A DUAL DIFFERENTIABLE EXACT PENALTY FUNCTION

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Replace x_j^i+ by x_j^i- in the first equation of (21) on page 15 and in the first equation on page 16. Replace u_j^i+ by u_j^i- in the second equation of (21) and the second equation on page 16.

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ABSTRACT

A new penalty function is associated with an inequality constrained nonlinear programming problem via its dual. This penalty function is globally differentiable if the functions defining the original problem are twice globally differentiable. In addition, the penalty parameter remains finite. This approach reduces the original problem to a simple problem of maximizing a globally differentiable function on the product space of a Euclidean space and the nonnegative orthant of another Euclidean space. Many efficient algorithms exist for solving this problem. For the case of quadratic programming, the penalty function problem can be solved effectively by successive overrelaxation (SOR) methods which can handle huge problems while preserving sparsity features.

AMS (MOS) Subject Classifications: 90C30, 90C20

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1. Introduction

It is well known that exterior penalty functions [6,13] in mathematical programming suffer from one of two difficulties. Either the Hessian of the penalty function becomes ill-conditioned as the penalty parameter approaches infinity [6,20], or the penalty function is nondifferentiable [13]. There have been, however, attempts at obtaining penalty functions which are both differentiable and for which the penalty parameter remains finite [8,3,4,1]. We present here a different and an extremely simple penalty function which, by taking advantage of the structure of the dual problem, results in a penalty function which is differentiable and for which the penalty parameter remains finite. The key idea behind the present approach is extremely simple and is best illustrated by the following equality-constrained minimization problem

$$\underset{x\in R^n}{\text{minimize}} \quad f(x) \qquad \text{subject to} \quad h(x) = 0$$

where f and h are differentiable functions from the n-dimensional real Euclidean space R^n into R and R^k respectively. The classical exterior penalty problem for this problem is

$$\underset{x\in R^n}{\text{minimize}} \quad f(x) + \frac{\alpha}{2}\|h(x)\|^2$$

where α is a positive penalty parameter and $\|\cdot\|$ denotes the 2-norm. At stationary points of the penalty problem we have

$$\nabla f(x) + \alpha \nabla h(x)^T h(x) = 0$$

where $\nabla f(x)$ is the $n\times 1$ gradient of f, $\nabla h(x)$ is the $k\times n$ Jacobian of h and the superscript T denotes the transpose. In order for this condition to approach the stationarity conditions for the minimization problem, which are

$$\nabla f(x) + \nabla h(x)^T u = 0,\ h(x) = 0$$

where u is an $k\times 1$ vector of Lagrange multipliers, the quantity $\alpha h(x)$ must approach u. Since $h(x) = 0$, it turns out that <u>in general</u> α must approach ∞. There are exceptions. For example if $u = 0$ then α need not approach ∞. This is an exceptional case which does not hold in general for the original minimization problem. <u>However</u>, if we consider the Wolfe dual [22,15] to an <u>inequality</u> constrained minimization problem, then the optimal Lagrange multiplier associated with the equality constraint of the dual is zero provided that the Hessian of the Lagrangian is nonsingular at the optimum. Hence for the exterior penalty problem associated with Wolfe dual we can show (Theorems 1 to 4) that under rather natural conditions the penalty parameter remains finite. Hence we can obtain a globally differentiable penalty function with a finite penalty parameter. Because our penalty problem formulation depends in an essential manner on the dual problem, our results are local results in the absence of convexity, and become global results if convexity is assumed. Because our penalty function is smooth and its parameter is finite it has important computational implications. For example, fast methods of smooth optimization could be used to directly optimize the differentiable penalty function (Algorithm 1), or the function may be used as in [12] in enlarging the convergence region

of fast but locally convergent algorithms [9,11]. In addition, for positive definite quadratic programming problems, our penalty function can be used to derive a successive overrelaxation (SOR) algorithm without the need to invert the underlying positive definite matrix of the problem (Algorithm 2). SOR algorithms have proved to be successful in solving linear programming problems [17] and have the potential for solving enormous problems that cannot be tackled by pivotal methods while at the same time preserving the sparsity of the problem.

Besides this Introduction, this paper contains two sections. In Section 2 we treat the general nonlinear programming problem while in Section 2 we specialize to the quadratic programming case to obtain sharper results. Section 1 contains theorems relating stationary points, local and global optima of the nonlinear inequality constrained problem to those of the penalty problem. We also give a simple gradient projection algorithm for optimizing the penalty function. In Section 3 we have similar results for the quadratic programming case. We also present an SOR method for quadratic programming which is a generalization of the SOR method used with successful computational results on linear programming [17].

We briefly describe our notation. All vectors in R^n will be column vectors unless transposed to a row vector by the superscript T. R^n_+ will denote the nonnegative orthant $\{x | x \in R^n, x \geq 0\}$. For x in R^n, x_i, $i=1,\ldots,n$, will denote its ith component, while x_+ will denote a vector in R^n with components $(x_+)_i = \max\{x_i, 0\}$, $i=1,\ldots,n$ and $\|x\|$ will denote the Euclidean norm $(x^T x)^{\frac{1}{2}}$. For an $m \times n$ real matrix A, A_i

will denote the ith row, $A_{\bullet j}$ the jth column, and if $I \subset \{1,\ldots,m\}$, $J \subset \{1,\ldots,n\}$ then A_I will denote the submatrix with rows A_i, $i \in I$, A_J will denote the submatrix with columns $A_{\bullet j}$, $j \in J$, and A_{IJ} will denote the submatrix with elements A_{ij}, $i \in I$ and $j \in J$. For a differentiable function $f:R^n \to R$, $\nabla f(x)$ will denote the $n \times 1$ gradient vector, while for a differentiable function $g:R^n \to R^m$, $\nabla g(x)$ will denote the $m \times n$ Jacobian matrix. For a twice differentiable function $L:R^n \times R^m \to R$, $\nabla_x L(x,u)$ will denote the $n \times 1$ gradient with respect to x, $\nabla_u L(x,u)$ will denote $m \times 1$ gradient with respect to u, $\nabla^2 L(x,u)$ will denote $(n+m) \times (n+m)$ Hessian with respect to both x and u whose submatrix components are denoted as follows

$$\nabla^2 L(x,u) = \begin{bmatrix} \nabla_{xx} L(x,u) & \nabla_{xu} L(x,u) \\ \nabla_{ux} L(x,u) & \nabla_{uu} L(x,u) \end{bmatrix}$$

For a nonlinear programming problem such as (1) below, a point $(\bar{x},\bar{u}) \in R^{n+m}$ satisfying the Karush-Kuhn-Tucker conditions (1′) is said to be a <u>KKT point</u>, while $\bar{x}$ is said to be a <u>stationary point</u> of (1). Whenever a point $(\bar{x},\bar{u})$ is a KKT point, the differentiability of f and g at $\bar{x}$ is implicitly assumed.

Theorem 1 (Equivalence of stationary points of (1), (2) and (4))

Let f and g be twice continuously differentiable at $\bar{x}$. Then

(a) $\langle (\bar{x},\bar{u})$ is a stationary point of (2) and $\nabla_{xx}L(\bar{x},\bar{u})^{-1}$ exists $\rangle \Rightarrow \langle (\bar{x},\bar{u})$ is a KKT point of (1) $\rangle \Rightarrow \langle (\bar{x},\bar{u})$ is a stationary point of (4) for any γ $\rangle$

(b) $\langle (\bar{x},\bar{u})$ is a stationary point of (2) $\rangle \Leftarrow \langle (\bar{x},\bar{u})$ is a KKT point of (1) $\rangle \Leftarrow \langle (\bar{x},\bar{u})$ is a stationary point of (4), $\gamma \neq 0$ and $\frac{1}{\gamma}$ is not an eigenvalue of $\nabla_{xx}L(\bar{x},\bar{u})$ $\rangle$

Proof

The proof follows directly by writing the Karush-Kuhn-Tucker conditions [15] (1'), (2') and (4') for problems (1), (2) and (4) respectively as follows

$$\nabla_x L(\bar{x},\bar{u}) = 0,\ g(\bar{x}) \leqq 0,\ \bar{u}^T g(\bar{x}) = 0,\ \bar{u} \geqq 0 \qquad (1')$$

$$\left.\begin{aligned} &\text{For some } \bar{v} \in R^n: \\ &\nabla_x L(\bar{x},\bar{u}) - \nabla_{xx}L(\bar{x},\bar{u})\bar{v} = 0 \\ &g(\bar{x}) - \nabla g(\bar{x})\bar{v} \leqq 0 \\ &\bar{u}^T(g(\bar{x}) - \nabla g(\bar{x})\bar{v}) = 0 \\ &\bar{u} \geqq 0 \\ &\nabla_x L(\bar{x},\bar{u}) = 0 \end{aligned}\right\} \qquad (2')$$

2. The General Nonlinear Programming Problem

We consider here the problem

$$\underset{x\in R^n}{\text{minimize}} \quad f(x) \qquad \text{subject to} \quad g(x) \leqq 0 \tag{1}$$

where f is a function from the n-dimensional real Euclidean space R^n into the reals and g is from R^n into R^m. Associated with this problem is the Wolfe dual [22,15]

$$\begin{aligned} &\underset{(x,u)\in R^{n+m}}{\text{maximize}} \quad L(x,u) \qquad \text{subject to} \quad \nabla_x L(x,u) = 0,\ u \geqq 0 \\ &\text{where} \quad L(x,u) := f(x) + u^T g(x) \end{aligned} \tag{2}$$

Our penalty function is derived from (2) by constructing an exterior penalty function for the equality constraints only. Thus we define the penalty function

$$\theta(x,u,\gamma) := L(x,u) - \frac{\gamma}{2}\|\nabla_x L(x,u)\|^2 \tag{3}$$

and consider the penalty problem

$$\begin{aligned} &\underset{(x,u)\in R^{n+m}}{\text{maximize}} \quad \theta(x,u,\gamma) \\ &u \geqq 0 \end{aligned} \tag{4}$$

which is differentiable on R^{n+m} when f and g are differentiable on R^n. We shall relate various stationary and solution points of problems (1), (2) and (4). We begin with a simple but useful result.

$$\left.\begin{aligned} (I - \gamma\nabla_{xx}L(\bar{x},\bar{u}))\nabla_x L(\bar{x},\bar{u}) &= 0 \\ g(\bar{x}) - \gamma\nabla g(\bar{x})\nabla_x L(\bar{x},\bar{u}) &\leqq 0 \\ \bar{u}^T(g(\bar{x}) - \gamma\nabla g(\bar{x})\nabla_x L(\bar{x},\bar{u})) &= 0 \\ \bar{u} &\geqq 0 \end{aligned}\right\rangle \qquad (4')$$

□

In the next result we establish, under appropriate assumptions, the local concavity of $\theta(x,u,\gamma)$ in <u>both</u> the variables x and u.

<u>Theorem 2</u> (Negative semidefiniteness and definiteness of $\nabla^2\theta(\bar{x},\bar{u},\gamma)$)

Let $(\bar{x},\bar{u})$ be a KKT point of (1), let f and g be twice continuously differentiable at $\bar{x}$ and let $\nabla_{xx}L(\bar{x},\bar{u})$ be positive definite with minimum eigenvalue $\bar{\rho} > 0$. Then for $\gamma \geqq \frac{1}{\bar{\rho}}$, $(\bar{x},\bar{u})$ is a stationary point of (4) and the Hessian $\nabla^2\theta(\bar{x},\bar{u},\gamma)$ with respect to (x,u) is negative semidefinite. If in addition $\gamma > \frac{1}{\bar{\rho}}$ and $\nabla g(\bar{x})$ has linearly independent rows, then $\nabla^2\theta(\bar{x},\bar{u},\gamma)$ is negative definite and hence $(\bar{x},\bar{u})$ is a strict local maximum of (4).

<u>Proof</u>

By Theorem 1, $(\bar{x},\bar{u})$ satisfies the KKT conditions (4') for problem (4). We have from (3) when f and g are differentiable at x that

$$\nabla\theta(x,u,\gamma) = \begin{bmatrix} (I - \gamma\nabla_{xx}L(x,u))\nabla_x L(x,u) \\ \\ g(x) - \gamma\nabla g(x)\nabla_x L(x,u) \end{bmatrix} \qquad (5)$$

Recalling that $\nabla_x L(\bar{x},\bar{u}) = 0$ we have that

$$\nabla^2\theta(\bar{x},\bar{u},\gamma) = \begin{bmatrix} \nabla_{xx}L(\bar{x},\bar{u})(I-\gamma\nabla_{xx}L(\bar{x},\bar{u})) & (I-\gamma\nabla_{xx}L(\bar{x},\bar{u}))\nabla g(\bar{x})^T \\ \nabla g(\bar{x})(I-\gamma\nabla_{xx}L(\bar{x},\bar{u})) & -\gamma\nabla g(\bar{x})\nabla g(\bar{x})^T \end{bmatrix} \tag{6}$$

Define

$$C := \nabla_{xx}L(\bar{x},\bar{u}) \quad \text{and} \quad A := \nabla g(\bar{x}) \tag{7}$$

then

$$\nabla^2\theta(\bar{x},\bar{u},\gamma) = \begin{bmatrix} C(I-\gamma C) & (I-\gamma C)A^T \\ A(I-\gamma C) & -\gamma AA^T \end{bmatrix} = \begin{bmatrix} C & A^T \\ A & 0 \end{bmatrix} - \gamma \begin{bmatrix} C \\ A \end{bmatrix} \begin{bmatrix} C & A^T \end{bmatrix}$$

and for $\gamma \geq \frac{1}{\bar{\rho}}$ we have that

$$\begin{aligned} (x^T\ u^T)\nabla^2\theta(\bar{x},\bar{u},\gamma)\begin{pmatrix} x \\ u \end{pmatrix} &= x^TCx + 2x^TAu - \gamma\|Cx+A^Tu\|^2 \\ &= -x^TCx + 2x^T(Cx+A^Tu) - \gamma\|Cx+A^Tu\|^2 \\ &\leq -\bar{\rho}\|x\|^2 + 2\|x\|\ \|Cx+A^Tu\| - \gamma\|Cx+A^Tu\|^2 \\ &= -\bar{\rho}(\|x\| - \tfrac{1}{\bar{\rho}}\|Cx+A^Tu\|)^2 - (\gamma - \tfrac{1}{\bar{\rho}})\|Cx+A^Tu\|^2 \\ &\leq 0 \end{aligned}$$

Hence $\nabla^2\theta(\bar{x},\bar{u},\gamma)$ is positive semidefinite for $\gamma \geq \frac{1}{\bar{\rho}}$. If $\begin{pmatrix} x \\ u \end{pmatrix} \neq 0$ then we consider two cases:

Case I: $Cx + A^Tu \neq 0$. For this case it follows from $\gamma > \frac{1}{\bar{\rho}}$ that $(x^T\ u^T)\nabla^2\theta(\bar{x},\bar{u},\gamma)\begin{pmatrix} x \\ u \end{pmatrix} < 0$.

Case II: $Cx + A^T u = 0$ and $\binom{x}{u} \neq 0$. For this case we have that $x \neq 0$, else $u^T A = 0$, $u \neq 0$, which contradicts the assumption that the rows of A are linearly independent. Hence

$$(x^T \; u^T)\nabla^2\theta(\bar{x},\bar{u},\gamma)\binom{x}{u} = -x^T Cx < 0$$

where the last inequality follows from the assumption that C is positive definite.

Thus in either case $(x^T \; u^T)\nabla^2\theta(\bar{x},\bar{u},\gamma)\binom{x}{u} < 0$ for $(x,u) \neq 0$ and $\nabla^2\theta(\bar{x},\bar{u},\gamma)$ is negative definite for $\gamma > \frac{1}{\bar{\rho}}$ and $(\bar{x},\bar{u})$ is a strict local maximum of (4) [6,13]. □

The assumption in Theorem 2 that $\nabla g(\bar{x})$ has full row rank is restrictive, but apparently it is the best we can do if we require that $\nabla^2\theta(\bar{x},\bar{u},\gamma)$ be negative definite. A natural relaxation is to merely ask for conditions that ensure that $(\bar{x},\bar{u})$ is a strict local maximum of (4). It turns out that such a relaxation can be reflected in replacing the linear independence of the rows of $\nabla g(\bar{x})$ by the less stringent requirement of the linear independence of the gradients of the active constraints only as follows.

Theorem 3 (Strict local maximum of $\theta(x,u,\gamma)$)

The last sentence of Theorem 2 can be replaced by the following: If in addition $\gamma > \frac{1}{\bar{\rho}}$ and $\nabla g_i(\bar{x})$ are linearly independent for $i \in J$ where

$$J = \{i \,|\, g_i(\bar{x})=0,\ i=1,\ldots,m\} \tag{8}$$

then $(\bar{x},\bar{u})$ is a strict local maximum of (4).

Proof

Let $A_J = \nabla g_J(\bar{x})$. From the proof of Theorem 2, by replacing A by A_J, we have that $\nabla^2_{JJ}\theta(\bar{x},\bar{u},\gamma)$ is negative definite for $\gamma > \frac{1}{\bar{\rho}}$ where

$$\nabla^2_{JJ}\theta(\bar{x},\bar{u},\gamma) := \begin{bmatrix} C(I-\gamma C) & (I-\gamma C)A_J^T \\ A_J(I-\gamma C) & -\gamma A_J A_J^T \end{bmatrix} = \begin{bmatrix} C & A_J^T \\ A_J & 0 \end{bmatrix} - \gamma \begin{bmatrix} C \\ A_J \end{bmatrix} \begin{bmatrix} C & A_J^T \end{bmatrix} \tag{9}$$

We establish now that $(\bar{x},\bar{u})$ is a strict local maximum by (4) by establishing the second order sufficient optimality condition [6,13]. Note from (5) that $\nabla_u\theta(\bar{x},\bar{u},\gamma) = g(\bar{x})$, and since the optimal multiplier associated with the nonnegativity constraint $u \geqq 0$ is $-\nabla_u\theta(\bar{x},\bar{u},\gamma)$, hence the second order sufficient optimality condition for (4) is then

$$0 \neq \begin{pmatrix} x \\ u \end{pmatrix} = \begin{pmatrix} x \\ u_E = 0 \\ u_G \geqq 0 \\ u_H \end{pmatrix} \Rightarrow (x^T\ u_E^T\ u_G^T\ u_H^T)\nabla^2\theta(\bar{x},\bar{u},\gamma) \begin{pmatrix} x \\ x_E \\ u_G \\ u_H \end{pmatrix} < 0 \tag{10}$$

where

$$E = \{i \mid \bar{u}_i = 0,\ g_i(\bar{x}) < 0\}$$
$$G = \{i \mid \bar{u}_i = 0,\ g_i(\bar{x}) = 0\}$$
$$H = \{i \mid \bar{u}_i > 0,\ g_i(\bar{x}) = 0\}$$

Since $J = G \cup H$ it follows that the second order condition (10) can be rewritten as

$$0 \neq \begin{pmatrix} x \\ u_G \geqq 0 \\ u_H \end{pmatrix} \Rightarrow (x^T\ u_J^T)\nabla^2_{JJ}\theta(\bar{x},\bar{u},\gamma) \begin{pmatrix} x \\ u_J \end{pmatrix} < 0 \tag{11}$$

Condition (11) is automatically satisfied for $\gamma > \frac{1}{\bar{\rho}}$ because we have already established that $\nabla^2_{JJ}\theta(\bar{x},\bar{u},\gamma)$ is negative definite for $\gamma > \frac{1}{\bar{\rho}}$. □

So far no convexity assumptions have been made anywhere and consequently all our results are local results. We can globalize some of our results if we assume that f is uniformly strictly convex and g is convex on R^n. In fact we can show then that for each local solution $(x(\gamma), u(\gamma))$ of (4), $x(\gamma)$ is the unique global solution of (1). In particular we have the following.

Theorem 4 (Stationary points of (4) as global solutions of (1) and (2))

Let f and g be convex and twice continuously differentiable on R^n, let

$$y^T\nabla^2 f(x)y \geq \nu \|y\|^2 \quad \text{for all} \quad x, y\in R^n \quad \text{and some} \quad \nu > 0, \tag{12}$$

and let $\gamma > \frac{1}{\nu}$. For every stationary point $(x(\gamma), u(\gamma))$ of (4), $x(\gamma)$ is independent of γ and $x(\gamma) = \bar{x}$, where $\bar{x}$ is the unique solution of (1).

Proof

For x, y in R^n and $u\in R^m$, $u \geq 0$ we have that

$$y^T\nabla_{xx}L(x,u)y \geq y\nabla^2 f(x)y \geq \nu\|y\|^2 \tag{13}$$

Hence $\nabla_{xx}L(x,u)$ is positive definite for all $u \geq 0$ and its smallest eigenvalue $\rho(x,u)$ satisfies the inequality $\rho(x,u) \geq \nu$. By Theorem 1(b) every stationary point $(x(\gamma), u(\gamma))$ satisfies the KKT conditions (1′) of

(1). Since f is strictly convex and g is convex, $x(\gamma)$ must equal the unique solution $\bar{x}$ of (1) and $(\bar{x},u(\gamma))$ must solve (2) [15]. □

We note that problem (4) can be used directly to construct an algorithm for solving the original problem. For example we can easily prescribe a Levitin-Poljak gradient projection algorithm [14] or a superlinearly convergent quasi-Newton algorithm [10,7,9,11,21]. The key observation to make here is that the projection operation here is an extremely simple one, namely projection on $R^n \times R^m_+$. We give below the simplest gradient projection algorithm for solving (4) and its convergence to a KKT point of (1).

Algorithm 1 (Gradient projection algorithm for (4))

Choose $\gamma > 0$ and any $(x^0,u^0) \in R^n \times R^m_+$. Having (x^i,u^i) compute (x^{i+1},u^{i+1}) as follows:

$$\text{Direction choice: } p^i = (I-\gamma\nabla_{xx}L(x^i,u^i))\nabla_x L(x^i,u^i)$$

$$q^i = (u^i+g(x^i)-\gamma\nabla g(x^i)\nabla_x L(x^i,u^i))_+ - u^i$$

$$\text{Stepsize choice: } (x^{i+1},u^{i+1}) = (x^i+\lambda^i p^i, u^i+\lambda^i q^i)$$

where λ^i is chosen such that

$$\theta(x^i+\lambda^i p^i,u^i+\lambda^i q^i,\gamma) = \max_{\lambda}\{\theta(x^i+\lambda p^i,u^i+\lambda q^i,\gamma) \mid u^i+\lambda q^i \geqq 0\}$$

where θ is defined by (3).

By standard convergence results [14] and by Theorem 1 we have.

Theorem 5 (Convergence of Algorithm 1)

Let f and g be thrice differentiable on R^n. Each accumulation point $(\bar{x},\bar{u})$ of the sequence $\{(x^i,u^i)\}$ generated by the gradient projection Algorithm 1, such that $\frac{1}{\gamma}$ is not an eigenvalue of $\nabla_{xx}L(\bar{x},\bar{u})$, is a KKT point of (1).

3. The Quadratic Programming Problem

In this section we specialize our results to the quadratic programming problem and obtain some sharper results. However the principal purpose of this section is to describe an SOR method for solving the quadratic programming problem which does not require the inversion of the matrix defining the quadratic term [17]. This should substantially widen the applicability of SOR methods to mathematical programming problems which have hitherto been limited principally to the minimization of quadratic functions on the nonnegative orthant [16,17,18]. The principal advantages of SOR methods are their ability to handle extremely large problems and to preserve sparsity.

We shall consider here the quadratic program

$$\underset{x\in R^n}{\text{minimize}} \quad \tfrac{1}{2}x^TCx + d^Tx \qquad \text{subject to} \quad Ax \leq b \tag{14}$$

where C is an $n\times n$ symmetric matrix, A is an $m\times n$ matrix, d is in R^n and b is in R^m. The dual to this problem obtained from (2) is

$$\underset{(x,u)\in R^{n+m}}{\text{maximize}} \quad \tfrac{1}{2}x^TCx + d^Tx + u^T(Ax-b) \qquad \text{subject to} \quad Cx + d + A^Tu = 0,\ u \geq 0 \tag{15}$$

We note in passing that the standard quadratic programming dual [5,15] obtained by substituting from the equality constraint into the objective function of (15)

$$\underset{(x,u)\in R^{n+m}}{\text{maximize}} \quad -\tfrac{1}{2}x^TCx - b^Tu \qquad \text{subject to} \quad Cx + d + A^Tu = 0,\ u \geq 0 \tag{16}$$

cannot be used to obtain a differentiable exact penalty function because the optimal multiplier associated with the equality constraint in (15) is zero when C is nonsingular, whereas it is equal to x in (16) also when C is nonsingular [15].

The penalty function associated with (15) is

$$\phi(x,u,\gamma) := \frac{1}{2}x^TCx + d^Tx + u^T(Ax-b) - \frac{\gamma}{2}\|Cx+A^Tu+d\|^2 \tag{17}$$

and the associated penalty problem is

$$\begin{array}{l}\text{maximize} \\ (x,u)\in R^{n+m} \\ u \geqq 0\end{array} \quad \phi(x,u,\gamma) \tag{18}$$

We have as an immediate consequence of Theorems 2 and 3 the following.

Theorem 6 (Concavity and strict concavity of $\phi(x,u,\gamma)$)

Let C be positive definite with minimum eigenvalue $\bar{\rho} > 0$. Then for $\gamma \geqq \frac{1}{\bar{\rho}}$, $\nabla^2\phi(x,u,\gamma)$ is negative semidefinite and hence $\phi(x,u,\gamma)$ is a concave function of (x,u) on R^{n+m}. If in addition $\gamma > \frac{1}{\bar{\rho}}$ and A has linearly independent rows, then $\nabla^2\phi(x,u,\gamma)$ is negative definite and hence $\phi(x,u,\gamma)$ is a strictly concave function on R^{n+m}. If $\gamma > \frac{1}{\bar{\rho}}$ and only A_i, $i\in J$ are linearly independent where

$$J = \{i \,|\, A_i\bar{x}=b_i,\ i=1,\ldots,m\}$$

and $(\bar{x},\bar{u})$ is a KKT point of (1), then $(\bar{x},\bar{u})$ is a strict global maximum solution of (18).

Corollary 1 Let $\{x|Ax\leqq b\}$ be nonempty, let C be positive definite with least eigenvalue $\bar{\rho} > 0$. Then for each $\gamma \geqq \frac{1}{\bar{\rho}}$, problem (18) is a concave quadratic maximization problem which possesses a solution $(x(\gamma), u(\gamma))$ with $x(\gamma)$ independent of γ and $x(\gamma) = \bar{x}$ where $\bar{x}$ is the unique global solution of (14).

With the help of the SOR scheme of [16] we can solve iteratively the quadratic program (18) in $R^n \times R^m_+$ and thereby obtain a solution to (14). It will be convenient for that purpose to have the following expressions at hand

$$\nabla\phi(x,u,\gamma) = \begin{bmatrix} (I-\gamma C)(Cx+A^T u+d) \\ Ax - b - \gamma A(Cx+A^T u+d) \end{bmatrix} \tag{19}$$

$$\nabla^2\phi(x,u,\gamma) = \begin{bmatrix} C(I-\gamma C) & (I-\gamma C)A^T \\ A(I-\gamma C) & -\gamma AA^T \end{bmatrix} \tag{20}$$

An SOR method for solving the quadratic program (18) with relaxation factor $\omega\in(0,2)$ can be given as follows then

$$\left.\begin{aligned} x_j^{i+1} &= x_j^i - \frac{\omega}{(\nabla_{xx}\phi(x^i,u^i,\gamma))_{jj}} \nabla_{x_j}\phi(x_1^{i+1},\ldots,x_{j-1}^{i+1},x_j^i,\ldots,x_n^i,u^i,\gamma) \\ & \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad j=1,\ldots,n \\ u_j^{i+1} &= \left(u_j^i - \frac{\omega}{(\nabla_{uu}\phi(x^i,u^i,\gamma))_{jj}} \nabla_{u_j}\phi(x^{i+1},u_1^{i+1},\ldots,u_{j-1}^{i+1},u_j^i,\ldots,u_m^i,\gamma)\right)_+ \\ & \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad j=1,\ldots,m \end{aligned}\right\} \tag{21}$$

We spell out our SOR scheme in detail now.

Algorithm 2 (SOR scheme for (18))

Choose $\omega\in(0,2)$, $\gamma > \max_j \left\{ \frac{C_{jj}}{\|C_j\|^2} \,\middle|\, C_j \neq 0 \right\}$, $\frac{1}{\gamma} \neq$ an eigenvalue of C and $(x^0,u^0) \in R^n \times R^m_+$. Having (x^i,u^i) compute (x^{i+1},u^{i+1}) as follows:

$$x_j^{i+1} = x_j^i - \frac{\omega}{C_{jj}-\gamma\|C_j\|^2}((I_j-\gamma C_j)(\sum_{\ell=1}^{j-1} C_{\cdot\ell}x_\ell^{i+1} + \sum_{\ell=j}^{n} C_{\cdot\ell}x_\ell^i + A^T u^i + d))$$

$\leftarrow$ Set to 1 if $C_j = 0$ $\rightarrow$ $\leftarrow$ For $j > 1$ only $\rightarrow$

$j=1,\ldots,n$

$$u_j^{i+1} = (u_j^i - \frac{\omega}{-\gamma\|A_j\|^2}(A_j x^{i+1} - b_j - \gamma A_j(Cx^{i+1} + \sum_{\ell=1}^{j-1}(A^T)_{\cdot\ell}u_\ell^{i+1} + \sum_{\ell=j}^{m}(A^T)_{\cdot\ell}u_\ell^i + d)))_+$$

$\leftarrow$ For $j > 1$ only $\rightarrow$

$j=1,\ldots,m$

Remark 1

The only implicit assumption in Algorithm 2 is that $A_j \neq 0$, $j=1,\ldots,m$. This assumption imposes no restrictions whatsoever, since all constraints $A_j x \leq b_j$ of (14) for which $A_j = 0$ are either inconsistent $(b_j < 0)$ or else can be discarded.

Remark 2

Note that in Algorithm 2 only linear arrays are needed in distinction from rectangular arrays. That is, we need to access the rows and columns of C and A one at a time. Thus, if the problem is of enormous size and very sparse, then only the nonzero elements need be stored, and this sparsity unlike pivotal algorithms is never lost.

We can now use the convergence theorems of [16] and the theorems of this paper to obtain the following convergence result for the SOR Algorithm 2.

Theorem 7 (Monotonicity and convergence of the SOR Algorithm 2)

For the sequence $\{(x^i,u^i)\}$, $i=1,2,\ldots,$ generated by Algorithm 2

$$\phi(x^{i+1},u^{i+1},\gamma) \geq \phi(x^i,u^i,\gamma),\ i=0,1,\ldots. \tag{22}$$

and each accumulation point $(\bar{x},\bar{u})$ of the sequence $\{(x^i,u^i)\}$ is a KKT point of the original quadratic program (14). If in addition C is positive semidefinite then $\bar{x}$ is a global solution of (14).

Proof

Inequality (22) follows from (9) of [16] and by Theorem 2.1 of [16] $(\bar{x},\bar{u})$ is a stationary point of (17). By Theorem 1, $(\bar{x},\bar{u})$ is a KKT point of (14). When C is positive semidefinite $\bar{x}$ is a global minimum solution of (14) by the sufficiency of the KKT conditions [15]. □

We note that Theorem 7 does not ensure the existence of an accumulation $(\bar{x},\bar{u})$ of the sequence $\{(x^i,u^i)\}$ of Algorithm 2. To ensure that at least one accumulation point exists we need to impose some sort of qualification similar to that of Theorem 2.2 of [16] which will ensure the boundedness of the iterates $\{(x^i,u^i)\}$ of Algorithm 2. In particular we have the following.

Theorem 8 (Boundedness of the iterates of the SOR Algorithm 2)

Let C be positive definite with minimum eigenvalue $\bar{\rho} > 0$, let $\gamma > \frac{1}{\bar{\rho}}$ and let either (i) A have linearly independent columns and there exists an $\hat{x}$ satisfying the constraint qualification $A\hat{x} < b$ or (ii) let A have linearly independent rows. Then the sequence $\{(x^i,u^i)\}$, $i=1,2,\ldots,$ generated by the SOR Algorithm 2 is bounded and $\lim_{i\to\infty} x^i = \bar{x}$, where $\bar{x}$ is the unique global solution of (14).

Proof

By Theorem 6 the constant Hessian $\nabla^2\phi(x,u,\gamma)$ defined by (20) is negative semidefinite. We shall assume that the sequence $\{(x^i,u^i)\}$

generated by Algorithm 2 is unbounded and exhibit a contradiction. Without loss of generality suppose that $\|(x^i,u^i)\| \neq 0$ and $\{\|x^i,u^i\|\} \to \infty$. Define $z := \binom{x}{u}$, $M := \nabla^2\phi(x,u,\gamma)$ and $q := \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} := \begin{pmatrix} (I-\gamma C)d \\ -b-\gamma Ad \end{pmatrix}$. Then

$$\phi(x,u,\gamma) = \phi(z,\gamma) = \frac{1}{2}z^TMz + q^Tz$$

It follows from (22) and Algorithm 2 for $i=1,2,\ldots,$ that $u^i \geqq 0$ and

$$\frac{\phi(z^0,\gamma)}{\|z^i\|^2} \leqq \frac{\phi(z^i,\gamma)}{\|z^i\|^2} = \frac{1}{2}\frac{z^{i^T}Mz^i}{\|z^i\|^2} + \frac{1}{\|z^i\|}q^T\frac{z^i}{\|z^i\|}.$$

By the Bolzano-Weierstrass Theorem we get that $\left\{\frac{z^i}{\|z^i\|}\right\}$ has an accumulation point $\bar{y}$ on the unit sphere in R^{n+m} satisfying $0 \leqq \frac{1}{2}\bar{y}^TM\bar{y}$ and $\bar{y} = \binom{\bar{x}}{\bar{u}}$ with $\bar{x}\in R^n$ and $\bar{u}\in R^m_+$. Since M is negative semidefinite it follows that $\bar{y}^TM\bar{y} = 0$ and hence $M\bar{y} = 0$. Since we also have that

$$\frac{\phi(z^0,\gamma)}{\|z^i\|} \leqq \frac{\phi(z^i,\gamma)}{\|z^i\|} = \frac{1}{2}\frac{z^{i^T}Mz^i}{\|z^i\|} + \frac{q^Tz^i}{\|z^i\|} \leqq \frac{q^Tz^i}{\|z^i\|}$$

it follows that $0 \leqq q^T\bar{y}$. We thus have

$$M\bar{y} = 0,\ q^T\bar{y} \geqq 0,\ 0 \neq \bar{y} = \binom{\bar{x}}{\bar{u}},\ \bar{u} \geqq 0 \tag{23}$$

or equivalently

$$\begin{pmatrix} C(I-\gamma C) & (I-\gamma C)A^T \\ A(I-\gamma C) & -\gamma AA^T \end{pmatrix} \begin{pmatrix} \bar{x} \\ \bar{u} \end{pmatrix} = 0,\ q_1^T\bar{x} + q_2^T\bar{u} \geqq 0,\ \bar{u} \geqq 0,\ (\bar{x},\bar{u}) \neq 0 \tag{24}$$

From the generalized Gordan theorem of the alternative [19] (24) is equivalent to either

the rows of $[C(I-\gamma C)\quad (I-\gamma C)A^T]$ are linearly dependent (25)

or

$$\left.\begin{aligned} C(I-\gamma C)v + (I-\gamma C)A^Tw &= (I-\gamma C)d \\ A(I-\gamma C)v - \gamma AA^Tw &> -b-\gamma Ad \\ \text{has no solution } (v,w) &\text{ in } R^{n+m} \end{aligned}\right\} \tag{26}$$

Because $\gamma > \frac{1}{\bar{\rho}}$ it follows that $I - \gamma C$ is negative definite and that $C(I-\gamma C)$ is nonsingular which contradicts (25). We will show now that (26) also leads to a contradiction. By hypothesis we have that $A\hat{x} < b$ for the case when the columns of A are linearly independent and consequently there exists a w satisfying

$$A^Tw = d + C\hat{x}$$

and hence

$$A\hat{x} = AC^{-1}(A^Tw-d) < b$$

that is

$$AC^{-1}d - AC^{-1}A^Tw + b > 0.$$

For the case when the rows of A are linearly independent the last inequality also holds for some w because $AC^{-1}A^T$ is nonsingular. Consequently

$$AC^{-1}((I-\gamma C)d - (I-\gamma C)A^Tw) - \gamma AA^Tw > -b - \gamma Ad$$

By defining

$$v = (I-\gamma C)^{-1}C^{-1}((I-\gamma C)d - (I-\gamma C)A^T w)$$

we get

$$C(I-\gamma C)v + (I-\gamma C)A^T w = (I-\gamma C)d$$

$$A(I-\gamma C)v - \gamma AA^T w > - b - \gamma Ad$$

These last two relations contradict (26). Consequently the sequence $\{(x^i,u^i)\}$ is bounded and must have at least one accumulation point. For each accumulation point $(\tilde{x},\tilde{u})$, $\tilde{x}$ must equal the unique solution $\bar{x}$ of (14). Since $\{x^i\}$ is also bounded it must converge to $\bar{x}$ [2]. □

At this time we do not have any computational experience for the SOR Algorithm 2 for solving the general quadratic programming problem (14). However, for the case when matrix $C = \varepsilon I$ where ε is a positive number and $\gamma = \frac{1}{\varepsilon}$, the penalty problem (18) becomes

$$\underset{\substack{u\in R^m \\ u \geqq 0}}{\text{Maximize}} \; -\frac{1}{2}\|A^T u+d\|^2 - \varepsilon b^T u \tag{27}$$

This is precisely the dual of the quadratic program perturbation of [17] associated with the linear program

$$\underset{x\in R^n}{\text{Minimize}} \; d^T x \quad \text{subject to} \quad Ax \leqq b \tag{28}$$

and which was solved quite successfully by the SOR method proposed here. Thus for at least this special class of quadratic programs computational experience is very encouraging. It is hoped that this experience will carry over to the more general case.

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