Solution of Finite-Dimensional Variational Inequalities Using Smooth Optimization with Simple Bounds[1]

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Abstract. The variational inequality problem is reduced to an optimization problem with a differentiable objective function and simple bounds. Theoretical results are proved, that relate stationary points of the minimization problem to solutions of the variational inequality problem. Perturbations of the original problem are studied and an algorithm that uses the smooth minimization approach for solving monotone problems is defined.

Key words. Variational inequalities, box constrained optimization, complementarity.

1 Introduction

Let Ω be a nonempty, closed and convex subset of $I\!R^n$ and $F : I\!R^n \to I\!R^n$. The finite-dimensional variational inequality problem, denoted by VIP, is to find a vector $x \in \Omega$ such that

$$\langle F(x), w - x\rangle \geq 0, \text{ for all } w \in \Omega. \tag{1}$$

This problem has many interesting applications and its solution using special techniques has been considered extensively in the literature; see, for example, (Ref. 1) and references therein. The linear and nonlinear complementarity problems are particular cases of (1). In these cases Ω is the positive orthant of $I\!R^n$. See (Refs. 2–4). In the most recent surveys, both classical and interior-point tecniques; see, for example, (Refs. 5–7) are studied. If F is a gradient, (1) is the first order optimality condition of the minimization of the potential function over Ω.

The VIP can be formulated as the problem of solving a system of nonlinear equations and also as an optimization problem. A lot of research along these lines has been done recently, especially for the complementarity problem. See (Refs. 8–14).

Our approach in this paper is to formulate the VIP as an equivalent bound constrained smooth optimization problem. Differentiable bound constrained minimization is a well developed area of practical optimization and many methods and reliable software are available for large-scale problems. See, (Refs. 15–16). It is generally accepted that solving box constrained problems has, in practice, a similar degree of difficulty than solving unconstrained problems. This motivated the authors to find equivalences between variational and complementarity problems and box constrained minimization problems.

Formulation of the VIP as an optimization problem goes back to Auslender (Ref. 17) who introduced the gap function $g : I\!R^n \to I\!R^n$ given by

$$g(x) = \max_{y\in\Omega}\{\langle F(x), x - y\rangle\}.$$

Later, Hearn (Ref. 18) used this function for convex programming problems. The gap function provides a minimax formulation of the VIP, that leads to a nonsmooth optimization problem. Related formulations and references can be found in (Ref. 1), where it is mentioned (page 165) that the question of whether it is possible to formulate the VIP as a differentiable mathematical program when $F'(x)$ (the Jacobian of F at x) is not symmetric remains unanswered. Fukushima (Ref. 14) gave a positive answer to this question. He proposed a differentiable merit function such that any global minimizer subject to the feasible set Ω with optimal value zero is a solution of the VIP. The main result in his paper states that a sufficient condition for a stationary point of the optimization problem to be a solution of the VIP is the positive definiteness of $F'(x)$ on Ω. Thus, in this case, any constrained minimization algorithm can be applied to solve the problem. A drawback of the proposal is that the projection on Ω is required in the implementation of any algorithm for minimizing the merit function. So, the practicality of the method depends on the complexity of Ω. In (Refs. 19-21) the general projection steps are replaced by quadratic programming programs. In (Refs. 21–22) the VIP is formulated as an unconstrained smooth minimization problem, but the problem of calculating potentially difficult projections for computing the merit function remains. All these formulations have to solve subproblems with nontrivial constraints or to calculate projections.

In (Ref. 10), problem (1) is considered in the particular case where Ω is a bounded polytope, given in the standard form $Ax = b$, $x \geq 0$. The optimization problem associated to (1) is, in this case,

$$\min f(x,y,z) \equiv \|F(x) + A^T y - z\|^2 + \rho_1 \|Ax - b\|^2 + \rho_2 (x^T z)^p,$$
$$\text{s.t. } x \geq 0, \; z \geq 0. \tag{2}$$

where $\rho_1, \rho_2, p > 0$ are arbitrary. It is proved that, if $p > 1$, $F \in C^1(I\!R^n)$ is monotone and Ω is bounded, every stationary point of (2) is a solution of (1). This result was motivated by previous results for convex programming (Ref. 23) and linear complementarity (Ref. 9). For the nonlinear complementarity problem, Moré (Ref. 13) formulated a smooth optimization problem and gave a condition on $F'(x_*)$ that implies that the stationary point x_* is a global solution of the problem.

The essential features of our approach to the variational inequality problem are:

(a) Any efficient algorithm for smooth box constrained minimization problems can be used. In particular, we can use algorithms that do not use matrix factorizations at all, allowing us to deal with large scale problems. Special algorithms for dealing with nonsmoothness do not need to be devised.

(b) Unlike the approach of (Refs. 21–22), the computation of the merit function is straightforward and projections on convex sets are not necessary in order to compute neither the objective function nor the derivatives.

(c) The merit function preserves all the derivatives of the functions that define the VIP. Consequently, the global and local convergence properties depend of the algorithm chosen for box constrained minimization. This feature is very important, since it enables the use of algorithms that require high-order derivatives or their approximations, such as the tensor methods in (Ref. 24).

Our definition of the feasible set Ω in (1) is

$$\Omega = \{x \in I\!R^n \mid g(x) \leq 0, Ax = b, \bar{x} \geq 0\} \tag{3}$$

where $g = (g_1, \ldots, g_m)^T$, $g_i \in C^1(I\!R^n)$ is convex for all $i = 1, \ldots, m$, $A \in I\!R^{q \times n}$ and $\bar{x} = (x_1, \ldots, x_s)^T$. We associate to (1)-(3) a box constrained minimization problem and we prove, in Section 2, that, under a local monotonicity condition, stationary points of this problem are solutions of (1). In Section 3 we consider perturbations of the original problem, that allow us to deal with monotone functions, instead of strictly monotone ones. In Section 4 we describe an algorithm for variational inequalities, using perturbations and we show numerical examples. Finally, in Section 5, we state some conclusions and lines for future research.

Notation. We will denote $\|\cdot\|$ the Euclidean norm of $I\!R^n$ and its associated matricial norm.

If $g(x) = (g_1(x), \ldots, g_m(x))^T$, we denote

$$g_i'(x) = \nabla g_i(x)^T$$

for all $i = 1, \ldots, n$ and

$$g'(x) = (\nabla g_1(x), \ldots, \nabla g_m(x))^T.$$

As usually, $\nabla^2 g_i$ will denote the Hessian matrix of g_i. If B is a real $n \times n$ matrix, $B \geq 0$ ($B > 0$) means that B is positive semidefinite (positive definite).

We call

$$I\!R^n_+ = \{x \in I\!R^n \mid x \geq 0\}.$$

The notation $[x]_i$ will be used to indicate the $i - th$ coordinate of x. However, if it is clear from the context, we will also denote this coordinate x_i.

We denote $\{e_1, \ldots, e_n\}$ the canonical basis of $I\!R^n$.

If $v \in I\!R^s, \bar{0} = (0, \ldots, 0)^T \in I\!R^{n-s}$, we denote

$$(v, 0)^t = (v^T, \bar{0}^T)^T.$$

2 Equivalence Results

We consider the VIP defined by (1) and (3) with $F, g_1, \ldots, g_m \in C^1(I\!R^n)$ and g_i convex for all i. The associated merit function to the VIP is defined by

$$f(x, y, z, u, v) = \|F(x) + g'(x)^T y + A^T u - (v, 0)^t\|^2$$

$$+ \rho_1 \|z + g(x)\|^2 + \rho_2 \|Ax - b\|^2 + \rho_3 [(y^T z)^p + (\bar{x}^T v)^p], \tag{4}$$

where $\rho_1, \rho_2, \rho_3, p > 0$. Since the function $(y^T z)^p + (\bar{x}^T v)^p$ is a polynomial for all $p = 1, 2, \ldots$, the differentiability properties of f are determined by those of g and F when p is a natural number. Although the integrality of p is not required for the theoretical results, we think that this is the interesting case, from a practical point of view. Moreover, the case $p = 1$ is especially interesting because it allows us to reduce the linear variational inequality problem (where F and g are affine functions) to box constrained quadratic minimization.

We say that Ω satisfies a *constraint qualification* (Ref. 25) if at least one of the following conditions hold:

(a) g_i is an affine function for all $i = 1, \ldots, m$;
(b) there exists $z \in \Omega$ such that $g_i(z) < 0$ for all $i = 1, \ldots, m$, $z_i > 0$ for all $i = 1, \ldots, s$.

The minimization problem with simple bounds associated to the VIP is

$$\min\ f(x, y, z, u, v) \text{ s.t. } \bar{x} \geq 0, y \geq 0, z \geq 0, v \geq 0. \tag{5}$$

Theorem 2.1 is based on Proposition 2.2 of (Ref. 1) and relates global minimizers of (5) to solutions of the VIP .

Theorem 2.1. If Ω satisfies a constraint qualification and x_* is a solution of the VIP then there exist $z_*, y_* \in I\!R^m_+$, $u_* \in I\!R^q$, $v_* \in I\!R^s_+$ such that $(x_*, y_*, z_*, u_*, v_*)$ is a global minimizer of (5) and $f(x_*, y_*, z_*, u_*, v_*) = 0$. Conversely, if $(x_*, y_*, z_*, u_*, v_*)$ is such that $y_* \geq 0, z_* \geq 0, \bar{x}_* \geq 0, v_* \geq 0$

and $f(x_*, y_*, z_*, u_*, v_*) = 0$ (thus being a global minimizer of (5)) then x_* is a solution of the VIP .

Example 2.1. The constraint qualification condition cannot be removed for proving that given any solution x_* of the VIP, there exist y_*, z_*, u_*, v_* such that $f(x_*, y_*, z_*, u_*, v_*) = 0$. Consider $n = m = 1$, $q = s = 0$, $\rho_1 = \rho_3 = 1$, $g(x) = x^2$, $F(x) \equiv 1$. Here the only feasible point 0 is a solution of the VIP but $f(0, y, z, u, v) \geq 1$ for all y, z, u, v.

¿From Theorem 2.1 we deduce that, if a reliable algorithm for finding global minimizers is available, we can use it to solve the variational inequality problem with Ω defined by (3). In fact, if $f(x_*, y_*, z_*, u_*, v_*) = 0$ at a global minimizer of (5), then x_* is a solution of the VIP . If Ω satisfies a constraint qualification, and the global minimizers do not exist or, if at a global minimizer, we have $f(x_*, y_*, z_*, u_*, v_*) > 0$, then the VIP has no solutions.

However, global minimizers are very hard to find, especially in large-scale problems. Most efficient large-scale algorithms for box constrained optimization are guaranteed to converge only to stationary points of the problem. Therefore, it is necessary to relate stationary points of (5) to solutions of the VIP . The following example shows that, even for monotone functions F, stationary points of (5) can fail to be global minimizers.

Example 2.2. Consider $n = 1$, $\Omega = \{x \in I\!R \mid x \geq 0\}$, $F(x) \equiv 1$. Clearly, the unique solution of this VIP is $x_* = 0$. However, in this case, we have

$$f(x, v) = |1 - v|^2 + \rho(xv)^p.$$

If $\rho = 1, p = 1$ the point $(2, 0)^T$ is stationary but, obviously, it is not a solution of (1).

¿From now on, we assume that $g_1, \ldots, g_m \in C^2(I\!R^n)$ and we denote P a matrix whose columns form a basis of the null space of A. Moreover, Q will be a matrix whose columns form a basis of the subspace

$$\{x \in I\!R^n \mid Ax = 0, \;\; x_1 = \ldots = x_s = 0\}.$$

In the following theorem we give a sufficient condition that guarantees that a stationary point is a solution of the variational inequality problem.

Theorem 2.2. If $(x_*, y_*, z_*, u_*, v_*) \in I\!R^n \times I\!R^m_+ \times I\!R^m_+ \times I\!R^q \times I\!R^s_+$ is a stationary point of (5) with $p > 1$ and

$$P^T[F'(x_*) + \sum_{i=1}^{m}[y_*]_i \nabla^2 g_i(x_*)]P > 0,$$

then x_* is a solution of the VIP .

Proof. Let $(x_*, y_*, z_*, u_*, v_*)$ be a stationary point of (5). We call

$$H = F'(x_*) + \sum_{i=1}^{m}[y_*]_i \nabla^2 g_i(x_*), \tag{6}$$

$$w_1 = F(x_*) + g'(x_*)^T y_* + A^T u_* - (v_*, 0)^t, \tag{7}$$

$$w_2 = g(x_*) + z_*, \tag{8}$$

$$w_1^T = (\bar{w}_1^T, \hat{w}_1^T),$$

$$\bar{w}_1^T = ([w_1]_1, \ldots, [w_1]_s),$$

$$\hat{w}_1^T = ([w_1]_{s+1}, \ldots, [w_1]_n).$$

Then, there exist $\alpha \in I\!R^s_+, \beta \in I\!R^s_+, \gamma \in I\!R^m_+, \mu \in I\!R^m_+$ such that

$$2Hw_1 + 2\rho_1 g'(x_*)^T w_2 + 2\rho_2 A^T(Ax_* - b) + p\rho_3(\bar{x}_*^T v_*)^{p-1}(v_*, 0)^t - (\alpha, 0)^t = 0, \tag{9}$$

$$2g'(x_*)w_1 + p\rho_3(y_*^T z_*)^{p-1} z_* - \gamma = 0, \tag{10}$$

$$2\rho_1 w_2 + p\rho_3(y_*^T z_*)^{p-1} y_* - \mu = 0, \tag{11}$$

$$Aw_1 = 0, \tag{12}$$

$$-2\bar{w}_1 + p\rho_3(\bar{x}_*^T v_*)^{p-1}\bar{x}_* - \beta = 0, \tag{13}$$

$$\bar{x}_*^T \alpha = 0, \tag{14}$$

$$y_*^T \gamma = 0, \tag{15}$$

$$z_*^T \mu = 0, \tag{16}$$

$$v_*^T \beta = 0, \tag{17}$$

$$\bar{x}_* \geq 0, v_* \geq 0, y_* \geq 0, z_* \geq 0, \alpha \geq 0, \beta \geq 0, \gamma \geq 0, \mu \geq 0. \tag{18}$$

By (10) and (11), we have that

$$2g'(x_*)w_1 = -p\rho_3(y_*^T z_*)^{p-1} z_* + \gamma$$

and

$$2\rho_1 w_2 = -p\rho_3(y_*^T z_*)^{p-1} y_* + \mu.$$

Therefore, by (16) and (15),

$$4\rho_1 w_1^T g'(x_*)^T w_2 =$$

$$[-p\rho_3(y_*^T z_*)^{p-1} z_* + \gamma]^T[-p\rho_3(y_*^T z_*)^{p-1} y_* + \mu] = p^2\rho_3^2(y_*^T z_*)^{2p-1} + \gamma^T \mu. \tag{19}$$

On the other hand, by (13),

$$2\bar{w}_1 = p\rho_3(\bar{x}_*^T v_*)^{p-1}\bar{x}_* - \beta. \tag{20}$$

Pre-multiplying (9) by $2w_1^T$, we obtain, using (19) and (12), that

$$4w_1^T H w_1 + p^2\rho_3^2(y_*^T z_*)^{2p-1} + \gamma^T\mu + 2w_1^T[p\rho_3(\bar{x}_*^T v_*)^{p-1}(v_*, 0)^t] - 2w_1^T(\alpha, 0)^t = 0.$$

So, by (20), (14) and (17),

$$0 = 4w_1^T H w_1 + p^2\rho_3^2(y_*^T z_*)^{2p-1} + \gamma^T \mu$$
$$+2p\rho_3(\bar{x}_*^T v_*)^{p-1}\bar{w}_1^T v_* - [p\rho_3(\bar{x}_*^T v_*)^{p-1}\bar{x}_* - \beta]^T \alpha$$
$$= 4w_1^T H w_1 + p^2\rho_3^2(y_*^T z_*)^{2p-1} + \gamma^T \mu + p^2\rho_3^2(\bar{x}_*^T v_*)^{2p-1} + \alpha^T \beta.$$

Therefore, by (18), (12) and $P^T H P \geq 0$,

$$w_1^T H w_1 = 0, \tag{21}$$

$$y_*^T z_* = 0, \tag{22}$$

$$\bar{x}_*^T v_* = 0, \tag{23}$$

$$\mu^T \gamma = 0 \tag{24}$$

and

$$\alpha^T \beta = 0. \tag{25}$$

Since $P^T H P > 0$, (12) and (21) imply that

$$w_1 = 0. \tag{26}$$

By (8), (9), and (26), we have:

$$2\rho_1 g'(x_*)^T (g(x_*) + z_*) + 2\rho_2 A^T (Ax_* - b) + p\rho_3 (\bar{x}_*^T v_*)^{p-1} (v_*, 0)^t - (\alpha, 0)^t = 0. \tag{27}$$

So, since $p > 1$, (23) implies that

$$2\rho_1 g'(x_*)^T (g(x_*) + z_*) + 2\rho_2 A^T (Ax_* - b) - (\alpha, 0)^t = 0. \tag{28}$$

Now, by (8), (11), (22) and $p > 1$, we have:

$$2\rho_1 [g(x_*) + z_*] - \mu = 0. \tag{29}$$

Define

$$I = \{i \in \{1, \dots, m\} \mid [z_*]_i = 0\}.$$

If $i \notin I$, then $[z_*]_i \neq 0$. So, by (16), $\mu_i = 0$. Therefore, by (29),

$$g_i(x_*) + [z_*]_i = 0 \text{ for all } i \notin I \tag{30}$$

Moreover, by (29),

$$g_i(x_*) = \frac{\mu_i}{2\rho_1} \geq 0 \text{ for all } i \in I. \tag{31}$$

By (30) and (28), we obtain:

$$2\rho_1 \sum_{i \in I} g_i(x_*) \nabla g_i(x_*) + 2\rho_2 A^T (Ax_* - b) - (\alpha, 0)^t = 0. \tag{32}$$

Let x_0 be an arbitrary point of the nonempty set Ω. We write

$$\bar{x}_0 = ([x_0]_1, \dots, [x_0]_s)^T, \hat{x}_0 = ([x_0]_{s+1}, \dots [x_0]_n)^T.$$

Pre-multiplying (32) by $x_* - x_0$, we obtain:

$$2\rho_1 \sum_{i \in I} g_i(x_*) g_i'(x_*)(x_* - x_0) + 2\rho_2 \|Ax_* - b\|^2 - \bar{x}_*^T \alpha + \bar{x}_0^T \alpha = 0.$$

So, by (14) and $\bar{x}_0 \geq 0$,

$$2\rho_1 \sum_{i \in I} g_i(x_*) g_i'(x_*)(x_* - x_0) + 2\rho_2 \|Ax_* - b\|^2 \leq 0. \tag{33}$$

But, since g_i is convex, we have that

$$g_i'(x_*)(x_* - x_0) \geq g_i(x_*) - g_i(x_0) \text{ for all } i.$$

So, by (33),

$$2\rho_1 \sum_{i \in I} g_i(x_*)[g_i(x_*) - g_i(x_0)] + 2\rho_2 \|Ax_* - b\|^2 \leq 0.$$

Therefore, by (31), since $g_i(x_0) \leq 0$ for all i, we have that

$$2\rho_1 \sum_{i \in I} g_i(x_*)^2 + 2\rho_2 \|Ax - b\|^2 \leq 2\rho_1 \sum_{i \in I} g_i(x_*) g_i(x_0) \leq 0.$$

So,

$$\|Ax_* - b\| = 0 \tag{34}$$

and $g_i(x_*) = 0$ for all $i \in I$. This implies that $g_i(x_*) + [z_*]_i = 0$ for all $i \in I$. So, by (30),

$$g(x_*) + z_* = 0. \tag{35}$$

By (7), (26), (35), (34), (22) and (23), we have that $f(x_*, y_*, z_*, u_*, v_*) = 0$, as we wanted to prove. □

Example 2.3. The fact that $F'(x) > 0$ for all x does not guarantee the *existence* of stationary points of (5). Consider the VIP defined by $n = m = 1$, $q = s = 0$, $\rho_1 = \rho_3 = 0$, $g(x) = x^2$, $F(x) = x + 1$. Here the VIP has the unique solution 0. However, using arguments analogous to the ones used in the first part of the proof of Theorem 2.2, it can be shown that (5) has no stationary points for $p > 1$. So, the existence of stationary points of (5) is not automatically guaranteed by the existence and unicity of solutions of the VIP .

The following theorem shows that the hypotheses of Theorem 2.2 can be relaxed if the set defined by the linear constraints is bounded. This result generalizes for the nonlinearly constrained problem the main results of (Refs. 10 and 23).

Theorem 2.3. Assume that the region

$$\Upsilon = \{x \in I\!R^n \mid Ax = b, \bar{x} \geq 0\}$$

is bounded, $(x_*, y_*, z_*, u_*, v_*) \in I\!R^n \times I\!R^m_+ \times I\!R^m_+ \times I\!R^q \times I\!R^s_+$ is a stationary point of (5) with $p > 1$,

$$P^T[F'(x_*) + \sum_{i=1}^m [y_*]_i \nabla^2 g_i(x_*)]P \geq 0$$

and

$$Q^T[F'(x_*) + \sum_{i=1}^m [y_*]_i \nabla^2 g_i(x_*)]Q > 0.$$

Then, x_* is a solution of the VIP.

Proof: As in Theorem 2.2, we obtain (7)–(25). Now, by (12), w_1 is in the null-space of A. By (20), (18) and (23), $\bar{w}_1 \leq 0$. Since Υ is nonempty and bounded, it follows that $\bar{w}_1 = 0$. Therefore, (26) follows from $Q^T H Q > 0$. The rest of the proof follows as in Theorem 2.2. □

The following theorem extends the conclusion of Theorem 2.2 for the case $p = 1$. However, an additional condition is necessary.

Theorem 2.4. If $(x_*, y_*, z_*, u_*, v_*) \in I\!R^n \times I\!R^m_+ \times I\!R^m_+ \times I\!R^q \times I\!R^s_+$ is a stationary point of (5), with $p = 1$,

$$P^T[F'(x_*) + \sum_{i=1}^m [y_*]_i \nabla^2 g_i(x_*)]P > 0,$$

and $\nabla g_1(x_*), \ldots, \nabla g_m(x_*), a_1, \ldots, a_q, e_{i_1}, \ldots, e_{i_\ell}$ are linearly independent, where $A^T = (a_1, \ldots, a_q)$, and $i_1, \ldots, i_\ell$ are the indices $j \in \{1, \ldots, s\}$ such that $[x_*]_j = 0$, then x_* is a solution of the VIP.

Proof. The equations (26), (22) and (23), are obtained exactly as in Theorem 2.2. Now, by (27) with $p = 1$, we have that

$$2\rho_1 g'(x_*)^T(g(x_*) + z_*) + 2\rho_2 A^T(Ax_* - b) + p\rho_3(v_*, 0)^t - (\alpha, 0)^t = 0. \quad (36)$$

Now, if $[\bar{x}_*]_i > 0$, we have, by (23), that $[v_*]_i = 0$ and, by (14), that $\alpha_i = 0$. Therefore,

$$p\rho_3(v_*, 0)^t - (\alpha, 0)^t = \sum_{\nu=1}^{\ell} (p\rho_3[v_*]_{i_\nu} + \alpha_{i_\nu})e_{i_\nu}. \quad (37)$$

Replacing (37) in (36), we obtain, by the linear independence of the vectors considered in the hypothesis, that $z_* + g(x_*) = 0$ and $Ax_* - b = 0$. This completes the proof. $\square$

In the following theorem we give the sufficient conditions that correspond to the case $p = 1$ when Υ is bounded.

Theorem 2.5. Assume that Υ (defined in Theorem 2.3) is bounded. If $(x_*, y_*, z_*, u_*, v_*) \in \mathbb{R}^n \times \mathbb{R}^m_+ \times \mathbb{R}^m_+ \times \mathbb{R}^q \times \mathbb{R}^s_+$ is a stationary point of (5), with $p = 1$,

$$P^T[F'(x_*) + \sum_{i=1}^{m}[y_*]_i \nabla^2 g_i(x_*)]P \geq 0,$$

$$Q^T[F'(x_*) + \sum_{i=1}^{m}[y_*]_i \nabla^2 g_i(x_*)]Q > 0,$$

and $\nabla g_1(x_*), \ldots, \nabla g_m(x_*), a_1, \ldots, a_q, e_{i_1}, \ldots, e_{i_\ell}$ are linearly independent, where $A^T = (a_1, \ldots, a_q)$, and $i_1, \ldots, i_\ell$ are the indices $j \in \{1, \ldots, s\}$ such that $[x_*]_j = 0$, then x_* is a solution of the VIP.

Proof. The expressions (6)-(26) follow as in the proof of Theorem 2.3. The rest of the proof is as in Theorem 2.4. $\square$

Due to the convexity of g, the results stated in Theorems 2.2, 2.3, 2.4 and 2.5 hold replacing $F'(x_*) + \sum_{i=1}^{m}[y_*]_i \nabla^2 g_i(x_*)$ by $F'(x_*)$. In particular, the following corollaries can be stated.

Corollary 2.1. Assume that $(x_*, y_*, z_*, u_*, v_*) \in \mathbb{R}^n \times \mathbb{R}^m_+ \times \mathbb{R}^m_+ \times \mathbb{R}^q \times \mathbb{R}^s_+$ is a stationary point of (5) with $p > 1$. If $P^T F'(x_*)P > 0$ then x_* is a solution of the VIP. If Υ (defined as in Theorem 2.3) is bounded, $P^T F'(x_*)P \geq 0$ and $Q^T F'(x_*)Q > 0$, then x_* is a solution of the VIP. In particular, the conclusion also follows if Υ is bounded, $F'(x_*) \geq 0$ and $s = n$.

Corollary 2.2. Suppose that $(x_*, y_*, z_*, u_*, v_*) \in \mathbb{R}^n \times \mathbb{R}^m_+ \times \mathbb{R}^m_+ \times \mathbb{R}^q \times \mathbb{R}^s_+$ is a stationary point of (5) with $p = 1$. Assume, further, that $P^T F'(x_*)P \geq 0$, $Q^T F'(x_*)Q > 0$, and $\nabla g_1(x_*), \ldots, \nabla g_m(x_*), a_1, \ldots, a_q, e_{i_1}, \ldots, e_{i_\ell}$ are linearly independent, where $A^T = (a_1, \ldots, a_q)$, and $i_1, \ldots, i_\ell$ are the indices $j \in \{1, \ldots, s\}$ such that $[x_*]_j = 0$. Then x_* is a solution of the VIP .

The condition of linear independence of *all* the gradients $\nabla g_i(x_*)$ in Theorem 2.4 seems strange, since it involves, not only active constraints, but also constraints where $g_i(x_*) < 0$. (Observe that this condition holds in the very important case of complementarity problems, where $\Omega = I\!R^n_+$.) However, it cannot be easily removed, as the following example shows.

Example 2.4. Consider the variational inequality problem defined by $F : I\!R^1 \to I\!R^1$, $F(x) = x$ and

$$\Omega = \{x \in I\!R^1 \mid -x \leq 0,\ x - 2 \leq 0\}.$$

Clearly, 0 is the unique solution of this problem. With $p = 1$, $\rho_1 = 1$, $\rho_3 = 1$, $m = 2$, $q = s = 0$, the merit function of (5) is

$$f(x, y, z, u, v) = (x - y_1 + y_2)^2 + (-x + z_1)^2 + (x - 2 + z_2)^2 + y_1 z_1 + y_2 z_2\ .$$

If $x_* = 1$, $y_* = (3, 2)^T$ and $z_* = (0, 0)^T$, we verify, after some trivial calculations, that $(x_*, y_*, z_*, 0, 0)$ is a stationary point of (5) but x_* is not a solution of the VIP . Observe that, in this problem, not only the mapping F is strictly monotone, but also it is linear and the set Ω is a bounded polytope.

Example 2.5. A variational inequality problem with $F'(x) > 0$ for all x can have no solutions, even if all the points of Ω are regular. However, in this case, by Theorem 2.2, (5) has no stationary points for all $p \geq 1$. This is the case, for example, of the problem defined by $F(x) = e^x$ with $\Omega = (-\infty, 0]$.

A sufficient condition that guarantees that stationary points of (5) exist and can be found by standard minimization techniques is the boundedness of the level sets of (5). In the next theorem we prove that this condition holds for nonlinear complementarity problems if F is a *uniform P-function.* Let us denote $F = (F_1, \ldots F_n)^T$. A mapping $F : I\!R^n \to I\!R^n$ is said to be a uniform P-function if there exists $\varepsilon > 0$ such that for all $x, w \in I\!R^n$, we have

$$\max_i \{(F_i(x) - F_i(w))(x_i - w_i)\} \geq \varepsilon \|x - w\|^2 \tag{38}$$

It can be proved that strongly monotone functions are P-uniform. See (Ref. 1). Assume now that we deal with the nonlinear complementarity problem, for which the function f in (5) takes the form

$$f(x, v) = \|F(x) - v\|^2 + \rho(x^T v)^p, \tag{39}$$

where, as in (5), $p > 0$.

Theorem 2.6. If F is P-uniform, the level sets of $f(x, v)$, given by (39), on $I\!R^n_+ \times I\!R^n_+$ are bounded.

Proof. Given $c > 0$, define

$$S = \{(x, v) \in I\!R^n_+ \times I\!R^n_+ \mid f(x, v) \leq c\}.$$

If $(x, v) \in S$, then

$$\|F(x) - v\|^2 \leq c \text{ and } \rho(x^T v)^p \leq c.$$

So,

$$x_i v_i \leq (c/\rho)^{1/p} \text{ and } |F_i(x) - v_i| \leq \sqrt{c} \tag{40}$$

for all $i = 1, \ldots, n$.

But, by (38),

$$\varepsilon\|x\|^2 \leq \max_i\{(F_i(x) - F_i(0))x_i\} = \max_i\{x_i v_i + (F_i(x) - v_i)x_i - F_i(0)x_i\}$$

So, by (40),

$$\varepsilon\|x\|^2 \leq (c/\rho)^{1/p} + \sqrt{c}\|x\| + \|F(0)\|\|x\|.$$

Therefore, if $\|x\| \neq 0$,

$$\varepsilon\|x\| \leq (c/\rho)^{1/p}\frac{1}{\|x\|} + \sqrt{c} + \|F(0)\|.$$

So, if $\|x\| \geq 1$, we have that

$$\|x\| \leq d'$$

where

$$d' = (c/\rho)^{1/p} + \sqrt{c} + \|F(0)\|.$$

Thus, we proved that, if $(x, v) \in S$, then

$$\|x\| \leq d \equiv \max\{1, d'\}.$$

Now, by (40) and the continuity of F,

$$\|v\| \leq \|F(x) - v\| + \|F(x)\| \leq \sqrt{c} + \max_{\|x\| \leq d} \|F(x)\|.$$

So, the proof is complete. $\square$

3 Perturbed Problems

In some situations, we can guarantee that, when F is (not necessarily strictly) monotone, stationary points of the merit function are solutions of the variational inequality problem. Some of these situations are listed below:

(a) When Ω is a bounded polytope in the standard form and $p > 1$ (Ref. 10);

(b) When we have a linear complementarity problem ($F(x) = Mx + q$), $\{x \in \mathbb{R}^n \mid Mx + q \geq 0, x \geq 0\} \neq \emptyset$ and $p > 1$ (Ref. 9).

In general, we can have stationary points of the associated problem that are not solutions of the original variational problem, even for F monotone and convex with $p > 1$. Consider, for example, the following problem:

Example 3.1. Let $F : \mathbb{R}^1 \to \mathbb{R}^1$ be given by $F(x) = -1$ if $x \leq 1$ and $F(x) = (x-1)^2 - 1$ if $x \geq 1$, $\Omega = \mathbb{R}^1_+$. Observe that F is monotone and convex. The associated variational inequality problem has the unique solution $x_* = 2$. The merit function (with $p = 2, \rho_1 = \rho_2 = 1$) is, in this case, given by

$$f(x, v) = (-1 - v)^2 + (xv)^2 \text{ if } x \leq 1,$$

$$f(x, v) = [(x-1)^2 - 1 - v]^2 + (xv)^2 \text{ if } x \geq 1.$$

Now, $(0,0)^T$ is a stationary point of the problem (5) that corresponds to this function.

Given a sequence of strictly positive ε_k such that $\varepsilon_k \downarrow 0$, we can associate a family of perturbed problems, replacing $F(x)$ by $F(x) + \varepsilon_k x$. We define, for all $x \in \mathbb{R}^n$,

$$F_k(x) = F(x) + \varepsilon_k x$$

We call VIP(k) the problem of finding $x_k \in \Omega$ such that

$$\langle F_k(x), w - x \rangle \geq 0 \text{ for all } w \in \Omega.$$

The following theorems relate the solutions of the perturbed problems to the solution of the VIP .

Theorem 3.1. If VIP(k) admits a solution for all $k \in \mathbb{N}$ and the sequence of solutions $\{x_k\}$ is bounded, then every limit point of $\{x_k\}$ is a solution of the VIP.

Proof. Since $\{x_k\}$ is bounded, it admits a convergent subsequence. Let K_1 be an infinite subset of $I\!N$, and $x_* \in \Omega$ such that

$$\lim_{k \in K_1} x_k = x_*.$$

If $w \in \Omega$, since x_k is a solution of VIP(k), we have that

$$\langle F(x_k) + \varepsilon_k x_k, w - x_k \rangle \geq 0 \text{ for all } k \in I\!N.$$

So, taking limits for $k \in K_1$, we obtain that

$$\langle F(x_*), w - x_* \rangle \geq 0.$$

Since $w \in \Omega$ is arbitrary, x_* is a solution of the VIP . □

A condition that guarantees existence and unicity of the variational inequality problem is strong monotonicity, see Corollary 3.2 of (Ref. 1). A function $F : I\!R^n \to I\!R^n$ is strongly monotone (modulus ε) if $\varepsilon > 0$ and

$$\langle F(w) - F(x), w - x \rangle \geq \varepsilon \|w - x\|^2$$

for all $x, w \in I\!R^n$. Obviously, strong monotonicity implies strict monotonicity.

If F is monotone, then F_k is strongly monotone and the solution x_k of VIP(k) exists and is unique for all $k \in I\!N$. Therefore, if Ω satisfies a constraint qualification, there exist $(x_k, y_k, z_k, u_k, v_k)$ feasible for (5) such that $f_k(x_k, y_k, z_k, u_k, v_k) = 0$ for all $k \in I\!N$, where f_k is the merit function associated to VIP(k).

Theorem 3.2. Assume that F is monotone and that the set of solutions of the VIP is not empty. Then, $\{x_k\}$ converges to the unique minimum norm solution of the VIP .

Proof. Let $\bar{x}$ be a solution of the VIP . Since $\bar{x} \in \Omega$ and x_k is a solution of VIP(k), we have that, for all $k \in I\!N$,

$$\langle F(x_k) + \varepsilon_k x_k, \bar{x} - x_k \rangle \geq 0.$$

So, since $\langle F(\bar{x}), x_k - \bar{x} \rangle \geq 0$, we have, using the monotonicity of F, that

$$0 \leq \langle F(x_k) - F(\bar{x}), x_k - \bar{x} \rangle \leq \varepsilon_k \langle x_k, \bar{x} - x_k \rangle - \langle F(\bar{x}), x_k - \bar{x} \rangle \leq \varepsilon_k \langle x_k, \bar{x} - x_k \rangle$$

$$\leq \varepsilon_k(\|x_k\|\|\bar{x}\| - \|x_k\|^2) = \varepsilon_k\|x_k\|(\|\bar{x}\| - \|x_k\|)$$

Therefore,

$$\|x_k\| \leq \|\bar{x}\| \text{ for all } k \in I\!N. \tag{41}$$

Hence, the sequence $\{x_k\}$ is bounded. By Theorem 3.1, every limit point of $\{x_k\}$ is a solution of the VIP . However, by (41) limit points of $\{x_k\}$ must be minimum norm solutions of the VIP . Now, by Proposition 3.1 of (Ref. 1) the set of solutions of the monotone VIP is convex and its minimum norm solution is unique. Therefore, the sequence converges to the minimum norm solution of the VIP . □

4 Algorithm

The algorithm presented in this section is motivated by the perturbation results proved in Section 3. Assume that there exists $b \leq 0$ such that for all $x \in I\!R^n$, if $r \in I\!R$ is the real part of an eigenvalue of $F'(x)$, we have that $r \geq b$. Thus, if $T > -b$, the function $F(x) + T(x - a)$ is strongly monotone. Moreover, if $a \in \Omega$ and T is large enough, the variational inequality problem associated to this function has a solution that will be close to a, and the stationary point of (5) will be the solution of this variational inequality problem. So, using any minimization algorithm for box constraints, we should probably be able to find a solution $(x(T), y(T), z(T), u(T), v(T))$ of the perturbed problem up to any desired precision. This fortunate situation will extend to all $t \leq T$ such that $F(x) + t(x - a)$ is strongly monotone, for each of which a solution $(x(t), y(t), z(t), u(t), v(t))$ should be computed using standard minimization methods. Roughly speaking, if T_0 is the infimum t such that $F(x) + t(x - a)$ is strongly monotone, the points $\{x(t), t > T_0\}$ will probably form a curve in $I\!R^n$ that can be computationally traced. Many times, solutions of the variational inequality problem associated to $t < T_0$ could also be obtained using minimization. Let us call T_1 the infimum t such that the "curve" that begins at $x(T)$ can be traced. If $T_1 = 0$, we are done. If $T_1 > 0$, many alternatives are possible, all of them connected to homotopy tracing methods for resolution of nonlinear systems. See (Ref. 26). In the algorithm presented, we suggest to change the homotopy when a very rough approximation of the singular point is computed, using a as the last computed point $x(t)$ of the curve and computing a new T. The algorithm is stated below. We make a very high level description, so that the main steps of the algorithm can be understood.

We will call $P(a,t)$ the minimization problem associated to a VIP defined by (3) and the operator $F(a,t,x) \equiv F(x) + t(x-a)$. That is, $P(a,t)$ is

$$\min f_{a,t}(x,y,z,u,v)$$

$$\text{s.t. } \bar{x} \geq 0, y \geq 0, z \geq 0, v \geq 0,$$

where

$$f_{a,t}(x,y,z,u,v) = \|F(x) + t(x-a) + g'(x)^T y + A^T u - (v,0)^t\|^2$$

$$+\rho_1\|z + g(x)\|^2 + \rho_2\|Ax - b\|^2 + \rho_3[(y^T z)^p + (\bar{x}^T v)^p],$$

and $\rho_1, \rho_2, \rho_3, p > 0$. Clearly, $P(a,0)$ is problem (5).

Algorithm 4.1.
Let T be a (large) positive number, $a \in \Omega$. Set

$$x_0 \leftarrow a, \;\; y_0 \leftarrow 0, \;\; z_0 \leftarrow -g(x_0), \;\; u_0 \leftarrow 0, \;\; v_0 \leftarrow 0,$$

Phase 1. This includes Steps 1-2 below.

Step 1: *Try to solve (5)*
Using a box-constrained minimization algorithm, with initial approximation $(x_0, y_0, z_0, u_0, v_0)$, find a stationary point $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v})$ of (5) such that

$$f(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) \leq f(x_0, y_0, z_0, u_0, v_0). \tag{42}$$

Step 2: *Stop if the solution was found*
If $f(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) = 0$, then stop. A global minimizer of (5) was found.
Otherwise, begin the homotopic process setting $t \leftarrow T$.

Phase 2. This includes Steps 3-4 below.

Step 3: *Try to solve $P(a,t)$*
Using a box-constrained minimization algorithm, with initial approximation $(x_0, y_0, z_0, u_0, v_0)$, find a stationary point $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v})$ of $P(a,t)$.

Step 4: *If Step 3 failed, increase t*
If $f_{a,t}(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) > 0$, then increase $t \leftarrow 2t$ and repeat Step 3.

Else, set

$$(x_*, y_*, z_*, u_*, v_*) \leftarrow (\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}),$$

$$t_c \leftarrow t, \quad t_- \leftarrow 0$$

and continue with Phase 3.

Phase 3. This includes Steps 5-9 below.

Step 5: *Solve the minimization problem for t_-*

Using a box-constrained minimization algorithm, with initial approximation $(x_0, y_0, z_0, u_0, v_0) \leftarrow (x_*, y_*, z_*, u_*, v_*)$, find a stationary point $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v})$ of P_{a,t_-}.

Step 6: *Test if a solution of (5) was found*

If $f_{a,t_-}(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) = 0$ and $t_- = 0$, a global solution of (5) was found. Stop.

Step 7: *Test if a new point on the homotopic curve was found*

If $f_{a,t_-}(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) = 0$ but $t_- > 0$, set

$$(x_*, y_*, z_*, u_*, v_*) \leftarrow (\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}),$$

$$t_c \leftarrow t_-, \quad t_- \leftarrow 0,$$

and go to Step 5.

Step 8: *Increase t_-*

If $f_{a,t_-}(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) > 0$ and $t_c - t_- > 0.01 t_c$, set

$$t_- \leftarrow \frac{t_c + t_-}{2}$$

and go to Step 5.

Step 9: *Change the homotopy*

If $f_{a,t_-}(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) > 0$ but $t_c - t_- \leq 0.01 t_c$, set

$$a \leftarrow x_*, \quad (x_0, y_0, z_0, u_0, v_0) \leftarrow (x_*, y_*, z_*, u_*, v_*)$$

and return to Step 1.

To adjust the parameters of the algorithm, we used the nonlinear complementarity problem called "Singular-Broyden" (Refs. 27–29). According to (Refs. 28 and 29), this problem is hard, since different merit functions tend to find stationary points that are not global minimizers. The merit function (4) was used with $\rho_3 = 2$, $p = 1$. (The second and third term of (4) are not present, since $\Omega = I\!R^n_+$ in this case.) The problems $P(a,t)$ were solved using the box-constrained minimization algorithm introduced in (Ref. 16) (called BOX from now on). The executions of BOX were stopped when one of the following stopping criteria was achieved:

(a) Objective function value less than 10^{-8};

(b) Euclidian norm of the projected gradient less than 10^{-5};

(c) Trust region radius less than 10^{-5};

(d) Number of iterations greater than 100;

(e) Number of functional evaluations greater than 200;

(e) $f_{k-1} - f_k \le \kappa \max \{f_j - f_{j-1}, j = 1, \dots, k\}$, where f_j is the objective function value of $P(a,t)$ at iteration j.

An execution of BOX was declared "successful", when

$$\max \{| \min \{\bar{x}_i, [F(\bar{x})]_i\}|\} \le 10^{-4}, i = 1, \dots, n\}, \tag{43}$$

where $\bar{x}$ is the final point computed by BOX. When (43) holds, the same procedure as in the case $f_t(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}) = 0$ described in Algorithm 4.1 is followed.

We tried to solve Singular-Broyden with $n = 10$ using the box-constrained minimization method using different randomly generated starting points. The initial approximations (x_0, v_0) were generated as follows: for all $i = 1, \dots, n$ $[x_0]_i = 0$ and $[v_0]_i > 0$ with probability 0.5. When $[x_0]_i > 0$ ($[v_0]_i > 0$), $[x_0]_i$ ($[v_0]_i$) was generated randomly in $[0, 5]$. First, $\kappa = 0.001$ was used with 5000 initial points. The total number of major iterations was 25445, with 34746 functional evaluations and 96590 minor iterations (used by the internal quadratic solver). This process used one hour and twenty minutes in our computer (PC 486, 66 MHz). However, no global solution was found.

Completely different results were obtained setting $\kappa = 0$. In this case, we used the first 100 initial points considered above. In 78 cases the algorithm converged because a small projected gradient or a very small functional value was obtained. In 21 cases, 500 functional evaluations were not sufficient to achieve convergence. In one case, the box constrained method stopped because the trust region radius turned out to be very small. The global minimizer was obtained in 16 cases. Therefore, it seems that, for this problem, the probability of converging to a global solution, starting from a random initial point is 16%. In this set of experiments, 4637 major iterations and 19317 functional evaluations were performed.

With $n = 20$ and $\kappa = 0$ the results using random points were qualitatively analogous to the case $n = 10$. A global solution was obtained in 3 out of 100 cases. The total number of iterations of BOX was 6688 and the function was evaluated 31332 times.

Based on the results using random initial points, tried to solve the problem for $n = 10$ using Algorithm 4.1, with $\kappa = 0$. We used $T = 10$. Two homotopies were necessary to reach a solution. Using the first one, we cannot trace the curve for $t < 0.76$, so the solution of $P(a, 0.76)$ was used to generate a different homotopy, that succeeded very quickly.

Then, Algorithm 4.1 was used for solving the same problem ($n = 10$) with $\kappa = 0.001$. The results were much better in this case, only one homotopy was sufficient for getting a solution of the nonlinear complementarity problem.

Based on the results for $n = 10$, we ran Algorithm 4.1 for Singular-Broyden with $n = 20$ only with $\kappa = 0.001$. In this case, three homotopies were necessary to reach a global solution. The first one, that uses $a = 0$, gets stuck when $t \approx 3.63$. It is replaced but the one that has the solution obtained for $t \approx 3.63$ as basic point. In this case, it is necessary to increase t up to 1280 to obtain the first successful point of the second homotopy. However, this one fails for $t < 0.26$, and is replaced by a third one that succeeds quickly. Trajectories of the succesful solutions for different values of t for these problems are shown in Tables 1–3 in (Ref. 30).

5 Final Remarks

Our main objective in this paper was to exploit the characteristics of a smooth minimization problem with simple bounds associated to the variational inequality problem. The minimization problem is globally equivalent to the VIP in the sense that if the objective function at the minimum is zero, then the corresponding point is a solution of the VIP and, conversely, under regularity, any solution of the VIP must be a global minimizer with null objective function value. The most important feature of the merit function is that it has all the derivatives of the functions that define the operator F and the constraints. This feature allows us to use any algorithm for box constrained minimization, exploiting the great development attained by this area of practical optimization. In particular, methods that use high order derivatives can be applied, if they are available. Obviously, in these cases the chances of obtaining a global minimizer grow, since the set of high order stationary points is smaller than the set of first order stationary points.

We proved that first order stationary points of the minimization problem are solutions of the VIP under some "local-monotonicity" conditions and showed a sufficient condition under which the minimization problem associated to the nonlinear complementarity problem has bounded level sets. The study of perturbed problems, by means of which monotone problems are approximated by strongly monotone ones, suggested us to define an algorithm based on an homotopy approach. Due to the theoretical results proved, the algorithm finds solutions when the monotone problem is solvable but some experiments suggest that the solution of the VIP can also be found in many other interesting situations.

Further properties of the smooth minimization problem associated to the VIP must be exploited. Some of them are the following:

(a) Since it is possible to use high order minimization methods, it follows that high order stationary points of the minimization problems can be obtained. New sufficient conditions should be discovered, under which high order stationary points are solutions of the VIP.

(b) Global optimization algorithms for solving the minimization problem should be developed, at least for special cases such as the nonlinear and even the linear complementarity problem.

(c) Different smooth optimization problems must be analyzed and its relation to the one proposed here must be studied. In particular, the merit function for the VIP that is suggested by Moré's approach to nonlinear complementarity (Ref. 13) should be compared with our merit function.

(d) Weaker sufficient conditions for the optimality of stationary points in complementarity problems should be studied.

(e) Since the optimality conditions of nonlinear programming with convex feasible region are variational inequality problems, our approach should be exploited in connection to general minimization problems with convex constraints. This can be done in two ways, either by direct application of a box constrained minimizer to (5) (where F is the gradient of the objective function), or using (5) as a merit problem to provide a sequential quadratic algorithm with global convergence properties. The possibility of attacking nonlinear programming problems directly through (5) is attractive since in this problem we do not need to develop ad hoc estimators of penalization or Lagrange multipliers and its solution can be obtained using matrix-free algorithms. Examples in the case where the feasible region is a bounded polytope have been given in (Ref. 10).

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