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Enlarging the Region of Convergence of Newton's Method for Constrained Optimization[1]

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Abstract. In this paper, we consider Newton's method for solving the system of necessary optimality conditions of optimization problems with equality and inequality constraints. The principal drawbacks of the method are the need for a good starting point, the inability to distinguish between local maxima and local minima, and, when inequality constraints are present, the necessity to solve a quadratic programming problem at each iteration. We show that all these drawbacks can be overcome to a great extent without sacrificing the superlinear convergence rate by making use of exact differentiable penalty functions introduced by Di Pillo and Grippo (Ref. 1). We also show that there is a close relationship between the class of penalty functions of Di Pillo and Grippo and the class of Fletcher (Ref. 2), and that the region of convergence of a variation of Newton's method can be enlarged by making use of one of Fletcher's penalty functions.

Key Words. Constrained minimization, Newton's method, differentiable exact penalty functions, superlinear convergence.

1. Introduction

We consider Newton's method for the constrained optimization problem

(ECP) minimize $f(x)$,
subject to $h(x) = 0$,

where $f: R^n \to R$, $h: R^n \to R^m$. It consists of the iteration

$$x_{k+1} = x_k + \Delta x_k, \qquad \lambda_{k+1} = \lambda_k + \Delta\lambda_k, \tag{1}$$

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where $(\Delta x_k, \Delta\lambda_k) \in R^{n+m}$ is obtained by solving the system of equations

$$\begin{bmatrix} \nabla^2_{xx} L(x_k, \lambda_k) & \nabla h(x_k) \\ \nabla h(x_k)' & 0 \end{bmatrix} \begin{bmatrix} \Delta x_k \\ \Delta\lambda_k \end{bmatrix} = -\begin{bmatrix} \nabla_x L(x_k, \lambda_k) \\ h(x_k) \end{bmatrix}, \tag{2}$$

with $L: R^{n+m} \to R$ being the Lagrangian function

$$L(x, \lambda) = f(x) + \lambda' h(x). \tag{3}$$

If started sufficiently close to a local minimum-Lagrange multiplier pair (x^*, λ^*) satisfying the sufficiency conditions

$$\nabla_x L(x^*, \lambda^*) = 0, \qquad h(x^*) = 0,$$

$$\nabla h(x^*) \text{ has rank } m,$$

$$z'\nabla^2_{xx} L(x^*, \lambda^*) z > 0, \qquad \forall z \neq 0,\ \nabla h(x^*)'z = 0,$$

the method is well defined and converges to (x^*, λ^*) superlinearly.

Recent work has been directed toward extensions to handle inequality constraints and modifications aimed at enlarging the region of convergence of the method. The paper by Mayne and Polak (Ref. 3) is characteristic in this respect, while the work of Powell (Refs. 4 and 5) has similar aims within the context of quasi-Newton versions of iteration (1)–(2). These papers are based on the use of an exact but nondifferentiable penalty function to enforce monotonic descent and combinations with first-order linearization methods of the type first introduced and analyzed by Pshenichnyi (Refs. 6 and 7) [a method of this type was rediscovered in weaker form by Han (Ref. 8), and a related method was proposed by Mayne and Maratos (Ref. 9)]. Inequality constraints are dealt with by solving quadratic programming subproblems in place of linear systems of equations as in Wilson (Ref. 10) and Pshenichnyi (Ref. 6).

The purpose of this paper is to show that the region of convergence of Newton's method can be enlarged by making use of differentiable exact penalty functions. One such function, due to Di Pillo and Grippo (Ref. 1), is given by

$$P(x, \lambda; c, \alpha) = L(x, \lambda) + (c/2)|h(x)|^2 + (\alpha/2)|\nabla_x L(x, \lambda)|^2, \tag{4}$$

where $c > 0$ and $\alpha > 0$ are scalar parameters. It has been shown in Ref. 1 that, if c is chosen sufficiently large, then (x^*, λ^*) is a strict local minimum of P. We show that, near (x^*, λ^*), the solution of the system (2) satisfies an equation of the form

$$\begin{bmatrix} \Delta x_k \\ \Delta\lambda_k \end{bmatrix} = -B(x_k, \lambda_k; c, \alpha) \nabla P(x_k, \lambda_k; c, \alpha),$$

where $B(\cdot,\cdot;c,\alpha)$ is a continuous $(n+m)\times(n+m)$ matrix satisfying, for all $c>0$, $\alpha>0$,

$$B(x^*,\lambda^*;c,\alpha)=[\nabla^2 P(x^*,\lambda^*;c,\alpha)]^{-1}.$$

As a result, iteration (1) may be viewed as a consistent approximation (see Ref. 11) of Newton's method for minimizing $P(\cdot,\cdot;c,\alpha)$ with respect to (x,λ). Based on this fact, one can introduce in iteration (1) a stepsize procedure based on descent of the objective function P, and combine the iteration with the steepest-descent method (for example) to enforce convergence from poor starting points.

Similar results are shown for exact penalty functions of the form

$$P(x,\lambda;c,M)=L(x,\lambda)+(c/2)|h(x)|^2+(1/2)|M(x)\nabla_x L(x,\lambda)|^2, \tag{5}$$

where $c>0$ and $M(\cdot)$ is a continuous $m\times n$ matrix such that $M(x^*)\nabla h(x^*)$ is invertible (Ref. 1).

The advantage that the penalty functions (4), (5) offer over, for example, the penalty function (cf. Tapia, Ref. 12)

$$(1/2)|h(x)|^2+(1/2)|\nabla_x L(x,\lambda)|^2 \tag{6}$$

is that, under mild conditions, a local maximum-Lagrange multiplier pair is also a local minimum of (6), but not of (5) (Ref. 1). We show that the same is true for the penalty function (4), provided α is chosen sufficiently small. Thus, use of (4) and (5) provides a built-in preference toward constrained local minima versus local maxima, while this is not true for the penalty function (6).

Extensions to inequality constraints are also given in this paper and are based on the use of exact penalty functions obtained from (4) and (5) by converting inequality constraints to equality constraints through the use of squared slack variables. The resulting Newton-like methods do not require solution of quadratic programming subproblems, but rather employ systems of linear equations similar to those arising in the equality constrained case and involving only the active and nearly active constraints.

The paper is structured as follows. In Section 2, we review some properties of the exact penalty functions (4) and (5). The material here is based primarily on the work of Refs. 1 and 13. Two new observations are made. First, we show that a local maximum-Lagrange multiplier pair of (ECP) satisfying the second-order sufficiency conditions for optimality cannot be a local minimum of the penalty function (4) if α is sufficiently small. Second, we show that an exact penalty function introduced by Fletcher (Refs. 2, 14, 15) and further utilized and extended by Mukai and Polak (Ref. 16) and Glad and Polak (Ref. 17) can be obtained from the penalty function (5) for a special choice of the matrix $M(x)$. As a result, it follows that the methods of Fletcher (Ref. 15) and Mukai and Polak (Ref. 16) may be viewed as second-order methods for minimizing the penalty function (5) with respect to (x, λ). This suggests that the Newton-like methods of this paper exhibit similar convergence behavior near a solution as those of Refs. 15 and 16. At the same time, they are somewhat simpler in terms of computational burden per iteration, since they do not require a matrix inversion for each function evaluation.

In Section 3, we consider the Newton iteration (1)–(2) for equality constrained problems and show that, asymptotically, it approaches Newton's method for minimizing both penalty functions (4) and (5). Consistent approximations to Newton's method for minimizing the penalty functions have also been suggested and tested by Di Pillo, Grippo, and Lampariello (Ref. 13), following related ideas of Fletcher (Ref. 15). These methods asymptotically approach the Newton iteration (1)–(2), but this close connection was apparently not recognized by the authors of Ref. 13.

In Section 3, we also consider problems with inequality constraints. The corresponding algorithms treat inequality constraints by an implicit active set strategy, whereby constraints perceived by the algorithm to be active at the solution are treated as equalities, while the remaining constraints are ignored and their Lagrange multipliers are set to zero. In this approach, there is no need to solve a quadratic program at each iteration. In this connection, it is worth noting that extension of methods based on Fletcher's ideas to inequality constrained problems has proved to be quite difficult. For example, Glad and Polak (Ref. 17) require a restrictive linear independence assumption on the gradients of the constraint functions in order to prove global convergence for their method. Furthermore, the method requires at each iteration the solution of a system of linear equations involving the gradients of *all* the constraints.

In Section 4, we consider a variation of the Newton iteration (1)–(2) and show that it represents a consistent approximation to Newton's method for minimizing a member of the class of Fletcher's penalty functions.

The results of limited computational experiments conducted by the author, and briefly described in Section 5, are in general agreement with those of Ref. 13 and suggest that Newton-like methods based on the penalty functions (4) and (5) are useful and at least competitive with methods based on nondifferentiable exact penalty functions. In this connection, it is worth noting that the pair (x_{k+1}, λ_{k+1}) generated by the Newton iteration (1) need not decrease the value of nondifferentiable exact penalty functions, even if (x_k, λ_k) is arbitrarily close to a solution as observed by Maratos (Ref. 18). While this difficulty can be overcome by means of devices such as those employed by Mayne and Polak (Ref. 3) and Chamberlain *et al.* (Ref.

19), it may be viewed as a rather fundamental limitation of nondifferentiable exact penalty functions.

We note that it is possible to enlarge similarly the region of convergence of quasi-Newton versions of iteration (1)–(2) (Refs. 14, 12, 20, 21) by making use of the penalty functions (4) and (5), but this subject is beyond the scope of the present paper. A detailed account is given in Refs. 22 and 28.

The notation employed in the paper is as follows. All vectors are finite dimensional and will be considered to be column vectors. A prime denotes transposition. The usual norm on the Euclidean space R^n is denoted by $|\cdot|$, i.e.,

$$|x| = (x'x)^{1/2}, \qquad \text{for all } x \in R^n.$$

For a mapping $h: R^n \to R^m$, $h = (h_1, \ldots, h_m)'$, we denote by $\nabla h(x)$ the $n \times m$ matrix with columns the gradients $\nabla h_1(x), \ldots, \nabla h_m(x)$. Whenever there is danger of confusion, we explicitly indicate the argument of differentiation: for example $\nabla_x L(x^*, \lambda^*)$ denotes the gradient of L with respect to x evaluated at the pair (x^*, λ^*).

2. Differentiable Exact Penalty Functions

Equality Constraints. Consider first the equality constrained problem

(ECP) minimize $f(x)$,

subject to $h(x) = 0$,

where $f: R^n \to R$, $h: R^n \to R^m$, and $m \le n$. *We assume throughout that f and h are three times continuously differentiable on R^n.* For $c > 0, \alpha > 0$, and $M(\cdot)$ being a twice continuously differentiable $m \times n$ matrix, the penalty functions (4) and (5) can be written as

$$P(x, \lambda; c, \alpha) = L(x, \lambda) + (1/2)\nabla L(x, \lambda)' K(c, \alpha) \nabla L(x, \lambda), \tag{7}$$

$$P(x, \lambda; c, M) = L(x, \lambda) + (1/2)\nabla L(x, \lambda)' K[c, M(x)] \nabla L(x, \lambda), \tag{8}$$

where

$$K(c, \alpha) = \begin{bmatrix} \alpha I & 0 \\ 0 & cI \end{bmatrix}, \tag{9}$$

$$K[c, M(x)] = \begin{bmatrix} M(x)'M(x) & 0 \\ 0 & cI \end{bmatrix}, \tag{10}$$

I is the identity matrix of appropriate dimension, and

$$\nabla L(x, \lambda) = \begin{bmatrix} \nabla_x L(x, \lambda) \\ \nabla_\lambda L(x, \lambda) \end{bmatrix} = \begin{bmatrix} \nabla_x L(x, \lambda) \\ h(x) \end{bmatrix}. \tag{11}$$

We refer to any pair (x^*, λ^*) satisfying the first-order necessary optimality condition

$$\nabla L(x^*, \lambda^*) = 0$$

as a *K–T pair*; and we refer to any pair (x^*, λ^*) for which the gradient of P is zero as a *critical point of P*.

We denote by X^* the open set of points x for which $\nabla h(x)$ has rank m,

$$X^* = \{x \mid \nabla h(x) \text{ has rank } m\}. \tag{12}$$

Special attention will be given to K–T pairs (x^*, λ^*) satisfying the following second-order sufficiency assumption.

Assumption S. The K–T pair (x^*, λ^*) satisfies

$$z'\nabla^2_{xx}L(x^*, \lambda^*)z > 0, \qquad \forall z \neq 0, \nabla h(x^*)'z = 0,$$

and the matrix $\nabla h(x^*)$ has rank m.

We have, from (7)–(10),

$$\nabla P(x, \lambda; c, \alpha) = \{I + \nabla^2 L(x, \lambda)K(c, \alpha)\}\nabla L(x, \lambda), \tag{13}$$

$$\nabla P(x, \lambda; c, M) = \{I + (1/2)\nabla^2 L(x, \lambda)K[c, M(x)] + (1/2)\nabla[K[c, M(x)]\nabla L(x, \lambda)]\}\nabla L(x, \lambda), \tag{14}$$

where the Hessian $\nabla^2 L(x, \lambda)$ is given by

$$\nabla^2 L(x, \lambda) = \begin{bmatrix} \nabla^2_{xx}L(x, \lambda) & \nabla h(x) \\ \nabla h(x)' & 0 \end{bmatrix}. \tag{15}$$

By differentiating these relations at a K–T pair $(x^*, \lambda^*)[\nabla L(x^*, \lambda^*) = 0]$, we obtain

$$\nabla^2 P(x^*, \lambda^*; c, \alpha) = \nabla^2 L(x^*, \lambda^*) + \nabla^2 L(x^*, \lambda^*)K(c, \alpha)\nabla^2 L(x^*, \lambda^*), \tag{16}$$

$$\nabla^2 P(x^*, \lambda^*; c, M) = \nabla^2 L(x^*, \lambda^*) + \nabla^2 L(x^*, \lambda^*)K[c, M(x^*)]\nabla^2 L(x^*, \lambda^*). \tag{17}$$

The following proposition gives the properties of the penalty function (7) that are of interest for our purposes.

Proposition 2.1. (a) Let X be a compact subset of the set X^* of (12), and Λ a compact subset of R^m. There exists a scalar $\bar{\alpha} > 0$ and, for each $\alpha \in (0, \bar{\alpha}]$, a scalar $\bar{c}(\alpha) > 0$ such that, for all c, α with

$$\alpha \in (0, \bar{\alpha}], \qquad c \geq \bar{c}(\alpha),$$

every critical point of $P(\cdot, \cdot, c, \alpha)$ belonging to $X \times \Lambda$ is a K–T pair of (ECP). If $\nabla^2_{xx}L(x, \lambda)$ is positive semidefinite for all $(x, \lambda) \in X \times \Lambda$, then $\bar{\alpha}$ can be chosen to be any positive scalar.

(b) If (x^*, λ^*) is a K–T pair of (ECP) satisfying Assumption S, then for every $\alpha > 0$ there exists a $\bar{c}(\alpha) > 0$ such that, for all $c \geq \bar{c}(\alpha)$, (x^*, λ^*) is a strict local minimum of $P(\cdot, \cdot; c, \alpha)$. Furthermore, $\nabla^2 P(x^*, \lambda^*; c, \alpha)$ is positive definite.

(c) Let (x^*, λ^*) be a K–T pair of (ECP) for which there exists $z \in R^n$ such that

$$\nabla h(x^*)'z = 0 \quad \text{and} \quad z'\nabla^2_{xx}L(x^*, \lambda^*)z < 0.$$

Then, there exists $\bar{\alpha} > 0$ such that, for all $\alpha \in (0, \bar{\alpha})$ and $c > 0$, (x^*, λ^*) is not an unconstrained local minimum of $P(\cdot, \cdot; c, \alpha)$.

Proof. (a) At any critical point of P in $X \times \Lambda$, we have $\nabla P = 0$ which, using (13) and (15), can be written as

$$\begin{bmatrix} I + \alpha \nabla^2_{xx}L & c\nabla h \\ \alpha \nabla h' & I \end{bmatrix} \begin{bmatrix} \nabla_x L \\ h \end{bmatrix} = 0. \tag{18}$$

Let $\bar{\alpha} > 0$ be such that, for all $\alpha \in (0, \bar{\alpha}]$, the matrix $(I + \alpha \nabla^2_{xx}L)$ is positive definite on $X \times \Lambda$. If $\nabla^2_{xx}L$ is positive semidefinite on $X \times \Lambda$, then $\bar{\alpha}$ can be taken to be any positive scalar. From the first equation of the system (18), we obtain

$$\nabla_x L = -c(I + \alpha \nabla^2_{xx}L)^{-1}\nabla h h. \tag{19}$$

Substitution in the second equation yields

$$[\alpha c \nabla h'(I + \alpha \nabla^2_{xx}L)^{-1}\nabla h - I]h = 0. \tag{20}$$

For any $\alpha \in (0, \bar{\alpha})$, we can choose $\bar{c}(\alpha) > 0$ such that, for all $c \geq \bar{c}(\alpha)$, the matrix on the left above is positive definite on $X \times \Lambda$. For such c and α, we obtain from (20)

$$h = 0,$$

and from (19)

$$\nabla_x L = 0.$$

Hence, for such c and α, all critical points of $P(\cdot, \cdot; c, \alpha)$ in $X \times \Lambda$ are K–T pairs of (ECP).

(b) See Ref. 1, Theorem 1.

(c) A straightforward calculation using (9), (15), and (16) yields

$$\nabla^2 P(x^*, \lambda^*; c, \alpha) = \begin{bmatrix} \nabla^2_{xx} L(x^*, \lambda^*) + c\nabla h(x^*)\nabla h(x^*)' & \nabla h(x^*) \\ \nabla h(x^*)' & 0 \end{bmatrix}$$

$$+\alpha \begin{bmatrix} \nabla^2_{xx} L(x^*, \lambda^*) \\ \nabla h(x^*)' \end{bmatrix} [\nabla^2_{xx} L(x^*, \lambda^*), \nabla h(x^*)].$$

For any $z \in R^n$ such that

$$\nabla h(x^*)'z = 0 \quad \text{and} \quad z'\nabla^2_{xx} L(x^*, \lambda^*)z < 0,$$

we have

$$[z', 0]\nabla^2 P(x^*, \lambda^*; c, \alpha)\begin{bmatrix} z \\ 0 \end{bmatrix} = z'\nabla^2_{xx} L(x^*, \lambda^*)z + \alpha|\nabla^2_{xx} L(x^*, \lambda^*)z|^2.$$

Let

$$\bar{\alpha} = -z'\nabla^2_{xx} L(x^*, \lambda^*)z/|\nabla^2_{xx} L(x^*, \lambda^*)z|^2.$$

Then, for all $\alpha \in (0, \bar{\alpha})$, we have

$$[z', 0]\nabla^2 P(x^*, \lambda^*; c, \alpha)\begin{bmatrix} z \\ 0 \end{bmatrix} < 0.$$

Hence, for such α, (x^*, λ^*) cannot be a local minimum of $P(\cdot, \cdot; c, \alpha)$. □

Note that the proof of Proposition 2.1(a) suggests that α should be taken small enough so that $(I + \alpha\nabla^2_{xx} L)$ is positive definite on $X \times \Lambda$ and that, for small α, one should choose c so that $[\alpha c I - (\nabla h'\nabla h)^{-1}]$ is positive definite on $X \times \Lambda$ [cf. (19), (20)]. This suggests that a reduction in α aimed at avoiding a situation where a local maximum of (ECP) is also a local minimum of P should be accompanied by an increase in c, so as to keep the product αc roughly constant. A more precise substantiation of this rule of thumb will be given in the next section.

Analogous results for the penalty function (8) are given in the following proposition (see Refs. 1, 13, 22 for the proof).

Proposition 2.2. Let X be a compact subset of X^* and Λ a compact subset of R^m, and assume that $M(x)\nabla h(x)$ is a nonsingular $m \times m$ matrix for all $x \in X$.

(a) There exists a $\bar{c} > 0$ such that, for all $c \geq \bar{c}$, if $(x^*, \lambda^*) \in X \times \Lambda$ is a local minimum of $P(\cdot, \cdot; c, M)$, then x^* is a local minimum of (ECP), and if $(x^*, \lambda^*) \in X \times \Lambda$ is a critical point of $P(\cdot, \cdot; c, M)$, then (x^*, λ^*) is a K–T pair of (ECP).

(b) If x^* is the unique global minimum of f over

$$X \cap \{x \mid h(x) = 0\},$$

x^* lies in the interior of X, λ^* lies in the interior of Λ, and

$$\nabla L(x^*, \lambda^*) = 0,$$

there exists a $\bar{c} > 0$ such that, for all $c \geq \bar{c}$, (x^*, λ^*) is the unique global minimum of $P(\cdot, \cdot; c, M)$ over $X \times \Lambda$.

(c) Let (x^*, λ^*) be a K–T pair of (ECP) satisfying Assumption S. Then, there exists a $\bar{c} > 0$ such that, for all $c \geq \bar{c}$, (x^*, λ^*) is a strict local minimum of $P(\cdot, \cdot; c, M)$ and $\nabla^2 P(x^*, \lambda^*; c, M)$ is positive definite.

The results of Propositions 2.1 and 2.2 might lead one to hypothesize that, if $X^* = R^n$, then all the critical points of P are K–T pairs of (ECP). This is not true, however. Even under quite favorable circumstances, both $P(\cdot, \cdot; c, \alpha)$ and $P(\cdot, \cdot; c, M)$ can have, for an infinite set of values of c and α, critical points that are unrelated to K–T pairs of (ECP). According to Propositions 2.1 and 2.2, these spurious critical points move toward infinity as $c \to \infty$. We illustrate this situation by an example.

Example 2.1. Let $n = m = 1$ and

$$f(x) = (1/6)x^3, \qquad h(x) = x.$$

Here, $X^* = R$; and, for

$$M(x) \triangleq \sqrt{\alpha},$$

we have

$$P(x, \lambda; c, \alpha) = P(x, \lambda; c, M) = (1/6)x^3 + \lambda x + (c/2)x^2 + (\alpha/2)|x^2/2 + \lambda|^2.$$

Here, $\{x^* = 0, \lambda^* = 0\}$ is the unique K–T pair. Critical points of P are obtained by solving the equations

$$\nabla_x P = x^2/2 + \lambda + cx + \alpha x(x^2/2 + \lambda) = 0,$$

$$\nabla_\lambda P = x + \alpha(x^2/2 + \lambda) = 0.$$

From the second equation, we obtain

$$\lambda = -x/\alpha - x^2/2;$$

and substitution in the first equation yields, after a straightforward calculation,

$$x(x - c + 1/\alpha) = 0.$$

By solving these equations, we obtain that the critical points of P are

$$\{x^* = 0, \lambda^* = 0\}$$

and

$$\{x(c, \alpha) = c - 1/\alpha, \lambda(c, \alpha) = (1 - c^2\alpha^2)/2\alpha^2\}.$$

It can be seen that, for all $c > 0$ and $\alpha > 0$ with $c\alpha \neq 1$, the critical point $[x(c, \alpha), \lambda(c, \alpha)]$ is not a K–T pair of (ECP). On the other hand, for every $\alpha > 0$, we have

$$\lim_{c \to \infty} x(c, \alpha) = \infty \quad \text{and} \quad \lim_{c \to \infty} \lambda(c, \alpha) = -\infty,$$

which is consistent with the conclusions of Propositions 2.1 and 2.2.

The next example shows that, if $\nabla^2_{xx}L$ is not positive semidefinite on $X \times \Lambda$, then the upper bound $\bar{\alpha}$ in Propositions 2.1(a) and 2.1(c) cannot be chosen arbitrarily.

Example 2.2. Let $n = 2$, $m = 1$ and

$$f(x_1, x_2) = -(1/2)x_1^2, \qquad h(x_1, x_2) = x_2.$$

Here,

$$\{x_1^* = 0,\ x_2^* = 0,\ \lambda^* = 0\}$$

is the unique K–T pair (a global maximum), and $X^* = R^2$. Take $\alpha = 1$. We have, for every $c > 0$,

$$\begin{aligned} P(x, \lambda; c, 1) &= -(1/2)x_1^2 + \lambda x_2 + (c/2)x_2^2 + (1/2)x_1^2 + (1/2)\lambda^2 \\ &= \lambda x_2 + (c/2)x_2^2 + (1/2)\lambda^2. \end{aligned}$$

Since P is independent of x_1, any vector of the form

$$\{x_1 = y, x_2 = 0, \lambda = 0\},$$

with $y \in R$, is a critical point of P; and, of these, only the vector

$$\{x_1^* = 0,\ x_2^* = 0,\ \lambda^* = 0\}$$

is a K–T pair of (ECP). Also, for all $c \geq 1$, every critical point of P is a local minimum including the local maximum

$$\{x_1^* = 0,\ x_2^* = 0,\ \lambda^* = 0\}$$

of (ECP).

More general penalty functions than (7) and (8) are given by

$$P_\tau(x, \lambda; c, \alpha) = L(x, \lambda) + (1/2)\nabla L(x, \lambda)' K_\tau(\lambda, c, \alpha)\nabla L(x, \lambda), \tag{21}$$

$$P_\tau(x, \lambda; c, M) = L(x, \lambda) + (1/2)\nabla L(x, \lambda)' K_\tau(\lambda, c, M(x))\nabla L(x, \lambda), \tag{22}$$

where $\tau \geq 0$ is a scalar and

$$K_\tau(\lambda, c, \alpha) = \begin{bmatrix} \alpha I & 0 \\ 0 & (c + \tau|\lambda|^2)I \end{bmatrix}, \tag{23}$$

$$K_\tau(\lambda, c, M) = \begin{bmatrix} M(x)'M(x) & 0 \\ 0 & (c + \tau|\lambda|^2)I \end{bmatrix}. \tag{24}$$

When $\tau = 0$, the functions (21) and (22) reduce to the penalty functions (7) and (8). For $\tau > 0$, the functions (21) and (22) contain the extra term

$$(\tau/2)|\lambda|^2|h(x)|^2. \tag{25}$$

This term guarantees that P_τ is bounded below with respect to (x, λ) if $f(x)$ is bounded below with respect to x. It appears that this extra term results in better numerical stability when minimizing computationally P_τ with respect to (x, λ) by using standard descent methods, as suggested by Di Pillo, Grippo, and Lampariello (Ref. 13), who considered the very similar extra term $(\tau/2)[\lambda' h(x)]^2$ in place of (25). This was also confirmed by the author's numerical experiments. It is straightforward to show that the results of Proposition 2.1 also hold for the penalty function $P_\tau(x, \lambda; c, \alpha)$ for all $\tau > 0$. The results of Proposition 2.2 also hold for $P_\tau(x, \lambda; c, M)$ as shown in Ref. 13 for the slightly different penalty function mentioned earlier.

Relation with Fletcher's Penalty Function. For $x \in X^*$, let us select

$$M(x) = [\nabla h(x)' \nabla h(x)]^{-1} \nabla h(x)' \tag{26}$$

in the penalty function (8). Then,

$$M(x)\nabla h(x) = I,$$

and we have

$$P(x, \lambda; c, M) = f(x) + \lambda' h(x) + (c/2)|h(x)|^2 + (1/2)|M(x)\nabla f(x) + \lambda|^2. \tag{27}$$

Define

$$\hat{P}(x; c) = \min\{P(x, \lambda; c, M) \mid \lambda \in R^m\}. \tag{28}$$

The minimum is attained at $\hat{\lambda}(x)$ satisfying

$$0 = \nabla_\lambda P[x, \hat{\lambda}(x); c, M] = h(x) + M(x)\nabla f(x) + \hat{\lambda}(x),$$

or equivalently

$$\hat{\lambda}(x) = -h(x) - [\nabla h(x)'\nabla h(x)]^{-1}\nabla h(x)'\nabla f(x).$$

Substitution in (27), (28) yields

$$\hat{P}(x; c) = f(x) - \nabla f(x)'\nabla h(x)[\nabla h(x)'\nabla h(x)]^{-1}h(x) + [(c-1)/2]|h(x)|^2.$$

It follows that

$$\hat{P}(x; c+1) = f(x) + \lambda(x)'h(x) + (c/2)|h(x)|^2, \tag{29}$$

where

$$\lambda(x) = -[\nabla h(x)'\nabla h(x)]^{-1}\nabla h(x)'\nabla f(x). \tag{30}$$

The penalty function (29), (30) was first introduced by Fletcher (Ref. 2).

It is clear from the preceding analysis that any unconstrained method for the minimization of $\hat{P}(x; c+1)$ with respect to x is equivalent to a method for the minimization of the penalty function $P(x, \lambda; c+1, M)$ of (27) with $M(x)$ given by (26). This suggests that the second-order methods of Refs. 13, 15, 16, 17, as well as those of this paper, should exhibit quite similar convergence characteristics.

Extension to Inequality Constraints. An extension of the penalty function (8) to inequality constraints has been given in Ref. 23 by using the device of converting inequalities to equalities via squared slack variables. We provide a similar generalization for the penalty function (21). For simplicity, we will consider problems with inequality constraints exclusively. Obvious adjustments are needed to provide extensions to the case where additional equality constraints are present.

Consider the problem

$$\text{(ICP)} \qquad \text{minimize} \quad f(x), \qquad \text{subject to} \quad g(x) \leq 0,$$

where $f: R^n \to R$, $g: R^n \to R^m$, $g = (g_1, \ldots, g_r)'$ are three times continuously differentiable functions. An equivalent equality constrained problem is given by

$$\begin{aligned} &\text{minimize} \quad f(x), \\ &\text{subject to} \quad g_j(x)+z_j^2=0, \qquad j=1,\ldots,r, \end{aligned} \tag{31}$$

involving the additional vector

$$z=(z_1,\ldots,z_r)'.$$

Consider the penalty function (7) for this problem:

$$P(x, z, \mu; c, \alpha)=f(x)+\sum_{j=1}^{m}\{\mu_j[g_j(x)+z_j^2]+(c/2)[g_j(x)+z_j^2]^2\}$$
$$+(\alpha/2)|\nabla_x L(x, \mu)|^2+2\alpha\sum_{j=1}^{m} z_j^2\mu_j^2, \tag{32}$$

where

$$L(x, \mu)=f(x)+\mu' g(x)=f(x)+\sum_{j=1}^{r}\mu_j g_j(x).$$

Minimization of P with respect to (x, z, μ) can be carried out by minimizing first with respect to z and by subsequently minimizing the resulting function with respect to (x, μ). A straightforward calculation shows that

$$P^+(x, \mu; c, \alpha) \triangleq \min_z P(x, z, \mu; c, \alpha)$$
$$=f(x)+(\alpha/2)|\nabla_x L(x, \mu)|^2+(1/2c)\sum_{j=1}^{r} Q_j(x, \mu; c, \alpha), \tag{33}$$

where

$$Q_j(x, \mu; c, \alpha)=[\max\{0, \mu_j+2\alpha\mu_j^2+cg_j(x)\}]^2$$
$$-(\mu_j+2\alpha\mu_j^2)^2-4\alpha c\mu_j^2 g_j(x). \tag{34}$$

The minimum in (33) is attained at

$$z_j^2(x, \mu; c, \alpha)=\max\{0, -(\mu_j+2\alpha\mu_j^2)/c-g_j(x)\}, \qquad j=1,\ldots,r.$$

Thus, minimization of P can be carried out by minimizing instead the function P^+ of (33) which does not involve the additional variables z_j.

Properties of interest of the penalty function P^+ can be obtained by applying Proposition 2.1 to problem (31) and the penalty function (32). In particular, let (x^*, μ^*) be a K–T pair of (ICP) satisfying the sufficiency assumption below.

Assumption S$^+$. There holds

$$\nabla L(x^*, \mu^*) = 0,\ \mu^* \geq 0,\ \mu_j^* g_j(x^*) = 0, \qquad \forall j = 1, \ldots, r,$$

$$\mu_j^* > 0, \qquad \forall j \in A(x^*) = \{i \mid g_i(x^*) = 0\},$$

$$z' \nabla_{xx}^2 L(x^*, \mu^*) z > 0, \qquad \forall z \neq 0, \text{ with } \nabla g_j(x^*)' z = 0,\ j \in A(x^*).$$

It is easy to show using Proposition 2.1 that, given any $\alpha > 0$, there exists $\bar{c}(\alpha) > 0$ such that (x^*, μ^*) is a strict local minimum of $P^+(\cdot, \cdot; c, \alpha)$ for all $c \geq \bar{c}(\alpha)$, and $\nabla^2 P^+(x^*, \mu^*; c, \alpha)$ is positive definite. Furthermore, if (x^*, μ^*) is a local maximum-Lagrange multiplier pair satisfying second-order sufficiency conditions analogous to Assumption S$^+$, then there exists $\bar{\alpha} > 0$ such that, for all $\alpha \in (0, \bar{\alpha})$ and $c > 0$, (x^*, μ^*) cannot be a local minimum of $P^+(\cdot, \cdot; c, \alpha)$. This establishes the validity of a solution method based on unconstrained minimization of P^+.

A similar procedure may be used to obtain an inequality constrained version of the penalty function P_τ of (21) for $\tau > 0$. It has the form

$$P_\tau^+(x, \mu; c, \alpha) = f(x) + (\alpha/2)|\nabla_x L(x, \mu)|^2 + [1/2(c + \tau|\mu|^2)] \sum_{j=1}^{r} Q_j(x, \mu; c, \alpha, \tau), \tag{35}$$

where

$$Q_j(x, \mu; c, \alpha, \tau) = [\max\{0, \mu_j + 2\alpha\mu_j^2 + (c + \tau|\mu|^2) g_j(x)\}]^2 - (\mu_j + 2\alpha\mu_j^2)^2 - 4\alpha(c + \tau|\mu|^2)\mu_j^2 g_j(x), \qquad j = 1, \ldots, r.$$

It is also possible to obtain in a similar manner an inequality constrained version of the penalty function $P_\tau(\cdot, \cdot; c, M)$ of (22). As shown by Di Pillo and Grippo (Ref. 23), a special choice of M used in conjunction with problem (31) yields the penalty function

$$P_\tau^+(x, \mu; c, \eta) = f(x) + \mu' g(x) + [(c + \tau|\mu|^2)/2]|g(x)|^2 + (\eta/2)|\nabla g(x)' \nabla_x L(x, \mu)|^2 - \sum_{j=1}^{r} \frac{[\min\{0, (c + \tau|\mu|^2) g_j(x) + \mu_j + 4\eta\mu_j \nabla g_j(x)' \nabla_x L(x, \mu)\}]^2}{2(c + \tau|\mu|^2 + 16\eta\mu_j^2)}, \tag{36}$$

where

$$c > 0, \qquad \tau \geq 0, \qquad \eta > 0$$

are scalar parameters.

Penalty functions for problems like (ICP), but with the additional constraint $x \geq 0$, are given in Bertsekas (Ref. 22).

3. Newton's Method for Solving the Necessary Optimality Conditions as a Method for Minimizing the Exact Penalty Functions

Consider first the equality constrained problem (ECP). Denote, for every k,

$$z_k = \begin{bmatrix} x_k \\ \lambda_k \end{bmatrix},$$

and write $P(z_k; c, \alpha)[P(z_k; c, M)]$ in place of $P(x_k, \lambda_k; c, \alpha)[P(x_k, \lambda_k; c, M)]$. Newton's method for solving the system of necessary conditions

$$\nabla L(x_k, \lambda_k) = 0$$

consists of the iteration

$$z_{k+1} = z_k + d_k, \tag{37}$$

where

$$d_k = -[\nabla^2 L(x_k, \lambda_k)]^{-1} \nabla L(x_k, \lambda_k). \tag{38}$$

It is well known [see, e.g., Poljak (Ref. 24)] that, if (x^*, λ^*) is a K–T pair satisfying Assumption S, then $\nabla^2 L(x^*, \lambda^*)$ is invertible. As a result, iteration (37)–(38) is well defined in a neighborhood of (x^*, λ^*). By well-known results on Newton's method (see, e.g., Ref. 11), (x^*, λ^*) is a point of attraction of the iteration and the rate of convergence is at least quadratic (recall that f and h are assumed three times continuously differentiable).

By using (16) and Proposition 2.1(b), we have that, for any K–T pair (x^*, λ^*) satisfying Assumption S and any $\alpha > 0$, there exists $\bar{c}(\alpha) > 0$ such that, for all $c \geq \bar{c}(\alpha)$, the matrix

$$\begin{aligned} \nabla^2 P(x^*, \lambda^*; c, \alpha) &= \nabla^2 L(x^*, \lambda^*) + \nabla^2 L(x^*, \lambda^*) K(c, \alpha) \nabla^2 L(x^*, \lambda^*) \\ &= [I + \nabla^2 L(x^*, \lambda^*) K(c, \alpha)] \nabla^2 L(x^*, \lambda^*) \end{aligned} \tag{39}$$

is positive definite. Since $\nabla^2 L(x^*, \lambda^*)$ is invertible, it follows that $[I + \nabla^2 L(x^*, \lambda^*) K(c, \alpha)]$ is also invertible for $c \geq \bar{c}(\alpha)$. Hence, for such c and (x_k, λ_k) sufficiently close to (x^*, λ^*), the matrix

$$B(x_k, \lambda_k; c, \alpha) = [\nabla^2 L(x_k, \lambda_k)]^{-1} \{I + \nabla^2 L(x_k, \lambda_k) K(c, \alpha)\}^{-1} \tag{40}$$

is well defined. By using (13), (38), (40), we obtain that the Newton direction d_k can also be written as

$$d_k = -B(x_k, \lambda_k; c, \alpha) \nabla P(x_k, \lambda_k; c, \alpha). \tag{41}$$

From (39) and (40), it follows that

$$B(x^*, \lambda^*; c, \alpha) = \nabla^2 P(x^*, \lambda^*; c, \alpha)^{-1}. \tag{42}$$

In view of (41), (42), it follows that

$$\lim_{(x_k,\lambda_k)\to(x^*,\lambda^*)} \frac{|[B(x_k,\lambda_k;c,\alpha)-\nabla^2 P(x^*,\lambda^*;c,\alpha)^{-1}]\nabla P(x_k,\lambda_k;c,\alpha)|}{|\nabla P(x_k,\lambda_k;c,\alpha)|}=0. \tag{43}$$

This shows that the Newton direction (38) approaches asymptotically the direction used by Newton's method as applied to minimization of $P(\cdot,\cdot;c,\alpha)$.

We now consider an algorithm which combines the Newton iteration (37)–(38), a scaled steepest-descent method with a positive-definite scaling matrix D, and the Armijo stepsize rule with parameters $\sigma \in (0,\frac{1}{2})$, $\beta \in (0,1)$, and unity initial stepsize. The algorithm consists of the iteration

$$z_{k+1}=z_k+\beta^{m_k}p_k, \tag{44}$$

where m_k is the first nonnegative integer m for which

$$P(z_k;c,\alpha)-P(z_k+\beta^m p_k;c,\alpha)\geq -\sigma\beta^m p_k'\nabla P(z_k;c,\alpha). \tag{45}$$

The direction p_k is the Newton direction (38)

$$p_k=d_k \tag{46}$$

if $\nabla^2 L(x_k,\lambda_k)$ is invertible and[3]

$$-d_k'\nabla P(z_k;c,\alpha)\geq\gamma|\nabla P(z_k;c,\alpha)|^3, \tag{47}$$

where γ is a positive scalar (with typically very small value). Otherwise, p_k is the scaled steepest-descent direction

$$p_k=-D\nabla P(z_k;c,\alpha). \tag{48}$$

The algorithm (44)–(48) is not necessarily the most efficient for any given problem, but rather represents an example of how the preceding analysis can be used to enlarge the region of convergence of Newton's method. Additional algorithms are given in Ref. 22.

It is a routine matter to show, based on the analysis given thus far [cf. (43)] and standard results of unconstrained minimization methods [see, e.g., Ortega and Rheinboldt (Ref. 11), Dennis and Moré (Ref. 25)], that the following proposition holds true.

Proposition 3.1. (a) Every limit point of a sequence $\{z_k\}$ generated by iteration (44) is a critical point of $P(\cdot,\cdot;c,\alpha)$.

(b) Let $z^*=(x^*,\lambda^*)$ be a K–T pair of (ECP) satisfying Assumption

[3] We are using the third power of $|\nabla p|$ in (47), instead of the usual second power, in order to avoid assuming that γ is sufficiently small in proving superlinear convergence.

S, and assume that $c \geq \bar{c}$, where $\bar{c}$ is as in Proposition 2.1(b). If z^* is a limit point of a sequence $\{z_k\}$ generated by iteration (44), then $\{z_k\}$ actually converges to z^*. Furthermore, the rate of convergence is at least Q-quadratic, i.e.,

$$\limsup_{k\to\infty} \frac{|z_{k+1} - z^*|}{|z_k - z^*|^2} < \infty.$$

In addition, there exists an integer $\bar{k}$ such that, for all $k \geq \bar{k}$, p_k is given by the Newton direction d_k and the stepsize equals unity [$m_k = 0$ in (44)]. If z_0 is sufficiently close to z^*, then the same is true for all k.

Analogous results can be shown for the.Newton iteration (37)–(38) in connection with the penalty functions $P(\cdot, \cdot; c, M)$, $P_\tau(\cdot, \cdot; c, \alpha)$, and $P_\tau(\cdot, \cdot; c, M)$. Take, for example, the latter. We have from (22), (24)

$$\begin{aligned}\nabla P_\tau(x, \lambda; c, M) = \{&I + (1/2)\nabla^2 L(x, \lambda)K_\tau[\lambda, c, M(x)] \\ &+ (1/2)\nabla[K_\tau[\lambda, c, M(x)]\nabla L(x, \lambda)]\}\nabla L(x, \lambda),\end{aligned}$$

while, for any K–T pair (x^*, λ^*), we have

$$\begin{aligned}\nabla^2 P_\tau(x^*, \lambda^*; c, M) = &\nabla^2 L(x^*, \lambda^*) \\ &+ \nabla^2 L(x^*, \lambda^*)K_\tau[\lambda^*, c, M(x^*)]\nabla^2 L(x^*, \lambda^*). \quad (49)\end{aligned}$$

Consider the matrix

$$\begin{aligned}A_\tau(x, \lambda; c, M) = I &+ (1/2)\nabla^2 L(x, \lambda)K_\tau[\lambda, c, M(x)] \\ &+ (1/2)\nabla[K_\tau[\lambda, c, M(x)]\nabla L(x, \lambda)]. \quad (50)\end{aligned}$$

We have, for a K–T pair (x^*, λ^*),

$$A_\tau(x^*, \lambda^*; c, M) = I + \nabla^2 L(x^*, \lambda^*)K_\tau[\lambda^*, c, M(x^*)], \quad (51)$$

and it follows from (49), (51) that

$$\nabla^2 P_\tau(x^*, \lambda^*; c, M) = A_\tau(x^*, \lambda^*; c, M)\nabla^2 L(x^*, \lambda^*). \quad (52)$$

If (x^*, λ^*) satisfies Assumption S, then by Proposition 2.2(c) there exists a $\bar{c} > 0$ such that, for all $c \geq \bar{c}$, $\nabla^2 P_\tau(x^*, \lambda^*; c, M)$ is positive definite. Since $\nabla^2 L(x^*, \lambda^*)$ is invertible, it follows from (52) that, for all $c \geq \bar{c}$, $A_\tau(x^*, \lambda^*; c, M)$ is also invertible, Hence, for each $c \geq \bar{c}$, there is a neighborhood of (x^*, λ^*) within which both $\nabla^2 L(x, \lambda)$ and $A_\tau(x, \lambda; c, M)$ are invertible. For all (x_k, λ_k) in this neighborhood, the matrix

$$B_\tau(x_k, \lambda_k; c, M) = [\nabla^2 L(x_k, \lambda_k)]^{-1}[A_\tau(x_k, \lambda_k; c, M)]^{-1} \quad (53)$$

is well defined; and, in view of (38), (48), (50), we have

$$d_k = -B_\tau(x_k, \lambda_k; c, M)\nabla P_\tau(x_k, \lambda_k; c, M). \quad (54)$$

We also have from (52), (53)

$$B_\tau(x^*, \lambda^*; c, M) = \nabla^2 P_\tau(x^*, \lambda^*; c, M)^{-1}. \tag{55}$$

It follows as earlier from (54), (55) that the Newton direction d_k approaches asymptotically the direction used by Newton's method as applied to minimization of $P_\tau(\cdot, \cdot; c, M)$.

Similarly as earlier, we can combine the Newton iteration (37)–(38) with a scaled steepest-descent method and the Armijo rule to obtain a method for minimizing $P_\tau(\cdot, \cdot; c, M)$. The statement of this algorithm is exactly the same as (44)–(48), except that $P(\cdot, \cdot; c, \alpha)$ is replaced by $P_\tau(\cdot, \cdot; c, M)$. The convergence results of Proposition 3.1 hold for this algorithm as well.

Extension to Inequality Constraints. We first consider an extension of the Newton iteration (37)–(38) to the inequality constrained problem (ICP) which does not involve solution of a quadratic programming problem as in Wilson (Ref. 10) and Robinson (Ref. 26). Fix

$$c > 0, \qquad \tau \geq 0, \qquad \alpha > 0,$$

and define, for each $(x, \mu) \in R^{n+r}$,

$$A^+(x, \mu) = \{j \mid \mu_j + 2\alpha\mu_j^2 + (c + \tau|\mu|^2)g_j(x) > 0, j = 1, \ldots, r\}, \tag{56}$$

$$A^-(x, \mu) = \{j \mid \mu_j + 2\alpha\mu_j^2 + (c + \tau|\mu|^2)g_j(x) \leq 0, j = 1, \ldots, r\}. \tag{57}$$

For a given (x, μ), assume (by reordering indices if necessary) that $A^+(x, \mu)$ contains the first p indices where p is an integer with $0 \leq p \leq r$. Define

$$g_+(x) = \begin{bmatrix} g_1(x) \\ \vdots \\ g_p(x) \end{bmatrix}, \qquad g_-(x) = \begin{bmatrix} g_{p+1}(x) \\ \vdots \\ g_r(x) \end{bmatrix}, \tag{58}$$

$$\mu_+ = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_p \end{bmatrix}, \qquad \mu_- = \begin{bmatrix} \mu_{p+1} \\ \vdots \\ \mu_r \end{bmatrix}, \tag{59}$$

$$L_+(x, \mu) = f(x) + \mu_+' g_+(x). \tag{60}$$

We note that p, g_+, g_-, μ_+, μ_-, L_+ depend on (x, μ), but to simplify notation we do not show explicitly this dependence.

In the extension of Newton's method that we consider, given (x, μ), we denote the next iterate by $(\hat{x}, \hat{\mu})$, where

$$\hat{\mu} = (\hat{\mu}_1, \ldots, \hat{\mu}_r).$$

We also write

$$\hat{\mu}_+ = \begin{bmatrix} \hat{\mu}_1 \\ \vdots \\ \hat{\mu}_p \end{bmatrix}, \qquad \hat{\mu}_- = \begin{bmatrix} \hat{\mu}_{p+1} \\ \vdots \\ \hat{\mu}_r \end{bmatrix}. \tag{61}$$

The iteration, roughly speaking, consists of setting the multipliers of the inactive constraints $[j \in A^-(x, \mu)]$ to zero, and by treating the remaining constraints as equalities. More precisely, we set

$$\hat{\mu}_- = 0, \tag{62}$$

and obtain $\hat{x}$, $\hat{\mu}_+$ by solving the system

$$\begin{bmatrix} \nabla^2_{xx} L_+(x, \mu) & \nabla g_+(x) \\ \nabla g_+(x)' & 0 \end{bmatrix} \begin{bmatrix} \hat{x} - x \\ \hat{\mu}_+ - \mu_+ \end{bmatrix} = -\begin{bmatrix} \nabla_x L_+(x, \mu) \\ g_+(x) \end{bmatrix}, \tag{63}$$

assuming, of course, that the matrix on the left above is invertible.

We consider the following combination of the Newton iteration (62), (63) with the Armijo rule and a scaled steepest-descent method for minimizing the penalty function $P_\tau^+(\cdot, \cdot; c, \alpha)$ of (35). Let

$$\sigma \in (0, \tfrac{1}{2}), \qquad \beta \in (0, 1), \qquad \gamma > 0,$$

and let D be a positive–definite matrix. Given (x, μ), the next iterate $(\bar{x}, \bar{\mu})$ is given by

$$\begin{bmatrix} \bar{x} \\ \bar{\mu} \end{bmatrix} = \begin{bmatrix} x \\ \mu \end{bmatrix} + \beta^{\bar{m}} \begin{bmatrix} p_x \\ p_\mu \end{bmatrix}, \tag{64}$$

where $\bar{m}$ is the first nonnegative integer m for which

$$P_\tau^+(x, \mu; c, \alpha) - P_\tau^+(x + \beta^m p_x, \mu + \beta^m p_\mu; c, \alpha) \geq -\sigma \beta^m p' \nabla P_\tau^+(x, \mu; c, \alpha). \tag{65}$$

The direction

$$p = (p_x, p_\mu)$$

is given by the Newton direction obtained from (62), (63):

$$p = \begin{bmatrix} p_x \\ p_\mu \end{bmatrix} = \begin{bmatrix} \hat{x} - x \\ \hat{\mu} - \mu \end{bmatrix}, \tag{66}$$

if the matrix on the left of (63) is invertible and

$$-(\hat{x} - x)' \nabla_x P_\tau^+(x, \mu; c, \alpha) - (\hat{\mu} - \mu)' \nabla_\mu P_\tau^+(x, \mu; c, \alpha) \geq \gamma |\nabla P_\tau^+(x, \mu; c, \alpha)|^3. \tag{67}$$

Otherwise,

$$p = -D\nabla P_\tau^+(x, \mu; c, \alpha). \tag{68}$$

Based on known results for unconstrained minimization methods, it can be shown that any limit point of a sequence generated by the method described above is a critical point of P_τ^+. There remains to show, similarly as for equality constrained problems, that the direction generated by the Newton iteration (62), (63) approaches asymptotically the Newton direction for minimizing P_τ^+ as (x, μ) approaches a K–T pair (x^*, μ^*) satisfying Assumption S^+ [cf. (43)]. A quadratic convergence rate result analogous to the one of Proposition 3.1(b) then follows.

Consider a K–T pair (x^*, μ^*) of (ICP) satisfying Assumption S^+. In view of the strict complementarity assumption [$\mu_j^* > 0$, if $g_j(x^*) = 0$], for each

$$c > 0, \qquad \tau \geq 0, \qquad \alpha > 0,$$

there exists a neighborhood of (x^*, μ^*) within which we have

$$A^+(x, \mu) = A(x^*) = \{j \mid g_j(x^*) = 0, j = 1, \ldots, r\}. \tag{69}$$

Within this neighborhood, the Newton iteration (62), (63) reduces to the Newton iteration for solving the system of necessary conditions

$$\nabla_x L_+(x, \mu) = 0, \qquad g_+(x) = 0,$$

corresponding to the equality constrained problem

$$\begin{aligned} &\text{minimize} \quad f(x), \\ &\text{subject to} \quad g_+(x) = 0. \end{aligned}$$

Based on this fact, it is easy to see that (x^*, μ^*) is a point of attraction of the iteration (62), (63) and the rate of convergence is at least quadratic. Let c, τ, α be such that $\nabla^2 P_\tau^+(x^*, \mu^*; c, \alpha)$ is positive definite. We will show that, in a neighborhood of (x^*, μ^*) within which (69) holds, we have

$$\begin{bmatrix} \hat{x} - x \\ \hat{\mu} - \mu \end{bmatrix} = -[H_\tau(x, \mu; c, \alpha)]^{-1} \nabla P_\tau^+(x, \mu; c, \alpha), \tag{70}$$

where $H_\tau(\cdot, \cdot; c, \alpha)$ is a continuous matrix satisfying

$$H_\tau(x^*, \mu^*; c, \alpha) = \nabla^2 P_\tau^+(x^*, \mu^*; c, \alpha). \tag{71}$$

We show this fact for $\tau = 0$.

Consider the $(n+r)\times(n+r)$ matrix

$$H=\left[\begin{array}{c|c|c} \nabla^2_{xx}L_+ + c\nabla g_+\nabla'_{g_+} + \alpha\nabla^2_{xx}L_+\nabla^2_{xx}L_+ & \nabla g_+ + \alpha\nabla^2_{xx}L_+\nabla g_+ & \alpha\nabla^2_{xx}L\nabla g_- + \alpha E \\ \hline \nabla g'_+ + \alpha\nabla g'_+\nabla^2_{xx}L_+ & \alpha\nabla g'_+\nabla g_+ & \alpha\nabla g'_+\nabla g_- \\ \hline \alpha\nabla g'_-\nabla^2_{xx}L & \alpha\nabla g'_-\nabla g_+ & \alpha\nabla g'_-\nabla g_+ + F \end{array}\right], \tag{72}$$

where all derivatives are evaluated at a point (x, μ) in a neighborhood of (x^*, μ^*) within which (69) holds, the $(r-p)\times(r-p)$ diagonal matrix F is given by

$$F=\begin{bmatrix} -(1+4\alpha\mu_{p+1})(1+2\alpha\mu_{p+1})/c-4\alpha g_{p+1} & & 0 \\ & \ddots & \\ 0 & & -(1+4\alpha\mu_r)(1+2\alpha\mu_r)/c-4\alpha g_r \end{bmatrix}, \tag{73}$$

and the $n\times(r-p)$ matrix E is given by

$$E=[-\nabla^2 g_{p+1}\nabla_x L - 2\mu_{p+1}\nabla g_{p+1} \mid \cdots \mid -\nabla^2 g_r\nabla_x L - 2\mu_r\nabla g_r]. \tag{74}$$

The function P^+ of (33), (34) can also be written as

$$P^+(x, \mu; c, \alpha) = L_+(x, \mu) + (c/2)|g_+(x)|^2 + (\alpha/2)|\nabla_x L(x, \mu)|^2 - \sum_{j=p+1}^{r} [(\mu_j + 2\alpha\mu_j^2)^2/2c + 2\alpha\mu_j^2 g_j(x)]. \tag{75}$$

By differentiating this expression, we obtain

$$\nabla P^+(x, \mu; c, \alpha) = \begin{bmatrix} \nabla_x L_+ + c\nabla g_+ g_+ + \alpha\nabla^2_{xx}L\nabla_x L - 2\alpha \sum_{j=p+1}^{r} \mu_j^2\nabla g_j \\ g_+ + \alpha\nabla g'_+\nabla_x L \\ \alpha\nabla g'_-\nabla_x L + F\mu_- \end{bmatrix}, \tag{76}$$

where F is given by (73). We now observe that the solution $(\hat{x}-x, \hat{\mu}_+ - \mu_+)$ of the system (63) also satisfies

$$\left[\begin{array}{c|c} \nabla^2_{xx}L_+ + c\nabla g_+\nabla g'_+ + \alpha\nabla^2_{xx}L_+\nabla^2_{xx}L_+ & \nabla g_+ + \alpha\nabla^2_{xx}L_+\nabla g_+ \\ \hline \nabla g'_+ + \alpha\nabla g'_+\nabla^2_{xx}L_+ & \alpha\nabla g'_+\nabla g_+ \end{array}\right]\begin{bmatrix} \hat{x}-x \\ \hat{\mu}_+ - \mu_+ \end{bmatrix} = -\begin{bmatrix} \nabla_x L_+ + c\nabla g_+ g_+ + \alpha\nabla^2_{xx}L_+\nabla_x L_+ \\ g_+ + \alpha\nabla g'_+\nabla_x L_+ \end{bmatrix}. \tag{77}$$

By using (72)–(74) and (76), (77), it is straightforward to verify that

$$H\begin{bmatrix} \hat{x}-x \\ \hat{\mu}_+ - \mu_+ \\ \hat{\mu}_- - \mu_- \end{bmatrix} = \nabla P^+(x, \mu; c, \alpha),$$

and hence the vector $(\hat{x}, \hat{\mu})$ generated by (62), (63) satisfies [cf. Eq. (70)]

$$\begin{bmatrix} \hat{x}-x \\ \hat{\mu}-\mu \end{bmatrix} = -H^{-1}\nabla P^{+}(x, \mu; c, \alpha).$$

Denote by H^* the matrix H of (72) evaluated at (x^*, μ^*). Taking into account the fact that

$$\nabla_x L(x^*, \mu^*) = 0 \quad \text{and} \quad \mu_j^* = 0, \; j = p+1, \ldots, r,$$

it is easy to verify that

$$H^* = \nabla^2 P^{+}(x^*, \mu^*; c, \alpha).$$

We have shown therefore that, for $\tau = 0$, (70) and (71) hold with $H_\tau(x, \mu; c, \alpha)$ being the matrix (72). The proof for the case where $\tau > 0$ is similar but very tedious, as the reader may surmise from the analysis of the case where $\tau = 0$. We will omit the details.

It is also possible to construct an algorithm analogous to (64)–(68) in connection with the penalty function $P_\tau^{+}(\cdot, \cdot; c, \eta)$ of (36), and to show similar convergence results. The detailed analysis is again very tedious and will be omitted.

It is worth noting that, if the algorithm (64)–(68) is modified at the expense of a slight loss in reliability so that the test (67) is replaced by

$$-(\hat{x}-x)'\nabla_x P_\tau^{+}(x, \mu; c, \alpha) - (\hat{\mu}-\mu)'\nabla_\mu P_\tau^{+}(x, \mu; c, \alpha) > 0,$$

then, *near a K–T pair* (x^*, μ^*) *satisfying Assumption* S^+, *it is not necessary to compute the gradient matrix* $\nabla g_-(x)$ *corresponding to the inactive constraints.*

To see this, note that computation of the Newton direction [cf. (62), (63)] does not require knowledge of $\nabla g_-(x)$. Next, with the aid of (76), observe that, if $\mu_- = 0$ [and hence also $(\hat{\mu}_- - \mu_-) = 0$], then computation of the inner products in (65) and (67) also does not require knowledge of $\nabla g_-(x)$. If the algorithm converges to a *K–T* pair (x^*, μ^*) satisfying Assumption S^+, then the Newton iteration will be accepted and the set of inactive constraints will remain the same for all iterations after some index. After this index, we will have $\mu_- = 0$, and there will be no need for computing $\nabla g_-(x)$, with potentially significant computational savings resulting.

Choice of Parameters. The choice of the parameters c and α in the penalty function $P(\cdot, \cdot; c, \alpha)$ and c in the penalty function $P(\cdot, \cdot; c, M)$ is crucial for the success of the overall method. The function $P(\cdot, \cdot; c, M)$ seems more attractive in this regard, since only one parameter choice is necessary. On the other hand, the function $P(\cdot, \cdot; c, \alpha)$ is simpler and, if α is chosen properly, just as effective. Basically, α should be chosen sufficiently small in order for the method to avoid spurious critical points of P or local maxima of (ECP) [cf. Proposition 2.1(a) and 2.1(c)]. The parameter c should be chosen sufficiently large to ensure that a K–T pair (x^*, λ^*) satisfying Assumption S will be a strict local minimum of P and spurious critical points of P are avoided [cf. Proposition 3.1(a) and 3.1(b)]. We can gain some insight regarding the proper range of values for c by considering a problem with quadratic objective function and linear constraints:

$$\text{minimize} \quad f(x) = \tfrac{1}{2}x'Hx,$$

$$\text{subject to} \quad N'x = 0,$$

where we assume that $f(x) > 0$ for all $x \neq 0$ with $N'x = 0$, and that N has rank m. This corresponds to the case where the K–T pair $\{x^* = 0, \lambda^* = 0\}$ satisfies Assumption S.

Consider the penalty function

$$P(x, \lambda; c, M) = (1/2)x'Hx + \lambda'N'x + (c/2)|N'x|^2 + (1/2)|M(Hx + N\lambda)|^2,$$

where M is a $p \times n$ matrix with $m \leq p \leq n$ and such that MN has rank m. We are interested in conditions on c and M that guarantee that $\nabla^2 P$ is positive definite. Consider the function

$$\tilde{P}(x; c, M) = \min_{\lambda} P(x, \lambda; c, M).$$

Since P is positive definite quadratic in λ for every x, the minimization above can be carried out explicitly, and the minimizing vector is given by

$$\hat{\lambda}(x) = -(N'M'MN)^{-1}(N' + N'M'MH)x.$$

Substitution in the expression for $\tilde{P}$ yields

$$\tilde{P}(x; c, M) = \tfrac{1}{2}x'[H + HM'MH + cNN' - (N + HM'MN) \times (N'M'MN)^{-1}(N' + N'M'MH)]x.$$

It is clear that $\nabla^2 P$ is positive definite iff

$$\nabla^2 \tilde{P}(x; c, M) > 0.$$

Consider the matrices

$$E_M = M'MN(N'M'MN)^{-1}N', \qquad \hat{E}_M = I - E_M. \tag{78}$$

A straightforward calculation shows that P may also be written as

$$\tilde{P}(x; c, M) = \tfrac{1}{2}x'[\hat{E}_M'H\hat{E}_M - E_M'HE_M + cNN' - N(N'M'MN)^{-1}N']x$$
$$+ \tfrac{1}{2}(MHx)'[I - MN(N'M'MN)^{-1}N'M'](MHx).$$

The matrix $[I - MN(N'M'MN)^{-1}N'M']$ is a projection matrix and is therefore positive semidefinite. Hence, the second term in the right side above is nonnegative, and it follows that, in order that $\nabla^2\tilde{P}(x; c, M) > 0$, it is sufficient that

$$x'[\hat{E}_M'H\hat{E}_M - E_MHE_M + cNN' - N(N'M'MN)^{-1}N']x > 0, \qquad \forall x \neq 0. \tag{79}$$

Consider the subspaces

$$\mathscr{C} = \{x \,|\, N'x = 0\}, \qquad \mathscr{C}^\perp = \{N\xi \,|\, \xi \in R^m\}.$$

For any $x \in R^n$, we have, using (78),

$$N'E_Mx = N'x, \qquad N'\hat{E}_Mx = N'(I - E_M)x = 0.$$

Hence,

$$\hat{E}_Mx \in \mathscr{C}, \qquad \forall x \in R^n. \tag{80}$$

We have also

$$N'x = N'Ex,$$

where E is given by

$$E = N(N'N)^{-1}N'.$$

In view of (78), this implies that

$$E_Mx = E_MEx.$$

By using the above two equations, we can write (79) as

$$(\hat{E}_Mx)'H(\hat{E}_Mx) + (Ex)'[cNN' - E_M'HE_M - N(N'M'MN)^{-1}N'](Ex) > 0,$$
$$\forall x \neq 0.$$

In view of the fact $\hat{E}_Mx \in \mathscr{C}$ [cf. (80)] and the hypothesis $z'Hz > 0$, $\forall z \neq 0$, with $z \in \mathscr{C}$, the first term above is nonnegative. Hence, the relation above will hold iff

$$c > \max\left\{\frac{z'[E_M'HE_M + N(N'M'MN)^{-1}N']z}{z'NN'z} \,\middle|\, |z| = 1, z \in \mathscr{C}^\perp\right\}. \tag{81}$$

This in turn implies that the matrix $\nabla^2 P$ will be positive definite if c satisfies (81).

Consider now the case

$$M = \sqrt{\alpha I},$$

for which we have

$$P(x, \lambda; c, M) = P(x, \lambda; c, \alpha).$$

Since every vector $z \in \mathscr{C}^{\perp}$ can be represented as

$$z = N\xi,$$

where

$$\xi \in R^m \quad \text{and} \quad E_M = N(N'N)^{-1}N',$$

relation (81) is easily shown to be equivalent to

$$c\alpha(N'N)^2 - \alpha N'HN - N'N > 0, \tag{82}$$

or, by right and left multiplication with $(N'N)^{-1}$,

$$c\alpha I - \alpha(N'N)^{-1}(N'HN)(N'N)^{-1} - (N'N)^{-1} > 0.$$

This relation suggests rules for the selection of the parameters c and α. Given α, one should select c sufficiently large so that (82) holds. If the value of α is not sufficiently small to the extent that unconstrained minimization yields critical points of P which are not local minima of (ECP), then α must be reduced, but *this reduction must be accompanied by a corresponding increase of c so that* (82) *holds. A good rule of thumb is therefore to increase c so as to keep the product $c\alpha$ roughly constant.*

In some cases, it may be desirable to have an automatic scheme for increasing c while the method is in progress. Such a scheme is given in Refs. 13 and 22 in the spirit of the one in Ref. 16. It may be desirable to also have a similar scheme for decreasing α automatically. There are several possibilities along these lines, but their investigation is beyond the scope of the present paper.

As a final remark, we mention that it may be advantageous to exploit the *a priori* knowledge that Lagrange multipliers corresponding to inequality constraints are nonnegative. Thus, instead of minimizing P_τ^+ subject to no constraints on (x, μ), it is possible to use special methods that can handle efficiently simple constraints in order to minimize P_τ^+ subject to $\mu \geq 0$. This eases the problem of selection of an appropriate value for the parameter α, since by enforcing the constraint $\mu \geq 0$ we preclude the possibility that the method will converge to a K–T pair with a negative Lagrange multiplier such as the usual type of local maximum. When f and g_j are convex functions, then for all x and $\mu \geq 0$ the matrix $\nabla_{xx}^2 L$ is positive semidefinite and the appropriate extension of Proposition 2.1(a) shows that any positive value of α is suitable. Thus, *for convex programming problems, the selection of the parameter α presents no difficulties as long as minimization of P_τ^+ is carried out subject to the constraint $\mu \geq 0$.*

4. A Variation of Newton's Method as a Method for Minimizing a Penalty Function of Fletcher

Define, in connection with (ECP), for $x \in X^*$

$$\tilde{\lambda}(x) = [\nabla h(x)'\nabla h(x)]^{-1}[h(x) - \nabla h(x)'\nabla f(x)]; \tag{83}$$

and, for $c > 0$, consider the penalty function

$$\tilde{P}(x; c) = f(x) + \tilde{\lambda}(x)'h(x) + (c/2)|h(x)|^2, \tag{84}$$

belonging to the class introduced by Fletcher (Ref. 2).

Note that $\tilde{P}$ can also be written as

$$\tilde{P}(x; c) = f(x) + \lambda(x)'h(x) + (1/2)h(x)'(cI + [\nabla h(x)'\nabla h(x)]^{-1})h(x),$$

where $\lambda(x)$ is given by (30), so it is slightly different from the function (29) considered earlier. We mention also that the penalty function (85) can be derived from the penalty function

$$L(x, \lambda) + (1/2)h(x)'(cI - [\nabla h(x)'\nabla h(x)]^{-1})h(x) + (1/2)|M(x)\nabla_x L(x, \lambda)|^2,$$

where

$$M(x) = [\nabla h(x)'\nabla h(x)]^{-1/2}\nabla h(x)',$$

in the same way as $\hat{P}(\cdot\,; c)$ was derived from the penalty function (8) [cf. (26)–(28)].

For $x_k \in X^*$, consider the iteration (Refs. 7 and 27)

$$x_{k+1} = x_k - \{E(x_k) + [I - E(x_k)]\nabla_{xx}^2 L[x_k, \tilde{\lambda}(x_k)]\}^{-1}\nabla_x L[x_k, \tilde{\lambda}(x_k)], \tag{85}$$

where, for all $x \in X^*$, $E(x)$ is defined by

$$E(x) = \nabla h(x)[\nabla h(x)'\nabla h(x)]^{-1}\nabla h(x)'. \tag{86}$$

It is shown in Pshenichnyi and Danilin (Ref. 7, pp. 208, 209) that, if (x^*, λ^*) is a K–T pair of (ECP) satisfying Assumption S, then

$$\tilde{\lambda}(x^*) = \lambda^*$$

and

$$E(x^*) + [I - E(x^*)]\nabla_{xx}^2 L(x^*, \lambda^*) = \nabla p(x^*)', \tag{87}$$

where the function $p: X^* \to R^n$ is defined by

$$p(x) = \nabla_x L[x, \tilde{\lambda}(x)].$$

Furthermore, the matrix $\nabla p(x^*)$ is invertible. As a result, iteration (85) is well defined for x_k sufficiently close to x^* and may be viewed as a consistent approximation of Newton's method,

$$x_{k+1} = x_k - [\nabla p(x_k)']^{-1} p(x_k),$$

for solving the nonlinear system

$$p(x) = 0.$$

The vector x^* is easily seen to be a solution of this system.

Actually, iteration (85) is closely related to the Newton iteration (1)–(2). In fact, we will show that, for every vector $\lambda_k \in R^m$, x_{k+1} as given by (85) satisfies, together with some vector λ_{k+1}, the system of equations

$$\begin{bmatrix} \nabla^2_{xx} L[x_k, \tilde{\lambda}(x_k)] & \nabla h(x_k) \\ \nabla h(x_k)' & 0 \end{bmatrix} \begin{bmatrix} x_{k+1} - x_k \\ \lambda_{k+1} - \lambda_k \end{bmatrix} = - \begin{bmatrix} \nabla_x L(x_k, \lambda_k) \\ h(x_k) \end{bmatrix}. \tag{88}$$

The similarity of this system with system (2) is evident. In fact, if the constraints are all linear, the two systems are identical. Note that we can also write (88) as

$$\nabla^2_{xx} L[x_k, \tilde{\lambda}(x_k)](x_{k+1} - x_k) + \nabla h(x_k)\lambda_{k+1} = -\nabla f(x_k), \tag{89}$$

$$\nabla h(x_k)'(x_{k+1} - x_k) = -h(x_k), \tag{90}$$

so x_{k+1} and λ_{k+1} are entirely independent of λ_k. From (90), we have

$$\begin{aligned} &\nabla h(x_k)[\nabla h(x_k)\nabla h(x_k)']^{-1}\nabla h(x_k)'(x_{k+1} - x_k) \\ &\quad = -\nabla h(x_k)[\nabla h(x_k)'\nabla h(x_k)]^{-1} h(x_k), \end{aligned} \tag{91}$$

while from (99) we obtain

$$\begin{aligned} &-\nabla h(x_k)[\nabla h(x_k)'\nabla h(x_k)]^{-1}\nabla h(x_k)'\nabla^2_{xx} L[x, \tilde{\lambda}(x_k)](x_{k+1} - x_k) - \nabla h(x_k)\lambda_{k+1} \\ &\quad = \nabla h(x_k)[\nabla h(x_k)'\nabla h(x_k)]^{-1}\nabla h(x_k)'\nabla f(x_k). \end{aligned} \tag{92}$$

By adding (89), (91), (92), and by making use of (83), we obtain

$$\{E(x_k) + [I - E(x_k)]\nabla^2_{xx} L[x_k, \tilde{\lambda}(x_k)]\}(x_{k+1} - x_k) = -\nabla_x L[x_k, \tilde{\lambda}(x_k)], \tag{93}$$

where $E(\cdot)$ is defined by (86). It can be seen that (85) and (93) are identical, so it follows that x_{k+1} can alternatively be obtained by solving the Newton-like system (88).

In view of (87), we can write

$$E(x_k) + [I - E(x_k)]\nabla^2_{xx} L[x_k, \tilde{\lambda}(x_k)] = \nabla p(x_k)' + A(x_k), \tag{94}$$

where $A(\cdot)$ is a continuous matrix such that

$$\lim_{x \to x^*} A(x) = 0. \tag{95}$$

We also have

$$\nabla p(x)' = \nabla[\nabla f(x) + \nabla h(x)\tilde{\lambda}(x)]' \\ = \nabla^2_{xx}L[x, \tilde{\lambda}(x)] + \nabla h(x)\nabla\tilde{\lambda}(x)'; \tag{96}$$

and from (93)–(96), we obtain

$$\{\nabla^2_{xx}L[x, \tilde{\lambda}(x_k)] + \nabla h(x_k)\nabla\tilde{\lambda}(x_k)' + A(x_k)\}(x_{k+1} - x_k) = -\nabla_x L[x_k, \tilde{\lambda}(x_k)]. \tag{97}$$

From (84), by differentiation we obtain

$$\nabla\tilde{P}(x_k; c) = \nabla_x L[x_k, \tilde{\lambda}(x_k)] + \nabla\tilde{\lambda}(x_k)h(x_k) + c\nabla h(x_k)h(x_k), \tag{98}$$

which in view of (90) yields

$$\nabla\tilde{P}(x_k; c) = \nabla_x L[x_k, \tilde{\lambda}(x_k)] - [\nabla\tilde{\lambda}(x_k)\nabla h(x_k)' + c\nabla h(x_k)\nabla h(x_k)'](x_{k+1} - x_k). \tag{99}$$

From (97) and (99), it follows that (85) can be written as

$$H(x_k; c)(x_{k+1} - x_k) = -\nabla\tilde{P}(x_k; c), \tag{100}$$

where

$$H(x_k; c) = \nabla^2_{xx}L[x_k, \tilde{\lambda}(x_k)] + \nabla h(x_k)\nabla\tilde{\lambda}(x_k)' + \nabla\tilde{\lambda}(x_k)\nabla h(x_k)' \\ + c\nabla h(x_k)\nabla h(x_k)' + A(x_k). \tag{101}$$

Now, by using (95), (101) and by differentiating (98), we obtain

$$H(x^*; c) = \nabla^2\tilde{P}(x^*; c).$$

Thus, we see that iteration (100), which is equivalent to iteration (85), can be viewed as a consistent approximation to Newton's method for minimizing the penalty function $\tilde{P}(\cdot\,; c)$ of (84). Similarly as in the previous section, we can construct a descent method with global convergence properties for minimizing $\tilde{P}(\cdot\,; c)$, which near x^* has the form (85) and attains a quadratic rate of convergence. A superlinearly convergent variable metric version of iteration (85) using line search based on descent of the penalty function (84) is described in Ref. 28.

5. Computational Experience

The method described by (64)–(68) and its version corresponding to the penalty function $P^+_\tau(\cdot\,, \cdot\,; c, \eta)$ of (36) was implemented and tested with a few example problems. For inequality constrained problems, local maxima typically have negative Lagrange multipliers associated with active constraints. Now, the Newton iteration (63) ignores all constraints j for which

$$\mu_j + 2\alpha\mu_j^2 + (c + \tau|\mu|^2)g_j(x) \le 0. \tag{102}$$

This means that, if α is sufficiently small, then within a neighborhood of a local-maximum Lagrange multiplier pair (x^*, μ^*) for which strict complementarity holds ($\mu_j^* < 0$ if $g_j(x^*) = 0$), *all* constraints are ignored by the Newton iteration (63) which then becomes an iteration of Newton's method for unconstrained minimization of $f(x)$. Thus, even though the method may be initially attracted to a local-maximum Lagrange multiplier pair and may approach it during several iterations while it attempts to reach the feasible region, it has the ability to eventually recognize such local maxima and to take large steps away from them. This behavior was confirmed in our experiments. Similar observations hold for the method corresponding to the penalty function (36).

For illustration purposes, we provide some results for a problem in which the scaling matrix D for the steepest-descent iteration was chosen to be diagonal, with the terms on the diagonal chosen by experimentation on the basis of the diagonal terms of the Hessian matrix $\nabla^2 P_\tau^+$. We did not experiment with any schemes for the automatic adjustment of c and α. The problem is

$$\text{minimize} \quad x_1,$$
$$\text{subject to} \quad x_1^2 + x_2^2 \le 1.$$

It has two K–T pairs,

$$\{x_1^* = 1, x_2^* = 0, \mu^* = -\tfrac{1}{2}\} \qquad \text{(global maximum)}$$

and

$$\{x_1^* = -1, x_2^* = 0, \mu^* = \tfrac{1}{2}\} \qquad \text{(global minimum)}.$$

For $\alpha = 0.01$, $c = 100$, and a broad range of starting points and values of τ, the method (64)–(68) each time converged to the global minimum. Similar results were also obtained for $\alpha = 0.1$, $c = 10$, and other values of α, c such that $\alpha < 1$ and $\alpha c = 1$ (compare with (82) and the note following the proof of Proposition 2.1). For $\alpha > 1$, the method converged sometimes to the global maximum and sometimes to the global minimum [cf. (102) and the subsequent discussion]. For $c = 10$ and $\alpha = 0.01$, the method sometimes did not converge to a point which is a K–T pair, indicating that a larger value of c is necessary. We list in Table 1 the number of Newton and steepest-descent iterations needed to obtain convergence to the global minimum within at least five significant digits for each coordinate for the case where $\alpha = 0.01$, $c = 100$, and for a variety of starting points. The

Table 1. Numerical results, $c = 100$, $\alpha = 0.01$.

Starting point	τ	Number of Newton iterations	Number of steepest descent iterations	Total number of iterations
(−100, −100, 50)	0	11	0	11
(100, 100, −50)	0	12	3	15
(−0.2, −0.2, 10)	0	3	7	10
(1.1, 0.1, −0.5)	0	5	2	7
(−1.1, −0.1, 0.5)	0	2	0	2
(−100, −100, 50)	10	11	0	11
(100, 100, −50)	10	12	3	15
(−0.2, −0.2, 10)	10	5	7	12
(1.1, 0.1, −0.5)	10	4	3	7
(−1.1, −0.1, 0.5)	10	2	0	2

number of iterations for other values of c and α, such that $c < 100$, $0.01 < \alpha < 1$, $\alpha c = 1$, was roughly comparable. As one would expect, lower values of c tend to have a beneficial effect on the performance of the method, particularly when the starting point is near the constraint boundary but far from the solution. This can be attributed to ill-conditioning associated with large values of c.

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