking into account other factors such as the relative "cost-effectiveness" of any schedule of changes in any model parameter.

Referring back to Table 4, we note that the Lagrange multiplier u_2^* is much greater than u_1^* . Recalling the "sensitivity" interpretation of Lagrange multipliers, which holds under the present conditions, it follows that $u_1^* = -\partial Z^*/\partial K_1$ and $u_2^* = -\partial Z^*/\partial K_2$. This conclusion is consistent with the result obtained in Table 5, and it means that the work load constraint g_2 is by far the more effective in determining the minimum number of expected time-weighted shortages at the current value of the parameters, e.g., a small increase in K_2 will have a greater effect on reducing Z^* than a small increase in K_1 . Nonetheless, a user must again simultaneously consider the comparative costs involved in making finite changes, in conjunction with their expected effects, to arrive at an optimal marginal improvement based on this first order information. The sensitivity information is valuable, but requires some care in exploiting.

Table 6 gives the estimates of the first derivatives of the optimal reorder quantities Q_i and reorder points r_i with respect to each of the problem parameters. This is extremely detailed information which gives an indication of how the components of the solution vector itself will change as the various parameters change. In particular, this information

TABLE 6
SOLUTION POINT SENSITIVITY

PARTIALS	ITEM i		
	1	2	3
$\partial Q_i / \partial K_2$	- 47.3187	- 18.7610	- 14.9065
$\partial r_i / \partial K_2$	5.2265	6.1961	9.9671
$\partial Q_i / \partial c_1$	-208.8688	15.3140	14.3755
$\partial r_i / \partial c_1$	- 31.7918	- 10.3425	- 20.0020
$\partial Q_i / \partial \sigma_2$	- .8469	.2271	- .1084
$\partial r_i / \partial \sigma_2$	- .1273	1.0337	- .4919
$\partial Q_i / \partial c_2$	8.1908	- 4.9719	3.8522
$\partial r_i / \partial \sigma_2$	- 2.6783	- 7.2676	- 7.1087
$\partial Q_i / \partial \sigma_3$	- 1.2374	- .4033	.5843
$\partial r_i / \partial \sigma_3$	- .2611	- .3839	.0446
$\partial Q_i / \partial c_3$	- .1670	.4442	- .4251
$\partial r_i / \partial c_3$	- 2.3072	- 3.1702	- 12.1523

can be used to obtain a first order estimate of the solution vector of a problem involving different parameter values, having obtained a solution for a given set of parameters.

The partial derivatives of the Lagrange multipliers with respect to the parameters are given in Table 7. Again, these can be used to obtain first order estimates of the Lagrange multipliers of a problem with different parameter values. In particular, the relative effects of the constraints on the optimal value of problems involving different parameter values can be estimated. Furthermore, it can be shown that the partial derivatives of the multipliers with respect to K_1 and K_2 yield the second partial derivatives of the optimal value function with respect to the parameters K_1 and K_2 , under the present conditions. Thus, the kind of information given in Table 7 can be used to provide a second order estimate of the optimal value function Z^* for different values of these parameters.

To illustrate and test the application of the type of information provided here, the first partial derivatives with respect to c_1 of the optimal value function Z^* , the solution components Q_i and r_i , and the Lagrange multipliers u_1 and u_2 , were used to give a first order (Taylor's Series) estimate of the corresponding solution values associated with the problem where the given value of c_1 was increased by one dollar. These estimates were compared with the respective values of the solution obtained by actually solving the perturbed problem. The results are summarized in Table 8. Though the perturbation is large (the parameter being increased by 100% of its current value), the estimates are seen to be extremely accurate with the exception of the estimated reorder quantity Q_1 . Many uses could be made of the estimated solution; e.g., should it be desirable to solve the perturbed problem accurately, it would be

TABLE 7

L.M. SENSITIVITY

OPTIMAL L.M. DERIVATIVES		
PARTIALS	CONSTRAINT i	
	1: INVESTMENT	2: WORKLOAD
$\partial u_i^* / \partial K_2$	-.0002	-.1382
$\partial u_i^* / \partial c_1$	.0006	.1635
$\partial u_i^* / \partial \sigma_2$	.0000	.0006
$\partial u_i^* / \partial c_2$	.0002	.0489
$\partial u_i^* / \partial \sigma_3$	.0000	.0020
$\partial u_i^* / \partial c_3$	.0003	.0323

computationally extremely advantageous to use the estimated solution as a starting point.

The complete exploitation of this sensitivity analysis information now available will depend largely on user interest and ingenuity.

TABLE 8
FIRST ORDER ESTIMATES FOR A UNIT
INCREASE OF PARAMETER c_1

QUANTITY $F(\epsilon^1)$	ESTIMATE $F(\epsilon^1)_1^\dagger$	ACTUAL	% ABS. ERROR
$z^*(\epsilon^1)$	15.159	14.996	1.08
$Q_1(\epsilon^1)$	324	412	21.36
$r_1(\epsilon^1)$	221	229	3.49
$Q_2(\epsilon^1)$	261	257	1.56
$r_2(\epsilon^1)$	267	268	.37
$Q_3(\epsilon^1)$	299	297	.67
$r_3(\epsilon^1)$	417	420	.71
$u_1(\epsilon^1)$	.0058	.0057	1.75
$u_2(\epsilon^1)$	.7865	.7671	1.94

$$\begin{aligned}
 {}^\dagger F(\epsilon^1)_1 &= F(\epsilon^0) + (\epsilon^1 - \epsilon^0)^T \nabla_{\epsilon} F(\epsilon^0) \\
 &= F(\epsilon^0) + (1) \partial F(\epsilon^0) / \partial c_1 .
 \end{aligned}$$

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APPENDIX A

SUBROUTINES SENS, LMULT AND PRESEN

```

0001      SUBROUTINE SENS                                016680
C                                                    016690
C                                                    016700
C              15 MARCH 1972                        016710
C THIS VERSION OF THE SENSITIVITY ANALYSIS SUBROUTINE IS USED TO 016720
C COMPUTE THE DIRECTIONAL DERIVATIVES OF X AND F WITH RESPECT TO 016730
C CERTAIN PARAMETERS CODED IN THE ARRAY PAR(20). THE DIRECTIONAL 016740
C DERIVATIVES ARE ESTIMATED FOR ONE PARAMETER AT A TIME WITH NPAP BEING 016750
C THE NUMBER OF PARAMETERS INVOLVED IN THE SENSITIVITY ANALYSIS. THE 016760
C USE OF THE PARAMETERS PAR(20) MUST BE CONSISTENT THROUGHOUT THE 016770
C USER'S SUBROUTINES.                                016780
C THE SUBROUTINE IS USED FOR A SENSITIVITY ANALYSIS AT THE FINAL SUB- 016790
C PROBLEM OR FOR A SENSITIVITY ANALYSIS AT EACH SUBPROBLEM ALONG THE 016800
C MINIMIZING TRAJECTORY. DPAR(20) IS THE ARRAY OF DIFFERENCING 016810
C INTERVALS CORRESPONDING TO THE PARAMETERS PAR(20). DPAR(20) IS 016820
C ASSIGNED VALUES IN SUBROUTINE PARDEF.              016830
C THIS APPROACH TO SENSITIVITY ANALYSIS IS DUE TO A. V. FIACCO. THE 016840
C FIRST VERSION WAS CODED BY R. CAUSEY. THE SECOND VERSION WAS CODED 016850
C BY W. C. MYLANDER. THIS IS THE THIRD VERSION WHICH IS AN EXTENSION 016860
C OF THE SECOND VERSION TO PERMIT SENSITIVITY ANALYSIS ALONG THE 016870
C MINIMIZING TRAJECTORY. AND WAS CODED BY R. L. ARMACOST. 016880
C IMPLICIT REAL*8(A-H,O-Z)                          016890
C REAL*8 RHOIN,PATIO,EPST,THETA0,XEP1,XEP2          016900
C COMMON/SHARE/X(20),DEL(20),A(20,20),N,M,MN,NP1,NM1 016910
C COMMON/EQUAL/H,M1,M2                              016920
C COMMON/CPTNS/NT1,NT2,NT3,NT4,NT5,NT6,NT7,NT8,NT9,NT10 016930
C COMMON/VALUE/F,G,PC,PSIGMA,FJ(40),UHQ            016940
C COMMON/CST/DELX(20),DELY(20),RHOIN,PATIO,EPST,THETA0, 016950
C INTCL,MUMIN,X1(20),X2(20),X3(20),X4(20),X5(20),X6(20),X7(20),X8(20),X9(20),X10(20),X11(20),X12(20),X13(20),X14(20),X15(20),X16(20),X17(20),X18(20),X19(20),X20(20),X21(20),X22(20),X23(20),X24(20),X25(20),X26(20),X27(20),X28(20),X29(20),X30(20),X31(20),X32(20),X33(20),X34(20),X35(20),X36(20),X37(20),X38(20),X39(20),X40(20),X41(20),X42(20),X43(20),X44(20),X45(20),X46(20),X47(20),X48(20),X49(20),X50(20),X51(20),X52(20),X53(20),X54(20),X55(20),X56(20),X57(20),X58(20),X59(20),X60(20),X61(20),X62(20),X63(20),X64(20),X65(20),X66(20),X67(20),X68(20),X69(20),X70(20),X71(20),X72(20),X73(20),X74(20),X75(20),X76(20),X77(20),X78(20),X79(20),X80(20),X81(20),X82(20),X83(20),X84(20),X85(20),X86(20),X87(20),X88(20),X89(20),X90(20),X91(20),X92(20),X93(20),X94(20),X95(20),X96(20),X97(20),X98(20),X99(20),X100(20),X101(20),X102(20),X103(20),X104(20),X105(20),X106(20),X107(20),X108(20),X109(20),X110(20),X111(20),X112(20),X113(20),X114(20),X115(20),X116(20),X117(20),X118(20),X119(20),X120(20),X121(20),X122(20),X123(20),X124(20),X125(20),X126(20),X127(20),X128(20),X129(20),X130(20),X131(20),X132(20),X133(20),X134(20),X135(20),X136(20),X137(20),X138(20),X139(20),X140(20),X141(20),X142(20),X143(20),X144(20),X145(20),X146(20),X147(20),X148(20),X149(20),X150(20),X151(20),X152(20),X153(20),X154(20),X155(20),X156(20),X157(20),X158(20),X159(20),X160(20),X161(20),X162(20),X163(20),X164(20),X165(20),X166(20),X167(20),X168(20),X169(20),X170(20),X171(20),X172(20),X173(20),X174(20),X175(20),X176(20),X177(20),X178(20),X179(20),X180(20),X181(20),X182(20),X183(20),X184(20),X185(20),X186(20),X187(20),X188(20),X189(20),X190(20),X191(20),X192(20),X193(20),X194(20),X195(20),X196(20),X197(20),X198(20),X199(20),X200(20),X201(20),X202(20),X203(20),X204(20),X205(20),X206(20),X207(20),X208(20),X209(20),X210(20),X211(20),X212(20),X213(20),X214(20),X215(20),X216(20),X217(20),X218(20),X219(20),X220(20),X221(20),X222(20),X223(20),X224(20),X225(20),X226(20),X227(20),X228(20),X229(20),X230(20),X231(20),X232(20),X233(20),X234(20),X235(20),X236(20),X237(20),X238(20),X239(20),X240(20),X241(20),X242(20),X243(20),X244(20),X245(20),X246(20),X247(20),X248(20),X249(20),X250(20),X251(20),X252(20),X253(20),X254(20),X255(20),X256(20),X257(20),X258(20),X259(20),X260(20),X261(20),X262(20),X263(20),X264(20),X265(20),X266(20),X267(20),X268(20),X269(20),X270(20),X271(20),X272(20),X273(20),X274(20),X275(20),X276(20),X277(20),X278(20),X279(20),X280(20),X281(20),X282(20),X283(20),X284(20),X285(20),X286(20),X287(20),X288(20),X289(20),X290(20),X291(20),X292(20),X293(20),X294(20),X295(20),X296(20),X297(20),X298(20),X299(20),X300(20),X301(20),X302(20),X303(20),X304(20),X305(20),X306(20),X307(20),X308(20),X309(20),X310(20),X311(20),X312(20),X313(20),X314(20),X315(20),X316(20),X317(20),X318(20),X319(20),X320(20),X321(20),X322(20),X323(20),X324(20),X325(20),X326(20),X327(20),X328(20),X329(20),X330(20),X331(20),X332(20),X333(20),X334(20),X335(20),X336(20),X337(20),X338(20),X339(20),X340(20),X341(20),X342(20),X343(20),X344(20),X345(20),X346(20),X347(20),X348(20),X349(20),X350(20),X351(20),X352(20),X353(20),X354(20),X355(20),X356(20),X357(20),X358(20),X359(20),X360(20),X361(20),X362(20),X363(20),X364(20),X365(20),X366(20),X367(20),X368(20),X369(20),X370(20),X371(20),X372(20),X373(20),X374(20),X375(20),X376(20),X377(20),X378(20),X379(20),X380(20),X381(20),X382(20),X383(20),X384(20),X385(20),X386(20),X387(20),X388(20),X389(20),X390(20),X391(20),X392(20),X393(20),X394(20),X395(20),X396(20),X397(20),X398(20),X399(20),X400(20),X401(20),X402(20),X403(20),X404(20),X405(20),X406(20),X407(20),X408(20),X409(20),X410(20),X411(20),X412(20),X413(20),X414(20),X415(20),X416(20),X417(20),X418(20),X419(20),X420(20),X421(20),X422(20),X423(20),X424(20),X425(20),X426(20),X427(20),X428(20),X429(20),X430(20),X431(20),X432(20),X433(20),X434(20),X435(20),X436(20),X437(20),X438(20),X439(20),X440(20),X441(20),X442(20),X443(20),X444(20),X445(20),X446(20),X447(20),X448(20),X449(20),X450(20),X451(20),X452(20),X453(20),X454(20),X455(20),X456(20),X457(20),X458(20),X459(20),X460(20),X461(20),X462(20),X463(20),X464(20),X465(20),X466(20),X467(20),X468(20),X469(20),X470(20),X471(20),X472(20),X473(20),X474(20),X475(20),X476(20),X477(20),X478(20),X479(20),X480(20),X481(20),X482(20),X483(20),X484(20),X485(20),X486(20),X487(20),X488(20),X489(20),X490(20),X491(20),X492(20),X493(20),X494(20),X495(20),X496(20),X497(20),X498(20),X499(20),X500(20),X501(20),X502(20),X503(20),X504(20),X505(20),X506(20),X507(20),X508(20),X509(20),X510(20),X511(20),X512(20),X513(20),X514(20),X515(20),X516(20),X517(20),X518(20),X519(20),X520(20),X521(20),X522(20),X523(20),X524(20),X525(20),X526(20),X527(20),X528(20),X529(20),X530(20),X531(20),X532(20),X533(20),X534(20),X535(20),X536(20),X537(20),X538(20),X539(20),X540(20),X541(20),X542(20),X543(20),X544(20),X545(20),X546(20),X547(20),X548(20),X549(20),X550(20),X551(20),X552(20),X553(20),X554(20),X555(20),X556(20),X557(20),X558(20),X559(20),X560(20),X561(20),X562(20),X563(20),X564(20),X565(20),X566(20),X567(20),X568(20),X569(20),X570(20),X571(20),X572(20),X573(20),X574(20),X575(20),X576(20),X577(20),X578(20),X579(20),X580(20),X581(20),X582(20),X583(20),X584(20),X585(20),X586(20),X587(20),X588(20),X589(20),X590(20),X591(20),X592(20),X593(20),X594(20),X595(20),X596(20),X597(20),X598(20),X599(20),X600(20),X601(20),X602(20),X603(20),X604(20),X605(20),X606(20),X607(20),X608(20),X609(20),X610(20),X611(20),X612(20),X613(20),X614(20),X615(20),X616(20),X617(20),X618(20),X619(20),X620(20),X621(20),X622(20),X623(20),X624(20),X625(20),X626(20),X627(20),X628(20),X629(20),X630(20),X631(20),X632(20)

```

0033	50 FORMAT(45H) PARAMETER VALUE DIFFERENCING INTERVAL /	017230
	1 (1A,2X,G14.5,6X,G14.5))	017240
0034	WRITE(6,55)	017250
0035	55 FORMAT(//)	017260
	C EVALUATE F, G AND H.	017270
0036	CALL FSTNT(7,F)	017280
0037	IF(MMZ.EQ.0) GO TO 85	017290
0038	DO 80 J=1,NPMZ	017300
0039	CALL FSTNT(J,RJ(J))	017310
0040	80 CONTINUE	017320
0041	IF(NXOPG.EQ.3) GO TO 85	
0042	CALL PRESEN(DU,KTEST)	
	C COMPUTE DEL F.	017330
0043	85 CALL GRAC(0)	017340
0044	DO 90 I=1,N	017350
0045	X3H(I) = DEL(I)	017360
0046	90 CONTINUE	017370
	C COMPUTE (DEL)**2 P - STORED IN A.	017380
0047	CALL SECOR(2)	017390
	C PERFORM THE L-U DECOMPOSITION OF A.	017400
0048	DO 100 I=1,N	017410
0049	DELX(I)=C.0	017420
0050	100 CONTINUE	017430
0051	NPENT3	017440
0052	NT3=1	017450
0053	CALL INVER5(1)	017460
	C CHECK TO MAKE SURE AN ORTHOGONAL MOVE IS NOT ATTEMPTED.	017470
0054	DO 110 I=1,N	017480
0055	IF(DELX(I).EQ.0.C) GO TO 110	017490
0056	WRITE(6,105)	017500
0057	105 FORMAT(64H) THE MATRIX OF SECOND PARTIALS IS NOT POSITIVE DEFINITE	017510
	1. SENSITIVITY ANALYSIS IS TERMINATED)	017520
	GO TO 272	017530
0058	110 CONTINUE	017540
0059	DO 120 I=1,NPAR	017550
0060	X2H(I) = PAR(I)	017560
0061	120 CONTINUE	017570
0062	DO 200 J=1,NPAR	017580
0063	IF(NXKLP5.EQ.0) GO TO 115	
0064	IF(KTEST(J).EQ.0) GO TO 200	
0065	115 IF(NXKLP4.EQ.0) GO TO 121	
0066	CALL LMULT(1,DELMU,DEM,DU)	
0067	C COMPUTE D(DEL P)/DA(J) AND D(F)/DA(J) USING CENTRAL DIFFERENCING.	017590
0068	121 PAR(J) = FAF(J) + DPAP(J)	017600
0069	CALL FSTNT(3,DF)	017610
0070	IF(W.EQ.0) GO TO 126	017620
0071	DO 125 I=1,M	017630
0072	CALL FSTNT(1,RJ(I))	017640
0073	IF(RJ(I).GT.AVAL) GO TO 125	017650
0074	123 DPAP(J)=C.1*DPAP(J)	017660
0075	PAR(J) = X2H(J)	017670
0076	WRITE(6,124) J,DPAP(J)	017680
0077	124 FORMAT(16H RESETTING DPAP(,1,2V3H)= ,G14.5)	017690
0078	IF(DPAR(J).EQ.0.) GO TO 231	017700
0079	GO TO 121	017710
0080	125 CONTINUE	017720
0081	126 IF(MZ.EQ.0) GO TO 128	017730
0082	DO 127 I=1,MZ	017740
0083	MZPI=M+1	017750
0084	CALL FSTNT(MZPI,PJ(MZPI))	017760
0085	127 CONTINUE	017770
0086	128 IF(NXKPA.EQ.0) GO TO 129	
0087	CALL LMULT(1,DELMU,DEM,DU)	
0088	129 CALL GRAC(2)	
0089	DO 130 I=1,N	017780
0090	DELX(I)=DELX0(I)	017800
0091	130 CONTINUE	017810
0092	DEM=2.C*DPAP(J)	017820
0093	PAR(J)=PAR(J) - DEM	017830
0094	CALL FSTNT(0,VAL)	017840
0095	IF(W.EQ.0) GO TO 136	017850
0096	DO 135 I=1,M	017860
0097	CALL FSTNT(1,RJ(I))	017870
0098	IF(RJ(I).GT.AVAL) GO TO 135	017880
0099	GO TO 123	017890
0100	135 CONTINUE	017900
0101	136 IF(MZ.EQ.0) GO TO 139	017910
0102	DO 137 I=1,MZ	017920
0103	MZPI=M+1	017930
0104	CALL FSTNT(MZPI,PJ(MZPI))	017940
0105	137 CONTINUE	017950

```

0106      138 IF(NEXCF4.F0.C) GO TO 139
0107      CALL LMULT(2,DELMU,DEM,DU)
0108      139 CALL GFAD(2)
0109      DF=(DF-VAL)/DEM
0110      DO 140 I=1,N
0111      DELX(I)=(DELX(I) - DELX0(I))/DEM
0112      140 CONTINUE
0113      PAR(J) = X2H(J)
C HAVING ALREADY FACTORED A, SOLVE A*X=B FOR X,
C WHERE B=DFELX AND X=DX/DA(J).
0114      CALL INVER(2)
C PRINT OUT DX/DA(J)
0115      WRITE(6,150) J
0116      150 FORMAT(47H X-DERIVATIVES ARE WITH RESPECT TO PARAMETER ,I2)
0117      DO 170 I=1,M,6
0118      II=MING(I+5,N)
0119      WRITE(6,160) ((JJ,DELX(JJ)),JJ=I,II)
0120      160 FORMAT(44H DX(,I2,2H)=,G14,7)
0121      170 CONTINUE
0122      IF(NEXCF4.F0.C) GO TO 375
0123      IF(M.F0.C) GO TO 301
0124      CALL LMULT(3,DELMU,DEM,DU)
0125      WRITE(6,155) J
0126      350 FORMAT(41H U-DERIVATIVES WITH RESPECT TO PARAMETER ,I2)
0127      DO 351 I=1,M,6
0128      II=MING(I+5,M)
0129      WRITE(6,152) ((JJ,DU(JJ)),JJ=I,II)
0130      152 FORMAT(64H DU(,I2,2H)=,G14,7)
0131      351 CONTINUE
0132      301 IF(M2.F0.C) GO TO 375
0133      CALL LMULT(4,DELMU,DEM,DU)
0134      WRITE(6,160) J
0135      360 FORMAT(41H W-DERIVATIVES WITH RESPECT TO PARAMETER ,I2)
0136      DO 361 I=1,M2,6
0137      II=MING(I+5,M2)
0138      WRITE(6,162) ((JJ,DU(JJ+M)),JJ=I,II)
0139      362 FORMAT(64H DW(,I2,2H)=,G14,7)
0140      361 CONTINUE
0141      375 CONTINUE
C COMPUTE DF/DA(J).
0142      DO 130 I=1,N
0143      DF = DF + X3H(I)*DELX(I)
0144      130 CONTINUE
C PRINT DF/DA(J).
0145      * WRITE(6,190) DF
0146      190 FORMAT(17X,13HDF(X(I))/DA= ,G14,6/10H *****)
0147      200 CONTINUE
0148      GO TO 202
0149      201 WRITE(6,100) J
0150      106 FORMAT(1H ,21HTERMINATING PARAMETER,13,16H DUE TO DPAR = 0 /)
0151      GO TO 200
0152      202 NT3=NP
0153      CALL REJECT
0154      DO 205 I=1,N
0155      DELX(I) = DELTX(I)
0156      205 DELX(I) = DELT(I)
0157      RETURN
0158      END

```

017970
017980
017990
018000
018010
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018030
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018080
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019220
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019280
019290
019300
019310

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0001      SUBROUTINE LMULT(IND,DELMU,DEM,DU)
0002      IMPLICIT REAL*8(A-H,O-Z)
0003      REAL*8 AHCIN,RATIO,EPSI,THETA0,XEP1,XEP2
0004      COMMON/SHARE/X(20),DFI(20),A(20,20),N,M,MN,NP1,NM1
0005      COMMON/VALUE/F,G,PG,ESIGMA,RJ(40),RHO
0006      COMMON/EOAL/ H, M1, M2
0007      COMMON/CRST/DELX(20),DELY(20),PHOIN,RATIO,EPSI,THETA0,
      INTCTA,NUMINI,X1(20),X2(20),X3(20),XF2(20),XF1(20),PRI,
      ZPP2,P1,F1,RJ1(40),DOTT,PGFAD(20),DIAG(20),
      SPEV3,ADLX,RSIG1,G1,NPHASE,NSATIS
      DIMENSION DELMU(40),DU(40)
      MMZ = M + M2
      GO TO (1,2,3,3), IND

      C IND = 0
      DO 100 I=1,MMZ
0011      100 DELMU(I) = 0.
0012      RETURN
0013

      C IND = 1
0014      1 DO 50 I=1,MMZ
0015      50 DELMU(I) = RJ(I)
0016      RETURN

      C IND = 2
0017      2 DO 60 I=1,MMZ
0018      60 DELMU(I) = (DELMU(I) - RJ(I))/DEM
0019      RETURN

      C IND = 3
0020      3 DO 70 I=1,MMZ
0021      CALL GRAD1(I)
0022      CALL RESTNT(I,VAL)
0023      SUM = 0.
0024      DO 71 JJ=1,N
0025      71 SUM = SUM + DEL(JJ)*DELY(JJ)
0026      IF(IND.EQ.4) GO TO 80
0027      DU(I) = -(SUM + DELMU(I))*RHO/(VAL**2)
0028      GO TO 70
0029      80 DU(I) = 2.0*(SUM + DELMU(I))/RHO
0030      70 CONTINUE
0031      RETURN
0032      END

```

```

0001      SUBROUTINE PROCFN(DU,KTEST)
0002      IMPLICIT REAL*8(A-H,C-Z)
0003      COMMON/SHAPE/X(20),DEL(20),A(20,20),N,M,MN,NP1,NM1
0004      COMMON/VALUE/F,G,F0,F1,SIGMA,RJ(40),RHO
0005      COMMON/FOCAL/H, H1,M2
0006      COMMON/SEN/PA0(20),DPA0(20),NPAR,ISENS
0007      DIMENSION GX(40),DU(40),KTEST(20),KLIST(20)
0008      MPMZ = M + M2
0009      FTEST = C*(C1 + CABS(F))
0010      DO 100 J=1,NPAR
0011      KTEST(J) = 0
0012      PAR(J) = PAR(J) + DPAR(J)
0013      CALL FSTNT(0,DF)
0014      IF(MPMZ.EQ.0) GO TO 20
0015      DO 10 I=1,MPMZ
0016      CALL FSTNT(I,DU(I))
0017      CONTINUE
0018      20      DEM = 2. + DPAR(J)
0019      PAR(J) = PAR(J) - DEM
0020      CALL FSTNT(0,XF)
0021      IF(MPMZ.EQ.0) GO TO 40
0022      DO 30 I=1,MPMZ
0023      CALL FSTNT(I,GX(I))
0024      CONTINUE
0025      40      DFPS = (DF - XF)/DEM
0026      IF(MPMZ.EQ.0) GO TO 60
0027      DO 50 I=1,MPMZ
0028      DU(I) = (DU(I) - GX(I))/DEM
0029      SUM = DFPS
0030      IF(V.EQ.0) GO TO 80
0031      DO 70 I=1,M
0032      SUM = SUM - RHC/RJ(I)*DU(I)
0033      80      IF(MZ.EQ.0) GO TO 95
0034      TSUM = 0.
0035      DO 90 I=1,MZ
0036      IK = I+M
0037      TSUM = TSUM + RJ(IK)*DU(IK)
0038      SUM = SUM + TSUM * 2./RHO
0039      95      DEL(J) = SUM
0040      PAR(J) = PAR(J) + DPAR(J)
0041      DTEST = DABS(DEL(J))
0042      IF(DTEST.GT.FTEST) KTEST(J) = 1
0043      100     CONTINUE
0044      WRITE(6,603)
0045      600     FORMAT(22X,'34OPTIMAL VALUE FUNCTION SENSITIVITY' //)
0046      DO 200 I=1,NPAR,5
0047      II=MIN(I+4,NPAR)
0048      WRITE(6,601) ((JJ,DEL(JJ)), JJ=I,II)
0049      601     FORMAT(5(7H DF/DA(,12,2H)=,G14.7))
0050      200     CONTINUE
0051      JJ = 0
0052      DO 250 J=1,NPAR
0053      IF(KTEST(J).EQ.0) GO TO 250
0054      JJ = JJ + 1
0055      KLIST(JJ) = J
0056      250     CONTINUE
0057      IF(JJ.EQ.0) GO TO 300
0058      WRITE(6,602)
0059      602     FORMAT(/51H DETAILED SENSITIVITY RESULTS FOLLOW FOR PARAMETERS )
0060      WRITE(6,603) (KLIST(I), I=1,JJ)
0061      603     FORMAT(1H 40(12,2H ,))
0062      WRITE(6,604)
0063      604     FORMAT(/)
0064      RETURN
0065      300     WRITE(6,605)
0066      605     FORMAT(4H THERE ARE NO DETAILED SENSITIVITY RESULTS //)
0067      RETURN
0068      END

```

APPENDIX B

USER SUBROUTINES FOR SCHRADY-CHOE PROBLEM

```

0001      SUBROUTINE READIN
0002      IMPLICIT REAL*8(A-H,O-Z)
0003      COMMON/INV/BETA(20),PHI(20),DENSE(20),IDENT(20),NI
0004      COMMON/SEN/PAR(20),OPAR(20),NPAR,ISENS
0005      901  FORMAT(15,A,F12.6)
0006      READ(5,901) NI,PAR(1),PAR(2)
0007      WRITE(6,901) NI,PAR(1),PAR(2)
0008      DO 100 I=1,NI
0009      READ(5,901) IDENT(I),(PAR(4*I-2+J),J=1,4)
0010      WRITE(6,901) IDENT(I),(PAR(4*I-2+J),J=1,4)
0011      100  CONTINUE
0012      NPAR = 4*NI+2
0013      RETURN
0014      END

0001      SUBROUTINE RESTNT(IN,VAL)
0002      IMPLICIT REAL*8(A-H,O-Z)
0003
0004      COMMON/SHAPE/X(20),DEL(20),A(20,20),N,M,MN,NP,NI
0005      COMMON/INV/BETA(20),PHI(20),DENSE(20),IDENT(20),NI
0006      COMMON/SEN/PAR(20),OPAR(20),NPAR,ISENS
0007      VAL = 0.
0008      IF(IN.EQ.0) GO TO 300
0009      IF(IN.EQ.1) GO TO 100
0010      200  DO 250 I=1,NI
0011      IJ = 2*I-1
0012      QO = X(IJ)
0013      IF(QO.LE.0.) GO TO 180
0014      250  VAL = VAL + PAR(4*I+2)/QO
0015      VAL = PAR(2) - VAL
0016      RETURN
0017      180  VAL = -1.0
0018      RETURN
0019      100  DO 150 I=1,NI
0020      IJ1 = 2*I
0021      IJ = IJ1 - 1
0022      PR = X(IJ1)
0023      IF(PR.LE.0.) GO TO 180
0024      QO = X(IJ)
0025      IF(QO.LT.0.) GO TO 180
0026      150  VAL = VAL + PAR(4*I+1)*(PR+QO/2.-PAR(4*I-1))
0027      VAL = PAR(1) - VAL
0028      RETURN
0029      300  DO 350 I=1,NI
0030      IJ1 = 2*I
0031      IJ = IJ1 - 1
0032      QO = X(IJ)
0033      PR = X(IJ1)
0034
0035      UU = PAR(4*I-1)
0036
0037      SS = PAR(4*I)
0038
0039      DELTA = PR - UU
0040      ZN = DELTA / SS
0041      CALL ANDTR(ZN,F1,DEN)
0042      PHI(I) = F1
0043      DENSE(I) = DEN
0044      BETA(I) = 0.5*((SS+SS*DELTA*DELTA)*PHI(I)-SS*DELTA*DENSE(I))
0045      350  VAL = VAL + BETA(I)/QO
0046      RETURN
0047      END

```

```

0001      SUBROUTINE GRAD1(IN)
0002      IMPLICIT REAL*8(A-H,O-Z)
0003      COMMON/SHARE/X(20),DEL(20),A(20,20),N,M,MN,NP1,NM1
0004      COMMON/INV/BETA(20),PHI(20),DENSE(20),IDENT(20),NI
0005      COMMON/SEN/PAR(20),OPAR(20),NPAR,ISENS
0006      IF(IN.EQ.0) GO TO 300
0007      IF(IN.EQ.1) GO TO 100
0008      DO 250 I=1,NI
0009      IJ1 = 2*I
0010      IJ = IJ1 - 1
0011      QQ = X(IJ)
0012      DEL(IJ1) = 0.
0013      250 DEL(IJ) = PAR(4*I+2)/QQ/QQ
0014      RETURN
0015      100 DO 150 I=1,NI
0016      IJ1 = 2*I
0017      IJ = IJ1 - 1
0018      DEL(IJ1) = -PAR(4*I+1)
0019      150 DEL(IJ) = DEL(IJ1)/2.
0020      RETURN
0021      300 DO 350 I=1,NI
0022      IJ1 = 2*I
0023      IJ = IJ1 - 1
0024      QQ = X(IJ)
0025      RR = X(IJ1)
0026      UU = PAR(4*I-1)
0027      SS = PAR(4*I)
0028      DELTA = RR - UU
0029      ZN = DELTA / SS
0030      CALL ANDR(ZN,F1,DEN)
0031      PHI(I) = F1
0032      DENSE(I) = DEN
0033      BETA(I) = 0.5*((SS*SS+DELTA*DELTA)*PHI(I)-SS*DELTA*DENSE(I))
0034      DEL(IJ1) = (DELTA*PHI(I)-SS*DENSE(I))/QQ
0035      350 DEL(IJ) = -BETA(I)/QQ/QQ
0036      RETURN
0037      END
0038
0001      SUBROUTINE MATR1X(IN,IKK)
0002      IMPLICIT REAL*8(A-H,O-Z)
0003      COMMON/SHARE/X(20),DEL(20),A(20,20),N,M,MN,NP1,NM1
0004      COMMON/INV/BETA(20),PHI(20),DENSE(20),IDENT(20),NI
0005      COMMON/SEN/PAR(20),OPAR(20),NPAR,ISENS
0006      IF(IN.EQ.0) GO TO 300
0007      IF(IN.EQ.1) GO TO 100
0008      DO 250 I=1,NI
0009      IJ = 2*I-1
0010      QQ = X(IJ)
0011      250 A(IJ,IJ) = -2.*PAR(4*I+2)/QQ**3
0012      RETURN
0013      100 IKK = 1
0014      RETURN
0015      300 DO 350 I=1,NI
0016      IJ1 = 2*I
0017      IJ = IJ1 - 1
0018      QQ = X(IJ)
0019      RR = X(IJ1)
0020      UU = PAR(4*I-1)
0021      SS = PAR(4*I)
0022      DELTA = RR - UU
0023      ZN = DELTA / SS
0024      CALL ANDR(ZN,F1,DEN)
0025      PHI(I) = F1
0026      DENSE(I) = DEN
0027      BETA(I) = 0.5*((SS*SS+DELTA*DELTA)*PHI(I)-SS*DELTA*DENSE(I))
0028      A(IJ,IJ) = 2.*BETA(I)/QQ**3
0029      A(IJ,IJ1) = -(DELTA*PHI(I)-SS*DENSE(I))/QQ/QQ
0030      350 A(IJ1,IJ1) = PHI(I)/QQ
0031      RETURN
0032      END
0033
0001      SUBROUTINE ANDR(XX,PHI,DENSE)
0002      IMPLICIT REAL*8(A-H,O-Z)
0003      AX = 0.455(XX)
0004      T = 1.57/(1.3+0.2316419*AX)
0005      DENSE = C.3492423*DEXP(-XX*XX/2.)
0006      PHI = DENSE*T*((1.330274*T - 1.021256)*T+1.781478)*T
0007      I = 0.3505638*T + 0.3193815
0008      IF(XX) 1,2
0009      1 PHI = 1.0 - PHI
0010      2 RETURN
0011      END

```

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