WHEN ARE THE (UN)CONSTRAINED STATIONARY POINTS OF THE IMPLICIT LAGRANGIAN GLOBAL SOLUTIONS?

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Abstract. Mangasarian and Solodov [*Mathematical Programming, Vol. 62, pp. 277–297, 1993*] proposed to solve nonlinear complementarity problems by seeking the unconstrained global minima of a new merit function which they called *implicit Lagrangian.* A crucial point in such an approach is to determine conditions which guarantee that every unconstrained stationary point of the implicit Lagrangian is a global solution, since standard unconstrained minimization techniques are only able to locate stationary points. Some authors partially answered this question by giving sufficient conditions which guarantee this key property. In this paper we settle the issue by giving a necessary and sufficient condition for a stationary point of the implicit Lagrangian to be a global solution and, hence, a solution of the nonlinear complementarity problem. We show that this new condition easily allows us to recover all previous results and to establish new sufficient conditions. We then consider a constrained reformulation based on the implicit Lagrangian in which nonnegative constraints on the variables are added to the original unconstrained reformulation. This is motivated by the fact that often, in applications, the function which defines the complementarity problem is defined only on the nonnegative orthant. We consider the KKT-points of this new reformulation and show that the same necessary and sufficient condition which guarantees, in the unconstrained case, that every unconstrained stationary point is a global solution, also guarantees that every KKT-point of the new problem is a global solution.

Key words: Nonlinear complementarity problems, unconstrained minimization, bound constrained optimization, global minima, stationary points, implicit Lagrangian.

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1 Introduction

Consider the *nonlinear complementarity problem*, denoted by NCP(F), which is to find a vector in $\mathbb{R}^n$ satisfying the conditions

$$x_i \geq 0, \quad F_i(x) \geq 0, \quad x_i F_i(x) = 0 \qquad \forall i \in I := \{1, \dots, n\},$$

where $F : \mathbb{R}^n \to \mathbb{R}^n$ is a continuously differentiable function.

In 1993, Mangasarian and Solodov [12] introduced a new and interesting approach for the solution of NCP(F) which is based on the so-called *implicit Lagrangian*

$$M(x) := \sum_{i \in I} \varphi(x_i, F_i(x)),$$

where $\varphi : \mathbb{R}^2 \to \mathbb{R}$ is defined by

$$\varphi(a,b) := ab + \frac{1}{2\alpha}\left(\max{}^2\{0, a - \alpha b\} - a^2 + \max{}^2\{0, b - \alpha a\} - b^2\right)$$

and where $\alpha > 1$ is any fixed parameter. Mangasarian and Solodov [12] proved that M is a continuously differentiable, nonnegative function having the property

$$M(x) = 0 \Longleftrightarrow x \text{ solves NCP}(F).$$

If we assume that NCP(F) has at least one solution, this implies that a vector $x^* \in \mathbb{R}^n$ solves NCP(F) if and only if it is a global minimizer of the unconstrained minimization problem

$$\min_{x \in \mathbb{R}^n} M(x). \tag{1}$$

However, unconstrained minimization procedures applied to problem (1) are in general only able to find stationary points of M. An open question raised by Mangasarian and Solodov [12] is the following: Under what assumptions is a stationary point of M a solution of NCP(F)? A first answer to this question was given by Yamashita and Fukushima [18]: They proved that if x^* is a stationary point of M such that the Jacobian matrix $F'(x^*)$ is positive definite, then x^* solves NCP(F). Independently and based on a more general approach, the same result was obtained by Kanzow [10]. Recently Jiang [9] implicitly showed that the positive definiteness of $F'(x^*)$ can be replaced by the weaker assumption that $F'(x^*)$ is a P-matrix.

In this paper we settle the issue by giving a necessary and sufficient condition for a stationary point of the implicit Lagrangian to be a global solution and, hence, a solution of the nonlinear complementarity problem. We show that this new condition easily allows us to recover all previously known results and to establish new sufficient conditions.

We then consider a new constrained reformulation, based on the implicit Lagrangian, in which nonnegative constraints on the variables are added to the original unconstrained reformulation (1), thus obtaining the problem

$$\min_{x \geq 0} M(x). \tag{2}$$

It is obvious that also in this case, assuming that NCP(F) has a solution, solving the nonlinear complementarity problem is equivalent to finding a global minimum point of (2). This second approach is motivated by the fact that often, in applications, the function F is defined only on the nonnegative orthant. We consider the Karush-Kuhn-Tucker- (KKT-) points of this new reformulation and show that the same necessary and sufficient condition which guarantees, in the unconstrained case, that every unconstrained stationary point is a global solution, also guarantees that every KKT-point of (2) is a global solution.

The organization of the paper is as follows. In the next section we state some basic definitions and preliminary results. In Section 3 we introduce the notion of regular point and prove that an unconstrained stationary point of the implicit Lagrangian is a solution of NCP(F) if and only if it is regular; furthermore we give sufficient conditions for a point to be regular. Section 4 contains an analogous analysis for the constrained reformulation (2). We conclude with some final remarks in Section 5.

A few words about notation. We denote by $\mathbb{R}^n_+$ the nonnegative orthant. If $F : \mathbb{R}^n \to \mathbb{R}^n$ is a differentiable function, the Jacobian of F at a point $x \in \mathbb{R}^n$ is denoted by $F'(x)$. The index set $\{1, \ldots, n\}$ is always abbreviated by the capital letter I. If $x \in \mathbb{R}^n$ is an arbitrary vector and $J \subseteq I$, the vector $x_J \in \mathbb{R}^{|J|}$ consists of the elements $x_i, i \in J$. Similarly, given any matrix $A \in \mathbb{R}^{n\times n}, A = (a_{ij}), i, j \in I$, we denote by $A_{JJ} \in \mathbb{R}^{|J|\times|J|}$ the submatrix which has the elements $a_{ij}, i, j \in J$.

2 Preliminaries

We first restate the definition of some important classes of matrices.

Definition 2.1 *A matrix $A \in \mathbb{R}^{n\times n}$ is called*

(a) P-matrix $\iff \forall x \in \mathbb{R}^n, x \neq 0, \exists i \in I$ such that $x_i[Ax]_i > 0$;

(b) strictly semimonotone $\iff \forall x \in \mathbb{R}^n_+, x \neq 0, \exists i \in I$ such that $x_i[Ax]_i > 0$;

(c) S-matrix $\iff \exists x \in \mathbb{R}^n$ such that $x \geq 0$ and $Ax > 0$.

Obviously, every P-matrix is strictly semimonotone. Moreover, it is known that every strictly semimonotone matrix is an S-matrix. For some further properties of these classes of matrices, we refer the reader to the excellent book by Cottle, Pang and Stone [2].

We now recall two elementary, but important properties of the function φ. The proofs can be found in [12, 10].

Lemma 2.2 *φ is a nonnegative function and the following relationships hold:*

$$a \geq 0, b \geq 0, ab = 0 \iff \varphi(a, b) = 0 \iff \nabla\varphi(a, b) = 0.$$

Lemma 2.3 *The following inequality holds for all* $(a,b)^T \in \mathbb{R}^2$:

$$\frac{\partial \varphi}{\partial a}(a,b)\frac{\partial \varphi}{\partial b}(a,b) \geq 0.$$

We conclude this section by proving three further results that will be needed in the sequel.

Lemma 2.4 *The following inequality holds for all* $(a,b)^T \in \mathbb{R}^2_+$:

$$\frac{\partial \varphi}{\partial b}(a,b) \geq 0.$$

Proof. First note that

$$\frac{\partial \varphi}{\partial b}(a,b) = a + \frac{1}{\alpha}\left(-\alpha \max\{0, a-\alpha b\} + \max\{0, b-\alpha a\} - b\right). \tag{3}$$

Let $(a,b) \in \mathbb{R}^2_+$ be fixed and consider the following four cases.
Case 1: $a - \alpha b \geq 0$ and $b - \alpha a > 0$.
Since we also have $a \geq 0, b \geq 0$ and $\alpha > 1$, we therefore get $a \geq \alpha b \geq b$ and $b > \alpha a \geq a$, a contradiction. For this reason, this case cannot occur.
Case 2: $a - \alpha b \geq 0$ and $b - \alpha a \leq 0$.
Then it follows from (3) that

$$\alpha \frac{\partial \varphi}{\partial b}(a,b) = (\alpha^2 - 1)b \geq 0$$

since $\alpha > 1$ and $b \geq 0$.
Case 3: $a - \alpha b < 0$ and $b - \alpha a > 0$.
In this case, (3) reduces to

$$\frac{\partial \varphi}{\partial b}(a,b) = 0,$$

which is obviously nonnegative.
Case 4: $a - \alpha b < 0$ and $b - \alpha a \leq 0$.
Then $a \geq b/\alpha$ so that (3) becomes

$$\frac{\partial \varphi}{\partial b}(a,b) = a - b/\alpha \geq 0.$$

The assertion is therefore an immediate consequence of the cases 1 – 4. □

Lemma 2.5 *For all* $b \in \mathbb{R}$, *we have*

$$\frac{\partial \varphi}{\partial a}(0,b) = 0.$$

Proof. It is readily verified that

$$\frac{\partial \varphi}{\partial a}(a,b) = b + \frac{1}{\alpha}\left(\max\{0, a-\alpha b\} - a - \alpha \max\{0, b-\alpha a\}\right).$$

Hence we have

$$\alpha \frac{\partial \varphi}{\partial a}(0,b) = \alpha b + \max\{0, -\alpha b\} - \alpha \max\{0, b\}.$$

Now it can easily be verified by considering the two possible cases $b \geq 0$ and $b < 0$ separately that $\frac{\partial \varphi}{\partial a}(0,b) = 0$. □

Lemma 2.6 *For all $b \in \mathbb{R}$, we have*

$$\frac{\partial \varphi}{\partial b}(0,b) \leq 0.$$

Proof. Recalling the expression (3), we can write

$$\alpha \frac{\partial \varphi}{\partial b}(0,b) = \left(-\alpha \max\{0, -\alpha b\} + \max\{0, b\} - b\right)$$

which, by considering the two cases $b \geq 0$ and $b < 0$, is easily seen to be a nonpositive quantity. □

3 Unconstrained Stationary Points

In the remaining part of this paper we make use of the following notation:

$$\begin{aligned}
\frac{\partial \varphi}{\partial a}(x, F(x)) &:= \left(\frac{\partial \varphi}{\partial a}(x_1, F_1(x)), \ldots, \frac{\partial \varphi}{\partial a}(x_n, F_n(x))\right)^T \in \mathbb{R}^n, \\
\frac{\partial \varphi}{\partial b}(x, F(x)) &:= \left(\frac{\partial \varphi}{\partial b}(x_1, F_1(x)), \ldots, \frac{\partial \varphi}{\partial b}(x_n, F_n(x))\right)^T \in \mathbb{R}^n,
\end{aligned}$$

where $x \in \mathbb{R}^n$ is an arbitrary vector. Using this notation, we can write the gradient of M at x as

$$\nabla M(x) = \frac{\partial \varphi}{\partial a}(x, F(x)) + F'(x)^T \frac{\partial \varphi}{\partial b}(x, F(x)). \tag{4}$$

In order to prove the main result of this section, we need the following lemma.

Lemma 3.1 *Let $x^* \in \mathbb{R}^n$ be a stationary point of M. Then x^* is a solution of NCP(F) if and only if $\frac{\partial \varphi}{\partial b}(x^*, F(x^*)) = 0$.*

Proof. Since x^* is a stationary point of M, we get from (4):

$$\frac{\partial\varphi}{\partial a}(x^*, F(x^*)) + F'(x^*)^T \frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = 0. \tag{5}$$

Now assume that x^* solves NCP(F). Then $\varphi(x_i^*, F_i(x^*)) = 0$ for all $i \in I$, so that we have $\nabla\varphi(x_i^*, F_i(x^*)) = 0$ for all $i \in I$ by Lemma 2.2. This implies $\frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = 0$.

Conversely, assume that $\frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = 0$ holds. From (5), we then obtain $\frac{\partial\varphi}{\partial a}(x^*, F(x^*)) = 0$, i.e. $\nabla\varphi(x_i^*, F_i(x^*)) = 0$ for all $i \in I$. In view of Lemma 2.2, this implies $\varphi(x_i^*, F_i(x^*)) = 0$ for all $i \in I$ and therefore $M(x^*) = 0$. Hence x^* is a solution of NCP(F). □

We now give the definition of a regular point (with respect to the merit function M) which will be central in the subsequent analysis. Similar conditions, but for different merit functions, are considered by Pang and Gabriel [14], Moré [13], Ferris and Ralph [4] and De Luca, Facchinei and Kanzow [3]. To this end, we partition the index set $I = \{1, \ldots, n\}$ into the following subsets:

$$\begin{array}{rcll} \mathcal{C} & := & \{i \in I \mid \frac{\partial\varphi}{\partial b}(x_i, F_i(x)) = 0\} & (\underline{\text{c}}\text{omplementary indices}), \\ \mathcal{P} & := & \{i \in I \mid \frac{\partial\varphi}{\partial b}(x_i, F_i(x)) > 0\} & (\underline{\text{p}}\text{ositive indices}), \\ \mathcal{N} & := & \{i \in I \mid \frac{\partial\varphi}{\partial b}(x_i, F_i(x)) < 0\} & (\underline{\text{n}}\text{egative indices}). \end{array}$$

Note that these index sets depend on the particular vector x, but that this dependence is not reflected in our notation since the underlying vector will always be clear from the context.

Definition 3.2 *A point $x \in \mathbb{R}^n$ is called* regular *if for every nonzero $z \in \mathbb{R}^n$ with*

$$z_{\mathcal{C}} = 0, \quad z_{\mathcal{P}} > 0, \quad z_{\mathcal{N}} < 0, \tag{6}$$

there exists a vector $y \in \mathbb{R}^n$ such that

$$y_{\mathcal{C}} = 0, \quad y_{\mathcal{P}} \geq 0, \quad y_{\mathcal{N}} \leq 0 \tag{7}$$

and

$$y^T F'(x)^T z > 0. \tag{8}$$

We are now in the position to prove the main result of this section.

Theorem 3.3 *Let $x^* \in \mathbb{R}^n$ be a stationary point of M. Then x^* solves NCP(F) if and only if x^* is regular.*

Proof. If $x^* \in \mathbb{R}^n$ is a solution of NCP(F), then $\mathcal{P} = \mathcal{N} = \emptyset$ by Lemma 3.1, and hence there is no nonzero vector satisfying (6). To prove the converse result, first note that (5) holds since x^* is a stationary point of M by assumption. Hence we have

$$y^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*)) + y^T F'(x^*)^T \frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = 0 \tag{9}$$

for every $y \in \mathbb{R}^n$. Assume that x^* is not a solution of NCP(F), and define $z := \frac{\partial\varphi}{\partial b}(x^*, F(x^*))$. By Lemma 3.1, z is a nonzero vector. Moreover, it follows from the very definitions of the corresponding index sets that z satisfies the conditions (6). Since x^* is a regular point, there is a vector $y \in \mathbb{R}^n$ such that (7) and (8) hold. From Lemma 2.3, it follows that

$$\frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{P}} \geq 0, \frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{N}} \leq 0$$

and therefore

$$y^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*)) = y_{\mathcal{C}}^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{C}} + y_{\mathcal{P}}^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{P}} + y_{\mathcal{N}}^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{N}} \geq 0 \tag{10}$$

and

$$y^T F'(x^*)^T \frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = y^T F'(x^*)^T z > 0. \tag{11}$$

From (10) and (11), however, we get a contradiction to (9). Hence x^* is a solution of NCP(F). □

In the remaining part of this section we shall give several sufficient conditions for a stationary point to be a solution of NCP(F).

Proposition 3.4 *Let $x^* \in \mathbb{R}^n$ be a stationary point of M and assume that the Jacobian matrix $F'(x^*)$ is a P-matrix. Then x^* is a solution of NCP(F).*

Proof. In view of Theorem 3.3, it suffices to show that x^* is regular. Let $z \in \mathbb{R}^n$ be the vector in the Definition 3.2 of regular point. Since, by assumption, $F'(x^*)$ and therefore also $F'(x^*)^T$ is a P-matrix, there exists an index j for which $z_j[F'(x^*)^T z]_j > 0$. Let $y \in \mathbb{R}^n$ be the vector whose components are all 0 except for its j-th component, which is equal to z_j. It is then easy to see that this y satisfies the conditions (7). Furthermore we also have, by the definition of y,

$$y^T F'(x^*)^T z = y_j[F'(x^*)^T z]_j = z_j[F'(x^*)^T z]_j > 0$$

so that also (8) holds and x^* is a regular point. □

Note that Proposition 3.4 gives the result by Jiang [9]. Analogously the following corollary points out that also the result by Yamashita and Fukushima [18] is an easy consequence of Proposition 3.4.

Corollary 3.5 *Let $x^* \in \mathbb{R}^n$ be a stationary point of M and assume that the Jacobian matrix $F'(x^*)$ is positive definite. Then x^* is a solution of NCP(F).*

Proof. This follows immediately from Proposition 3.4 and the fact that every positive definite matrix is also a P-matrix. A different proof of Corollary 3.5 can be obtained by taking $y = z$ in Definition 3.2 of a regular point and by using Theorem 3.3. $\square$

We now give a new sufficient condition which includes and generalizes the results of Proposition 3.4 and Corollary 3.5. To this end we need some further notation. Let us set

$$\mathcal{D} := \mathcal{N} \cup \mathcal{P}$$

and define a diagonal matrix $T := diag(t_1, \ldots, t_{|\mathcal{D}|}) \in \mathbb{R}^{|\mathcal{D}| \times |\mathcal{D}|}$ by

$$t_i := \begin{cases} 1 & \text{if} \quad i \in \mathcal{P}, \\ -1 & \text{if} \quad i \in \mathcal{N}. \end{cases}$$

Theorem 3.6 *Let $x \in \mathbb{R}^n$ and assume that the matrix $TF'(x)_{\mathcal{D}\mathcal{D}}T$ is an S-matrix. Then x is a regular point.*

Proof. By the definition of an S-matrix, there is a vector $\tilde{y}_{\mathcal{D}} \in \mathbb{R}^{|\mathcal{D}|}$ such that

$$\tilde{y}_{\mathcal{D}} \geq 0 \text{ and } TF'(x)_{\mathcal{D}\mathcal{D}}T\tilde{y}_{\mathcal{D}} > 0. \tag{12}$$

Let $y \in \mathbb{R}^n$ be the unique vector defined by

$$y_{\mathcal{C}} = 0, y_{\mathcal{D}} = T\tilde{y}_{\mathcal{D}}.$$

Since $\tilde{y}_{\mathcal{D}} \geq 0$, we have

$$y_{\mathcal{P}} \geq 0 \text{ and } y_{\mathcal{N}} \leq 0$$

by the definition of the diagonal matrix T, i.e., the vector $y \in \mathbb{R}^n$ satisfies all the conditions in (7). Now let $z \in \mathbb{R}^n$ be an arbitrary vector such that $z \neq 0$ and

$$z_{\mathcal{C}} = 0, z_{\mathcal{P}} > 0, z_{\mathcal{N}} < 0.$$

Since $TT = I$, it is easy to see that

$$\begin{aligned} y^T F'(x)^T z &= y_{\mathcal{D}}^T F'(x)_{\mathcal{D}\mathcal{D}}^T z_{\mathcal{D}} \\ &= y_{\mathcal{D}}^T (TT) F'(x)_{\mathcal{D}\mathcal{D}}^T (TT) z_{\mathcal{D}} \\ &= (y_{\mathcal{D}}^T T)(TF'(x)_{\mathcal{D}\mathcal{D}}^T T)(T z_{\mathcal{D}}) \\ &= \tilde{y}_{\mathcal{D}}^T (TF'(x)_{\mathcal{D}\mathcal{D}}^T T)(T z_{\mathcal{D}}) \\ &> 0, \end{aligned}$$

where the last inequality follows from (12) and the fact that $(Tz_{\mathcal{D}}) > 0$. This proves that x is a regular point. $\square$

We recall that a matrix A is a P-matrix if and only if DAD is a P-matrix for every nonsingular diagonal matrix D and that every principal submatrix of a P-matrix is again a P-matrix. These properties, along with the fact that every P-matrix is also an S-matrix, clearly show that Proposition 3.4 (and hence Corollary 3.5) is a particular case of Theorem 3.6. We conclude this section by deducing from Theorem 3.6 another sufficient criterion for a stationary point of M to be a solution of NCP(F). Before stating this result, recall that a vector $x \in \mathbb{R}^n$ is said to be *feasible* if $x \geq 0$ and $F(x) \geq 0$.

Corollary 3.7 *Let $x^* \in \mathbb{R}^n$ be a feasible stationary point of M and assume that the Jacobian matrix $F'(x^*)$ is strictly semimonotone. Then x^* is a solution of NCP(F).*

Proof. Since x^* is feasible we have, by Lemma 2.4, that $\mathcal{N} = \emptyset$. Hence the matrix T used in Theorem 3.6 is just the identity matrix, and the assertion follows from Theorem 3.3 and Theorem 3.6 by noting that if $F'(x^*)$ is strictly semimonotone then $F'(x^*)_{\mathcal{DD}}$ is an S-matrix, see [2, Corollary 3.9.13]. □

4 Bound Constrained Reformulation

In many applications, in particular in those arising from economic equilibrium models, the function F of the nonlinear complementarity problem NCP(F) is not defined on the whole space $\mathbb{R}^n$. For these problems we cannot apply the unconstrained reformulation considered in the previous section. In these cases it may be more appropriate to try to solve the nonlinear complementarity problem by solving the constrained problem (2) that we recall here for convenience:

$$\min_{x \geq 0} M(x), \tag{13}$$

where we assume that F is defined and continuously differentiable on an open neighborhood of $\mathbb{R}^n_+$. Obviously, $x^* \in \mathbb{R}^n$ is a solution of NCP(F) if and only if $M(x^*) = 0$ and $x^* \geq 0$. So, again, the problem is to find a global solution of (13). Since there are nowadays many efficient algorithms for problems of the type (13) where all iterates remain feasible, the reformulation (13) of NCP(F) can be applied to those applications where F is not defined everywhere. In choosing an algorithm for solving problem (13) one should keep in mind that if x^* is a solution of NCP(F), then, since, as shown in the previous section, $\nabla M(x^*) = 0$, x^* is a *degenerate* solution of the bound constrained optimization reformulation (13). Hence, if one wants to guarantee a fast convergence rate, an appropriate minimization algorithm has to be selected. A suitable candidate is, for example, the algorithm proposed by Conn, Gould and Toint [1], as shown by Lescrenier [11]. However, whatever the algorithm selected and in view of the nonconvexity of the merit function M (see, however, Peng [16]), it will only be possible, in general, to find a KKT-point of (13). In this section we therefore investigate conditions which guarantee that every KKT-point of (13) is a global minimum of (13) and hence (if the solution set of NCP(F) is nonempty) a solution of the nonlinear complementarity problem itself. The surprising result of the analysis is that a KKT-point x^* of (13) is a global solution if and only if x^* is a regular point according to Definition 3.2. In particular, all the sufficient conditions stated in the previous section also guarantee that a KKT-point of problem (13) is a global solution.

We start by recalling the KKT-conditions of (13), which can be written as follows:

$$\begin{aligned} x &\geq 0, && (14)\\ \nabla M(x) &\geq 0, && (15)\\ x_i[\nabla M(x)]_i &= 0, \quad \forall i \in I. && (16) \end{aligned}$$

Given any KKT-point $x \in \mathbb{R}^n$, we partition the index set I into the following two subsets:

$$\begin{aligned} I_+ &:= \{i \in I \,|\, [\nabla M(x)]_i > 0\}, \\ I_0 &:= \{i \in I \,|\, [\nabla M(x)]_i = 0\}. \end{aligned}$$

Correspondingly, we shall consider partitions of vectors as $x = (x_+^T, x_0^T)^T$. We now state two preliminary results. The first one is the direct counterpart of Lemma 3.1 for the bound constrained reformulation of NCP(F).

Lemma 4.1 *Let $x^* \in \mathbb{R}^n$ be a KKT-point of (13). Then x^* solves NCP(F) if and only if* $\frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = 0$.

Proof. If x^* solves NCP(F) it follows from Lemma 2.2 that $\frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = 0$. So we only have to prove the reverse direction. Since x^* is a KKT-point of (13) satisfying $\frac{\partial\varphi}{\partial b}(x^*, F(x^*)) = 0$ by assumption, the KKT-conditions (14) – (16) reduce, taking into account the explicit expression (4) of the gradient of M, to

$$x^* \geq 0, \quad \frac{\partial\varphi}{\partial a}(x^*, F(x^*)) \geq 0, \quad x_i^* \frac{\partial\varphi}{\partial a}(x_i^*, F(x_i^*)) = 0 \qquad \forall\, i \in I.$$

Assume there exists an index $j \in I$ such that $\frac{\partial\varphi}{\partial a}(x_j^*, F(x_j^*)) \neq 0$. Then we have $x_j^* = 0$ because of (16). But by Lemma 2.5 we also have $\frac{\partial\varphi}{\partial a}(0, F_j(x^*)) = 0$, which is a contradiction, so that $\frac{\partial\varphi}{\partial a}(x^*, F(x^*)) = 0$. Therefore, by assumption and Lemma 2.2, we have $M(x^*) = 0$. This means that x^* solves NCP(F). $\square$

Lemma 4.2 *Assume that $x^* \in \mathbb{R}^n$ is a KKT-point of problem (13). Then we have* $\frac{\partial\varphi}{\partial b}(x_i^*, F_i(x^*)) \leq 0$ *for all $i \in I_+$.*

Proof. If $i \in I_+$ then, by (16), $x_i^* = 0$. Hence the thesis follows by Lemma 2.6. $\square$

We can now prove the main result of this section.

Theorem 4.3 *Let $x^* \in \mathbb{R}^n$ be a KKT-point of (13). Then x^* solves NCP(F) if and only if x^* is regular.*

Proof. If $x^* \in \mathbb{R}^n$ is a solution of NCP(F), then $\mathcal{P} = \mathcal{N} = \emptyset$ by Lemma 4.1, so that there is no nonzero vector satisfying (6). Hence x^* is a regular point.

To prove the converse result, let $x^* \in \mathbb{R}^n$ be a regular KKT-point of (13) and assume, by contradiction, that x^* is not a solution of NCP(F). Define $z := \frac{\partial\varphi}{\partial b}(x^*, F(x^*))$. By Lemma 4.1, z is a nonzero vector. Moreover, it follows from the very definition of the index sets $\mathcal{C}$, $\mathcal{P}$ and $\mathcal{N}$ that z satisfies the conditions (6). Since x^* is a regular point, there is a vector $y \in \mathbb{R}^n$ such that (7) and (8) hold. Since $x^*_+ = 0$ because of (16), we have $z_+ \leq 0$ by Lemma 4.2. In view of Definition 3.2, we therefore also have $y_+ \leq 0$. Hence, recalling (15), we can write

$$y^T \nabla M(x^*) = (y_+^T, y_0^T) \begin{pmatrix} [\nabla M(x^*)]_+ \\ [\nabla M(x^*)]_0 \end{pmatrix} = (y_+^T, y_0^T) \begin{pmatrix} [\nabla M(x^*)]_+ \\ 0 \end{pmatrix} = y_+^T [\nabla M(x^*)]_+ \leq 0. \tag{17}$$

On the other hand, by the definition of regular point, we have

$$y^T F'(x^*)^T z > 0, \tag{18}$$

and also, recalling Lemma 2.3 and (7)

$$y^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*)) = y_{\mathcal{C}}^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{C}} + y_{\mathcal{P}}^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{P}} + y_{\mathcal{N}}^T \frac{\partial\varphi}{\partial a}(x^*, F(x^*))_{\mathcal{N}} \geq 0. \tag{19}$$

But, taking into account that

$$\nabla M(x^*) = \frac{\partial\varphi}{\partial a}(x^*, F(x^*)) + F'(x^*)^T z,$$

relations (18) and (19) give a contradiction to (17). Hence x^* is a solution of NCP(F). □

For the sake of completeness, we restate here the following result which follows directly from Theorem 4.3 and the corresponding results of Section 3.

Corollary 4.4 *Let $x^* \in \mathbb{R}^n$ be a KKT-point of (13). Then:*
(a) If $F'(x^*)$ is a P-matrix, then x^* solves NCP(F).
(b) If $F'(x^*)$ is strictly semimonotone and x^* is feasible, then x^* solves NCP(F).

Since x^* is assumed to be a KKT-point of (13) in Corollary 4.4, we know that $x^* \geq 0$. Hence the feasibility condition of x^* in Corollary 4.4 (b) is more likely to be satisfied than in the corresponding result (Corollary 3.7) for the unconstrained reformulation.

After finishing this paper it was pointed out to the authors by Solodov [17] that Theorem 4.3 remains true also for the following bound constrained reformulation of NCP(F):

$$\min_{x \geq 0} N(x), \tag{20}$$

where

$$N(x) := \sum_{i \in I} \psi(x_i, F_i(x))$$

denotes the restricted implicit Lagrangian [12, 7] and

$$\psi(a, b) := ab + \frac{1}{2\alpha} \left(\max{}^2\{0, a - \alpha b\} - a^2 \right).$$

It is know that, for any parameter $\alpha > 0$, the function $N(x)$ is nonnegative on $\mathbb{R}^n_+$ and that $N(x) = 0$ for $x \in \mathbb{R}^n_+$ if and only if x solves NCP(F), see [12, 7]. Hence the global minimizers of (20) correspond to the solutions of NCP(F) if the solution set is nonempty. In order to see that Theorem 4.3 is true also for the constrained reformulation (20), one just has to show that the function ψ enjoys properties similar to those of the function φ. We omit the details here.

5 Summary and Discussion

In this paper we considered the implicit Lagrangian function and gave a necessary and sufficient condition for a stationary point to be a global solution and, hence, a solution of the nonlinear complementarity problem. We showed that this new condition, which we called *regularity*, easily allows us to recover previous results and to establish new sufficient conditions. We then considered a constrained reformulation based on the implicit Lagrangian in which nonnegative constraints on the variables are added to the original unconstrained reformulation. We proved that, also in this case, regularity guarantees that a KKT-point of the new problem is a global solution.

We think that the results reported in this work indicate that, from the theoretical point of view, the implicit Lagrangian based minimization reformulation of a nonlinear complementarity problem enjoys weaker properties than other recently proposed optimization reformulations see, e.g., [4, 9, 10], especially if compared to those based on the Fischer-function, see [3, 5, 8] and references therein. The main drawback of the implicit Lagrangian reformulation seems to be that a certain "degree of nonsingularity" is needed in order to guarantee that every stationary point is a solution of the nonlinear complementarity problem. So, as already noted by Yamashita and Fukushima [18], a minimization approach based on the implicit Lagrangian cannot handle monotone complementarity problems. This is also confirmed by the numerical experience reported in [8], where convergence to points which are not solutions was observed in practice in the case of monotone complementarity problems derived from strictly convex quadratic problems.

This point can be enlightened and made precise by the following analysis. We first recall that a matrix $A \in \mathbb{R}^{n\times n}$ is said to be *column sufficient* [2, p. 157] if, for every $x \in \mathbb{R}^n$, it satisfies the implication

$$(x_i[Ax]_i \leq 0 \text{ for all } i \in I) \Longrightarrow (x_i[Ax]_i = 0 \text{ for all } i \in I).$$

The matrix A is called *row sufficient* if its transpose is column sufficient.

Obviously, every positive semidefinite matrix is both row and column sufficient. Note also that all Jacobian matrices of a (strictly) monotone function are positive semidefinite and hence row sufficient. The following result indicates what is the degree of nonsingularity which is needed in order to guarantee that every stationary point of the implicit Lagrangian is a global solution. We recall that $\mathcal{D}$ denotes the index set defined before Theorem 3.6.

Proposition 5.1 *Let $x^* \in \mathbb{R}^n$ be a stationary point of M such that $F'(x^*)$ is row sufficient. If x^* is not a solution of NCP(F), then the principal submatrix $F'(x^*)_{\mathcal{D}\mathcal{D}}$ is singular.*

Proof. Since $x^* \in \mathbb{R}^n$ is a stationary point of M, we have

$$[\nabla M(x^*)]_i = \frac{\partial \varphi}{\partial a}(x_i^*, F_i(x^*)) + \left[F'(x^*)^T \frac{\partial \varphi}{\partial b}(x^*, F(x^*))\right]_i = 0 \quad \forall i \in I.$$

Premultiplying the ith equation by $\frac{\partial \varphi}{\partial b}(x_i^*, F_i(x^*))$ and taking into account Lemma 2.3, we obtain

$$\frac{\partial \varphi}{\partial b}(x_i^*, F_i(x^*)) \left[F'(x^*)^T \frac{\partial \varphi}{\partial b}(x^*, F(x^*))\right]_i = -\frac{\partial \varphi}{\partial a}(x_i^*, F_i(x^*)) \frac{\partial \varphi}{\partial b}(x_i^*, F_i(x^*)) \leq 0$$

for all $i \in I$. Since $F'(x^*)$ is row sufficient, $F'(x^*)^T$ is column sufficient. We therefore obtain

$$\frac{\partial \varphi}{\partial b}(x_i^*, F_i(x^*)) \left[F'(x^*)^T \frac{\partial \varphi}{\partial b}(x^*, F(x^*))\right]_i = 0 \quad \forall i \in I.$$

Since x^* is not a solution of NCP(F), we have $\mathcal{D} \neq \emptyset$. Since $\frac{\partial \varphi}{\partial b}(x^*, F(x^*))_{\mathcal{C}} = 0_{\mathcal{C}}$ and $\frac{\partial \varphi}{\partial b}(x_i^*, F_i(x^*)) \neq 0$ for all $i \in \mathcal{D}$ by definition of the index sets $\mathcal{C}$ and $\mathcal{D}$, we get

$$F'(x^*)^T_{\mathcal{D}\mathcal{D}} \frac{\partial \varphi}{\partial b}(x^*, F(x^*))_{\mathcal{D}} = 0_{\mathcal{D}}.$$

This shows that $F'(x^*)_{\mathcal{D}\mathcal{D}}$ must be singular. $\square$

Since in most of the cases $\mathcal{D} = I$, we see that the submatrix considered in the previous proposition is just the Jacobian itself.

Notwithstanding the drawbacks just described, we should also note that the limited numerical experience reported in [8, 10] seems to indicate that, when the conditions required for a stationary point of M to solve NCP(F) are satisfied, a minimization approach to the numerical solution of a nonlinear complementarity problem based on the implicit Lagrangian can be rather efficient. This may be due to the fact that the gradient of the implicit Lagrangian enjoys the favourable property of being piecewise smooth. It may also be interesting to point out that the implicit Lagrangian can be generalized to handle variational inequalities [15, 19]. So only a more extensive numerical testing and comparison of theoretical properties can settle the question of which merit function, if any, is better from the practical point of view.

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