Mathematical Programming 10 (1976) 287–311.
North-Holland Publishing Company

SENSITIVITY ANALYSIS FOR NONLINEAR PROGRAMMING USING PENALTY METHODS*

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Received 26 July 1974
Revised manuscript received 18 August 1975

In this paper we establish a theoretical basis for utilizing a penalty-function method to estimate sensitivity information (i.e., the partial derivatives) of a local *solution* and its associated Lagrange multipliers of a large class of nonlinear programming problems with respect to a general parametric variation in the problem functions. The local solution is assumed to satisfy the second order sufficient conditions for a strict minimum. Although theoretically valid for higher order derivatives, the analysis concentrates on the estimation of the first order (first partial derivative) sensitivity information, which can be explicitly expressed in terms of the problem functions. For greater clarity, the results are given in terms of the mixed logarithmic-barrier quadratic-loss function. However, the approach is clearly applicable to *any algorithm* that generates a once differentiable "solution trajectory".

1. Introduction

The primary purpose of this paper is the theoretical validation of a technique for estimating the sensitivity of a local solution of a general mathematical programming problems to a small parametric variation of the problem functions. The solution point in question is assumed to satisfy the second order sufficient conditions for strict (locally unique) local optimization [11, Theorem 4]. Although the approach allows, in theory, for the use of any procedure that generates the appropriate estimates of the first order Kuhn–Tucker parameters, it is structured here to provide an intimate correspondence with, and exploitation of, a particular penalty function algorithm. Although existence results are obtained for higher order derivatives, the analysis concentrates on the explicitly tractable first order (first partial derivative) sensitivity information.

The main results may be viewed as extensions of sensitivity results

* Supported by the U.S. Army Research Office, Durham.

and extrapolation results that were presented in [11] (in particular Theorems 6 and 17).

A number of authors have studied the variational behavior of the *solution value* or *the set of solution points* of a parametric mathematical programming problem. Most of these results, some of them known for some time, appear to be concerned with the continuity of these entities in terms of continuity properties of the point-to-set mapping that defines the constraint set as a function of the parameter. Results of this nature may be found in [2, 8, 9, 13 and 16]. Related results for problems having special structure may be found in the literature of parametric programming. At an elemental unstructured level, sufficient conditions such that any neighborhood of a compact set of local solution points (of a given mathematical programming problem) will eventually contain a local solution of a related sequence of problems were recently given by the author [10], in terms of the limiting behavior of the respective sequence of constraint sets.

The distinguishing feature of the sensitivity analysis given in [11, Theorem 6] was the inclusion of results pertaining to the *rate of change* of a solution point. It provided:

(1) a demonstration of the relationship of the second order sufficient optimality conditions (for a strict local solution) to the existence and behavior of first order variations of a local solution and the associated Lagrange multipliers, when the problem functions are subject to parametric variations,

(2) the explicit representation of the first partial derivatives of the local solution point and the associated Lagrange multipliers with respect to the problem parameters. The main results here first extend this theory to incorporate a larger class of parametric problems, and then synthesize this sensitivity theory with an extension of the penalty function extrapolation theory presented in [11, Theorem 17, in particular].

A generalization of the basic sensitivity results given in [11, Theorem 6] is obtained in Section 2 for a large class of nonlinear programming problems involving parametric variation. Essentially, first order (i.e., first derivative) sensitivity information is determined for a second order local solution and the associated Lagrange multipliers. Closely related results have also been obtained by Bigelow and Shapiro [3] and Robinson [19].

A basis for estimating the sensitivity information is established and explicitly related to the usual logarithmic-barrier quadratic-loss penalty function algorithm, in Section 3, giving rise to a procedure for calculating the desired estimates. Two small examples involving parameters are resolved using the indicated method, in Section 4. Also, higher order partial derivatives (with respect to the involved parameters) are shown to exist under appropriate differentiability assumptions on the problem functions, and other extensions (e.g., to parametric programming) are suggested. An indication of the status of computational implementation of the approach, and acknowledgements, are briefly summarized in Section 5. A few remarks concerning related results are given in Section 6.

2. First-order sensitivity analysis of a second order local solution

We give a generalization of a result presented in [11]. Consider the problem of determining a local solution $x(\epsilon)$ of

$$\text{P}(\epsilon) \qquad \begin{aligned} &\min_x f(x, \epsilon), \\ &\text{s.t.} \quad g_i(x, \epsilon) \geqslant 0 \quad (i = 1, ..., m), \qquad h_j(x, \epsilon) = 0 \quad (j = 1, ..., p), \end{aligned}$$

where $x \in \mathrm{E}^n$ and ϵ is a parameter vector in E^k.

The Lagrangian of $P(\epsilon)$ is defined as

$$L(x, u, w, \epsilon) \equiv f(x, \epsilon) - \sum_{i=1}^{m} u_i g_i(x, \epsilon) + \sum_{j=1}^{p} w_j h_j(x, \epsilon) . \qquad (2.1)$$

Throughout the paper, if there are no inequality constraints, simply suppress reference to the functions g_i and the associated multipliers u_i, and do likewise for the h_j and w_j if there are no equalities. In all cases, the gradient vector and Hessian matrix operators, respectively denoted by ∇ and ∇^2, are taken with respect to x.

We are interested in analyzing the behavior of a local solution $x(\hat{\epsilon})$ of $P(\hat{\epsilon})$ when $\hat{\epsilon}$ is subject to perturbation. For simplicity in notation, we shall assume that $\hat{\epsilon} = 0$ (without loss of generality). Conditions will be given that guarantee the existence of a local solution $x(\epsilon)$ of $P(\epsilon)$ in a neighborhood of $x(0)$ for ϵ in a neighborhood of 0, along with the associated optimal Lagrange multipliers $u(\epsilon)$ and $w(\epsilon)$. Under these conditions, the components of all these quantities are shown to be uniquely defined differentiable functions of ϵ in a neighborhood of $\epsilon = 0$.

We shall make critical use of the second order sufficient conditions for a locally unique solution of a mathematical programming problem.

These conditions are now well known, although they have only recently been seriously exploited. They are developed and verified in [11, Theorem 4] and in a number of papers (several of which are given as references in [11]). For the problem $P(0)$, the conditions may be stated as follows.

Lemma 2.1 (second order sufficient conditions for a local isolated minimizing point of problem $P(0)$). *If the functions defining problem $P(0)$ are twice continuously differentiable in a neighborhood of x^*, then x^* is a local isolated (locally unique) minimizing point of problem $P(0)$ if there exist (Lagrange multiplier) vectors $u^* \in \mathrm{E}^m$ and $w^* \in \mathrm{E}^p$ such that the first order Kuhn–Tucker conditions hold, i.e.,*

$$\begin{aligned} &g_i(x^*, 0) \geqslant 0 \quad (i = 1, ..., m)\,, \\ &h_j(x^*, 0) = 0 \quad (j = 1, ..., p)\,, \\ &u_i^* g_i(x^*, 0) = 0 \quad (i = 1, ..., m)\,, \\ &u_i^* \geqslant 0 \quad (i = 1, ..., m)\,, \end{aligned}$$

$$\nabla L(x^*, u^*, w^*, 0) \equiv \nabla f(x^*, 0) - \sum_{i=1}^{m} u_i^* \nabla g_i(x^*, 0) + \sum_{j=1}^{p} w_j^* \nabla h_j(x^*, 0) = 0$$

and further if $y^{\mathrm{T}} \nabla^2 L(x^*, u^*, w^*, 0)\, y > 0$ for all $y \neq 0$ such that

$$\begin{aligned} &y^{\mathrm{T}} \nabla g_i(x^*, 0) \geqslant 0 \quad \text{for all } i, \text{ where } g_i(x^*, 0) = 0\,, \\ &y^{\mathrm{T}} \nabla g_i(x^*, 0) = 0 \quad \text{for all } i, \text{ where } u_i^* > 0\,, \\ &y^{\mathrm{T}} \nabla h_j(x^*, 0) = 0 \quad (j = 1, ..., p)\,. \end{aligned}$$

These conditions are applicable whether or not constraints are present, and whether or not there exists a vector y as indicated. If there are no constraints, the above conditions are logically valid if reference to the constraints is suppressed. This leads to the well known sufficient conditions that x^* be an isolated local unconstrained minimizing point of $f(x, 0)$: $\nabla f(x^*, 0) = 0$ and $y^{\mathrm{T}} \nabla^2 f(x^*, 0)\, y > 0$ for all $y \neq 0$. If there are no $y \neq 0$ satisfying the indicated relationships with the constraint gradients and the first order Kuhn–Tucker conditions hold, then (x^*, u^*, w^*) again logically satisfies these second order conditions. As a point of interest it is observed that in such a case there must be n linearly independent binding-constraint gradients at x^*. For example, if $P(0)$ is a linear programming problem and the second order conditions hold at (x^*,u^*,w^*), then, since $\nabla^2 L \equiv 0$, there can be no $y \neq 0$ satisfying the given inequalities, i.e., x^* must be a vertex of the feasible region defined by the constraints of $P(0)$.

A slight strengthening of the second order strict sufficiency conditions at $(x^*, 0)$ and the appropriate differentiability assumptions lead to the following generalization of a result proved in [11, Theorem 6].

Theorem 2.1 (first-order sensitivity results for a second order local minimizing point x^*). *If*

(i) *the functions defining $P(\epsilon)$ are twice continuously differentiable in (x, ϵ) in a neighborhood of $(x^*, 0)$,*

(ii) *the second order sufficient conditions for a local minimum of $P(0)$ hold at x^*, with associated Lagrange multipliers u^* and w^*,*

(iii) *the gradients $\nabla g_i(x^*, 0)$ (for i such that $g_i(x^*, 0) = 0$) and $\nabla h_j(x^*, 0)$ (all j) are linearly independent, and*

(iv) *$u_i^* > 0$ when $g_i(x^*, 0) = 0$ ($i = 1, ..., m$) (i.e., strict complementary slackness),*

then

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

(c) *strict complementarity (with respect to $u(\epsilon)$ and the inequality constraints) and linear independence of the binding constraint gradients hold at $x(\epsilon)$ for ϵ near 0.*

Proof. (Part (a) follows if (b) is true. It is stated separately because it follows without differentiability in ϵ or assumption (iv).) The fact that x^* is a local isolated minimum of $P(0)$ follows from assumption (ii), which also implies that $\nabla L(x^*,u^*,w^*,0) = 0$. The uniqueness of u^* and w^* follows from this and assumption (iii).

The proof of (b) follows from a straightforward application of the implicit function theorem [14] to the first order necessary optimality conditions of $P(\epsilon)$, as follows.

Assumption (ii) implies the satisfaction of the Kuhn–Tucker first-order conditions

$$\begin{aligned} &\nabla L(x, u, w, \epsilon) = 0 \,, \\ &u_i g_i(x, \epsilon) = 0 \quad (i = 1, ..., m) \,, \\ &h_j(x, \epsilon) = 0 \quad (j = 1, ..., p) \,, \end{aligned} \tag{2.2}$$

at $(x, u, w, \epsilon) = (x^*, u^*, w^*, 0)$. Assumption (i) implies that the system of eqs. (2.2) is once continuously differentiable in all the arguments, so in particular, the Jacobian matrix of (2.2) with respect to (x,u,w) is well-defined. It follows that assumptions (ii), (iii) and (iv) imply the existence of the inverse of this matrix at $(x^*,u^*,w^*,0)$. (An immediate extension of [11, Theorem 14], and now a well-known result.)

The assumptions of the implicit function theorem with respect to eqs. (2.2) and the particular solution $(x^*,u^*,w^*,0)$ are satisfied and we can conclude that in a neighborhood of (x^*,u^*,w^*), for ϵ in a neighborhood of 0, there exists a unique once continuously differentiable function $[x(\epsilon), u(\epsilon), w(\epsilon)]$ satisfying (2.2), with $[x(0), u(0), w(0)] = (x^*,u^*,w^*)$. The satisfaction of (2.2) means that for ϵ near 0, $x(\epsilon)$ is a first-order Kuhn–Tucker point of problem $P(\epsilon)$, with associated Lagrange multipliers $u(\epsilon)$ and $w(\epsilon)$.

To complete the proof of (b), we first note that the binding constraint set at $x(0)$ remains the same for ϵ near 0. This is seen immediately for the equalities $h_j[x(\epsilon),\epsilon] = 0$, since $x(\epsilon)$ satisfies (2.2) near $\epsilon = 0$. For the inequalities, we have from (2.2) that $u_i(\epsilon)\, g_i[x(\epsilon),\epsilon] = 0$ $(i = 1, ..., m)$ near $\epsilon = 0$. If $g_i[x(0),0] = 0$ for some i, then $u_i(0) > 0$ (by strict complementary slackness), hence $u_i(\epsilon) > 0$ near $\epsilon = 0$ by continuity of $u(\epsilon)$ and we conclude that $g_i[x(\epsilon),\epsilon] = 0$. If $g_i[x(0),0] > 0$ for some i, then $g_i[x(\epsilon),\epsilon] > 0$ near $\epsilon = 0$ by continuity. Therefore, defining

$$B(\epsilon) \equiv \{i \mid g_i[x(\epsilon), \epsilon] = 0\} \,,$$

we have concluded that $B(\epsilon) = B(0)$ for ϵ near 0. (The argument also shows that strict complementary slackness is preserved for ϵ near 0, proving the first part of (c).)

We now assert that the second order sufficient optimality conditions (Lemma 2.1) hold at $[x(\epsilon), w(\epsilon), w(\epsilon)]$ for any ϵ near 0. We must show that there exists $\delta > 0$ such that for any ϵ such that $|\epsilon| < \delta$, it follows that $y^{\mathrm{T}}(\epsilon)\ \nabla^2 L[x(\epsilon), u(\epsilon), w(\epsilon)]\, y(\epsilon) > 0$ for any vector $y(\epsilon) \neq 0$ such that $y^{\mathrm{T}}(\epsilon) \nabla g_i[x(\epsilon),\epsilon] = 0$ for all $i \in B(0)$ and $y^{\mathrm{T}}(\epsilon)\ \nabla h_j[x(\epsilon),\epsilon] = 0$ for all j. This may be proved as follows. Suppose the assertion is false. Then there must exist $\epsilon_k > 0$ and $y^k \neq 0$ such that $\epsilon_k \to 0$, $(y^k)^{\mathrm{T}}\ \nabla g_i[x(\epsilon_k),\epsilon_k] = 0$ for all $i \in B(0)$, $(y^k)^{\mathrm{T}}\ \nabla h_j[x(\epsilon_x),\epsilon_k] = 0$ for all j, and $(y^k)^{\mathrm{T}}\ \nabla^2 L[x(\epsilon_k), u(\epsilon_k)\, w(\epsilon_k), \epsilon_k]\, y^k \leqslant 0$ for $k = 1,2, \ldots$. Without loss of generality, assume $\|y^k\| = 1$ for all k. Select a convergent subsequence of $\{y^k\}$, relabel the subsequence $\{y^k\}$ for convenience and call the limit $\bar{y}$. Taking limits as $k \to +\infty$ and recalling assumption (i) yields the conclusion that $\bar{y}^{\mathrm{T}}\ \nabla^2 L(x^*,u^*,w^*,0)\, \bar{y} \leqslant 0$ for some $\bar{y}$ such that $\|\bar{y}\| = 1$, $y^{\mathrm{T}}\ \nabla g_i(x^*,0) = 0$ for all $i \in B(0)$ and $y^{\mathrm{T}}\ \nabla h_j(x^*,0) = 0$ for all j. But this is a contradiction of assumption (ii) and the proof of the assertion is complete.

Since it was established that $[x(\epsilon),u(\epsilon),w(\epsilon)]$ uniquely solves (2.2) for ϵ near 0, it follows that $x(\epsilon)$ is a locally unique local minimum of $P(\epsilon)$ with associated unique Lagrange multipliers $u(\epsilon)$ and $w(\epsilon)$, completing the proof of part (b).

The preservation of strict complementary slackness was proved above. The preservation of the linear independence of the (say) $r + b$ binding constraint gradients at $x(\epsilon)$ for ϵ near 0 follows directly from the fact that an $(r + p)$ by $(r + p)$ Jacobian of the system of equations defined by the constraints that are binding at $x(0)$ must be nonsingular, along with the assumed continuity of the first derivatives.

Bigelow and Shapiro [3] have obtained a similar generalization and an extension for the problem with inequality constraints, removing the requirement of strict complementary slackness and showing the existence of directional derivatives of a solution and the associated Lagrange multipliers. Robinson [19] also has recently proved an analogous theorem under weaker assumptions (specifically, assumption (i) is replaced by the assumption that the second partial derivatives of the problem functions with respect to x are jointly continuous in (x,ϵ)), and demonstrated the resulting continuity of $(x(\epsilon),u(\epsilon),w(\epsilon))$ near $\epsilon = 0$. He also obtains bounds on the variation of $(x(\epsilon),u(\epsilon),w(\epsilon))$ for small changes in ϵ and uses these to determine convergence rates for a large class of algorithms.

The conditions of the theorem are assumed to hold in the remainder of this section.

With $(x,u,w) = [x(\epsilon),u(\epsilon),w(\epsilon)]$, eqs. (2.2) are identically satisfied for

ϵ near 0 and can be differentiated with respect to ϵ to yield explicit expressions for the first partial derivatives of this vector function. Define the matrices,

$$\mathrm{d}x/\mathrm{d}\epsilon = [\partial x_i/\partial \epsilon_j] \quad (i = 1, ..., n;\ j = 1, ..., k)\ ,$$
$$\mathrm{d}u/\mathrm{d}\epsilon \equiv [\partial u_i/\partial \epsilon_j] \quad (i = 1, ..., m;\ j = 1, ..., k)\ ,$$
$$\mathrm{d}w/\mathrm{d}\epsilon \equiv [\partial w_i/\partial \epsilon_j] \quad (i = 1, ..., p;\ j = 1, ..., k)\ .$$

For convenience, let $y(\epsilon) \equiv [x(\epsilon), u(\epsilon), w(\epsilon)]^{\mathrm{T}}$, and also define

$$\partial/\partial\epsilon(\nabla_x L) \equiv [\partial^2 L/\partial x_i \partial \epsilon_j]^{\mathrm{T}} \quad (i = 1, ..., n;\ j = 1, ..., k)\ ,$$
$$\partial g_i/\partial\epsilon \equiv [\partial g_i/\partial\epsilon_1, ..., \partial g_i/\partial\epsilon_k]^{\mathrm{T}} \quad (i = 1, ..., m)\ ,$$
$$\partial h_j/\partial\epsilon \equiv [\partial h_j/\partial\epsilon_1, ..., \partial h_j/\partial\epsilon_k]^{\mathrm{T}} \quad (j = 1, ..., p)\ .$$

It follows from the fact that the total derivative of (2.2) with respect to ϵ is zero for ϵ near 0 that

$$M(\epsilon)\ \mathrm{d}y(\epsilon)/\mathrm{d}\epsilon = N(\epsilon)\ , \tag{2.3}$$

where

$$M(\epsilon) \equiv \begin{bmatrix} \nabla^2 L & -\nabla g_1, ... -\nabla g_m & \nabla h_1, ..., \nabla h_p \\ u_1 \nabla^{\mathrm{T}} g_1 & g_1 \quad\quad 0 & \\ \vdots & \quad\ddots & 0 \\ u_m \nabla^{\mathrm{T}} g_m & 0 \quad\quad g_m & \\ \nabla h_1 & & \\ \vdots & 0 & 0 \\ \nabla h_p & & \end{bmatrix},$$

the Jacobian matrix of (2.2) with respect to (x,u,w), evaluated at $[y(\epsilon),\epsilon]$ and

$$N(\epsilon) \equiv \left[-\frac{\partial}{\partial\epsilon}(\nabla_x L), -u_1 \frac{\partial g_1}{\partial\epsilon}, ..., -u_m \frac{\partial g_m}{\partial\epsilon}, -\frac{\partial h_1}{\partial\epsilon}, ..., -\frac{\partial h_p}{\partial\epsilon} \right]^{\mathrm{T}},$$

the negative of the Jacobian matrix of (2.2) with respect to ϵ, evaluated at $[y(\epsilon),\epsilon]$. Since M is nonsingular for ϵ near 0, it follows that

$$\mathrm{d}y(\epsilon)/\mathrm{d}\epsilon = M^{-1}(\epsilon)\ N(\epsilon)\ , \tag{2.4}$$

where the quantities involved are defined above and ϵ is in a neighborhood of 0. In particular, we have that

$$\mathrm{d}y(0)/\mathrm{d}\epsilon = (M^*)^{-1}N^* \,, \tag{2.5}$$

where $y(0) = [x(0),u(0),w(0)]^{\mathrm{T}} \equiv (x^*,u^*,w^*)^{\mathrm{T}}$, $M^* = M(0)$ and $N^* = N(0)$. Also, since the quantities involved in (2.4) are all continuous in their arguments (from the assumptions of the theorem and the consequences of the implicit function theorem), (2.5) is also the limit of (2.4) as $\epsilon \to 0$, i.e.,

$$\lim_{\epsilon \to 0} \frac{\mathrm{d}y(\epsilon)}{\mathrm{d}\epsilon} = \frac{\mathrm{d}y(0)}{\mathrm{d}\epsilon} \,. \tag{2.6}$$

It is important to note that $\mathrm{d}y(\epsilon)/\mathrm{d}\epsilon$, a first-order estimate of the variation of an isolated local solution $x(\epsilon)$ of problem $P(\epsilon)$ and the associated unique Lagrange multipliers $u(\epsilon)$ and $w(\epsilon)$, *can be calculated* from (2.4) once $[x(\epsilon),u(\epsilon),w(\epsilon)]$ has been determined. In particular, $\mathrm{d}y(0)/\mathrm{d}\epsilon$, and hence a first order Taylor series approximation of $[x(\epsilon),u(\epsilon),w(\epsilon)]$ in a neighborhood of $\epsilon = 0$, is available from (2.5) once (x^*,u^*,w^*) is known. This is summarized in the following statement.

Corollary 2.1 (first order estimation of $[x(\epsilon),u(\epsilon),w(\epsilon)]$ near $\epsilon = 0$). *Under the assumptions of Theorem* 2.1, *a first order approximation of* $[x(\epsilon),u(\epsilon),w(\epsilon)]$ *in a neighborhood of* $\epsilon = 0$ *is given by*

$$\begin{bmatrix} x(\epsilon) \\ u(\epsilon) \\ w(\epsilon) \end{bmatrix} = \begin{bmatrix} x^* \\ u^* \\ w^* \end{bmatrix} + (M^*)^{-1}N^*\epsilon + o(\|\epsilon\|) \,, \tag{2.7}$$

where $(x^*,u^*,w^*) = [x(0),u(0),w(0)]$, $M^* = M(0)$, $N^* = N(0)$, *and* $M(\epsilon)$ *and* $N(\epsilon)$ *are defined as in* (2.3).

3. Approximation of first order sensitivity information using a penalty method algorithm

In the previous section, a first order analysis is given of the variation of a local isolated solution $x(\epsilon)$ of a general problem $P(\epsilon)$, along with the associated Lagrange multipliers $[u(\epsilon),w(\epsilon)]$, when ϵ is perturbed about $\epsilon = 0$. As indicated, once $(x^*,u^*,w^*) \equiv [x(0),u(0),w(0)]$ is available, $\mathrm{d}y(0)/\mathrm{d}\epsilon$ can be calcualted using (2.5) and hence $[x(\epsilon),u(\epsilon),w(\epsilon)]$ can be estimated (in some neighborhood of $\epsilon = 0$) using eq. (2.7).

Although this result is of considerable interest, in practice it is desirable to be able to estimate $\mathrm{d}y(0)/\mathrm{d}\epsilon$ without requiring prior determination of (x^*,u^*,w^*). It develops that the class of algorithms based on twice-differentiable penalty functions can readily be adapted to provide this estimate, *without additional assumptions.* Essentially, we formulate an appropriate penalty function for the problem $P(\epsilon)$, thus absorbing the problem parameter directly into the penalty-function. It follows that the assumptions of Theorem 2.1 guarantee the existence of a *trajectory* of unconstrained local minima of the penalty function converging to x^*. For changes in ϵ near $\epsilon = 0$, perturbations of this trajectory are shown to relate closely to perturbations of $x(\epsilon)$.

For convenience and to be more specific, the results will be given in terms of the logarithmic barrier function combined with a Courant quadratic penalty term to handle the equality constraints [11, p. 84]. For the problem $P(\epsilon)$, this function is written

$$W(x,\epsilon,r) \equiv f(x,\epsilon) - r \sum_{i=1}^{m} \ln g_i(x,\epsilon) + (\tfrac{1}{2}r) \sum_{j=1}^{p} h_j^2(x,\epsilon) , \qquad (3.1)$$

where r is a positive real parameter. The analysis can be carried out in a similar fashion for any twice-differentiable penalty function. Numerous interesting properties involving such penalty functions have been documented in [11] and elsewhere. For our present purposes, we shall prove the following results that are extensions of results obtained in [11, Theorems 6 and 17].

To avoid various trivial exceptions, it is assumed in the following that at least one constraint is present in $P(\epsilon)$.

Theorem 3.1 (approximation of first order sensitivity results and determination of estimates from $W(x,\epsilon,r)$). *If the assumptions of Theorem 2.1 hold, then in a neighborhood about* $(\epsilon,r) = (0,0)$ *there exists a unique once continuously differentiable vector function* $[x(\epsilon,r),u(\epsilon,r), w(\epsilon,r)]$ *satisfying*

$$\begin{aligned} &\nabla L(x,u,w,\epsilon) = 0 , && \\ &u_i g_i(x,\epsilon) = r && (i = 1, ..., m) , \\ &h_j(x,\epsilon) = w_j r && (j = 1, ..., p) , \end{aligned} \qquad (3.2)$$

with $[x(0,0),u(0,0),w(0,0)] = (x^*,u^*,w^*)$, *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* $W(x,\epsilon,r)$, *with* $g_i[x(\epsilon,r),\epsilon] > 0$ $(i = 1, ..., m)$ *and* $\nabla^2 W[x(\epsilon,r),\epsilon,r]$ *positive definite.*

Proof. The existence of $[x(\epsilon,r),u(\epsilon,r),w(\epsilon,r)]$ as described follows from the implicit function theorem [14] using the same argument as is used in Theorem 2.1 to prove part (b), noting that the Jacobian matrices of (3.2) and (2.2) coincide when $r = 0$.

The fact that $g_i[x(\epsilon,r),\epsilon] > 0$ for all i such that $g_i(x^*,0) > 0$ follows for all (ϵ,r) near $(0,0)$ since $g_i(x(\epsilon,r),\epsilon] \to g_i(x^*,0)$ as $(\epsilon,r) \to (0,0)$. For i such that $g_i(x^*,0) = 0$, the fact that $u_i(\epsilon,r) \to u_i^* > 0$ (the latter inequality deriving from the assumption of strict complementary slackness) as $(\epsilon,r) \to (0,0)$ implies from (3.2) that $g_i[x(\epsilon,r),\epsilon] = r/u_i(\epsilon,r) > 0$ for $r>0$ and (ϵ,r) near $(0,0)$. Thus, $g_i[x(\epsilon,r),\epsilon] > 0$ $(i = 1, ..., m)$ providing $r > 0$ and (ϵ,r) is sufficiently close to $(0,0)$.

By the definitions (3.1) of W and (2.1) of L we have that

$$\nabla W = f - \sum_{i=1}^{m} (r/g_i) \nabla g_i + \sum_{j=1}^{p} (h_j/r) \nabla h_j \,, \tag{3.3}$$

$$\nabla L = \nabla f - \sum_{i=1}^{m} u_i \nabla g_i + \sum_{j=1}^{p} w_j \nabla h_j \,. \tag{3.4}$$

Consequently, providing only that $g_i \neq 0$ (all i) and $r \neq 0$, so that W is well-defined, *any* solution (x,u,w) of the system (3.2) yields $\nabla W = \nabla L = 0$. In particular, this is true for $(x,u,w) = [x(\epsilon,r),u(\epsilon,r),w(\epsilon,r)]$ and we can conclude (using also the fact proved in the previous paragraph) that

$$W[x(\epsilon,r),\epsilon,r] \equiv \nabla L[x(\epsilon,r),u(\epsilon,r),w(\epsilon,r),\epsilon] = 0$$

for $r > 0$ and (ϵ,r) sufficiently close to $(0,0)$. Thus, the first order necessary condition that $x(\epsilon,r)$ be an unconstrained minimizing point of $W(x,\epsilon,r)$ is satisfied (for (ϵ,r) as indicated).

In the remainder of the proof assume, for convenience of notation, that all functions are evaluated at $[x(\epsilon,r),u(\epsilon,r),w(\epsilon,r)]$ unless otherwise specified. The positive definiteness of $\nabla^2 W$ for ϵ near 0 and $r > 0$ and small can be shown as follows.

We make use of the following facts. Differentiating (3.3) and (3.4) with respect to x and comparing yields

$$\nabla^2 W = \nabla^2 L + \sum_{i=1}^{m} (r/g_i^2)\, \nabla g_i\, \nabla^{\mathrm{T}} g_i + (1/r) \sum_{j=1}^{p} \nabla h_j\, \nabla^{\mathrm{T}} h_j$$

and pre- and post-multiplying by any vector Z and using (3.2) gives

$$Z^{\mathrm{T}} \nabla^2 W\, Z = Z^{\mathrm{T}} \nabla^2 L\, Z + \sum_{i=1}^{m} (u_i/g_i)\, (Z^{\mathrm{T}} \nabla g_i)^2 + (1/r) \sum_{j=1}^{p} (Z^{\mathrm{T}} \nabla h_j)^2 \,. \tag{3.5}$$

Also, recall that the second-order sufficient conditions, together with strict complementary slackness, imply that

$$\begin{aligned} &Z^{\mathrm{T}} \nabla^2 L\, (x^*,u^*,w^*,0)\, Z > 0 \quad \text{for } Z \neq 0 \text{ such that} \\ &Z^{\mathrm{T}} \nabla g_i(x^*,0) = 0 \quad \text{for all } i \in B^* \equiv \{i\text{: } g_i(x^*,0) = 0\} \,, \\ &Z^{\mathrm{T}} \nabla h_j(x^*,0) = 0 \quad (j = 1, ..., p) \,. \end{aligned} \tag{3.6}$$

Consider any sequence $\{\epsilon_k, r_k\}$ with $r_k > 0$ and $(\epsilon_k, r_k) \to (0,0)$. If suffices to show that $Z_k^{\mathrm{T}} \nabla W_k^2 Z_k > 0$ for k large, where $\{Z_k\}$ is an arbitrary sequence of unit vectors in E^n and $\nabla^2 W_k$ denotes the Hessian of W evaluated at (ϵ_k, r_k). For convenience, let

$$g_i^* \equiv g_i(x^*,0),\ h_j^* \equiv h_j(x^*,0), \ \text{ and } L^* \equiv L(x^*,u^*,w^*,0) \,.$$

Select a convergent subsequence of $\{Z_k\}$, relabel it $\{Z_k\}$ for convenience, and call the limit (unit vector) $\bar{Z}$. If $\bar{Z} \nabla g_i^* \neq 0$ for some $i \in B^*$ or if $\bar{Z} \nabla h_j^* \neq 0$ for some j, then taking limits in (3.5) with $Z = Z_k$ and $(\epsilon, r) = (\epsilon_k, r_k)$ and recalling the assumption of strict complementary slackness, yields the conclusion that $Z_k^{\mathrm{T}} \nabla^2 W_k Z_k \to +\infty$ as $k \to +\infty$. If $\bar{Z}^{\mathrm{T}} \nabla g_i^* = 0$ for all $i \in B^*$ and $\bar{Z}^{\mathrm{T}} \nabla h_j^* = 0$ for $j = 1, ..., p$, then we again take limits over the appropriate subsequence in (3.5) to conclude that

$$\liminf_k Z_k^{\mathrm{T}} \nabla^2 W_k Z_k \geqslant \liminf Z_k^{\mathrm{T}} \nabla^2 L_k Z_k = \bar{Z}^{\mathrm{T}} \nabla^2 L^* \bar{Z} > 0 \,,$$

because of (3.6) (assumption (ii)).
This shows that $Z^{\mathrm{T}} \nabla^2 W\, Z > 0$ for *all* $Z \neq 0$, providing $r > 0$ and (ϵ, r)

is close to (0,0), i.e., $\nabla^2 W$ is positive definite for all such (ϵ,r). This implies that $x(\epsilon,r)$ is a unique local minimizing point of $W(x,\epsilon,r)$ for any ϵ near 0 and $r > 0$ and small, completing the proof.

With $(x,u,w)^T = [x(\epsilon,r),u(\epsilon,r),w(\epsilon,r)]^T \equiv y(\epsilon,r)$, eqs. (3.2) are identically satisfied for (ϵ,r) in a neighborhood of (0,0). Using the chain rule, differentiation of (3.2) with respect to ϵ yields

$$M(\epsilon,r)\ \mathrm{d}y(\epsilon,r)/\mathrm{d}\epsilon = N(\epsilon,r)\ , \tag{3.7}$$

the precise analogy of (2.3), where the quantities in this equation correspond term by term with those appearing in (2.3), except that the $p \times p$ zero matrix (the last p rows and columns) that appeared in the Jacobian matrix $M(\epsilon)$ is now replaced in the new Jacobian matrix $M(\epsilon,r)$ by a $p \times p$ diagonal matrix with each diagonal element equal to $-r$. Corresponding to eqs. (2.4) and (2.5), respectively, we have, since $M(\epsilon,r)$ is nonsingular for (ϵ,r) near (0,0), that

$$\mathrm{d}y(\epsilon,r)/\mathrm{d}\epsilon = M^{-1}(\epsilon,r)\ N(\epsilon,r)\ , \tag{3.8}$$

$$\mathrm{d}y(0,0)/\mathrm{d}\epsilon = M^{-1}(0,0)\ N(0,0) = (M^*)^{-1}N^*\ , \tag{3.9}$$

where M^* and N^* are as defined in (2.5).

Since the systems of eqs. (2.2) and (3.2) coincide when $r = 0$, the conclusions of Theorems 2.1 and 3.1 imply that $y(\epsilon,0) = y(\epsilon)$ and $\mathrm{d}y(\epsilon,0)/\mathrm{d}\epsilon = \mathrm{d}y(\epsilon)/\mathrm{d}\epsilon$ for ϵ sufficiently close to 0. Hence, from Theorem 3.1 we can conlcude that for any $\bar{\epsilon}$ in a neighborhood of $\epsilon = 0$,

$$y(\epsilon,r) \to y(\bar{\epsilon},0) = y(\bar{\epsilon})\ , \tag{3.10}$$

$$\mathrm{d}y(\epsilon,r)/\mathrm{d}\epsilon \to \mathrm{d}y(\bar{\epsilon},0)/\mathrm{d}\epsilon = \mathrm{d}y(\bar{\epsilon})/\mathrm{d}\epsilon \tag{3.11}$$

as $(\epsilon,r) \to (\bar{\epsilon},0)$, with (ϵ,r) confined to a neighborhood of (0,0). In particular, for $(\epsilon,r) \to (0,0)$,

$$y(\epsilon,r) \to y(0,0) = y(0) = [x(0),u(0),w(0)]^T = (x^*,u^*,w^*)^T\ , \tag{3.12}$$

$$\mathrm{d}y(\epsilon,r)/\mathrm{d}\epsilon \to \mathrm{d}y(0,0)/\mathrm{d}\epsilon = \mathrm{d}y(0)/\mathrm{d}\epsilon = (M^*)^{-1}N^*\ . \tag{3.13}$$

Based on these results, it is apparent that we can estimate $y(\epsilon) = [x(\epsilon),u(\epsilon),w(\epsilon)]^T$ and $\mathrm{d}y(\epsilon)/\mathrm{d}\epsilon$ as closely as desired for ϵ near 0, by $y(\epsilon,r) = [x(\epsilon,r),u(\epsilon,r),w(\epsilon,r)]^T$ and $\mathrm{d}y(\epsilon,r)/\mathrm{d}\epsilon$, respectively, providing r is sufficiently close to 0. Having obtained a solution $y(\epsilon,r)$ of (3.2) for

(ϵ,r) sufficiently close to (0,0), $dy(\epsilon,r)/d\epsilon$ can be calculated from (3.8).

Though, in principle, any technique could be utilized that yields a solution of (3.2) near $(\epsilon,r) = (0,0)$, we have obviously formulated the system (3.2) – which should properly be viewed as a perturbation of the first order necessary conditions for a local minimizing point of problem $P(\epsilon)$ – such that it is satisfied by $[x(\epsilon,r),u(\epsilon,r),w(\epsilon,r)]$ for $r > 0$ if and only if the logarithmic-barrier quadratic-loss function $W(x,\epsilon,r)$ is minimized by $x(\epsilon,r)$ (with the multipliers $u(\epsilon,r)$ and $w(\epsilon,r)$ appropriately defined, as specified). Thus, the indicated algorithm is the usual penalty function procedure based on determining, for fixed ϵ, the unconstrained minimizing points $\{x(\epsilon,r_k)\}$ of $\{W(x,\epsilon,r_k)\}$ for $r_k > 0$ and $r_k \downarrow 0$, $k = 1,2,...,$ for x such that $g_i(x,\epsilon) > 0$ (all i) in an appropriate neighborhood of $x(0,0) = x^*$.

Having determined $x(\epsilon,r_k)$, an estimate of $x(\epsilon)$ when k is large, the Lagrange multipliers $(u(\epsilon),w(\epsilon))$ can be estimated from the relations $u_i(\epsilon,r_k) = r_k/g_i[x(\epsilon,r_k),\epsilon]$, $w_j(\epsilon,r_k) = h_j[x(\epsilon,r_k),\epsilon]/r_k$ (all i and j). It follows that the vector $y(\epsilon,r_k) = [x(\epsilon,r_k),u(\epsilon,r_k),w(\epsilon,r_k)]$ is a solution of (3.2) and $y(\epsilon,r_k) \to [x(\epsilon),u(\epsilon),w(\epsilon)]^T$ as $k \to \infty$. The first partial derivatives of $y(\epsilon,r_k)$ with respect to ϵ can then be obtained from eq. (3.8), and would constitute an estimate of $dy(\epsilon)/d\epsilon$ (according to (3.11)), providing k is large and ϵ is near 0.

An alternative to utilizing eq. (3.8) to calculate $dy(\epsilon,r)/d\epsilon$ is available, using the fact that the Hessian of $W(x,\epsilon,r)$ is nonsingular at a minimizing point $x(\epsilon,r)$. This will be seen to have the advantage of involving a smaller matrix inverse – that of the $n \times n$ Hessian of W rather than the $(n+m+p) \times (n+m+p)$ Jacobian matrix $M(\epsilon,r)$ appearing in (3.8) – *and requires only information that is readily available from the W function at a minimizing point.* In this approach, the penalty function is minimized to obtain $x(\epsilon,r)$, which determines $dx(\epsilon,r)/d\epsilon$ in terms of quantities available from $W[x(\epsilon,r),\epsilon,r]$ and its Hessian. The multipliers and their derivatives can then be calculated to satisfy (3.2), which determines these quantities as functions of x,ϵ, and r. The matrix $dx(\epsilon,r)/d\epsilon$ is obtained from the following result.

To avoid any ambiguity, denote by $\bar{x}(\epsilon,r)$ the trajectory of local minima of $W(x,\epsilon,r)$ whose existence is proved by the theorem. We showed that when $r > 0$

$$\bar{x}(\epsilon,r) \equiv x(\epsilon,r) \text{ and } d\bar{x}(\epsilon,r)/d\epsilon \equiv dx(\epsilon,r)/d\epsilon \tag{3.14}$$

for (ϵ,r) near (0,0). The following corollary is a direct consequence of

Theorems 2.1 and 3.1 and provides a basis for estimating changes in $x(\epsilon)$ by corresponding changes in $\bar{x}(\epsilon,r)$.

Corollary 3.1 (approximation of $x(\epsilon)$ and $\mathrm{d}x(\epsilon)/\mathrm{d}\epsilon$ by $\bar{x}(\epsilon,r)$ and $\mathrm{d}\bar{x}(\epsilon,r)/\mathrm{d}\epsilon$). *Under the assumptions of Theorem* 3.1, *for* (ϵ,r) *near* (0,0) *and* $r > 0$, *it follows that* $\bar{x}(\epsilon,r) \to x(\bar{\epsilon})$ *and* $\mathrm{d}\bar{x}(\epsilon,r)/\mathrm{d}\epsilon \to \mathrm{d}x(\bar{\epsilon})/\mathrm{d}\epsilon$ as $\epsilon \to \bar{\epsilon}$ *and* $r \to 0$, *and*

$$\mathrm{d}\bar{x}(\epsilon,r)/\mathrm{d}\epsilon = -\{\nabla^2 W[\bar{x}(\epsilon,r),\epsilon,r]\}^{-1}\, \partial/\partial\epsilon \{\nabla W[\bar{x}(\epsilon,r),\epsilon,r]\} \,. \tag{3.15}$$

Proof. Since the system of eqs. (2.2) and (3.2) coincide when $r = 0$, it follows from the conclusions of Theorem 2.1 and 3.1 that, for $r > 0$, and (ϵ,r) near (0,0),

$$\bar{x}(\epsilon,r) \to x(\bar{\epsilon},0) = x(\bar{\epsilon}) \,, \tag{3.16}$$

$$\mathrm{d}\bar{x}(\epsilon,r)/\mathrm{d}\epsilon \to \mathrm{d}x(\bar{\epsilon},0)/\mathrm{d}\epsilon = \mathrm{d}x(\bar{\epsilon})/\mathrm{d}\epsilon$$

as $\epsilon \to \bar{\epsilon}$ and $r \to 0$ (where convergence is component by component, in all cases). From the fact that $\nabla W[\bar{x}(\epsilon,r),\epsilon,r] = 0$ and $\bar{x}(\epsilon,r)$ is once continuously differentiable for any ϵ near 0 and $r > 0$ and small, it follows that

$$\nabla^2 W[\bar{x}(\epsilon,r),\epsilon,r]\, \mathrm{d}\bar{x}(\epsilon,r)/\mathrm{d}\epsilon + \partial/\partial\epsilon\ \nabla W[\bar{x}(\epsilon,r),\epsilon,r] = 0 \,,$$

and since we showed that $\nabla^2 W$ is positive definite for (ϵ,r) near (0,0) and $r > 0$, we obtain the expression given in (3.15) for $\mathrm{d}\bar{x}(\epsilon,r)/\mathrm{d}\epsilon$.

This result gives the basis for approximating $u(\bar{\epsilon})$ and $w(\bar{\epsilon})$ as well. With (ϵ,r) near (0,0) and $r > 0$, defining

$$\bar{u}_i(\epsilon,r) \equiv r/g_i[\bar{x}(\epsilon,r),\epsilon] \quad (i = 1, ..., n) \,, \tag{3.17}$$

$$\bar{w}_j(\epsilon,r) \equiv h_j[\bar{x}(\epsilon,r),\epsilon]/r \quad (j = 1, ..., p), \tag{3.18}$$

since

$$\nabla L[\bar{x}(\epsilon,r),\bar{u}(\epsilon,r),\bar{w}(\epsilon,r),\epsilon] = \nabla W[\bar{x}(\epsilon,r),\epsilon,r] = 0$$

it follows that $\bar{y}(\epsilon,r) \equiv [\bar{x}(\epsilon,r),\bar{u}(\epsilon,r),\bar{w}(\epsilon,r)]^{\mathrm{T}}$ is a solution of (3.2). Therefore, Theorems 2.1 and 3.1 imply that

$$\bar{u}_i(\epsilon,r) \to u_i(\bar{\epsilon},0) = u_i(\bar{\epsilon}) \quad (i = 1, ..., m) \,, \tag{3.19}$$

$$\bar{w}_j(\epsilon,r) \to w_j(\bar{\epsilon},0) = w_j(\bar{\epsilon}) \quad (j = 1, ..., p) \tag{3.20}$$

as $(\epsilon,r) \to (\bar{\epsilon},0)$.

Differentiation of (3.17) and (3.18) with respect to the s^{th} component of ϵ yields

$$\partial \bar{u}_i(\epsilon,r)/\partial\epsilon_s = (-r/g_i^2)\,\mathrm{d}g_i/\mathrm{d}\epsilon_s$$
$$= (-r/g_i^2)\,(\nabla^{\mathrm{T}} g_i \partial\bar{x}(\epsilon,r)/\partial\epsilon_s + \partial g_i/\partial\epsilon_s) \quad (i = 1, ..., m;\; s = 1, ..., k)\,, \tag{3.21}$$

$$\partial \bar{w}_j(\epsilon,r)/\partial\epsilon_s = (1/r)\,\partial h_j/\partial\epsilon_s$$
$$= (1/r)\,(\nabla^{\mathrm{T}} h_j \partial\bar{x}(\epsilon,r)/\partial\epsilon_s + \partial h_j/\partial\epsilon_s) \quad (j = 1, ..., p;\; s = 1, ..., k)\,, \tag{3.22}$$

where the functions are all evaluated at $[\bar{x}(\epsilon,r),\epsilon]$. The previous results also imply that the matrices whose components are given respectively by (3.21) and (3.22) converge component-wise as follows.

$$\mathrm{d}\bar{u}(\epsilon,r)/\mathrm{d}\epsilon \to \mathrm{d}u(\bar{\epsilon},0)/\mathrm{d}\epsilon = \mathrm{d}u(\bar{\epsilon})/\mathrm{d}\epsilon\,, \tag{3.23}$$

$$\mathrm{d}\bar{w}(\epsilon,r)\mathrm{d}\epsilon \to \mathrm{d}w(\bar{\epsilon},0)/\mathrm{d}\epsilon = \mathrm{d}w(\bar{\epsilon})/\mathrm{d}\epsilon \tag{3.24}$$

as $\epsilon \to \bar{\epsilon}$ and $r \to 0$.

Consequently, we can estimate $y(\epsilon)$ and $\mathrm{d}y(\epsilon)/\mathrm{d}\epsilon$ by $\bar{y}(\epsilon,r)$ and $\mathrm{d}\bar{y}(\epsilon,r)/\mathrm{d}\epsilon$ for (ϵ,r) sufficiently close to $(0,0)$ and $r > 0$. For any such (ϵ,r), *these quantities can all be calculated* once a local unconstrained minimizing point $\bar{x}(\epsilon,r)$ of $W(x,\epsilon,r)$ has been determined (in the region such that $g_i[x(\epsilon,r),\epsilon] > 0$ $(i = 1, ..., m)$), in a suitable open set containing $x(\epsilon,0)$.

Returning to the problem $P(0)$, it follows that *the usual penalty function approach* utilizing $W(x,0,r)$ to find a local solution of this problem can be used to approximate $y(0) = (x^*,u^*,w^*)^{\mathrm{T}}$ and $\mathrm{d}y(0)/\mathrm{d}\epsilon$. A minimizing sequence $\{\bar{x}(0,r_k)\}$ of $\{W(x,0,r_k)\}$ converging to x^* is guaranteed by Theorem 3.1 for $r_k > 0$ and small. The point $\bar{x}(0,r_k)$ may be considered an estimate of x^*. The quantities involved in the right-hand side of (3.15) can be evaluated at $\epsilon = 0$, $r = r_k$, once $\bar{x}(0,r_k)$ has been determined, yielding the estimate

$$\mathrm{d}x(0)/\mathrm{d}\epsilon \doteq \mathrm{d}\bar{x}(0,r_k)/\mathrm{d}\epsilon = \{\nabla^2 W[\bar{x}(0,r_k),0,r_k]\}^{-1}\partial/\partial\epsilon\{\nabla W[\bar{x}(0,r_k),0,r_k]\}\,. \tag{3.25}$$

The associated Lagrange multipliers $[u(\epsilon),w(\epsilon)]$ and their first partial derivatives at $\epsilon = 0$ can then be estimated from

$$u(0) \doteq \bar{u}(0,r_k)\,, \tag{3.26}$$

$$w(0) \doteq \bar{w}(0,r_k)\,, \tag{3.27}$$

$$\mathrm{d}u(0)/\mathrm{d}\epsilon \doteq \mathrm{d}\bar{u}(0,r_k)/\mathrm{d}\epsilon\,, \tag{3.28}$$

$$\mathrm{d}w(0)/\mathrm{d}\epsilon \doteq \mathrm{d}\bar{w}(0,r_k)/\mathrm{d}\epsilon\,, \tag{3.29}$$

where the respective quantities on the right are obtained from the relations (3.17), (3.18), (3.21) and (3.22) evaluated at $\epsilon = 0$, $r = r_k$.

It is important to note, from the point of view of computational implementation, that the inverse Hessian matrix $[\nabla^2 W]^{-1}$ of the penalty function W that is involved in calculating the estimate $\mathrm{d}\bar{x}(0,r_k)/\mathrm{d}\epsilon$ of $\mathrm{d}x(0)/\mathrm{d}\epsilon$ in (3.25), *will already be available* if one of the several popular variants of the Newton method [11,15], is used to compute the unconstrained minimizing point $\bar{x}(0,r_k)$ of $W(x,0,r_k)$. An estimate of this matrix will be available if a quasi-Newton method [11,15] is used. Thus, utilizing any of these well-known procedures for the unconstrained minimizations, much of the information required to calculate the sensitivity information by this technique will have already been generated in implementing the usual penalty function algorithm. (Of course, the second term $\partial/\partial\epsilon(\nabla W)$ appearing in (3.25) is known once the problem is specified and need only be evaluated at $[\bar{x}(0,r_k),0,r_k]$.)

The analogous observation holds for the calculation of the first partial derivatives of the problem functions at $\bar{x}(0,r_k)$ with respect to ϵ. Using the chain rule, we obtain

$$\mathrm{d}f[x(0,r_k),0]/\mathrm{d}\epsilon = [\mathrm{d}x/\mathrm{d}\epsilon]^{\mathrm{T}}\,\nabla f + \partial f/\partial\epsilon\,, \tag{3.30}$$

where

$$\mathrm{d}f/\mathrm{d}\epsilon \equiv [\mathrm{d}f/\mathrm{d}\epsilon_1, ..., \mathrm{d}f/\mathrm{d}\epsilon_k]^{\mathrm{T}} \quad \text{and}$$

$$\partial f/\partial\epsilon = [\partial f/\partial\epsilon_1, ..., \partial f/\partial\epsilon_k]^{\mathrm{T}}\,,$$

and all arguments are evaluated at $\epsilon = 0$, $r = r_k$. The vector of partials $\partial f/\partial\epsilon$ will be known once the problem is specified and need only be evaluated. The gradient ∇f will normally have already been calculated at $\bar{x}(0,r_k)$, in applying the usual penalty function algorithm. Thus, the work required to obtain the estimate

$$\mathrm{d}f[x(0),\epsilon]/\mathrm{d}\epsilon \doteq \mathrm{d}f[\bar{x}(0,r_k),0]/\mathrm{d}\epsilon$$

is considerably reduced. The same applies to the g_i and h_j, the derivatives of which appear in (3.21) and (3.22).

4. Examples and extensions

The application of the previous theoretical results for estimating sensitivity information may be illustrated by the following simple examples.

Example 1.

$$P_1(\epsilon) \qquad \begin{aligned} &\min x\,, \\ &\text{s.t. } x \geqslant \epsilon, \qquad x \in E^1\,. \end{aligned}$$

The solution of the problem is given uniquely by $x(\epsilon) = \epsilon$, for any ϵ. The hypotheses of Theorem 2.1 may be readily verified for this problem. (Note that the second order sufficient optimality conditions are satisfied in a logical sense, since there are no nonzero vectors orthogonal to the binding constraint gradients.) The Lagrangian (2.1) is given by $L(x,u,\epsilon) \equiv x - u(x - \epsilon)$ and the first order Kuhn–Tucker conditions yield $u(\epsilon) = 1$. We thus find

$$\mathrm{d}x(\epsilon)/\mathrm{d}\epsilon = 1, \qquad \mathrm{d}u(\epsilon)/\mathrm{d}\epsilon = 0 \qquad \text{for all } \epsilon\,.$$

The logarithmic barrier function (3.1) for this problem is $W(x,\epsilon,r) \equiv x - r\ln(x - \epsilon)$, uniquely minimized for $x > \epsilon$ and any $r > 0$ by $x(\epsilon,r) = \epsilon + r$. Hence, for any value of ϵ, $x(\epsilon,r) \to \epsilon = x(\epsilon)$ as $r \to 0$ and $\mathrm{d}x(\epsilon,r)/\mathrm{d}\epsilon \equiv 1 = \mathrm{d}x(\epsilon)/\mathrm{d}\epsilon$, illustrating the conclusions of Corollary 3.1. Also, since $u(\epsilon,r) \equiv r/g[x(\epsilon,r)]$, with $g[x(\epsilon,r)] \equiv x(\epsilon,r) - \epsilon = r$, we have that $u(\epsilon,r) = 1 = u(\epsilon)$ and $\mathrm{d}u(\epsilon,r)/\mathrm{d}\epsilon = 0 = \mathrm{d}u(\epsilon)/\mathrm{d}\epsilon$ for all r.

For this example, the solution $x(\epsilon)$ of $P(\epsilon)$ is unique and differentiable for *any* value of ϵ, and it is noted that the corresponding estimates using the penalty function are valid for *any* ϵ. This might have been anticipated by Theorems 2.1 and 3.1 and Corollary 3.1, since the required assumptions are satisfied for any ϵ.

Example 2.

$$P_2(\epsilon) \qquad \begin{aligned} &\min\ x_1 + \epsilon_1 x_2, \\ &\text{s.t. } g_1(x,\epsilon) \equiv -\epsilon_2^2\, x_1^2 + x_2 \geqslant 0\,, \\ &\phantom{\text{s.t. }} g_2(x,\epsilon) \equiv -x_1 \qquad \geqslant 0 \qquad (x \in E^2)\,. \end{aligned}$$

The first order Kuhn–Tucker conditions imply that the solution and the associated Lagrange multipliers are uniquely given by

$$x_1(\epsilon) = -1/2\epsilon_1\epsilon_2^2 , \qquad x_2(\epsilon) = 1/4\epsilon_1^2\epsilon_2^2 ,$$

$$u_1(\epsilon) = \epsilon_1 , \qquad u_2(\epsilon) = 0 ,$$

where $\epsilon = (\epsilon_1,\epsilon_2)$, for any value of ϵ such that $\epsilon_1 > 0$ and $\epsilon_1\epsilon_2 \neq 0$. We assume that the components of ϵ are so restricted in the following. It is easily verified that the second order conditions hold for $[x(\epsilon),u(\epsilon)]$ as given, and hence it is observed that all the hypotheses of Theorem 2.1 are satisfied for any value of ϵ as indicated.

It follows that

$$\frac{\mathrm{d}x(\epsilon)}{\mathrm{d}\epsilon} \equiv \left[\frac{\mathrm{d}x_1(\epsilon)}{\mathrm{d}\epsilon}, \frac{\mathrm{d}x_2(\epsilon)}{\mathrm{d}\epsilon}\right] = \begin{bmatrix} 1/2\epsilon_1^2\epsilon_2^2 , & -1/2\epsilon_1^3\epsilon_2^2 \\ 1/\epsilon_1\epsilon_2^3 , & -1/2\epsilon_1^2\epsilon_2^3 \end{bmatrix}$$

and

$$\frac{\mathrm{d}u(\epsilon)}{\mathrm{d}\epsilon} \equiv \left[\frac{\mathrm{d}u_1(\epsilon)}{\mathrm{d}\epsilon}, \frac{\mathrm{d}u_2(\epsilon)}{\mathrm{d}\epsilon}\right] = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} .$$

These matrices, whose coefficients give the desired first-order sensitivity information, can also be calculated directly from (2.4).

To estimate these quantities, we use the logarithmic barrier function (3.1), which for our example is

$$W(x,\epsilon,r) \equiv x_1 + \epsilon_1 x_2 - r \ln(x_2 - \epsilon_2^2 x_1^2) - r \ln(-x_1) .$$

As usual, $r > 0$ and the function is minimized over the set of points satisfying the constraints with strict inequality as $r \to 0$. From the requirement of stationarity, $\nabla W(x,\epsilon,r) = 0$, we find that $W(x,\epsilon,r)$ is minimized uniquely (over the indicated region) by

$$x_1(\epsilon,r) = \frac{-1 - (1 + 8\epsilon_1\epsilon_2^2 r)^{1/2}}{4\epsilon_1\epsilon_2^2}, \qquad x_2(\epsilon,r) = \epsilon_2^2 x_1^2(\epsilon,r) + \frac{r}{\epsilon_1} ,$$

for any $r > 0$. As expected from the theory, $x_1(\epsilon,r) \to -1/2\epsilon_1\epsilon_2^2 = x_1(\epsilon)$ and $x_2(\epsilon,r) \to 1/4\epsilon_1^2\epsilon_2^2 = x_2(\epsilon)$ as $r \to 0$.

The Lagrange multipliers associated with $x(\epsilon,r)$ are given by

$$u_1(\epsilon,r) = \frac{r}{g_1[x(\epsilon,r),\epsilon]} = \frac{r}{r/\epsilon_1} = \epsilon_1 ,$$

$$u_2(\epsilon,r) = \frac{r}{g_2[x(\epsilon,r),\epsilon]} = \frac{r}{-x_1(\epsilon,r)}\,.$$

It follows that $u_1(\epsilon,r) \equiv u_1(\epsilon)$ and $u_2(\epsilon,r) \to 0 = u_2(\epsilon)$ as $r \to 0$.

Calculating first derivatives with respect to ϵ we obtain

$$\frac{\mathrm{d}x_1(\epsilon,r)}{\mathrm{d}\epsilon_1} = \frac{-16\epsilon_1\epsilon_2^4(1+8\epsilon_1\epsilon_2^2 r)^{-1/2}\,r + 4\epsilon_2^2[1+(1+8\epsilon_1\epsilon_2^2 r)^{1/2}]}{16\epsilon_1^2\epsilon_2^4}\,,$$

$$\frac{\mathrm{d}x_1(\epsilon,r)}{\mathrm{d}\epsilon_2} = \frac{-32\epsilon_1^2\epsilon_2^3(1+8\epsilon_1\epsilon_2^2 r)^{-1/2}\,r + 8\epsilon_1\epsilon_2[1+(1+8\epsilon_1\epsilon_2^2 r)^{1/2}]}{16\epsilon_1^2\epsilon_2^4}\,.$$

It follows that $\mathrm{d}x_1(\epsilon,r)/\mathrm{d}\epsilon_1 \to 1/2\epsilon_1^2\epsilon_2^2 = \mathrm{d}x_1(\epsilon)/\mathrm{d}\epsilon_1$ and $\mathrm{d}x_1(\epsilon,r)/\mathrm{d}\epsilon_2 \to 1/\epsilon_1\epsilon_2^3 = \mathrm{d}x_1(\epsilon)/\mathrm{d}\epsilon_2$, as $r \to 0$.

One can also verify that

$$\frac{\mathrm{d}x_2(\epsilon,r)}{\mathrm{d}\epsilon_1} = 2\epsilon_2^2 x_1(\epsilon,r)\,\frac{\mathrm{d}x_1(\epsilon,r)}{\mathrm{d}\epsilon_1} - \frac{r}{\epsilon_1^2}\,,$$

$$\frac{\mathrm{d}x_2(\epsilon,r)}{\mathrm{d}\epsilon_2} = 2\epsilon_2^2 x_1(\epsilon,r)\,\frac{\mathrm{d}x_1(\epsilon,r)}{\mathrm{d}\epsilon_2} + 2\epsilon_2 x_1^2(\epsilon,r)\,.$$

Taking limits yields $\mathrm{d}x_2(\epsilon,r)/\mathrm{d}\epsilon_1 \to -1/2\epsilon_1^3\epsilon_2^2 = \mathrm{d}x_2(\epsilon)/\mathrm{d}\epsilon_2$ and $\mathrm{d}x_2(\epsilon,r)/\mathrm{d}\epsilon_2 \to -1/2\epsilon_1^2\epsilon_2^3 = \mathrm{d}x_2(\epsilon)/\mathrm{d}\epsilon_2$ as $r \to 0$, as desired. Thus, $\mathrm{d}x(\epsilon,r)/\mathrm{d}\epsilon \to \mathrm{d}x(\epsilon)/\mathrm{d}\epsilon$ as $r \to 0$, component by component, as concluded from the theory.

Finally, from the previous calculation of $u(\epsilon,r)$, we have that

$$\frac{\mathrm{d}u(\epsilon,r)}{\mathrm{d}\epsilon} = \begin{bmatrix} 1, \dfrac{r}{x_1^2(\epsilon,r)}\,\dfrac{\mathrm{d}x_1(\epsilon,r)}{\mathrm{d}\epsilon_1} \\[2ex] 0, \dfrac{r}{x_1^2(\epsilon,r)}\,\dfrac{\mathrm{d}x_1(\epsilon,r)}{\mathrm{d}\epsilon_2} \end{bmatrix} \to \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \frac{\mathrm{d}u(\epsilon)}{\mathrm{d}\epsilon}$$

as $r \to 0$, and the first order results are complete.

Note that, as in the previous example, the results are valid for a *set* of values of ϵ. In this case, the conditions implying existence and convergence of the quantities obtained above are satisfied as long as $\epsilon_1 > 0$ and $\epsilon_1\epsilon_2 \neq 0$. Thus, for both examples the results go well beyond the calculation and estimation of sensitivity information at a point (for a given value of ϵ), and essentially provide a "parametric analysis". The indicated functions exist for a large set of values of ϵ and the functions depending on the penalty parameter r converge pointwise in ϵ to their indicated limits as $r \to 0$.

These examples suggest that the theoretical results obtained in Sections 2 and 3 can be extended, under appropriate conditions, to allow for a parametric analysis (i.e., a sensitivity analysis in the large). Such would appear to follow, noting that the proofs of the main results hinge primarily on the implicit function theorem applied to the Kuhn–Tucker conditions of problem $P(0)$ and on an appropriate perturbation of those conditions. The respective results are valid in a neighborhood of *any* ϵ or (ϵ,r) for which the conditions (satisfying the hypotheses of the implicit function theorem) are assumed to hold. It appears that we need only invoke the analogous conditions for *every* ϵ or (ϵ,r) in the sets in which these parameters are allowed to vary, to establish the validity of the conclusions in a "neighborhood" of these sets. This argument remains to be investigated.

We conclude with two immediate extensions that may lead to additional developments of this theory.

The following corollary of Theorem 2.1 is an immediate implication of well-known extensions of the implicit function theorem [4,14].

Corollary 4.1 (existence of higher order derivatives). *If the conditions of Theorem* 2.1 *hold, with the assumed order of differentiability being* $k + 1$ $(k \geq 1)$, *then* $y(\epsilon) \equiv [x(\epsilon),u(\epsilon),w(\epsilon)]^{\mathrm{T}} \in C^k$ *in a neighborhood of* $\epsilon = 0$. *If the problem functions are analytic in* (x,ϵ) *in a neighborhood of* $(x^*,0)$, *then* $y(\epsilon)$ *is analytic in a neighborhood of* $\epsilon = 0$.

Proof. The existence and continuity of the higher order partial derivatives and analyticity results from the implicit function theorem and its extensions applied to the system of eq. (2.2) as in the proof of Theorem 2.1.

The following corollary of Theorem 3.1 is also, analogously, an immediate consequence of the same extensions if the implicit function theorem and the fact that the systems of eqs. (2.2) and (3.2) coincide when $r = 0$. The first part precisely parallels Corollary 4.1.

Corollary 4.2 (existence and convergence of higher order derivatives of $y(\epsilon,r)$). *If the assumptions of Theorem* 3.1 *hold and the assumed order of differentiability is* $k+1$ ($k \geqslant 1$), *then*

$$y(\epsilon,r) \equiv [x(\epsilon,r),u(\epsilon,r),w(\epsilon,r)]^{\mathrm{T}} \in C^k$$

in a neighborhood of $(\epsilon,r)=(0,0)$. *If the problem functions are analytic in* (x,ϵ) *in a neighborhood of* $(x^*,0)$, *then* $y(\epsilon,r)$ *is analytic in a neighborhood of* $(\epsilon,r)=(0,0)$. *Furthermore,*

$$y(\epsilon,r) \to y(\epsilon) \quad \text{and} \quad \mathrm{d}y^j(\epsilon,r)/\mathrm{d}\epsilon^j \to \mathrm{d}y^j(\epsilon)/\mathrm{d}\epsilon^j \quad (j=1,\dots,k)$$

as $r \to 0$, *for* (ϵ,r) *near* $(0,0)$.

Proof. The existence and continuity of the higher order partial derivatives and analyticity results from the implicit function theorem and its extensions applied to the system of eqs. (3.2) as in the proof of Theorem 3.1. From this and the fact that (2.2) and (3.2) coincide when $r=0$, we conclude that

$$y(\epsilon,r) \to y(\epsilon,0) = y(\epsilon)\ ,$$

$$\mathrm{d}^j y(\epsilon,r)/\mathrm{d}\epsilon^j \to \mathrm{d}^j y(\epsilon,0)/\mathrm{d}\epsilon^j = \mathrm{d}^j y(\epsilon)/\mathrm{d}\epsilon^j \quad (j=1,\dots,k)$$

as $r \to 0$, in a neighborhood of $(\epsilon,r)=(0,0)$.

These results are not pursued further in this paper. They could have application, e.g., in providing a basis for estimating the parametric vector function $x(\epsilon)$ by developing each component of $x(\epsilon)$ as a power series in ϵ, yielding the estimate $\hat{x}(\epsilon)$. This is precisely analogous to the extrapolation theory developed for estimating the course of a minimizing trajectory (in terms of the involved parameter) in penalty function methodology [11, Chapter 5 and Chapter 8, Section 8.4]. Similarly, $x(\epsilon,r)$ could be developed in a power series $\hat{x}(\epsilon,r)$ in (ϵ,r). For r near 0, $\hat{x}(\epsilon,r)$ may be an adequate estimate of $\hat{x}(\epsilon)$. To construct $\hat{x}(\epsilon,r)$, we could utilize the penalty function method based on $W(x,\epsilon,r)$ to obtain several values of $x(\epsilon,r)$ satisfying (3.2) for $r>0$ and fixed, corresponding to several values of ϵ in a suitable domain.

5. Computational implementation and acknowledgments

Garth McCormick primarily developed the basic sensitivity and extra-

polation theory presented in [11, Theorem 6 and Chapter 5]. As indicated, Theorems 2.1 and 3.1 are a generalization of some of these results. The idea of using the penalty function approach for estimating the sensitivity of a solution of a mathematical programming problem to perturbations emerged from discussions with McCormick and, subsequently, with Beverly Causey, who first implemented the technique [7] with an experimental computer program developed at the Research Analysis Corporation (RAC).

Charles Mylander, also at RAC, corrected and revised the Causey program, recoded this for computer implementation using the SUMT code, and gave a description of a computational procedure and the code in [17]. Recently, in a research study conducted under the author's direction at The George Washington University, Robert Armacost, coordinating with Mylander, further expanded the RAC-Mylander program and implemented it on the IBM 360/50 at The George Washington University Computer Center. Armacost obtained excellent results for several problems, including a number extracted from those reported in [5], introducing a variety of parametric perturbations in these problems. These results appear in a recent paper [1]. A users' guide to the use of the computer program (called SENS-SUMT) was prepared by Mylander and Armacost and appeared as a George Washington University technical paper [18].

The author is indebted to all the above for helpful discussions and insights. He also gratefully acknowledges the referees' thorough review, which resulted in several important corrections and modifications.

6. A note concerning related results

Zoutendijk [22] has suggested using a barrier function to incorporate a (scalar) parameter, primarily, it appears, to enforce satisfaction of a parametric constraint for all values of the parameter between specified bounds.

The barrier function involved is the inverse type (i.e., $\Sigma\ 1/g_i$) and the parametric barrier terms are integrated (mathematically) over the parameter space. This approach apparently has potential practical applications and has recently received some attention in the applied literature [12,20]. In fact, a very successful (and apparently the first) implementation of a generalization of the Zoutendijk idea was reported by Thornton and Schmit [21].

Though the idea of handling the parameter by way of a penalty function obviously coincides with the basic idea of the approach treated here, the motivation, formulation and intended application are apparently quite distinct. The author is unaware of any further developments based on Zoutendijk's suggestion.

More in the spirit of the present analysis, it is noted that Buys [6] has analyzed a parametric augmented Lagrangian (penalty) function for the equality constrained problem with "right-hand side" perturbation. In this case, because the penalty function is "exact", a local unconstrained minimum of this function yields a local solution of the given problem under certain conditions. Further, it follows that this penalty function is such that the local perturbation behavior of the penalty function minimum is also apparently exact, i.e., it coincides with the perturbation behavior of the corresponding solution of the given constrained problem. The results given in [6] are primarily concerned with the behavior of the optimal value function as a function of the right-hand side parameters.

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