Nonlinear Complementarity as Unconstrained and Constrained Minimization

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Dedicated to Phil Wolfe on his sixty-fifth birthday, in appreciation of his major contributions to Mathematical Programming.

Abstract. The nonlinear complementarity problem is cast as an unconstrained minimization problem that is obtained from an augmented Lagrangian formulation. The dimensionality of the unconstrained problem is the same as that of the original problem, and the penalty parameter need only be greater than one. Another feature of the unconstrained problem is that it has global minima of zero at precisely all the solution points of the complementarity problem without any monotonicity assumption. If the mapping of the complementarity problem is differentiable, then so is the objective of the unconstrained problem, and its gradient vanishes at all solution points of the complementarity problem. Under assumptions of nondegeneracy and linear independence of gradients of active constraints at a complementarity problem solution, the corresponding global unconstrained minimum point is locally unique. A Wolfe dual to a standard constrained optimization problem associated with the nonlinear complementarity problem is also formulated under a monotonicity and differentiability assumption. Most of the standard duality results are established even though the underlying constrained optimization problem may be nonconvex.

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1. Introduction

We shall be concerned here with the classical nonlinear complementarity problem [2, 3, 4, 10] of finding an x in the n-dimensional real space R^n such that

$$F(x) \quad 0, \;\; x \quad 0, \;\; xF(x) = 0 \qquad \text{(NCP)} \tag{1.1}$$

where $F\colon R^n \rightarrow R^n$. An obviously related constrained minimization problem is the following

$$\min_x \; \{xF(x) \big| F(x) \quad 0, \; x \quad 0\} \qquad \text{(MP)} \tag{1.2}$$

It is evident that the NCP is solvable if and only if the MP has a solution with a zero minimum value. Because of the special structure of MP, at a solution $\bar{x}$ such that $\bar{x}F(\bar{x}) = 0$, $\bar{x}$ plays the role of a multiplier for the constraints $F(x) \quad 0$, while $F(\bar{x})$ plays a similar role for the constraints $x \quad 0$. This is most easily seen if we assume that F is monotone (an assumption that will **not** be made in general for this paper, but only in Section 4). Thus, the following Kuhn-Tucker saddlepoint condition for MP with $\bar{u} = \bar{x}$ and $\bar{v} = F(\bar{x})$

$$\begin{aligned} &\bar{x}F(\bar{x}) - uF(\bar{x}) - v\bar{x} \quad \bar{x}F(\bar{x}) - \bar{u}F(\bar{x}) - \bar{v}\bar{x} \quad xF(x) - \bar{u}F(x) - \bar{v}x \\ &\qquad\qquad\qquad\qquad \forall (u, v) \in R^n_+ \times R^n_+, \; \forall x \in R^n \end{aligned} \tag{1.3}$$

follows directly from $\bar{x}F(\bar{x}) = 0$ and the monotonicity of F. The fact that the pair $\big(\bar{x}, \; F(\bar{x})\big)$ can be used as an optimal multiplier for MP, was first observed for the monotone differentiable case by Cottle [2, Chapter IV, Theorem 4] and Cottle and Dantzig [4, Theorem 1] to show that every constraint-qualification-satisfying local solution of MP (which incidentally is not a convex program, since neither its objective is convex nor the constraint function $F(x)$ is concave) is a global solution of (1.2) with a minimum value of zero and hence solves NCP. Motivated by this fact we were led to investigating an augmented Lagrangian formulation [19, 14, 1] for MP

$$L(x, u, v, \alpha) \colon = xF(x) + \frac{1}{2\alpha}\Big(\big\|\big(-\alpha F(x) + u\big)_+\big\|^2 - \big\|u\big\|^2 + \big\|\big(-\alpha x + v\big)_+\big\|^2 - \big\|v\big\|^2\Big) \tag{1.4}$$

where the norm is the 2-norm and $\big(z\big)_+$ denotes $\big(z_+\big)_i = \max\,\{z_i, 0\}, \; i = 1, \ldots, n$. With u replaced by x and v by $F(x)$ this led to the following unusual but very interesting **implicit Lagrangian** function

$$\begin{aligned} M(x, \alpha) \colon = xF(x) + \frac{1}{2\alpha}\Big(&\big\|\big(-\alpha F(x) + x\big)_+\big\|^2 - \big\|x\big\|^2 \\ &+ \big\|\big(-\alpha x + F(x)\big)_+\big\|^2 - \big\|F(x)\big\|^2\Big) \end{aligned} \tag{1.5}$$

It turns that this function is nonnegative on $R^n \times (1, \infty)$, and is zero if and only if x is a solution of the NCP without regard to whether F is monotone or not (Theorem 2.1 below). If F is differentiable on R^n, then so is $M(\cdot, \alpha)$, and its gradient vanishes at all solutions of NCP for $\alpha > 1$ (Corollary 2.2). Furthermore, at nondegenerate solution points of NCP at which the gradients of the active constraints are linearly independent, $M(x, \alpha)$ has a locally unique global minimum solution (Theorem 2.3). In a neighborhood of such points locally superlinearly convergent Newton Methods [5] can be applied (Remark 2.4). We note that in a similar vein, Di Pillo and Grippo [6, 7] solved for the multipliers in terms of the original variables of a constrained optimization problem to obtain exact penalty functions.

The paper is organized as follows. In Section 2 we establish the above results for the implicit Lagrangian $M(x, \alpha)$. In Section 3 we point out three other functions which also have zeros or unconstrained minima at solutions of NCP. One function $P(x, \alpha)$ (see (3.1)) is simply an asymptotic exterior penalty which merely has zeros at such points but not necessarily minimum points. Another function $E(x, \alpha)$ (see (3.2)) is an exact penalty, which, however, is nondifferentiable and is valid only for monotone F. The third is a simple function $Q(x, \alpha)$ (see (3.3)) based on the residuals of the NCP. Numerical comparisons of these three functions are made with $M(x, \alpha)$ on a simple one-dimensional nonmonotone complementarity problem and appear to favor $M(x, \alpha)$. In Section 4 we state a Wolfe dual (4.1) to MP (1.2) and derive most of the standard duality results, Theorems 4.2-4.4, for it under monotonicity and differentiability assumptions. It is interesting to note that these duality results, which in general require convexity of the primal problem, hold here despite the fact that MP (1.2) may have a nonconvex objective function and a nonconvex feasible region. Section 5 contains some concluding remarks and some open questions.

We describe our notation now and some concepts employed in the paper. For a row or column vector x in the n-dimensional space R^n with components x_i, $i = 1, \ldots, n$, x_+ will denote the orthogonal projection on the nonnegative orthant R^n_+, that is $\left(x_+\right)_i := \max\ \{x_i,\ 0\}$, $i = 1, \ldots, n$. The norm $\| \cdot \|$ will denote the 2-norm $(xx)^{\frac{1}{2}}$. Other norms will be subscripted such as $\|x\|_\infty := \max\limits_{1in} |x_i|$ and $\|x\|_1 := \sum\limits_{i=1}^{n} |x_i|$. A function $F: R^n \to R^n$ is said to be monotone on R^n if

$$(1.6) \qquad (y - x)\big(F(y) - F(x)\big)\ 0,\ \ \forall x, y \text{ in } R^n$$

The slightly unusual, but convenient, notation $F(x)^{-1}$ will denote $\left(F(x)^{-1}\right)_i = F_i(x)^{-1},\ i = 1,\ldots,n$. If F is differentiable at x, then $\nabla F(x)$ denotes the $n \times n$ Jacobian matrix, with rows $\nabla F_i(x),\ i = 1,\ldots,n$, where $\nabla F_i(x)$ is the $1 \times n$ gradient vector $\left(\dfrac{\partial F_i(x)}{\partial x_1},\ldots,\dfrac{\partial F_i(x)}{\partial x_n}\right)$, and $\nabla F(x)^T$ will denote the transpose of $\nabla F(x)$. For an $m \times n$ matrix A, A_i denotes the ith row, $i = 1,\ldots,m$. For $M(x,\alpha)\colon R^n \times R \to R, \nabla M(x,\alpha) := \left(\dfrac{\partial M(x,\alpha)}{\partial x_1},\ldots,\dfrac{\partial M(x,\alpha)}{\partial x_n}\right)$ and $\nabla^2 M(x,\alpha) := \left(\dfrac{\partial^2 M(x,\alpha)}{\partial x_i \partial x_j}\right),\ i,j = 1,\ldots,n$. For $L(x,u,v)\colon R^n \times R^n \times R^n \to R, \nabla_x L(x,u,v) := \left(\dfrac{\partial L(x,u,v)}{\partial x_1},\ldots,\dfrac{\partial L(x,u,v)}{\partial x_n}\right)$ and $\nabla_{xx} L(x,u,v) := \left(\dfrac{\partial^2 L(x,u,v)}{\partial x_i \partial x_j}\right),\ i,j = 1,\ldots,n$. For $f\colon X \subset R^n \to R$, $\arg\min_{x \in X} f(x)$ denotes the set of minimizers of $f(x)$ in X. The identity matrix of any order will be denoted by I. If $J \cup K$ is a partition of $\{1,\ldots,n\}$, then $F_J(x) := F_{i\in J}(x),\ F_K(x) := F_{i\in K}(x), \nabla F_J(x) := \nabla F_{i\in J}(x)$ and $I_J := I_{i\in J}$.

Finally, we note that by elementary arguments (just consider the individual cases $-\alpha F_i(x) + x_i\ \ 0$ and $-\alpha F_i(x) + x_i < 0$ separately, etc.) we have for $\alpha > 0$ that

$$(1.7)\qquad F(x)\ \ 0, x\ \ 0, xF(x) = 0 \Leftrightarrow x = \left(-\alpha F(x) + x\right)_+ \Leftrightarrow F(x) = \left(-\alpha x + F(x)\right)_+$$

2. Properties of the Implicit Lagrangian $M(x, \alpha)$

We first establish nonnegativity of the implicit Lagrangian $M(x, \alpha)$ and show that it vanishes only at solution points of the NCP. For convenience in the proofs we decompose $M(x, \alpha)$ as follows

$$(2.1a) \qquad M(x, \alpha) = \sum_{i=1}^{n} M_i(x, \alpha)$$

where

$$(2.1b) \quad M_i(x, \alpha) := x_i F_i(x) + \frac{1}{2\alpha}\Big(\big(-\alpha F_i(x) + x_i\big)_+^2 - x_i^2 + \big(-\alpha x_i + F_i(x)\big)_+^2 - F_i(x)^2\Big)$$

We state and prove our first principal result.

2.1 Theorem The implicit Lagrangian $M(x, \alpha)$ defined in (1.5) is nonnegative on $R^n \times (1, \infty)$. For $\alpha \in (1, \infty)$, $M(x, \alpha)$ vanishes if and only if x solves the NCP (1.1).

Proof Let $x \in R^n$, $\alpha \in (1, \infty)$ and let $F_i := F_i(x)$. Consider four cases:

Case 1: $-\alpha F_i + x_i \;\; 0, -\alpha x_i + F_i \;\; 0$

It follows that

$$x_i \;\; \alpha F_i \;\; \alpha^2 x_i \quad \text{and} \quad F_i \;\; \alpha x_i \;\; \alpha^2 F_i$$

Since $\alpha^2 > 1$ we have $x_i \;\; 0$ and $F_i \;\; 0$ and hence from (2.1b)

(2.2)

$$\begin{aligned} 2\alpha M_i(x, \alpha) &= 2\alpha x_i F_i + (\alpha^2 F_i^2 - 2\alpha x_i F_i + x_i^2) - x_i^2 + (\alpha^2 x_i^2 - 2\alpha x_i F_i + F_i^2) - F_i^2 \\ &= \alpha^2 F_i^2 + \alpha^2 x_i^2 - 2\alpha x_i F_i \\ &= (\alpha F_i - \alpha x_i)^2 + 2\alpha(\alpha - 1) x_i F_i \;\; 0 \end{aligned}$$

Case 2: $-\alpha F_i + x_i \;\; 0, -\alpha x_i + F_i < 0$

$$(2.3) \qquad 2\alpha M_i(x, \alpha) = (\alpha^2 - 1) F_i^2 \;\; 0$$

Case 3: $-\alpha F_i + x_i < 0, -\alpha x_i + F_i \;\; 0$

$$(2.4) \qquad 2\alpha M_i(x, \alpha) = (\alpha^2 - 1) x_i^2 \;\; 0$$

Case 4: $-\alpha F_i + x_i < 0, -\alpha x_i + F_i < 0$

It follows that

$$x_i < \alpha F_i < \alpha^2 x_i \text{ and } F_i < \alpha x_i < \alpha^2 F_i$$

Since $\alpha^2 > 1$ we have $x_i > 0$ and $F_i > 0$ and hence

$$(2.5) \qquad 2\alpha M_i(x,\alpha) = 2\alpha x_i F_i - x_i^2 - F_i^2 \left\langle \begin{array}{c} 2x_i^2 - x_i^2 - F_i^2 = x_i^2 - F_i^2 \\ \\ 2F_i^2 - x_i^2 - F_i^2 = F_i^2 - x_i^2 \end{array} \right\rangle \left|x_i^2 - F_i^2\right| \; 0$$

Since these four cases exhaust all possibilities it follows that $M(x,\alpha) = \sum_{i=1}^{n} M_i(x,\alpha)$ is nonnegative on $R^n \times (1,\infty)$.

Suppose now that x solves NCP (1.1) and let $\alpha \in (0,\infty)$. Hence by (1.7)

$$(2.6) \qquad xF(x) = 0, \;\; x = \big(-\alpha F(x) + x\big)_+, \;\; F(x) = \big(-\alpha x + F(x)\big)_+$$

It immediately follows that $M(x,\alpha) = 0$ for such x and $\alpha \in (0,\infty)$. This establishes the "if" part of the theorem. We now establish the "only if" part.

Suppose now that $M(x,\alpha) = 0$ for some $x \in R^n$ and $\alpha \in (1,\infty)$. It follows from the four cases above, since $M_i(x,\alpha) \; 0$, $i = 1,\ldots,n$, that

$$(2.7) \qquad M_i(x,\alpha) = 0, \; i = 1,\ldots,n$$

We again look at four cases $1', 2', 3'$ and $4'$ corresponding to the four cases 1, 2, 3, 4 above.

Case 1′ : It follows from $x_i \; 0$, $F_i \; 0$, (2.2), $\alpha > 1$ and $M_i(x,\alpha) = 0$, that $F_i = x_i$ and $x_i F_i = 0$. Hence $x_i = F_i = 0$.

Case 2′ : It follows from (2.3), $\alpha > 1$ and $M_i(x,\alpha) = 0$ that

$$F_i = 0, \;\; x_i > 0$$

Case 3′ : It follows from (2.4), $\alpha > 1$ and $M_i(x,\alpha) = 0$, that

$$x_i = 0, \;\; F_i > 0$$

Case 4′ : It follows from (2.5) and $M_i(x,\alpha) = 0$, that $x_i^2 = F_i^2$. Since $x_i > 0$ and $F_i > 0$ we also get that $x_i = F_i$. Using all these facts in (2.5) again we get that

$x_i = F_i = 0$ which contradicts the assumption of Case 4 that $-\alpha F_i + x_i < 0$. Hence this case is vacuous when $M(x,\alpha) = 0$ and $\alpha > 1$.

Combining the outcomes of Cases $1', 2'$ and $3'$ we have that x solves NCP (1.1) and the theorem is established. ∎

Theorem 2.1 establishes a one-to-one correspondence between solutions of the NCP (1.1) and global unconstrained minima of the implicit Lagrangian (1.5), all of which are zero in value. Note that no monotonicity or differentiability of F was assumed here. However, $M(x,\alpha)$ is differentiable if $F(x)$ is differentiable. We thus obtain the following immediate consequence of Theorem 2.1.

2.2 Corollary If F is differentiable at a solution $\bar{x}$ of NCP (1.1), then $\nabla M(\bar{x},\alpha) = 0$ for $\alpha \in (1,\infty)$.

In fact, Corollary 2.2 holds for $\alpha \in [0,\infty)$ as can be easily seen by evaluating $\nabla M(\bar{x},\alpha)$ (see (2.9) below) and noting by (1.7) and $\alpha > 0$ that $\bar{x} = \big(-\alpha F(\bar{x}) + \bar{x}\big)_+$ and $F(\bar{x}) = \big(-\alpha\bar{x} + F(\bar{x})\big)_+$.

We now establish the local uniqueness of global minimum solutions of $M(x,\alpha)$ at all nondegenerate solutions of the NCP at which the active constraints have linearly independent gradients.

2.3 Theorem Let $\bar{x}$ be a nondegenerate solution of NCP (1.1), that is $\bar{x} + F(\bar{x}) > 0$, let F be twice differentiable at $\bar{x}$, and let $\big\{\nabla F(\bar{x})_{j\in J},\ I_{k\in K}\big\}$ be linearly independent, where

$$J := \big\{j \big| F_j(\bar{x}) = 0\big\}, K := \big\{k \big| \bar{x}_k = 0\big\}. \tag{2.8}$$

Then $M(\bar{x},\alpha) = 0$ and $\bar{x}$ is a locally unique global minimum solution of $M(x,\alpha)$ for $\alpha \in (1,\ \infty)$.

Proof By Theorem 2.1, $M(\bar{x},\alpha) = 0$ and $\bar{x}$ is a global minimum solution of $M(x,\alpha)$ for $\alpha \in (1,\infty)$. We shall establish that $\bar{x}$ is a strict local minimum solution by showing that $\nabla^2 M(\bar{x},\alpha)$ is positive definite. Note that nondegeneracy (or strict complementarity) is used only to enable us to evaluate the Hessian of $M(x,\alpha)$ at $\bar{x}$. We first evaluate the gradient of $M(x,\alpha)$ at $\bar{x}$.

$$\begin{aligned}\alpha\nabla M(\bar{x},\alpha) &= \alpha\big(F(\bar{x})+\nabla F(\bar{x})^T\bar{x}\big)+\big(-\alpha\nabla F(\bar{x})^T+I\big)\big(-\alpha F(\bar{x})+\bar{x}\big)_+-\bar{x}\\ &\quad+\big(-\alpha I+\nabla F(\bar{x})^T\big)\big(-\alpha\bar{x}+F(\bar{x})\big)_+-\nabla F(\bar{x})^T F(\bar{x})\\ &=\big(-\alpha\nabla F(\bar{x})^T+I\big)\Big(\big(-\alpha F(\bar{x})+\bar{x}\big)_+-\bar{x}\Big)\\ &\quad+\big(-\alpha I+\nabla F(\bar{x})^T\big)\Big(\big(-\alpha\bar{x}+F(\bar{x})\big)_+-F(\bar{x})\Big)\end{aligned}\tag{2.9}$$

In order to evaluate the Hessian, Note the following as a consequence of nondegeneracy:

$$\nabla\big(-\alpha F(\bar{x})+\bar{x}\big)_+=\begin{bmatrix}-\alpha\nabla F_J(\bar{x})+I_J\\ 0_K\end{bmatrix}\tag{2.10a}$$

$$\nabla\big(-\alpha\bar{x}+F(\bar{x})\big)_+=\begin{bmatrix}0_J\\ -\alpha I_K+\nabla F_K(\bar{x})\end{bmatrix}\tag{2.10b}$$

Utilizing (2.10) in differentiating (2.9) and noting that $\bar{x}=\big(-\alpha F(\bar{x})+\bar{x}\big)_+$ and $F(\bar{x})=\big(-\alpha\bar{x}+F(\bar{x})\big)_+$ for $\alpha>0$ we have,

$$\begin{aligned}\alpha\nabla^2 M(\bar{x},\alpha) &= \big(-\alpha\nabla F(\bar{x})_J^T+I_J^T\big)\big(-\alpha\nabla F_J(\bar{x})+I_J\big)+\alpha\nabla F(\bar{x})^T-I\\ &\quad+\big(-\alpha I_K^T+\nabla F_K(\bar{x})^T\big)\big(-\alpha I_K+\nabla F_K(\bar{x})\big)+\alpha\nabla F(\bar{x})-\nabla F(\bar{x})^T\nabla F(\bar{x})\\ &=\alpha^2\nabla F(\bar{x})_J^T\nabla F_J(\bar{x})-\alpha\nabla F(\bar{x})_J^T I_J-\alpha I_J^T\nabla F_J(\bar{x})+I_J^T I_J+\alpha\nabla F(\bar{x})^T I\\ &\quad-I+\alpha^2 I_K^T I_K-\alpha I_K^T\nabla F_k(\bar{x})-\alpha\nabla F_K(\bar{x})^T I_K+\nabla F_K(\bar{x})^T\nabla F_K(\bar{x})\\ &\quad+\alpha I\nabla F(\bar{x})-\nabla F(\bar{x})^T\nabla F(\bar{x})\\ &=(\alpha^2-1)\big(\nabla F_J(\bar{x})^T\nabla F_J(\bar{x})+I_K^T I_K\big)\end{aligned}$$

Hence

$$\nabla^2 M(\bar{x},\alpha)=\big(\alpha-\frac{1}{\alpha}\big)\big(\nabla F_J(\bar{x})^T\ \ I_K^T\big)\begin{pmatrix}\nabla F_J(\bar{x})\\ I_K\end{pmatrix}\tag{2.11}$$

Since $\alpha>1$ and $\begin{pmatrix}\nabla F_J(\bar{x})\\ I_K\end{pmatrix}$ is nonsingular, it follows that $\nabla^2 M(\bar{x},\alpha)$ is positive definite and $\bar{x}$ is a strict local minimum solution of $M(x,\alpha)$. □

2.4 Remark Under the assumptions of Theorem 2.3, and if $\nabla F(x)$ is continuous in a neighborhood of $\bar{x}$, then the Newton method:

$$\nabla M(x^i,\alpha)+\nabla^2 M(x^i,\alpha)(x^{i+1}-x^i)=0\tag{2.12}$$

is well defined in a neighborhood of a nondegenerate solution $\bar{x}$ and converges superlinearly to $\bar{x}$ [18, Theorem 8.1.10].

We turn our attention now to other possible functions that may also have minima or zeros at solution points of NCP.

3. Other Unconstrained Minimization Equivalents of NCP

We consider now the following functions that can also be related to NCP (1.1) through unconstrained minimization or through their zeros:

$$P(x,\alpha) := xF(x) + \frac{\alpha}{2}\left\|\left(-F(x),\ -x\right)_+\right\|^2 \tag{3.1}$$

$$E(x,\alpha) := xF(x) + \alpha\left\|\left(-F(x),\ -x\right)_+\right\|_1 \tag{3.2}$$

$$Q(x,\alpha) := \left(xF(x)\right)^2 + \alpha\left\|\left(-F(x),\ -x\right)_+\right\|^2 \tag{3.3}$$

$P(x,\alpha)$ is an exterior penalty function [8] for MP (1.2) and as such will not have a global minimum at solutions of the NCP, but its global minimum solutions will approach NCP solutions as α tends to infinity. In fact, for $\alpha > 0$ we can summarize the properties of $P(x,\alpha)$ as follows:

(3.4a) $\bar{x}$ solves NCP $\Longrightarrow P(\bar{x},\alpha) = 0$
(3.4b) 〃 $\not\Longrightarrow \nabla P(\bar{x},\alpha) = 0$
(3.4c) 〃 $\not\Longrightarrow \bar{x} \in \arg\min\limits_{x\in R^n} P(x,\alpha)$
(3.4d) 〃 $\not\Longleftarrow P(\bar{x},\alpha) = 0$

In view of the failed implications (3.4b) - (3.4d), $P(x,\alpha)$ does not appear as an attractive unconstrained minimization reformulation of NCP. Some of these shortcomings can be alleviated by considering the exact penalty function [9] $E(x,\alpha)$, which has global minima of zero at solutions of NCP, *provided* F is monotone and α is sufficiently large as can be seen from the following simple result.

3.1 Theorem Let $F(x)$ be monotone on R^n and let $\bar{x}$ solve NCP (1.1). Then $\bar{x} \in \arg\min\limits_{x\in R^n} E(x,\alpha)$ for $\alpha\ \ \bar{\alpha} := \left\|\bar{x},\ F(\bar{x})\right\|_\infty$.

Proof For any x in R^n and $\alpha\ \ \bar{\alpha} := \left\|\bar{x},\ F(\bar{x})\right\|_\infty$.

$$\begin{aligned} E(\bar{x},\alpha) = \bar{x}F(\bar{x}) = -\bar{x}F(\bar{x}) \qquad & \text{(Since } \bar{x} \text{ solves NCP)} \\ xF(x) - \bar{x}F(x) - xF(\bar{x}) \qquad & \text{(By monotonicity of } F\text{)} \\ xF(x) + \bar{x}\left(-F(x)\right)_+ + F(\bar{x})(-x)_+ \qquad & \text{(Since } z\ \ (z)_+\text{)} \\ xF(x) + \left\|\bar{x},\ F(\bar{x})\right\|_\infty \cdot \left\|\left(-F(x),\ -x\right)_+\right\|_1 \qquad & \text{(By Cauchy-Schwarz)} \\ E(x,\alpha) \qquad & \end{aligned}$$

□

Note that the monotonicity of F plays a key role in the above theorem, which is unlike the situation with $M(x,\alpha)$ where no monotonicity is required. Furthermore, $E(x,\alpha)$ is not differentiable. We summarize the properties of $E(x,\alpha)$ below:

(3.5a) $\quad \bar{x}$ solves NCP $\Longrightarrow E(\bar{x},\alpha)=0$

(3.5b) $\quad$ " $\quad \Longrightarrow \bar{x} \in \arg\min\limits_{x\in R^n} E(x,\alpha)$ for $\alpha\ \ \bar{\alpha}$, F : monotone

(3.5c) $\quad$ " $\quad \not\Longleftarrow E(\bar{x},\alpha)=0.$

Finally we consider an obvious function which minimizes the residuals of NCP (1.1), that is $Q(x,\alpha)$. The motivation behind considering $Q(x,\alpha)$ is to obtain a function, besides $M(x,\alpha)$, for which there is a one-to-one correspondence between its zeros and solutions of NCP. In fact, $Q(x,\alpha)$ has many of the desirable properties of $M(x,\alpha)$, except that it tends to grow faster than $M(x,\alpha)$ because of the somewhat artificial squaring of the objective $xF(x)$. To get a feel of the magnitude of difference between $Q(x,\alpha)$ and $M(x,\alpha)$, as well as the other functions $E(x,\alpha)$ and $P(x,\alpha)$ we compared them on the following simple one-dimensional nonmonotone problem.

3.2 Example $F(x)=(x-1)^2\ \ 0,\ x\ \ 0,\ x(x-1)^2=0$. Solution points: 0, 1.

Figures 1a to 1d depict $M(x,2)$, $P(x,10)$, $E(x,2)$, and $Q(x,2)$ respectively. The penalty parameter α for $P(x,\alpha)$ was taken to be 10, large enough for $P(x,\alpha)$ to have a local minimum close enough to zero and to have another zero value on the negative x-axis close to zero. No essential changes in the other plots result in taking larger values of α. Figure 1a depicts two zeros of the function $M(x,2)$ at the two solution points 0 and 1 of Example 3.2, while Figure 1b depicts all the failed implications of (3.4): nonvanishing of the derivative at the solution point $x=0$ of Example 3.2, the solution point $x=0$ of Example 3.2 not being even a local minimum point, and the zero at $x=-0.381966$ not being a solution of Example 3.2. $P(x,10)$, however, does have zeros at both solution points 0 and 1 as asserted in implication (3.4a). Figure 1c shows similar shortcomings for $E(x,2)$ as well as its nondifferentiability at $x=0$. Figure 1d depicts $Q(x,2)$ which exhibits similar characteristics to $M(x,2)$, however, it grows more steeply over the same interval and thus appears considerably flatter than $M(x,2)$ over the interval [0,1]. What is probably most interesting to compare are the two functions $M(x,2)$ and $Q(x,2)$ over a slightly larger interval. This is done in Figures 2a and 2d. Both functions appear flat over [0,1] because of the increase in the range of the functions, but what is most striking is the actual range of the two functions over the interval [-10, 10]. The function $M(x,2)\ \ 100$ on this interval whereas $Q(x,2)$ exceeds

10^6 on the same interval. This is likely to cause computational difficulties if $Q(x, \alpha)$ were minimized to solve the NCP (1.1). Figures 2b and 2c indicate that both $P(x, 10)$ and $E(x, 2)$ tend to $-\infty$ as x tends to $-\infty$, which would again be computationally unstable.

The purpose of these comparisons of the four functions on this very simple example is not to make sweeping generalizations, but to point out the possible shortenings of some of these functions. These comparisons together with the results contained in Section 2, regarding the implicit Lagrangian $M(x, \alpha)$, make this function a worthy candidate for further study both in error bound analysis (as in [16, 17], for example) and the computational algorithms for solving the nonlinear complementarity problem.

4. A Dual to the Monotone Nonlinear Complementarity Problem

In this section we shall relate the monotone NCP (1.1) with differentiable $F(x)$ to the following Wolfe dual [20,13] of MP (1.2).

$$(4.1) \qquad \max_{x,u} \{-uF(x) - x\nabla F(x)^T(x-u) \big| F(x) + \nabla F(x)^T(x-u) \;\; 0,\ u \;\; 0\} \qquad \text{(DP)}$$

It is somewhat curious that the standard duality results [13] go through despite the fact that neither the objective function $xF(x)$ of MP (1.2) is convex in general under the monotonicity assumption on $F(x)$, nor is the feasible region of the same problem necessarily convex. These duality results depend critically on the monotonicity of F and the structure of MP (1.2) and makes use of Cottle's theorem [2, 4] which was referred to in Section 1. We state below Cottle's theorem in a slightly modified form and give its simple proof for completeness.

4.1 Theorem (Cottle [2, Chapter IV, Theorem 4], Cottle-Dantzig [4, Theorem 1]) Let $F(x)$ be differentiable and monotone on some open set containing R^n_+. If the point $(\bar{x}, \bar{u}, \bar{v})$ satisfies the Karush-Kuhn-Tucker conditions for MP (1.2)

$$(4.2) \;\; F(\bar{x}) + \nabla F(\bar{x})^T(\bar{x}-\bar{u}) - \bar{v} = 0, F(\bar{x}) \;\; 0, \bar{u}F(\bar{x}) = 0, \bar{u} \;\; 0, \bar{x} \;\; 0, \bar{v}\bar{x} = 0, \bar{v} \;\; 0 \qquad \text{(KKT)}$$

then $\bar{x}$ solves the NCP (1.1). Conversely if $\bar{x}$ solves the NCP (1.1), then $\big(\bar{x},\ \bar{u} = \bar{x},\ \bar{v} = F(\bar{x})\big)$ satisfy KKT conditions (4.2).

Proof If (4.2) hold then premultiplying the first equality by $(\bar{x} - \bar{u})$ and utilizing $\bar{u}F(\bar{x}) = 0,\ \bar{v}\bar{x} = 0$ gives

$$0 = (\bar{x}-\bar{u})F(\bar{x}) + (\bar{x}-\bar{u})\nabla F(\bar{x})^T(\bar{x}-\bar{u}) - (\bar{x}-\bar{u})\bar{v} = \bar{x}F(\bar{x}) + (\bar{x}-\bar{u})\nabla F(\bar{x})^T(\bar{x}-\bar{u}) + \bar{u}\bar{v}$$

Since each of three terms in the last sum is nonnegative and add up to zero, it follows that $\bar{x}F(\bar{x}) = 0$ and $\bar{x}$ solves NCP (1.1). The converse is obvious. $\square$

We establish Wolfe's weak duality theorem [20, 13] for the generally nonconvex MP (1.2) and its dual DP (4.1).

4.2 Weak Duality Theorem Let F be differentiable and monotone on R^n. If x is primal feasible, and (y, u) is dual feasible then

$$(4.3) \qquad xF(x) \;\; -uF(y) - y\nabla F(y)^T(y-u)$$

Proof

$$
\begin{aligned}
&xF(x) + uF(y) + y\nabla F(y)^T(y-u) \\
&\qquad\qquad = xF(x) + u\big(F(y) + \nabla F(y)^T(y-u)\big) + (y-u)\nabla F(y)^T(y-u) \\
&\qquad\qquad\ \ 0
\end{aligned}
$$

The last inequality follows from primal feasibility of x, dual feasibility of (y, u) and monotonicity of F. $\square$

Wolfe's strong duality now easily follows from Theorems 4.1 and 4.2.

4.3 Strong Duality Theorem Let F be differentiable and monotone. If $\bar{x}$ solves NCP (1.1) then the point $(x = \bar{x},\ u = \bar{x})$ solves the dual problem DP (4.1) and the dual maximum is zero.

Proof The point $(x = \bar{x},\ u = \bar{x})$ is dual feasible for (4.1), and since it achieves the upper bound of zero obtained by the Weak Duality Theorem 4.2 using the primal feasible point $\bar{x}$, the point $(x = \bar{x},\ u = \bar{x})$ is dual optimal. $\square$

We derive now a converse duality theorem [13] under a nonsingularity assumption on the following Hessian matrix, for any local solution $(\bar{x}, \bar{u})$ of the dual problem DP (4.1)

$$
(4.4) \qquad H(\bar{x}, \bar{u}) := \nabla F(\bar{x}) + \nabla F(\bar{x})^T + \sum_{i=1}^{n} (\bar{x} - \bar{u})_i \nabla^2 F_i(\bar{x})
$$

4.4 Converse Duality Theorem Let F be monotone and twice continuously differentiable on R^n. If $(\bar{x}, \bar{u})$ is a local solution of the dual problem DP (4.1) such that the Hessian $H(\bar{x}, \bar{u})$ (4.4) is nonsingular, then $\bar{x}$ solves the primal MP (1.2) with a zero minimum value and hence also the NCP (1.1).

Proof Since $(\bar{x}, \bar{u})$ is a local solution of DP (4.1) it satisfies, with some $\bar{v}$, the Fritz John conditions [13, Theorem 11.2.3] for the equivalent maximization problem

$$
(4.1a) \qquad \max_{x,u,v} \{L(x,u,v) \big| \nabla_x L(x,u,v) = 0,\ (u,v)\ \ 0\} \qquad \text{(DPa)}
$$

where the Lagrangian $L(x, u, v)$ is that of MP (1.2) and is defined by

$$
(4.5) \qquad L(x,u,v) := (x-u)F(x) - vx
$$

By the Fritz John conditions of (4.1a), $(\bar{x}, \bar{u}, \bar{v})$ and some $(\bar{r}_0, \bar{r}) \in R_+ \times R^n$, such that $(\bar{r}_0, \bar{r}) \neq 0$, satisfy

$$
(4.6) \qquad
\begin{aligned}
\bar{r}_0 \nabla_x L(\bar{x}, \bar{u}, \bar{v}) + \bar{r} \nabla_{xx} L(\bar{x}, \bar{u}, \bar{v}) &= 0 \\
\bar{r}_0 \nabla_u L(\bar{x}, \bar{u}, \bar{v}) + \bar{r} \nabla_{xu} L(\bar{x}, \bar{u}, \bar{v}) &\ \ 0 \\
\bar{u}(\qquad\qquad \text{〃} \qquad\qquad) &= 0 \\
\bar{r}_0 \nabla_v L(\bar{x}, \bar{u}, \bar{v}) + \bar{r} \nabla_{xv} L(\bar{x}, \bar{u}, \bar{v}) &\ \ 0 \\
\bar{v}(\qquad\qquad \text{〃} \qquad\qquad) &= 0 \\
\nabla_x L(\bar{x}, \bar{u}, \bar{v}) &= 0
\end{aligned}
$$

Since $\nabla_{xx} L(\bar{x}, \bar{u}, \bar{v}) = H(\bar{x}, \bar{u})$, it follows from the last and first equalities of (4.6) and the nonsingularity of $H(\bar{x}, \bar{u})$, that $\bar{r} = 0$ and $\bar{r}_0 > 0$. The remaining conditions of (4.6) degenerate to the KKT conditions (4.2) for MP (1.2) and hence by Theorem 4.1 $\bar{x}$ solves NCP (1.1) and MP (1.2) with minimum value zero. □

The following elementary properties of the dual problem are very simple to prove and their proofs are omitted.

4.5 Dual Problem DP 4.1 Properties Let F be differentiable and monotone on R^n.

(i) The dual objective is nonpositive on the dual feasible region.

(ii) If $(\bar{x}, \bar{u})$ is a solution of DP (4.1) such that the dual objective is zero and $\nabla F(\bar{x})$ is positive definite, then $\bar{x}$ solves NCP (1.1).

(iii) $\inf MP(1.2) \ \ -\sup DP(4.1) \ \ 0 \ \ -\inf \mathrm{MP}(1.2)$

(iv) $\inf MP(1.2) = \sup \mathrm{DP}(4.1)$ if and only if NCP (1.1) is solvable.

We conclude this section with a simple bound on the complementarity error in an interior point penalty solution to NCP (1.1).

4.6 Proposition Let F be differentiable and monotone on R^n, let $\alpha > 0$ and

$$
(4.7) \qquad x(\alpha) \in \arg\min \left\{ xF(x) - \alpha \sum_{i=1}^{n} \log F_i(x) \middle| F(x) > 0,\ x \ \ 0 \right\}
$$

Then

$$
(4.8) \qquad \alpha n \ \ x(\alpha) F\big(x(\alpha)\big) \ \ 0
$$

Proof The last inequality of (4.8) follows from $F\big(x(\alpha)\big) > 0$ and $x(\alpha)\ \ 0$. Since $x(\alpha)$ satisfies the optimality conditions

$$
\begin{aligned}
&F\big(x(\alpha)\big) + \nabla F\big(x(\alpha)\big)^T x(\alpha) - \alpha \sum_{i=1}^{n} \frac{\nabla F_i\big(x(\alpha)\big)}{F_i\big(x(\alpha)\big)}\ \ 0, \\
&x(\alpha)\Big(\qquad\qquad\qquad \text{''} \qquad\qquad\qquad \Big) = 0,\ x(\alpha)\ \ 0,
\end{aligned}
\tag{4.9}
$$

it follows that the point $\left(x = x(\alpha),\ u_i = \dfrac{\alpha}{F_i\big(x(\alpha)\big)},\ i = 1, \ldots, n\right)$ is dual feasible for DP (4.1) and by property 4.4(i) above

$$
\begin{aligned}
0\ \ &-\alpha n - x(\alpha)\nabla F(\big(x(\alpha)\big)^T \Big(x(\alpha) - \alpha F\big(x(\alpha)\big)^{-1}\Big) \\
&= -\alpha n + x(\alpha) F\big(x(\alpha)\big) && \text{By (4.9)}
\end{aligned}
$$

from which the first inequality of (4.8) follows. □

5. Concluding Remarks

The nonlinear complementarity problem has been reformulated as an unconstrained minimization of an implicit Lagrangian function in the same space as the original problem. The zero global minima of the implicit Lagrangian are in one-to-one correspondence with the nonlinear complementarity problem solution points. The correspondence is valid without any assumptions. When the nonlinear complementarity problem is differentiable so is the implicit Lagrangian. Thus the implicit Lagrangian appears to be a useful reformulation of the nonlinear complementarity problem that can be minimized to obtain solutions of the latter. Computational experiments are planned to test the effectiveness of this unconstrained minimization approach. Two interesting open questions remain:

5.1 Question: Under what assumptions is every (strict or nonstrict) local minimum solution of $M(x, \alpha)$ a global minimum solution of $M(x, \alpha)$? Are monotonicity and differentiability of $F(x)$ sufficient?

5.2 Question: Under what assumption is $M(x, \alpha)$ convex or pseudoconvex on R^n?

A Wolfe dual of a standard constrained minimization problem (associated with the nonlinear complementarity problem) is shown to be related through essentially all the standard duality results to the constrained minimization problem under monotonicity and differentiability (twice continuous differentiability) assumptions on the nonlinear complementarity problem. It would be interesting to investigate the computational potential of this dual problem, as well as the potential of both the implicit Lagrangian and the dual problem in generating residual bounds for the nonlinear complementarity problem in the spirit of [16, 17, 15, 11, 12].

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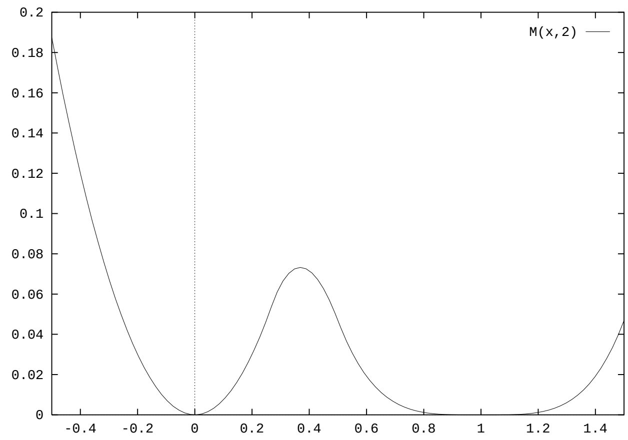

Figure 1a

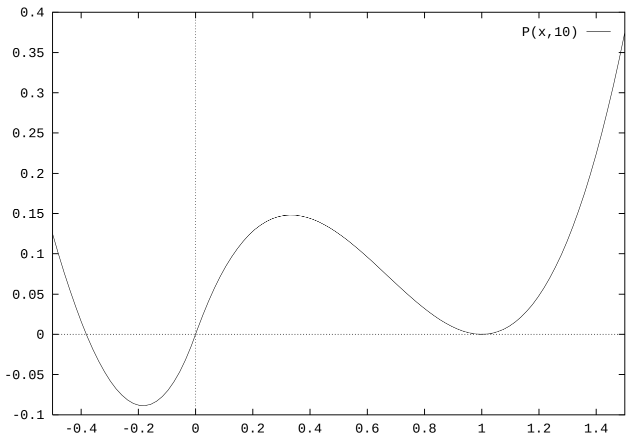

Figure 1b

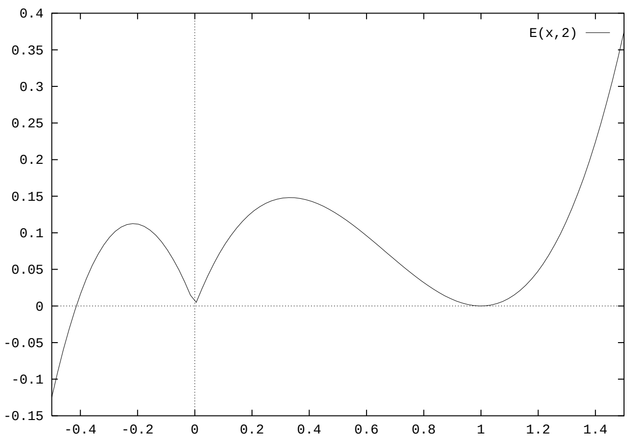

Figure 1c

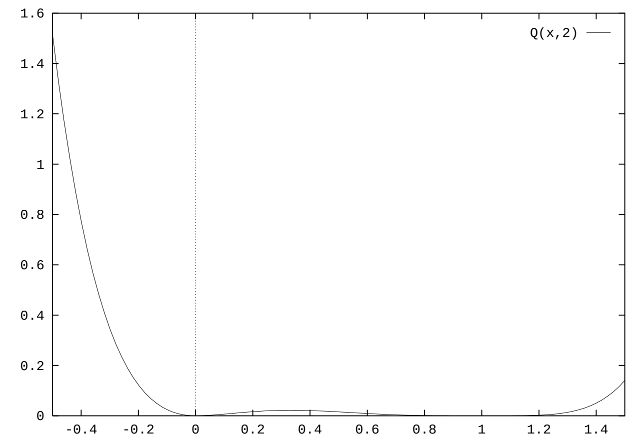

Figure 1d

Figure 1: The functions $M(x,2)$, $P(x,10)$, $E(x,2)$ and $Q(x,2)$ on the interval $[-0.5,\, 1.5]$ for the NCP: $(x-1)^2 \;\; 0,\;\; x \;\; 0,\;\; x(x-1)^2 = 0.$

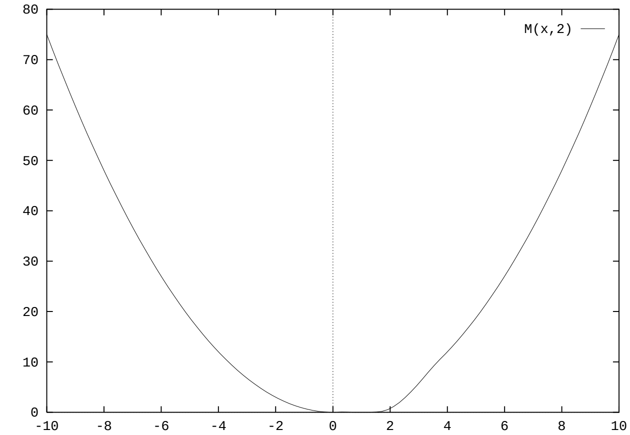

Figure 2a

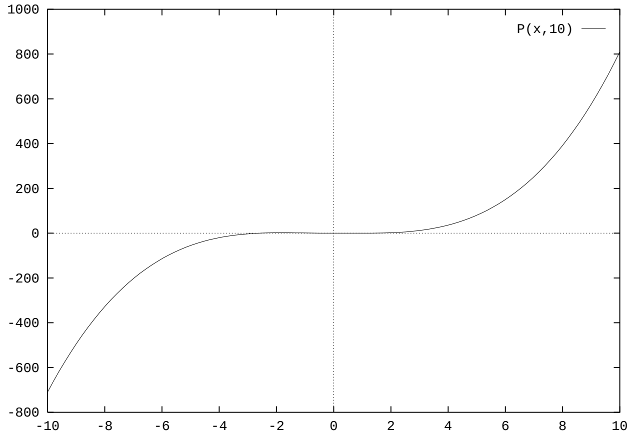

Figure 2b

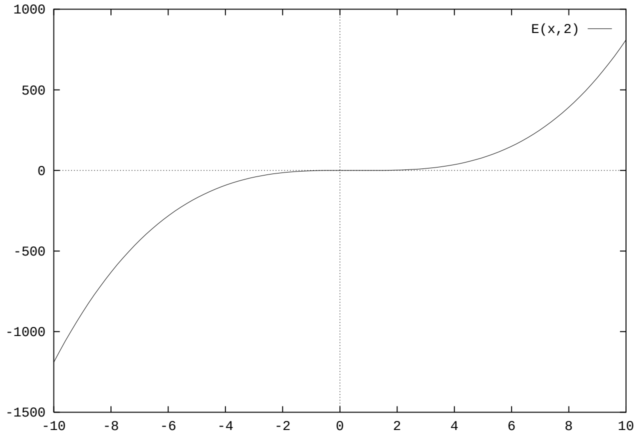

Figure 2c

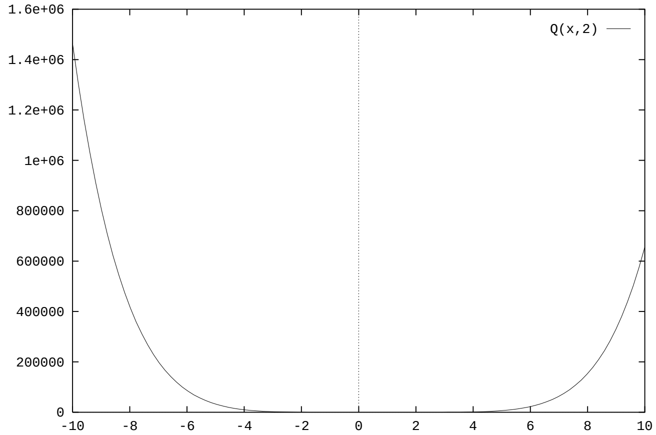

Figure 2d

Figure 2: The functions $M(x,2)$, $P(x,10)$, $E(x,2)$ and $Q(x,2)$ on the interval $[-10,\, 10]$ for the NCP: $(x-1)^2 \;\; 0,\;\; x \;\; 0,\;\; x(x-1)^2 = 0$.