Bound Constrained Smooth Optimization for Solving Variational Inequalities and Related Problems.

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Abstract

Variational inequalities and related problems may be solved via smooth bound constrained optimization. A comprehensive discussion of the important features involved with this strategy is presented. Complementarity problems and mathematical programming problems with equilibrium constraints are included in this report. Numerical experiments are commented. Conclusions and directions of future research are indicated.

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1 Introduction

Various reformulations of the variational inequality problem (VIP) in finite dimensional spaces as optimization problems have been proposed in the last ten years. In this paper

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we wish to survey bound constrained smooth optimization formulations for the VIP and related problems.

The VIP is to find a vector $x \in \Omega \in I\!R^n$ such that

$$F(x)^T \ (z - x) \ \geq 0 \ \forall \, z \in \Omega, \tag{1}$$

where $F : I\!R^n \rightarrow I\!R^n$ and Ω is a closed convex set.

This problem has many interesting applications and its solution using special techniques has been considered extensively in the literature. See [1, 31, 54, 35, 51] and references therein.

If Ω is the positive orthant of $I\!R^n$ we obtain, as particular cases, the linear and nonlinear complementarity problems, which will be denoted LCP and NCP respectively. The VIP, LCP and NCP have been formulated as equivalent optimization problems with or without constraints and also as equivalent systems of equations in $I\!R^n$ in many research papers.

Simple bounds in optimization problems were considered in detail in [13, 26, 50], where efficient algorithms are proposed. Smooth bound constrained optimization is a well developed area in practical optimization. Many useful methods exist and reliable software is available for solving large - scale problems that arise in applications. Therefore, the reformulation of the VIP as a smooth bound constrained optimization problem is particularly useful.

In all the reformulations of the VIP the solution is obtained finding a global optimizer of the equivalent optimization problem. However, global minimizers are very hard to find, especially for large - scale problems. Most efficient optimization algorithms are guaranteed to converge only to stationary points of the problem. Hence, it is necessary to establish results that relate stationary points of the equivalent optimization problems to the solutions of the VIP. Essentially, we need to find sufficient conditions on the VIP that guarantee that a stationary point of the equivalent optimization problem is a global minimizer. If the objective function of this problem is convex, the desired result holds, but it is not possible, in general, to reformulate the VIP as a convex mathematical program.

We consider the case where $F'(x)$ is not symmetric at the solution x of the VIP . If this matrix is symmetric, the VIP represents the necessary first order conditions of an optimization problem.

A necessary and sufficient condition for a vector x to be a solution of the VIP is that x solves the following optimization problem in Ω :

$$\text{Minimize}_z \ F(x)^T z \ \text{ subject } \ \text{ to } z \in \Omega \tag{2}$$

Since $F(x)$ is only known after solving the VIP, problem (2) is not useful from the practical point of view, but it gives insight on how to define merit functions that, minimized subject to bound constraints, provide us with solutions of the VIP.

In Section 2 we review a class of merit functions that inherit the differentiability of F and of the functions that define the region Ω, when this region can be characterized by a set of equalities and inequalities.

Remembering that LCP and NCP are particular cases of the VIP, these merit functions can be used for these problems. Due to the special structure of these problems the merit functions can be simplified and some assumptions on the problem data can be relaxed. Stronger results are obtained if F or g (the constraint function) are linear.

An important problem that can be cast as a smooth bound optimization problem is the minimization of a convex function subject to linear constraints and simple bounds. With this approach, neither Lagrange multipliers nor penalty parameters are necessary.

A very important question is that of the existence of solutions of the VIP and related problems. We are not going to treat this issue in this paper. An extensive analysis of this subject can be found in [35].

A relevant matter concerning the practical solution of the VIP using bound constrained optimization is the convergence of the sequences generated by the algorithms to stationary points of the optimization problems. In general, it is assumed that the level sets of the objective function are bounded. In Section 3 we discuss this property for some merit functions proposed in the literature for the VIP. Other possible strategies for generating bounded sequences are reviewed.

Other interesting problems that are not particular cases of the VIP exist, and can be considered as extensions or generalizations. These problems can also be reformulated as optimization problems and are considered in Section 4.

In Section 4 we also review how the approach studied in this work can be used as a tool for solving some integer programming, global optimization and bilevel programming problems. See [18].

Features concerning the advantages and disadvantages of different approaches for solving the VIP from the theoretical and practical view are commented throughout the paper.

In Section 5 some algorithms used for solving the problems are mentioned and a collection of numerical experiments is reviewed.

Final remarks and lines for future research are indicated in Section 6.

2 Bound Constrained Reformulations

In this section we review the merit functions used in [1, 27, 28, 29]. Theoretical and practical properties of these functions will be discussed and some smooth merit functions used by other authors will be commented [11, 25, 48, 49].

In [1] the VIP is studied for a region $\Omega \in I\!R^n$ defined by

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

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 $\bar{x} = (x_1, \ldots, x_s)^T$. The following merit function, motivated by the first order optimality conditions (KKT) of problem (2), is introduced,

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

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

where $\rho_1, \rho_2, \rho_3, p > 0$.

The smooth bound constrained minimization problem associated to the VIP is

$$\text{Minimize } f(x, y, z, u, v) \text{ subject to } \bar{x} \geq 0, y \geq 0, z \geq 0, v \geq 0. \tag{5}$$

Clearly, if p is a natural number, f inherits the differentiability properties of F and g.

Assuming a constraint qualification for Ω, a global minimizer of the merit function with zero function value exists if the first components corresponding to the x variables are a solution of the VIP. Reciprocally, any solution of the VIP can be extended to a solution of the optimization problem. If a reliable algorithm for finding global minimizers is available , we can use it to solve problem (5).

However, global minimizers are very hard to find, especially in large-scale problems. Most algorithms for bound constrained optimization are guaranteed to converge only to stationary points of the problem.

In [1] each of the next conditions are proved to be sufficient for a stationary point (x, y, z, u, v) of (5) to be a global optimizer with optimal value equal to zero and, therefore, for x to be a solution of the VIP .

(i) The matrix $F'(x) + \sum_{i=1}^m y_i \nabla^2 g_i(x)$ is positive definite in the null space of matrix A of (3). The number p in (4) is strictly greater than 1.

(ii) $F'(x) + \sum_{i=1}^m y_i \nabla^2 g_i(x)$ is positive semidefinite in the null space of matrix A and positive definite in the subspace $\{x \in I\!R^n \mid Ax = 0, \ \ \bar{x} = 0\}$. The region $\Upsilon = \{x \in I\!R^n \mid Ax = b, \bar{x} \geq 0\}$ is bounded and $p > 1$.

(iii) $F'(x) + \sum_{i=1}^m y_i \nabla^2 g_i(x)$ is positive definite in the null space of matrix A and $p = 1$. The set of vectors formed by all the rows of A, the gradients of the active constraints $\bar{x} \geq 0$ at x and all the gradients of the constraints g in the definition of Ω, is linearly independent.

(iv) $F'(x) + \sum_{i=1}^m y_i \nabla^2 g_i(x)$ is positive semidefinite in the null space of matrix A and positive definite in the subspace $\{x \in I\!R^n \mid Ax = 0, \ \ \bar{x} = 0\}$, the region $\Upsilon = \{x \in I\!R^n \mid Ax = b, \bar{x} \geq 0\}$ is bounded, $p = 1$ and the set of vectors formed by all the rows of A, the gradients of the active constraints $\bar{x} \geq 0$ at x and all the gradients of the constraints g in the definition of Ω, is linearly independent.

Due to the convexity of g, the conditions stated above hold replacing $F'(x)+\sum_{i=1}^m y_i \nabla^2 g_i(x)$ by $F'(x)$.

The condition of linear independence of *all* the gradients $\nabla g_i(x)$ in items (iii) and (iv) seems strange, since it involves, not only active constraints, but also constraints where $g_i(x) < 0$, but this happens in the very important case of complementarity problems, where $\Omega = I\!R^n_+$.

Monotonicity of F is a sufficient condition when the VIP is feasible and F and g are affine functions. See [2, 8].

The last two terms of the merit function (4) represent the slack complementarity conditions of problem (2). Instead of these terms, other authors use a term based on a class of functions $\Phi(a, b) : I\!R^2 \to I\!R$ called NCP functions such that

$$\Phi(a, b) = 0 \Leftrightarrow a \geq 0,\ b \geq 0 \text{ and } ab = 0.$$

The most popular NCP function is the Fischer-Burmeister function (FB), introduced in [23] and defined by

$$\Phi_1(a, b) = \sqrt{a^2 + b^2} - a - b. \tag{6}$$

In recent research [11] promising results for the algorithmic point of view have been proved for a merit function based on the penalized Fischer-Burmeister function (PFB),

$$\Phi_2(a, b) = \sqrt{a^2 + b^2} - a - b + \mu a_+ b_+, \tag{7}$$

where $\mu > 0$ and $a_+ = \max(0, a)$.

The merit functions based on the NCP functions mentioned above are at most of class C^1.

The linear and nonlinear complementarity problems (LCP and NCP), the nonlinear programming problem (NLP) and the KKT system are particular cases of (1). Hence, all the previous results can be applied to these problems. However, each of these problems has a specific structure that enables the achievement of stronger theoretical results.

In [27] the problem

$$\text{Minimize } f(x) \quad \text{subject to } Ax = b, \;\; x \geq 0$$

was reformulated as

$$\text{Minimize } \|\nabla f(x) + A^T\lambda - z\|^2 + (x^T z)^p \quad \text{subject to } x \geq 0, \; z \geq 0.$$

If f is strictly convex and $p > 1$, a stationary point of the bound constrained problem above provides a solution of the NLP. If the feasible set of the NLP is bounded, convexity is sufficient.

For a LCP, defined by

$$z = Mx + q, \;\; x^T z = 0, \;\; x, \; z \geq 0, \tag{8}$$

where $M \in I\!R^{n \times n}$ and $q \in I\!R^n$, similar results are obtained in [4, 28] for the following merit function

$$f(x, z) = \|Mx + q - z\|^2 + (x^T z)^2.$$

The weakest conditions for this merit function were established in [4]. The LCP has to be feasible and M must be a row-sufficient matrix. Also in [4] it is proved that, for the NCP, the sufficient condition is that F' is a row-sufficient and S-matrix.

Another important particular case of the VIP is the so called bounded variational inequality problem (BVIP), that was treated in [6]. In this case the region is a bounded box defined by $\Omega = \{x \,|a \leq x \leq b\}$. The merit function for the BVIP is

$$f(x, u, v) = \|F(x) - v + u\|^2 + \rho[(b - x)^T u)^p + (x - a)^T v)^p], \tag{9}$$

where $\rho, p > 0$. The associated minimization problem is

$$\text{Minimize } f(x, u, v) \quad \text{subject to } x \in \Omega. \tag{10}$$

A stationary point (x, u, v) of (10) provides a solution of the BVIP if $F'(x)$ is a row-sufficient matrix.

In [16] , for a merit function based on the NCP function (6), it is proved that it is sufficient for F' to be a P_0 matrix .

The mixed complementarity problem (MCP), is the VIP where the region Ω is a not necessarily bounded box. In [6, 7] this problem is reformulated as a bound constrained optimization problem with a rather different approach than the one reviewed up to this point. We will comment it in the next section.

The first smooth merit functions were introduced in [9, 30]. In [49] Moré defined a merit function for the NCP that uses the expression $\sum_{i=1}^{n}(x_i z_i)^2$ instead of $(x^T z)^2$ obtaining similar theoretical results. Also for the NCP, Mangasarian and Solodov [48], use the following merit function

$$f(x) = x^T F(x) + \frac{1}{2\alpha}[\|(-\alpha(F(x)+x)_+\|^2 - \|x\|^2$$

$$+\|(-\alpha x + F(x))_+\|^2 - \|F(x)\|^2],$$

where $\alpha > 1$ is arbitrary. The associated optimization problem is unconstrained. For more details see [25]. The merit functions based on the FB and PFB functions provide with the best theoretical results for the NCP. It is sufficient for F to be a P_0 function and the optimization problem is unconstrained. For minimizing these merit functions it may not be easy to apply general nonlinear programming algorithms because these are not C^2 funtions. In general, specific algorithms need to be designed in order to obtain good convergence results. The fact that the minimization problem is unconstrained may represent a drawback, specially for the solution of KKT systems, because some stationary points of the unconstrained problem may not be solutions of the system, hence the strategy can fail even when reformulating convex NLP. Fischer discussed this question in [24] and introduced bound constraints to avoid this undesirable feature. The merit function (4) is numerically tractable by any efficient bound constrained algorithm. We refer to [25] for an extensive discussion of the basic principles and properties of merit functions, specially for the NCP.

3 Compactification Strategies for the MCP

In this section we review the treatment given for the MCP in [6, 7] and discuss some interesting applications for the NCP and the solution of nonlinear systems of equations.

The basic idea is to reduce the MCP to a BVIP. Given a MCP where the box Ω is not necessarily bounded, a sufficiently large positive number L is chosen and a BVIP is proposed with the same function F of the MCP and a bounded box defined by

$$\Omega_{small} = \Omega \cap \{x \in I\!R^n \mid \|x\|_\infty \leq L\}$$

The result for the BVIP commented in Section 2 can be applied to this problem. The question now is whether the solution of this problem provides a solution of the original MCP. It is proved in [6] that if there exists a solution x of the original MCP such that $\|x\|_\infty < L$ and F is a *sufficient* function then any solution of the new BVIP is a solution of the original MCP. With this strategy, some assumptions on F can be relaxed. In [16] it is required for the MCP that the submatrix of F' related to the free variables at the solution is nonsingular, besides the assumption that $F'(x)$ is a P_0 matrix. The additional condition is not needed if the compactification strategy is applied to the new problem whith the merit function used in that paper but $F'(x)$ has to be a column-sufficient matrix.

For the NCP, using the merit function proposed in [4], it suffices that $F'(x)$ is a sufficient matrix, a weaker condition than monotonicity, that was shown not to be sufficient for the treatment given in that paper.

The compactification strategy can be applied to the solution of nonlinear systems. Suppose that we want to solve the nonlinear system of equations

$$F(x) = 0, \tag{11}$$

where $F : I\!R^n \to I\!R^n$ has continuous first derivatives. Usually, globally convergent algorithms for solving (11) rely on the unconstrained minimization problem

$$\text{Minimize } \|F(x)\|_2^2. \tag{12}$$

Most algorithms (for example, globalizations of Newton's method) have the property that every limit point of the iterates is stationary, that is:

$$\nabla \|F(x)\|_2^2 \equiv 2F'(x)^T F(x) = 0. \tag{13}$$

The most obvious drawbacks of this approach are:

(i) The algorithm might converge to a stationary point which is not a solution ($F'(x)$ being singular in this case).

(ii) Limit points of the generated sequence might not exist at all.

System (11) is a variational inequality problem where $\Omega = I\!R^n$, so the compactification strategy can be applied in this case and, if the function F is monotone, it is guaranteed that the difficulties mentioned above can be avoided. The issue in (ii) will be considered in the next section.

A drawback of the reduction to a BVIP is that the number of variables in the optimization problem is three times the number of variables in the original one. To overcome this disadvantage instead of a bounded box, a bounded simplex is used in [7] and, in this case, the number of variables is duplicated. This is the least possible increase in any reformulation of the MCP as a bound constrained optimization problem.

4 Merit functions and their level sets

Most efficient bound constrained optimization algorithms verify that any accumulation point of the generated sequence of approximate solutions is a stationary point of the optimization problem. Therefore, it is desirable to establish conditions under which accumulation points exist. For the problems we are discussing in this paper, the existence of these points depends basically on the merit functions . If it could be proved that the level sets of a given merit function are bounded, the existence of accumulation points would be guaranteed for the associated optimization problem. Unhappily, this is not the case for most merit functions that are currently used, unless some conditions are imposed to the original VIP. A sufficient condition in the case of the VIP is that the function F is a *uniform* P function. In [1] it is proved that this condition is sufficient for the merit function (4).

In [11] it was proved that, if for any sequence x^k in $I\!R^n$ there exists a component i of the vectors x^k such that $\limsup (x_i^k)_+ F_i(x^k)_+ = +\infty$ then the level sets of the merit function (7) are bounded. This seems to be the weakest condition on F established as far as we know for the NCP. It was proved in [6, 7] that the merit functions used in the compactification strategies discussed in the previous section have bounded level sets. The same results hold for the merit functions based on the NCP functions FB (see [5], PFB and Moré's merit function.

5 Extensions

Mangasarian and Pang introduced in [47] the extended linear complementarity problem (XLCP). Given $M, N \in I\!R^{m\times n}$ and a polyhedral set $\mathcal{C} \subset I\!R^m$, the extended linear complementarity problem associated to M, N and $\mathcal{C}$ is to find $x, y \in I\!R^n$ such that

$$Mx - Ny \in \mathcal{C}, \quad x^T y = 0, \ \ x, y \geq 0. \tag{14}$$

When $m = n$ and $\mathcal{C}$ is a single point in $I\!R^m$, this is the so called horizontal linear complementarity problem. In [3] two different representations of the polyhedral set $\mathcal{C}$ are considered. First, $\mathcal{C}$ is defined by a set of equalities and inequalities. So, without loss of generality,

$$\mathcal{C} = \{u \in I\!R^m \mid Au - b - z = 0, \quad z = (z_1^T, 0^T)^T, \ \ z_1 \in I\!R^p, z_1 \geq 0\}, \tag{15}$$

where $A \in I\!R^{\ell\times m}, b \in I\!R^{\ell}, z \equiv (z_1^T, 0^T)^T \in I\!R^{\ell}$. The other case is when the polyhedral set $\mathcal{C}$ can be defined in a parametric form, instead of the implicit form (15). In other words, $\mathcal{C}$ can be viewed as the image of a simple cone of $I\!R^s$, namely

$$\mathcal{C} = \{w \in I\!R^m \ \mid \ w = Lz + q, z = (z_1^T, z_2^T)^T, z_1 \in I\!R^{\nu}, z_1 \geq 0, z_2 \in I\!R^{s-\nu}\}. \tag{16}$$

The following bound constrained problems were proposed for the two cases:

$$\text{Minimize } (x^T y)^2 + \rho \|AMx - ANy - b - z\|^2$$

$$\text{subject to } x \geq 0,\ y \geq 0,\ z_1 \geq 0, \tag{17}$$

where $\rho > 0$ is an arbitrary constant and

$$\text{Minimize } (x^T y)^2 + \rho \|Mx - Ny - Lz - q\|^2$$

$$\text{subject to } \quad x \geq 0, y \geq 0, z_1 \geq 0. \tag{18}$$

It was proved that if the pair M, N has the *extended row- sufficiency* property with respect to the corresponding set $\mathcal{C}$, and the XLCP is feasible, any stationary point of the optimization problems mentioned above provides a solution of the XLCP. For more details, see [3].

The following bilinear program can be associated to (14):

$$\text{Minimize } x^T y \quad \text{subject to} \quad Mx - Ny \in \mathcal{C}, \quad x \geq 0, y \geq 0. \tag{19}$$

Methods for solving the horizontal linear complementarity problem based on (19) can be found, for example, in [10] and [56].

Proposition 2.2 of [47] relates stationary points of (19) to solutions of (14) when the polyhedral set is given in the form $\mathcal{C} = \{u \in I\!R^m \ \mid \ Au - b \geq 0\}$ where $A \in I\!R^{\ell \times m}$. This result, that was later generalized in [34], states that a stationary point of (19) is necessarily a solution of (14) if MN^T is copositive on the cone

$$\mathcal{R} \equiv \{v \in I\!R^m \mid v = A^T \lambda \quad \text{for some } \lambda \in I\!R^\ell_+\}.$$

From the global minimization point of view , (19) can be reduced to the minimization of a quadratic with positivity constraints. However, the conditions under which stationary points of this problem are global minimizers are stronger than the conditions required for (19).

Alternative bound constrained and unconstrained reformulations of the XLCP may be found in [53].

Another related problem, that is not a particular case of the VIP, is the so called generalized complementarity problem (GCP). It consists in finding $x \in I\!R^m$ such that

$$F(x) \in \mathcal{K}, \;\; G(x) \in \mathcal{K}^\circ, \;\; F(x)^T G(x) = 0, \tag{20}$$

where F and G are continuous functions from $I\!R^m$ to $I\!R^n$, $\mathcal{K}$ is a nonempty closed convex cone in $I\!R^n$, and $\mathcal{K}^\circ$ denotes the polar cone of $\mathcal{K}$.

In [2] the case $n = m$, $F, G \in C^1$ and $\mathcal{K}$ a polyhedral cone in R^n is considered. The cone may be defined by

$$\mathcal{K} = \{v \in I\!R^n \mid Av \geq 0, \;\; Bv = 0\}$$

and

$$\mathcal{K}^\circ = \{u \in I\!R^n \mid u = A^T\lambda_1 + B^T\lambda_2, \;\; \lambda_1 \geq 0\},$$

where $A \in I\!R^{p\times n}$ and $B \in I\!R^{s\times n}$.

The optimization problem proposed there is

$$\begin{array}{rl} \text{Minimize} & f(x, z, \lambda) \\ \text{subject to} & \left\{ \begin{array}{l} z^1 \geq 0, \\ \lambda^1 \geq 0. \end{array} \right. \end{array} \tag{21}$$

If $F, G \in C^1$, the matrix $G'(x)[F'(x)]^{-1}$ is positive definite in the null space of B and (x, λ, z) is a stationary point of (21) then, x is a solution of the GCP.

If F, G are affine functions and the GCP is feasible, a sufficient condition is that $G'F'^{-1}$ is positive semidefinite in the null space of B.

IF $\mathcal{K} = I\!R^n_+$, the sufficient condition is that $G'(x)[F'(x)]^{-1}$ is a row-sufficient S-matrix. If, in addition, F and G are affine just *row-sufficiency* is enough.

This problem is treated in [37, 45, 52, 54, 55]. In [52, 54, 55] the computation of the merit functions is difficult from the numerical point of view because it involves projections on convex sets. In [54] the same theoretical results as in [2] are obtained for a more general cone.

Using the same merit function of [45], a stronger result is obtained in [37] where the GCP is reformulated as a system of semismooth equations and an unconstrained differentiable optimization problem is given when $\mathcal{K}$ is the positive orthant. The conditions established to ensure that a stationary point x of the unconstrained minimization problem is a solution of the GCP are essentially that $F'(x)$ is nonsingular and that $D(G'(x)[F'(x)]^{-1})_{RR}D$ is an S_0-matrix, where D is a convenient nonsingular diagonal matrix and R is the set of indices for which (20) does not hold at x. This result extends the one in [45]. A trust-region method is proposed for solving the GCP based on these reformulations.

In [45] an unconstrained minimization reformulation of the GCP is considered such that the merit function is differentiable when $\mathcal{K} = I\!\!R^n_+$. The conditions that guarantee that a stationary point x of the merit function is a global minimizer are that $F'(x)$ is nonsingular and $G'(x)[F'(x)]^{-1}$ is a P_0-matrix. The authors suggest to use a first-order method for minimizing the merit function due to the fact that it is once but not twice continuously differentiable.

6 Applications

In this section we review some applications of the reformulation as smooth bound constrained optimization to other important and difficult problems of nonlinear programming.

The General Linear Complementarity Problem (GLCP) consists of finding vectors $z \in I\!\!R^n$ and $y \in I\!\!R^l$ such that

$$q + Mz + Ny \geq 0 \tag{22}$$

$$p + Rz + Sy \geq 0 \tag{23}$$

$$z \geq 0, \;\; y \geq 0, \;\; z^T(q + Mz + Ny) = 0 \tag{24}$$

where M, N, R and S are given matrices of orders $n \times n$, $n \times l$, $m \times n$ and $m \times l$ respectively and $q \in I\!\!R^n$, $p \in I\!\!R^m$ are given vectors. The GLCP has been studied by many authors as an ingredient for solving some optimization problems [32, 39, 40, 41, 42].

The GLCP can be solved in polynomial-time if M is a positive semidefinite matrix and $R = 0$ in its constraint (23) [43, 56]. This problem is denoted by PGLCP. The LCP was shown to be NP-hard when M is not a positive semidefinite matrix. See [43]. This fact motivated the search of techniques that reduce the LCP to a global optimization problem.

The following bound constrained minimization problem for the GLCP with $R = 0$ was introduced in [18]:

$$\begin{array}{lll} \text{Minimize} & f(z,y,w,v) \equiv & ||w - q - Mz - Ny||^2 + ||v - p - Sy||^2 + (\sum_{i=1}^{n}(z_i w_i)^g)^h \\ \text{subject to} & & z, w, y, v \geq 0 \end{array} \tag{25}$$

where $g, h \geq 1$ are real numbers such that $g > 1$ if $h = 1$. It was proved that a stationary problem of this NLP is a solution of the associated GLCP if the GLCP is feasible and the matrix M is *row-sufficient*.

A solution of the LCP exists if and only if the optimal value of the following bilinear programming problem (BLP) is zero.

$$\begin{array}{ll} \text{Minimize} & e^T z + q^T x + x^T(M - I)z \\ \text{subject to} & Mz \geq -q, \quad 0 \leq x \leq e \\ & z \geq 0 \end{array} \tag{26}$$

This BLP can be transformed into the following NLP [39].

$$\begin{array}{llll} \text{Minimize} & & & e^T z - e^T u \\ \text{subject to} & \begin{bmatrix} w \\ \beta \end{bmatrix} & = & \begin{bmatrix} q \\ e \end{bmatrix} + \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix} + \begin{bmatrix} M - I \\ 0 \end{bmatrix} z \\ & \alpha & = & q + Mz \\ & & & \begin{bmatrix} x \\ u \end{bmatrix}, \ z, \ \begin{bmatrix} w \\ \beta \end{bmatrix}, \ \alpha \geq 0 \\ & & & \begin{bmatrix} x \\ u \end{bmatrix}^T \begin{bmatrix} w \\ \beta \end{bmatrix} = 0 \end{array} \tag{27}$$

where the matrix corresponding to the complementary variables is positive semidefinite. We can find a solution to the LCP by computing a solution of the PGLCP with $e^T z - e^T u = 0$. If this constraint is added to the PGLCP the structure of the PGLCP is destroyed and the problem becomes NP-hard. A simple alternative used in [18] is to introduce the constraint

$$\gamma_0 = e^T z - e^T u$$

and a column with a variable $\lambda_0 \geq 0$ that is complementary to γ_0. This leads into a PGLCP.

It is proved in [18] that, if the original LCP is feasible, the PGLCP has a solution such that $\lambda_0 \leq 1$ and that if $\lambda_0 < 1$ a solution of the LCP is at hand.

This results motivated to solve the LCP by processing the PGLCP. Since the associated matrix is PSD, a solution to this PGLCP can be found by computing a stationary point of the associated nonlinear program with zero lower bounds . After finding such a point, there are two possible cases:

i) $\lambda_0 < 1$ and a solution of the LCP is obtained.

ii) $\lambda_0 = 1$ and a solution of the LCP may be available or not.

In the second case, if the term in the merit function related to the slack complementarity conditions is not zero, the stationary point obtained is not a solution of the LCP. Therefore, another stationary point of the associated nonlinear program has to be computed.

The main problem in this application is to get an initial point for the bound constrained that leads into a stationary point that is also a solution of the LCP. Recently there has been some work on the design of procedures that try to find a global minimum for an optimization problem by a clever choice of initial points. A heuristic procedure of this type has to be designed in order to fully exploit this approach for the solution of LCPs.

Mathematical programming problems with equilibrium constraints (MPEC) are nonlinear programming problems where the constraints have a form that is analogous to first-order optimality conditions of constrained optimization.

The problem is to

$$\text{Minimize } \; f(x,y)$$

subject to

$$h(x,y)=0, \;\; g(x,y)\le 0, \tag{28}$$

$$F(x,y)+[t'_y(x,y)]^T\lambda+[s'_y(x,y)]^T z=0, \tag{29}$$

$$t(x,y)=0, \tag{30}$$

$$z\ge 0, \;\; s(x,y)\le 0, \;\; z_i\;[s(x,y)]_i=0, i=1,\ldots,q, \tag{31}$$

where $[s(x,y)]_i$ is the $i-$th component of $s(x,y)$, $h(x,y)\in \mathbb{R}^{m_1}, g(x,y)\in \mathbb{R}^{\ell}$, $F(x,y)\in \mathbb{R}^m, t(x,y)\in \mathbb{R}^{m_2}, s(x,y)\in \mathbb{R}^q$ and all these functions are continuously differentiable.

The constraints (28) are called *ordinary* whereas the constraints (29,30,31) are called *equilibrium constraints*. If $F(x,y)$ is the gradient (with respect to y) of some potential function $P(x,y)$ then the equilibrium constraints are the Karush-Kuhn-Tucker (KKT) conditions of

$$\text{Minimize}_y \;\; P(x,y) \quad \text{subject to } t(x,y)=0, \; s(x,y)\le 0. \tag{32}$$

When, instead of (29,30,31), the constraints are (32), we are in presence of a *bilevel programming* problem.

Many NLP algorithms have the property that their accumulation points are stationary points of the squared norm of the residual of the constraints. Introducing slack variables $v\in \mathbb{R}^{m_2}, w\in \mathbb{R}^q$ in (29,30,31) the feasibility of the MPEC can be obtained by solving

$$\text{Minimize } \|h(x,y)\|^2+\|g(x,y)+v\|^2 \tag{33}$$

$$+\|F(x,y)+[t'_y(x,y)]^T\lambda+[s'_y(x,y)]^T z\|^2$$

$$+\|t(x,y)\|^2+\|s(x,y)+w\|^2+(\sum_{i=1}^{q}(w_i z_i)^r)^p \tag{34}$$

$$\text{subject to } v\ge 0, z\ge 0, w\ge 0. \tag{35}$$

where $r, p > 0$.

The constraints can also be written as

$$z \geq 0, \quad s(x,y) + w = 0, \quad w^T z = 0, w \geq 0, \tag{36}$$

The formulation (33) corresponds to the reformulation of nonlinear complementarity problems given in [49] and [1]. In [8] it was proved that the pair (x, y) is feasible if the following conditions hold:

(i) (x, y, v, w, λ, z) is a stationary point of (33, 34, 35);

(ii) The matrix $[F'_y(x,y)]^T + \sum_{i=1}^q [w]_i \nabla^2_{yy}[s(x,y)]_i$ is positive definite in the null-space of $t'_y(x,y)$;

(iii) $h(x,y) = 0$, $g(x,y) \leq 0$;

(iv) $t(x,y)$ is an affine function with respect to y and the functions $[s(x,y)]_i$ are convex with respect to y;

(v) There exists $\tilde{y}$ such that $t(x, \tilde{y}) = 0$;

(vi) $p \geq 1$, $r \geq 1$ and $p + r > 2$.

This result establishes sufficient conditions under which reasonable NLP algorithms find feasible points of MPEC. Very roughly speaking, the conditions "on the problem" say that the equilibrium constraints "look like" optimality conditions of a convex problem. The assumption $h(x,y) = 0, \; g(x,y) \leq 0$ has algorithmic consequences. It tells us that preserving feasibility of the ordinary constraints is important. It is not possible to guarantee feasibility of the ordinary constraints with the only assumption of stationarity of the sum of squares. Therefore, algorithms that maintain feasibility of the ordinary constraints at all the iterations should, perhaps, be preferred. When the ordinary constraints have a simple structure (for example, when they define boxes) to maintain their feasibility is simple, but the situation is different when the constraints are highly nonlinear.

The main difficulty in using ordinary NLP algorithms for solving the MPEC, is associated to the constraints (31). If $s_i(x,y) = 0$ the gradients that correspond to this active constraint and to $z_i s_i(x, y) = 0$ are linearly dependent. On the other hand, if $z_i = 0$, the gradient associated to the complementarity constraint $z_i s_i(x, y) = 0$ and the gradient associated to $z_i = 0$ are linearly dependent. Since, at any feasible point, either $z_i = 0$ or $s_i(x, y) = 0$, it turns out that the set of gradients of active constraints are linearly dependent for all the feasible points of MPEC. Many NLP algorithms depend strongly on the hypothesis of linearly independence of the gradients of active constraints, so their performance could be poor for MPEC or, perhaps, they could be inapplicable. This motivated many authors to introduce specific algorithms for solving MPEC. See [17] and references therein. All the feasible points of MPEC satisfy the Fritz-John optimality condition which, in consequence, is completely useless in this case. In [8] it was observed that many algorithms have the property of converging to points that satisfy an optimality condition (introduced in [48]) which is sharper than Fritz-John. The MPEC problem is a good example of the difference between Fritz-John and the sequential optimality condition AGP (approximate gradient projection), given in [48]. It was proved that the fulfillment of the AGP condition implies (under a "dual nondegeneracy" assumption) the fulfillment of AGP on a problem where positivity constraints are eliminated. In the new problem, not all the feasible points are Fritz-John points. As a consequence, there are good reasons to expect that the application of algorithms that converge to AGP points will behave well in MPEC problems.

If we want to use NLP algorithms for solving MPEC, we must choose a reformulation of the constraints that makes them suitable for NLP applications. In this paper the authors used straightforward reformulations that consist on squaring the complementarity constraints, maintaining the positivity of the variables. See [7, 49]. They showed that, in some situations, this reformulation is good, in the sense that stationary points of the squared violation of the constraints are, necessarily, feasible points. The same study must be done for other reformulations. Reformulations based on the Penalized-Fischer-Burmeister function are especially attractive, according to the experiments in [7, 11].

7 Numerical Experiments

In 1993, the authors of [27] were involved in the numerical comparison of bound constrained smooth solvers. With the aim of generating a family of structured and interesting problems, they considered the linear programming problem

$$\text{Minimize } c^T x \text{ subject to } Ax = b, \ x \geq 0$$

and they reformulated it in two different ways, as a box-constrained problem:

$$\text{Minimize } \|Ax - b\|^2 + \|c + A^T\pi - z\|^2 + x^T z \text{ s.t. } x \geq 0, z \geq 0 \tag{37}$$

and

$$\text{Minimize } \|Ax - b\|^2 + \|c + A^T\pi - z\|^2 + (x^T z)^2 \text{ s.t. } x \geq 0, z \geq 0. \tag{38}$$

They expected to find only local minimizers in both cases but, surprisingly, they found that the solution of (38) was always a global minimizer and, thus, a solution of the linear programming problem. This observation gave origin to the paper [27] and, thus, to the whole research that motivates this survey. Therefore, we can say that numerical experience is in the very beginning of this area of research.

In [27], the authors use the techniques discussed in Section 2 to solve the problem of finding estimators of parameters in problems that are modelled by large overdetermined linear systems of equations, subject to linear constraints and bounds on the variables.

In [28] the resolution of the LCP was tested. The motivation for the experiments presented in this paper, was to show that bound constrained optimization algorithms do not depend strongly on the conditions required for the problem in order to guarantee that stationary points are global minimizers. Various LCPs were tested such that the eigenvalues of the matrix M could be positive , zero and negative. The LCP was always succesfully solved when M was positive semidefinite and for more than 60 % of the problems that are not monotone a solution of the LCP is obtained. The efficiency of this approach is also discussed related to the performance of some classic problems found in the literature. These problems were tested for rather high dimensions considering the modest computer used. Even for problems where the matrix M is negative definite, an adjustment of the paramaters in the objective function was enough to obtain the solutions in many cases. The same was observed in tests for the HLCP.

In [29], where the VIP is treated, a comparison is made with an algorithm that uses projection-separation techniques introduced in [36]. This method relies strongly on the monotonicity required for the operator F of the VIP and this is confirmed by the numerical experiments. When F was not monotone the last algorithm always failed. This was not the case for the smooth bound constrained optimization approach. In general, the dependence of an algorithm on the problem properties should be taken in account when designing specific algorithms for complementarity and related problems if a robust algorithm is desired.

In [4] a new algorithm of the inexact-Newton type is introduced and applied to the horizontal nonlinear complementarity problem (HNLC), also introduced there. The numerical results presented intend to study the influence of dual degeneracy at the solution on the local convergence properties.

In [7] a comparison between the application of the compactification strategies to different merit functions is made with an extensive numerical experimentation.

In [2] the GCP is solved for a large number of problems and the experiments are compared with the results obtained in [37].

Finally, in [18] the package LANCELOT based on the algorithm introduced in [13] is used to solve the bound constrained optimization reformulations associated to bilinear programming problems, concave quadratic programming problems, knapsack problems and some difficult LCPs.

8 Final remarks

The main point about the reformulations of VIP-related problems analyzed here is that the associated optimization problems preserve all the smoothness of the data. Therefore, general optimization algorithms that deal well with "totally smooth" problems can be used to solve these reformulations and are probably effective. We mean not only Newton-like second derivative methods but also methods that use higher order derivatives, such as the tensor methods implemented in [12]. Usually, great effort is invested by developers of algorithms (and programmers!) in the implementation and improvement of general methods. This effort is justified by applications. To solve the reformulations studied in this survey will become even easier as far as the general smooth box-constrained technology is developed. On the other hand, reformulations that possess only first derivatives need the development of new solvers, if they are going to be competitive with Newton-like, or higher order, methods. Of course, these specific solvers could be so effective that could beat high-order solvers for completely smooth reformulations, but it is perhaps too soon to predict what is going to happen. As far as we know, all the experiments with totally smooth reformulations have been done with first-order solvers, so there is a lot of work that must still be done in practice.

It must be stressed that, as in many first-order reformulations, in the reformulations presented here, no advantage is taken from the structure of the "matrices" of data. If these matrices are highly structured, algorithms that use their structure must be much more effective. Perhaps, as so happens to occur with the solution of linear systems of equations, there is an intermediate stage of reformulations and methods, that allows one to use partially the structure, with the aim of accelerating the iterative box-solver. This "preconditioning idea" deserves future development. Preconditioning plays an important role in classical box-constrained solvers (for example, the default choice of LANCELOT includes a Hessian five-diagonal preconditioner) but we guess that some more clever and problem-oriented preconditioner could arise from the consideration of the original problem and could even have some influence in the choice of the reformulation.

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