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A feasible directions algorithm for nonlinear complementarity problems and applications in mechanics

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Abstract Complementarity problems are involved in mathematical models of several applications in engineering, economy and different branches of physics. We mention contact problems and dynamics of multiple bodies systems in solid mechanics. In this paper we present a new feasible direction algorithm for nonlinear complementarity problems. This one begins at an interior point, strictly satisfying the inequality conditions, and generates a sequence of interior points that converges to a solution of the problem. At each iteration, a feasible direction is obtained and a line search performed, looking for a new interior point with a lower value of an appropriate potential function. We prove global convergence of the present algorithm and present a theoretical study about the asymptotic convergence. Results obtained with several numerical test problems, and also application in mechanics, are described and compared with other well known techniques. All the examples were solved very efficiently with the present algorithm, employing always the same set of parameters.

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1 Introduction

We consider the nonlinear complementarity problem, (NCP):
Find $x \in \Re^n$ such that

$$x \geq 0, \;\; F(x) \geq 0 \text{ and } x^t F(x) = 0, \tag{1}$$

where $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$, is continuously differentiable.

Let be $\Omega := \{x \in \mathbb{R}^n | x \geq 0 \,,\, F(x) \geq 0\}$ the feasible set and Ω^0, the interior of Ω.

Several mathematical models in different disciplines, like engineering, physics and economics, lead to complementarity problems. This is the case of static and dynamic contact in solid mechanics, where there is a complementarity condition between the contact forces and the gap, see Christensen et al. (1998), Petersson (1995) and Tanoh et al. (2004). Limit Analysis and Plasticity models can also include a complementarity condition, see Zouain et al. (1993) and Tin-Loi (1999b). When this kind of mechanical models are employed for structural optimization, several authors employ mathematical programming problems with equilibrium constraints, MPEC, as in Tin-Loi (1999a). Models for free boundary problems can also involve complementarity conditions, see Leontiev et al. (2002). Optimality conditions of classical constrained optimization problems as well as bi-level programs, (Herskovits et al. 2000), or Nash-Cournot equilibrium include a complementarity condition. Further applications of complementarity problems are described in Ferris and Pang (1997).

The NCP can be also written as follows:

Find $x \in \mathbb{R}^n$ such that $x \geq 0$, $F(x) \geq 0$ and

$$x \bullet F(x) \equiv \begin{pmatrix} x_1 F_1(x) \\ \cdot \\ \cdot \\ \cdot \\ x_n F_n(x) \end{pmatrix} = \begin{pmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix}, \tag{2}$$

where $x \bullet F(x)$ represents a Hadamard product.

Considerable research effort was devoted by mathematicians and engineers to solve this problem, looking for robust and efficient techniques for real engineering applications. By employing an appropriate merit or potential function, the NCP can be solved employing unconstrained minimization techniques. However, this approach generally involves non-smooth functions. Another drawback is that the iterates can converge to a local minima of the potential function. See Mangasarian and Solodov (1993), Yamashita and Fukushima (1995), Geiger and Kanzow (1996), Kanzow (1996), Jiang and Qi (1997).

The so called NCP functions, $\psi : \mathbb{R}^2 \to \mathbb{R}$, are such that $\psi(a, b) = 0$ implies $a \geq 0, b \geq 0$ and $ab = 0$. Then, a solution of the NCP can be obtained by solving the following nonlinear system of equations in $\mathbb{R}^n$:

$$\begin{pmatrix} \psi(x_1, F_1(x)) \\ \cdot \\ \cdot \\ \cdot \\ \psi(x_n, F_n(x)) \end{pmatrix} = \begin{pmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix}. \tag{3}$$

Several numerical techniques to solve (3), with different NCP functions, were proposed. We mention Mangasarian (1973), Subramanian (1993), Kanzow (1994) and Chen and Mangasarian (1996).

The largely employed Fischer-Burmeister NCP function, (Fischer 1992) is defined as follows:

$$\psi_{FB}(a, b) = \sqrt{a^2 + b^2} - a - b \ .$$

However, this function is nonsmooth and requires special techniques to solve the nonlinear system, (Qi and Sun 1998).

The following potential function is derived from Fisher-Burmeister NCP function.

$$\phi_{FB}(x) = \frac{1}{2} \sum_{i=1}^{n} \psi_{FB}(x_i, F_i(x))^2.$$

This function has not derivatives at degenerated points. That is, when $x_i = 0$ and $F_i(x) = 0$ for some index i.

Another approach is based on interior point algorithms for nonlinear optimization, as path following methods and primal-dual interior point algorithms. See Ferris and Kanzow (2002), Wright (1997) and Tseng (1997).

Our approach is based on the iterative solution of the nonlinear system (2), without need of employing a NCP function. Given an initial feasible point, the present algorithm generates a sequence of feasible points such that the potential function

$$\phi(x) \equiv x^t F(x)$$

is reduced at each iteration. At each iteration a search direction is computed. This one is a descent direction with respect to the potential function and a feasible direction of the problem. A line search procedure ensures that the new point is in fact feasible and the potential lower. To define the search direction we employ some ideas proposed in Herskovits (1982, 1986) and also employed in the Feasible Direction Interior Point Algorithm for nonlinear optimization, FDIPA, described in Herskovits (1998).

As we know, there are not other strictly feasible techniques for NCPs. Feasibility is a requirement in several applications involving function that are not defined at infeasible points. Since all the points satisfy the constraints, it is not necessary to check feasibility for stopping the iterations.

These advantages are also relevant when employing feasible directions algorithms for constraint optimization in engineering applications, see Arora (2004), Herskovits et al. (2005) and Vanderplaats (1999).

The present technique is not based on the transformation of the complementarity problem in a constrained optimization problem, solved with a feasible directions technique, but it is a numerical technique that solves directly the complementarity problem without modifications. Our potential function is merely a measure of the error of (2).

We prove global convergence of the present method to a solution of the complementary problem as well as local superlinear convergence. Making stronger assumptions, quadratic asymptotic convergence is also proved.

We describe the numerical results obtained with several test problems and also two applications in mechanics, the contact analysis of an elastic membrane and a free boundary problem in a porous media. Even if all the points given by the present algorithm are strictly feasible, the problems are solved very efficiently when compared with other techniques. Our approach is also very robust, since a solution is always found with the same set of parameters.

In several applications, an initial feasible point can be found from the physics of the problem. When this is not the case, our suggestion consists on solving and auxiliary optimization problem as in Herskovits et al. (2005).

In the next section we give some preliminary concepts about nonlinear optimization and complementarity problems. The basic ideas of our approach are discussed in the subsequent section and a new algorithm is then defined. In Section 5, we prove global convergence, under an appropriate set of assumptions. Asymptotic convergence is studied in Section 6. Our numerical results with a set of test examples and with applications in mechanics are described in session 7. Finally we present our conclusions about the present approach.

2 Preliminary concepts

We introduce now the following definitions:

Definition 1 The vector $d \in \mathbb{R}^n$ is a **feasible direction** at $x \in \Omega$, if for some $\theta > 0$ we have $x + td \in \Omega$ for all $t \in [0, \theta]$.

Note that any vector is a feasible direction at $x \in \Omega^0$.

Definition 2 A vector field $d(x) \in \mathbb{R}^n$, with $x \in \Omega$, is a **uniformly feasible directions field** if for some $\Theta > 0$ and for any point $x \in \Omega$ we have $x + td(x) \in \Omega$ for all $t \in [0, \Theta]$.

Thus, a feasible direction d contains a non null feasible segment $[x; x + \theta(x)d]$, where θ depends on x. Definition 2 is more restrictive, since requires the existence of $\Theta > 0$ such that $\theta(x) \geq \Theta$ in Ω.

Definition 3 A vector $d \in \mathbb{R}^n$ is a Descent Direction of a real function ϕ at $x \in \mathbb{R}^n$ if there exists $\delta > 0$ such that $\phi(x + td) < \phi(x)$ for any $t \in (0, \delta)$.

The following propositions give conditions to check if a search direction is descent and feasible, see Bazaraa and Shetty (1979).

Proposition 1 *If ϕ is differentiable at x and $d \in \mathbb{R}^n$ such that $d^t \nabla \phi(x) < 0$, then d is a descent direction of ϕ.*

Proposition 2 *Let $d \in \mathbb{R}^n$ and $x \in \Omega$. If d satisfies the conditions:*

a) *$d_i > 0$ for all i such that $x_i = 0$ and*
b) *$d^t \nabla F_i(x) > 0$ for all i such that $F_i(x) = 0$,*

then d is a feasible direction of the NCP, at x.

3 Basic ideas of the present approach

We discuss now the basic ideas involved in the present technic. Let us consider the nonlinear system of equations (2). We have that

$$\nabla[x \bullet F(x)] = diag[F(x)] + diag(x)\nabla F(x) \tag{4}$$

where, given $v \in \mathbb{R}^n$, $diag(v) \in \mathbb{R}^{n \times n}$ is a diagonal matrix such that $diag(v)_{ii} \equiv v_i$ and the i-th row of $\nabla F(x)$ is $\nabla F_i(x)$.

A Newton - Raphson iteration to solve (2) is given by the following expression:

$$\left[diag\left(F\left(x^k\right)\right) + diag\left(x^k\right)\nabla F\left(x^k\right)\right]\left[x^{k+1} - x^k\right] = -x^k \bullet F\left(x^k\right).$$

Instead of taking x^{k+1} computed above, we define a search direction as $d_1^k = [x^{k+1} - x^k]$. Then, we have

$$\left[diag\left(F\left(x^k\right)\right) + diag\left(x^k\right)\nabla F\left(x^k\right)\right] d_1^k = -x^k \bullet F\left(x^k\right). \tag{5}$$

It is shown later that d_1^k is a descent direction of the potential function. However, d_1^k cannot be taken as a search direction of the present algorithm, since it is not always a feasible direction. In effect, it follows from (5) that $d_{1i}^k = 0$ when $x_i^k = 0$ and $d_1^{k^t}\nabla F_j(x^k) = 0$ when $F_j(x^k) = 0$. Then, the assumptions of Proposition 2 are not true at the boundary of Ω and $\theta = 0$ in Definition 1. Near the boundary θ will be very small.

Adding positive numbers in the right side of (5), we have the following linear system:

$$\left[diag\left(F\left(x^k\right)\right) + diag\left(x^k\right)\nabla F\left(x^k\right)\right] d^k = -x^k \bullet F\left(x^k\right) + \rho^k E,$$

where $\rho^k > 0$ and $E \equiv [1, 1, ..., 1]^t$, $E \in \mathbb{R}^n$.

If d^k is uniquely determined, it follows from Proposition 2 that d^k is a feasible direction. In effect,

i) When $x_i^k = 0$, it is $d_i^k = \frac{\rho^k}{F_i(x^k)} > 0$.
ii) When $F_i(x^k) = 0$, it is $\nabla F_i(x^k) d^k = \frac{\rho^k}{x_i^k} > 0$.

The vector d^k is then a perturbation of d_1^k proportional to ρ^k. As d_1^k is a descent direction, imposing convenient bounds on ρ^k, it is possible to ensure that d^k is a descent direction also.

In effect, since d_1 is a descent direction, we have that $d_1^{k^t} \nabla\phi(x^k) < 0$. We prove later that, taking $\rho^k \in \left(0, \frac{\phi(x^k)}{n}\right)$, it is

$$\nabla\phi\left(x^k\right)^t d^k = \left[1 - \frac{\rho^k n}{\phi\left(x^k\right)}\right] \nabla\phi\left(x^k\right)^t d_1^k < 0,$$

where $1 - \frac{\rho^k n}{\phi(x^k)} > 0$.

A new iterate is then obtained by performing an inexact line search procedure that looks for a new feasible point with a sufficient reduction of the potential function $\phi(x)$. We employ an extension of Armijo's line search that deals with inequality constraints, proposed by Herskovits (1986).

Line search procedures based on Wolfe's or Goldstein's inexact line search criteria can also be employed, (Bazaraa and Shetty 1979; Herskovits 1995, 1998). These are more efficient in practise.

The present iterations were obtained by introducing a perturbation in Newton's algorithm, that has quadratic rate of convergence. Then, working with a smaller perturbation will result in a faster convergence. Near a solution, we take $\rho^k = O(\phi^\beta(x^k))$ and discuss the cases, when $\beta \in (1, 2)$ and $\beta = 2$.

The numerical algorithm presented here requires an initial feasible point. In several applications, this point can be found from the physics of the problem. When this is not the case, a feasible point can be found with the help of the auxiliary mathematical program

$$\begin{aligned} &\max_{(x,z)} z \\ &\text{s. t. } F(x) \geq z, \\ &\qquad x \geq 0, \end{aligned} \tag{6}$$

where $z \in \mathbb{R}$ is an auxiliary variable. Solving this problem with a nonlinear programming algorithm, a feasible point is obtained once z becomes positive and the constraints are satisfied. If $F(x)$ is convex and the feasible region of (6) is not empty, the auxiliary problem has an unique solution.

4 FDA_NCP: feasible directions algorithm for NCP

The present algorithm is stated as follows:

Parameters:

$c > 0$, α, η, ν $\in (0, 1)$, $\beta \in (1, 2]$ and $\rho_0 < \alpha \min\{1, 1/(c^{\beta-1})\}$.

Initial Data: $x^0 \in \Omega^0$ such that $\phi(x^0) < c$ and $k = 0$.

Step 1 Calculation of the search direction.

Compute d^k by solving:

$$\begin{aligned} &\left[diag\left(F\left(x^k\right)\right) + diag\left(x^k\right) \nabla F\left(x^k\right)\right] d^k \\ &\quad = -x^k \bullet F\left(x^k\right) + \rho^k E, \end{aligned} \tag{7}$$

where $\rho^k = \rho^0 \left[\frac{\phi^\beta(x^k)}{n}\right]$.

Step 2 Line search.

Compute t^k, the first number of the sequence $\{1, \nu, \nu^2, ...\}$ satisfying

$$x^k + t^k d^k > 0 \tag{8}$$

$$F\left(x^k + t^k d^k\right) > 0 \tag{9}$$

$$\phi\left(x^k + t^k d^k\right) < \phi\left(x^k\right) + t^k \eta \nabla\phi\left(x^k\right)^t d^k \tag{10}$$

Step 3 Updates.

Set $x^{k+1} := x^k + t^k d^k$ and $k := k + 1$.

Go back to Step 1.

The present algorithm is very simple to implement and requires a computer effort similar to that of Newton method for nonlinear systems of equations.

In Fig. 1. we represent the Newton direction d_N^k and the search direction d^k at a point on the boundary of the feasible domain. In order to illustrate better the present algorithm, we include d_R^k, that restores feasibility, even if it is not explicitly computed.

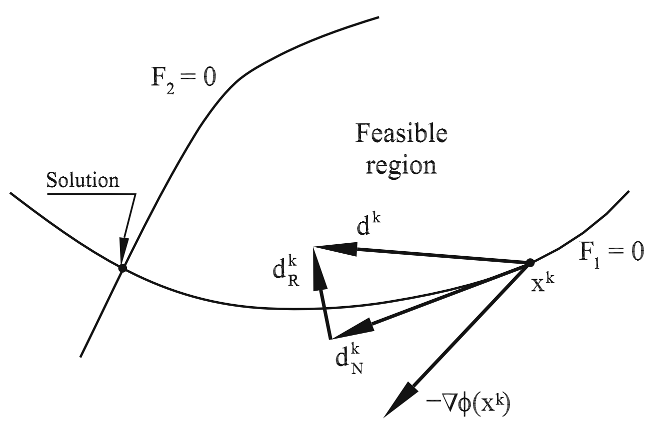

Fig. 1 Representation of directions

5 Study of global convergence

In this section we define a set of assumptions about the NCP and prove global convergence to a solution of the problem.

Assumption 1 The set

$$\Omega_c \equiv \{x \in \Omega | \phi(x) \leq c\},\ c > 0$$

is a compact set and has an interior Ω_c^0. Each $x \in \Omega_c^0$ satisfies $x > 0$ and $F(x) > 0$.

Assumption 2 The function $F(x)$ is continuously differentiable and $\nabla F(x)$ satisfies Lipschitz condition

$$\|\nabla F(y) - \nabla F(x)\| \leq \gamma_0 \|y - x\|,$$

for any $x, y \in \Omega_c$, where γ_0 is a positive real number.

Assumption 3 The matrix

$$diag(F(x)) + diag(x)\nabla F(x)$$

has an inverse in Ω_c.

The last assumption implies that x and $F(x)$ are not zero simultaneously for $x \in \Omega_c$. We also have that the linear system (7) has always a solution.

Since $\nabla F(x)$ is continuous, we have that the matrix in the last assumption has a continuous inverse in Ω_c. Thus, there exists a scalar $\kappa > 0$ such that

$$\|[diag(F(x)) + diag(x)\nabla F(x)]^{-1}\| \leq \kappa \tag{11}$$

for any $x \in \Omega_c$.

The following results prove that the search direction of the present algorithm is bounded, is a descent direction and constitutes an uniformly feasible directions field. These are valid for $\beta \in [1, 2]$.

Lemma 1 *For any $x^k \in \Omega_c$, the search direction d^k satisfies*

$$\|d^k\| \leq \kappa\phi(x^k). \tag{12}$$

Proof Let be $x^k \in \Omega_c$. We have,

$$\left\|-x^k \bullet F\left(x^k\right) + \rho^k E\right\|^2 = \left\|x^k \bullet F\left(x^k\right)\right\|^2 - 2\rho^k\phi\left(x^k\right) + n\left(\rho^k\right)^2.$$

Since $\left\|x^k \bullet F(x^k)\right\|^2 \leq \phi^2(x^k)$, we deduce

$$\left\|-x^k \bullet F(x^k) + \rho^k E\right\|^2 \leq (n-1)(\rho^k)^2 + (\phi(x^k) - \rho^k)^2.$$

From the definition of ρ^k given in the algorithm, we have $\rho^k \leq \frac{\phi(x^k)}{n}$. Then, we conclude that

$$\left\|-x^k \bullet F(x^k) + \rho^k E\right\| \leq \phi\left(x^k\right). \tag{13}$$

Considering now (7) and (11), we obtain the following bounds on $\|d^k\|$:

$$\left\|d^k\right\| \leq \kappa\left\| - x^k \bullet F\left(x^k\right) + \rho^k E\right\|. \tag{14}$$

Thus, the result follows from (13) and (14). □

As a consequence of the previous lemma, we deduce that

$$\|d^k\| \leq \kappa c. \tag{15}$$

Lemma 2 *The search direction d^k is a descent direction for $\phi(x)$ at any $x^k \in \Omega_c$ such that $\phi(x^k) > 0$.*

Proof We have that

$$\nabla\phi\left(x^k\right)^t = E^t\left[diag\left(F\left(x^k\right)\right) + diag\left(x^k\right)\nabla F\left(x^k\right)\right].$$

Then, it follows from (5) and (7) that

$$\nabla\phi\left(x^k\right)^t d_1^k = -\phi\left(x^k\right)$$

and

$$\nabla\phi^t\left(x^k\right) d^k = -\phi\left(x^k\right) + n\rho^k.$$

In consequence,

$$\nabla\phi^t\left(x^k\right) d^k = \left(1 - \frac{\rho^k n}{\phi\left(x^k\right)}\right)\nabla\phi^t(x^k)d_1^k < 0.$$

The result follows from Proposition 1. □

Lemma 3 *The search direction d^k, given by the present algorithm, constitutes a uniformly feasible directions field of the problem for $x^k \in \Omega_c$.*

Proof It follows from Assumption 2 that $\nabla(x \bullet F(x))$ satisfies Lipschitz condition in Ω_c. Let be γ a positive real number such that

$$\left\|\nabla(y \bullet F(y))_i - \nabla(x \bullet F(x))_i\right\| \leq \gamma\left\|y - x\right\|$$

for all $x, y \in \Omega_c$.

Let be $x^k \in \Omega_c$ and θ such that $[x^k, x^k + \tau d^k] \subset \Omega_c$ for $\tau \in [0, \theta]$. If follows from the Mean Value Theorem that

$$\left[\left(x^k + \tau d^k\right) \bullet F\left(x^k + \tau d^k\right)\right]_i \geq \left[x^k \bullet F\left(x^k\right)\right]_i$$
$$+ \tau\nabla\left[x^k \bullet F(x^k)\right]_i^t d^k - \tau^2\gamma\|d^k\|^2$$

for any $\tau \in [0, \theta]$ and $i = 1, 2, ..., n$. Since

$$\nabla\left[x^k \bullet F\left(x^k\right)\right]_i^t d^k = -\left[x^k \bullet F\left(x^k\right)\right]_i + \rho^k \tag{16}$$

it is

$$\left[\left(x^k+\tau d^k\right)\bullet F\left(x^k+\tau d^k\right)\right]_i \geq (1-\tau)\left[x^k\bullet F\left(x^k\right)\right]_i + \left(\rho^k-\tau\gamma\|d^k\|^2\right)\tau.$$

Then, for $\tau \leq \min\left\{1, \frac{\rho^k}{\gamma\|d^k\|^2}\right\}$, it is

$$\left[\left(x^k+\tau d^k\right)\bullet F\left(x^k+\tau d^k\right)\right]_i \geq 0$$

for $i = 1, 2, ..., n$. Considering now (15), for ρ^k defined in the algorithm, we have that the previous inequality is also true for

$$\tau \leq \min\left\{1, \frac{\rho_0}{\gamma n\kappa^2}\phi^{\beta-2}\left(x^k\right)\right\}. \tag{17}$$

Since $\beta \leq 2$, the present lemma is valid for

$$\theta = \min\left\{1, \frac{\rho^0 c^{\beta-2}}{\gamma n\kappa^2}\right\}.$$

□

Lemma 4 *There exists $\zeta > 0$ such that, for $x^k \in \Omega_c$, condition (10) is satisfied for any $t^k \in [0, \zeta]$.*

Proof Let be $t^k \in (0, \theta]$, where θ was obtained in the previous lemma. Applying the Mean Value theorem for $i = 1, 2, ..., n$ and do $x^{k+1} = x^k + t^k d^k$, we have

$$\left[x^{k+1}\bullet F\left(x^{k+1}\right)\right]_i \leq \left[x^k\bullet F\left(x^k\right)\right]_i + t^k\nabla\left[x^k\bullet F\left(x^k\right)\right]_i^t d^k + t^{k^2}\gamma\|d^k\|^2.$$

Summing the previous n inequalities and considering (16), we get:

$$\phi(x^{k+1}) \leq \left[1-\left(1-\frac{\rho^k n}{\phi\left(x^k\right)}\right)t^k\right]\phi(x^k) + nt^{k^2}\gamma\left\|d^k\right\|^2.$$

Then, if

$$\left[1-\left(1-\frac{\rho^k n}{\phi(x^k)}\right)t^k\right]\phi\left(x^k\right) + nt^{k^2}\gamma\|d^k\|^2 \leq \left[1-t^k\eta\left(1-\frac{\rho^k n}{\phi\left(x^k\right)}\right)\right]\phi(x^k)$$

is true, (10) is satisfied. Thus, it is enough to have

$$t^k \leq \frac{(1-\eta)\left(1-\frac{\rho^k n}{\phi(x^k)}\right)\phi\left(x^k\right)}{\gamma n\|d^k\|^2}.$$

As in the previous lemma, we get

$$t^k \leq (1-\eta)\left(1-\rho_0\phi^{\beta-1}\left(x^k\right)\right)\frac{\phi\left(x^k\right)^{-1}}{\gamma n\kappa^2}. \tag{18}$$

Then, the present lemma is true for

$$\zeta = \inf\left\{\frac{(1-\eta)\left(1-\rho^0 c^{\beta-1}\right)}{\gamma n\kappa^2 c}, \theta\right\},$$

where θ was obtained in Lemma 3. □

As a consequence of the two previous lemmas, we deduce that the number of steps required by Armijo's line search included in Step 2) of the algorithm is finite and bounded above. The following theorem proves global convergence of the present algorithm to a solution of the complementarity problem.

Theorem 1 *Given an initial feasible point, $x^0 \in \Omega_c$, the sequence $\{x^k\}$ generated by the present algorithm converges to x^*, a solution of problem (1).*

Proof It follows from the previous results that $x^k \in \Omega_c$ for $k = 1, 2, 3....$ Since Ω_c is a compact, $\{x^k\}$ has accumulation points in Ω_c. Let x^* be an accumulation point. Since the step length is always positive, we deduce that $\|d^k\| \to 0$. Considering (7), we deduce that $\{\phi(x^k)\} \to 0$. Thus, x^* is a solution of the problem. □

6 Study of asymptotic convergence

The search direction of the present algorithm is a perturbation of Newton's iteration for nonlinear systems of equations. Including a line search, Newton's method has quadratic convergence, provided that the step-length goes to one, (Dennis and Schnabel 1996). It is natural to expect better rates of convergence of our algorithm for smaller values of ρ^k.

As in Maratos effect, encountered in nonlinear constrained optimization, we cannot ensure that a unitary step-length is always obtained, see Herskovits and Santos (1998), Herskovits et al. (2005). In the present case, taking smaller values for ρ^k increases de possibility of having this effect.

Theorem 2 *Consider the sequence $\{x^k\}$ generated by the present algorithm that converges to a solution x^* of (1). Then,*

(i) *Taking $\beta \in (1, 2)$, then $t^k = 1$ for k large enough and the rate of convergence of the present algorithm is at least superlinear.*
(ii) *If $t^k = 1$ for k large enough and $\beta = 2$, then the rate of convergence is quadratic.*

Table 1 Test problems

No	Problems	n
1	Kojima-Josephy	4
2	Kojima-Shindo's	4
3	Nash-Cournot (Harker's)	5
4	Nash-Cournot (Harker's)	10
5	Nash-Cournot (Pang and Murphy's)	5
6	Nash-Cournot (Pang and Murphy's)	10
7	Mathiesen Modified	4
8	PNL Kanzow	5
9	PNL HS - 34	8
10	PNL HS - 35	4
11	PNL HS - 66	8
12	PNL HS - 76	7
13	NCP - 01	3
14	NCP - 02	3
15	NCP - 03	4
16	Chen and Ye	3

Proof Considering Theorem 1, we deduce from (17) and (18) that for k large enough, the step length obtained with Armijo's line search is $t^k = 1$.

Standard Newtons's method analysis procedures can be used to show that

$$\|x^{k+1} - x^*\| \leq \left(1 - t^k\right) \|x^k - x^*\| + \frac{\kappa \rho_0 \phi^\beta \left(x^k\right)}{\sqrt{n}} + O\left(\|x^k - x^*\|^2\right), \tag{19}$$

see Dennis and Schnabel (1996), for example.

It follows from the mean value theorem and Lipschitz condition that

$$\phi^\beta(y) \leq \phi^\beta(x) + \phi^{\beta-1}(\overline{x})\beta\sqrt{n}\, O(\|y - x\|),$$

where $\overline{x} = x + \epsilon(y - x)$ for some $\varepsilon \in (0, 1)$. Taking $x = x^*$, for all $y = x^k$ sufficiently near x^* it is

$$\phi^\beta\left(x^k\right) \leq \phi^{\beta-1}(\overline{x})\beta\sqrt{n}\, O\left(\|x^k - x^*\|\right).$$

(i) Then, for $\beta \in (1, 2)$, $\phi^\beta(x^k) = o(\|x^k - x^*\|)$. By substitution in (19) we get

$$\lim_{k\to\infty} \frac{\|x^{k+1} - x^*\|}{\|x^k - x^*\|} = 0.$$

Thus, the rate of convergence is superlinear.

(ii) The result for $\beta = 2$ is obtained in a similar way. □

Introducing a line search along an arc, as in (Herskovits and Santos 1998; Herskovits et al. 2005), it seems possible to avoid Maratos effect, even in the case when $\beta = 2$.

7 Numerical study

To study the numerical behavior of the present algorithm in practical applications we solve a set of test problems largely employed in mathematical programming literature.

Two applications in Mechanics are also solved. The first one is the solution of a numerical model of a

Table 2 Iterations

Alg	NCP-FDA				FB	
β	1.1		2		-	
Problem	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
1	13	0	8	0	6	11
2	1001	25683	21	47 ⋆	6	6
3	17	0	12	0	7	12
4	21	0	16	0	10	42
5	15	0	10	1	4	0
6	18	0	15	2	6	1
7	11	7	9	12	5	42
8	142	0	141	0	*	*
9	21	39	371	5152 ⋆	9	57
10	13	0	16	12 ⋆	8	62
11	17	16	147	1407 ⋆	29	711
12	12	1	15	13 ⋆	6	18
13	16	0	11	0	6	2
14	21	0	20	0	6	2
15	22	0	21	0	7	17
16	11	0	6	0	5	1

Table 3 Iterations for problem 17

Alg	NCP-FDA				FB	
β	1.1		2		-	
n	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
8	12	0	7	0	5	2
16	12	0	7	0	5	2
32	13	0	8	0	6	1
64	13	0	8	0	6	1
128	14	0	10	2	6	1
256	14	0	9	0	6	1
512	15	0	11	2	6	1
1024	15	0	10	0	6	1
2048	16	0	12	2	6	1

Table 5 Iterations for problem 19

Alg	NCP-FDA				FB	
β	1.1		2		-	
n	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
8	15	1	10	1	4	0
16	16	3	12	3	4	0
32	18	6	13	6	4	0
64	20	8	15	8	4	0
128	21	11	12	11	4	0
256	23	14	13	14	4	0
512	24	17	15	17	4	0
1024	26	20	16	20	4	0
2048	27	24	17	24	4	0

membrane with contact and, the second one, of a dam with percolation. In both application the usual notation in each of the corresponding disciplines is employed.

We take $\rho_0 = \alpha \min[1, \phi^{\beta-1}(x^k)]$ in the numerical implementation. In this way, extremely large deflections are avoided far of the solution and ρ_0 is constant when $\phi(x^k)$ is small. We study two cases, for $\beta = 1.1$ and $\beta = 2$, and take $\alpha = 0.25$, $\eta = 0.4$ and $\nu = 0.8$.

Our technique is compared with the algorithm described in Jiang and Qi (1997) which uses Newton iterations to solve (3) for $\Psi(a, b) = \Psi_{FB}(a, b)$. An Armijo's line search with $\phi_{FB}(x)$ as potential is included.

The present algorithm stops when $\phi(x^k) < 10^{-8}$, for all the examples. Employing Fischer-Burmeister function, feasibility must be also checked. A solution is accepted when $\phi(x^k) < 10^{-8}$ and $x_i^k > -10^{-8}$ and $F_i(x^k) > -10^{-8}$, for $i = 1, 2, ..., n$. The iterations required to solve the problems with the stopping criteria previously defined are presented in the corresponding tables, where "NCP-FDA" refers to the present method and "FB", to Newton iteration with Armijo's line search employed to minimize Fischer-Burmeister function. "Iter" represents the main iterations to solve the problem for the given stopping criteria and "Iter LS", the total number of extra function evaluations required by Armijo's line search. The symbol * indicates that convergence was not obtained and $\star$, that the unitary step length was not attained.

7.1 A collection of test problems

Problems 1 to 16 are listed in Table 1 , where n is the number of variables. The problems 1 to 9, 11 and 13 to 15 are NCPs, while problems 10, 12 and 16 are linear. Kojima-Josephy problem (Yamashita et al. 2004) has an unique nondegenerate solution. Kojima-Shindo's problem (Geiger and Kanzow 1996) has two solutions, one of them is degenerate. Nash-Cournot problems (Harker 1988; Murphy et al. 1982) have a single nondegenerate solution. Mathiesen modified (Jiang and Qi 1997) and Chen-Ye problems (Chen and Ye 2000) have several nondegenerate solutions. PNL Kanzow

Table 4 Iterations for problem 18

Alg	NCP-FDA				FB	
β	1.1		2		-	
n	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
8	13	0	8	0	4	0
16	15	0	10	0	5	0
32	17	0	12	0	5	0
64	20	1	15	2	5	0
128	22	4	17	5	5	0
256	24	7	20	9	5	0
512	26	10	22	12	5	0
1024	28	13	24	15	5	0
2048	30	16	27	19	5	0

Table 6 Iterations for problem 20

Alg	NCP-FDA				FB	
β	1.1		2		-	
n	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
8	17	0	14	0	7	16
16	20	0	16	0	7	29
32	23	0	19	0	8	54
64	25	0	22	0	10	122
128	28	0	24	0	9	77
256	30	1	27	1	15	334
512	33	1	30	1	7	39
1024	35	1	32	1	12	232
2048	38	2	35	2	10	139

Table 7 Iterations for the membrane in contact – obstacle ψ_1

Alg	NCP-FDA				FB	
β	1.1		2		-	
n	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
625	18	7	21	24	9	12
2500	20	19	24	41	11	42
5625	22	25	26	51	15	138
10000	24	47	29	76	19	202
15625	26	57	30	86	26	364
22500	27	64	32	100	35	363
30625	28	70	32	104	40	515

(Jiang and Qi 1997) has one degenerate solution. The examples 9 to 12 are Nonlinear Programs written as Complementarity Problems, (Hock and Schittkowski 1981). $F(x)$ in problems 13 to 15, (Yamashita et al. 2004), is monotone. Problems 14 and 15 has an unique degenerate solution.

For the results shown in Table 2, the initial points are the same as in the corresponding references. When this point is not feasible, a feasible initial point is obtained solving the auxiliary problem (6) with FAIPA, the Feasible Arc Interior Point Algorithm.

The iterations for Problem 2 described in Table 2 converge to a degenerate solution and the result with FB Function is better than with the present algorithm. However, making experiments with 1000 feasible initial points randomly obtained, FDA-NCP converged in all the cases while, with FB Function, convergence was not obtained for about 8% of the tests. In a similar study with Problem 1, it was observed 100% of convergence with the present algorithm and only 72% with FB function.

We present now the results for different values of n, with four sets of linear complementarity problems having $\nabla F(x)$ symmetric and positive definite. In consequence, $F(x)$ is monotonic and the solution is unique.

The initial point for Problem 17 (Geiger and Kanzow 1996), Problem 19 (Murty 1988; Xu 2000) and Problem 20 (Fathi 1979; Xu 2000) is $x^0 = [1, 1, ...1]$, $x^0 \in R^n$. For Problem 18 the initial point is $x^0 = [n, n-1, ...1]$. Tables 3, 4, 5, and 6 describe the iterations required by both techniques for different dimensions n. Problems 17–19 are very well conditioned, and the results are better with Fischer-Burmeister NCP function than with our approach. However, the number of iterations required with NCP-FDA remains almost unchanged for a larger dimension or a worst conditioning of the problem.

7.2 Two dimensions membrane in contact

We consider an elastic membrane subject to a vertical distributed loading with the boundary fixed and constrained to lie on one side of a rigid obstacle. Let Ω denote the open bounded set in $\mathbb{R}^2$ occupied by the undisturbed membrane, whose boundary is $\partial\Omega$. We call $f(x, y)$ the loading, $u(x, y)$ the transverse displacements of the membrane and $\psi(x, y)$ the shape of the obstacle, all these functions are defined in Ω. The fixed boundary is represented by $g(x, y)$, defined on $\partial\Omega$.The subsets in Ω with contact and without contact are designated by Ω^0 and Ω^+ respectively.

Table 8 Iterations for the membrane in contact - obstacle ψ_2

Alg	NCP-FDA				FB	
β	1.1		2		-	
n	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
625	13	3	16	15	8	16
2500	13	3	17	18	10	47
5625	13	5	17	20	12	82
10000	14	6	18	22	16	123
15625	14	6	18	24	16	141
22500	15	8	18	24	21	257
30625	24	7	19	27	22	314

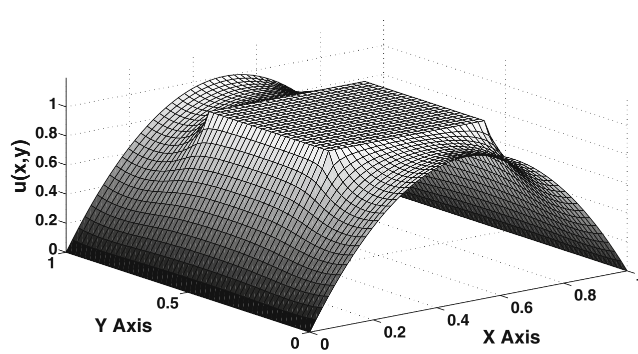

Fig. 2 Membrane shape for a 52 × 52 mesh - obstacle ψ_1

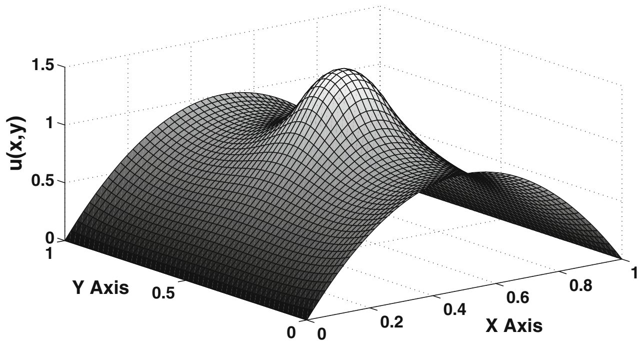

Fig. 3 Membrane shape for a 52 × 52 mesh - obstacle ψ_2

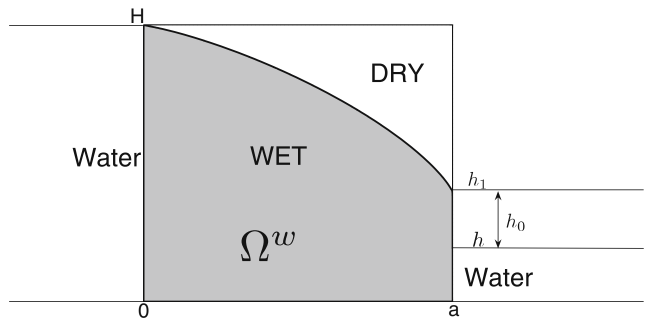

Fig. 4 The dike problem

We employ a linear elastic model described by the following equations:

$$-\Delta u(x, y) = f(x, y) \quad \text{in} \quad \Omega^+, \tag{20}$$

$$u(x, y) = \psi(x, y) \quad \text{in} \quad \Omega^0, \tag{21}$$

$$u(x, y) = g(x, y) \quad \text{on} \quad \partial\Omega. \tag{22}$$

Equation 20 represents the equilibrium, (21) the contact condition and (22) the boundary condition. The following inequalities must be also satisfied:

$$u(x, y) \geq \psi(x, y) \quad \text{in} \quad \Omega, \tag{23}$$

$$-\Delta u(x, y) \geq f(x, y) \quad \text{in} \quad \Omega, \tag{24}$$

where (23) prevents penetration in the obstacle and (24) imposes that the membrane is stretched.

The boundary between Ω^+ and Ω^0, that we call Γ, is unknown. Thus, the present is a free boundary problem that can be stated as the following complementarity problem:

Find $u(x, y) \in K$ such that:

$$\left\{ \begin{array}{c} u(x, y) - \psi(x, y) \geq 0 \\ -\Delta u(x, y) - f(x, y) \geq 0 \\ (u(x, y) - \psi(x, y))[-\Delta u(x, y) - f(x, y)] = 0 \end{array} \right. \tag{25}$$

where $K \equiv \{v(x, y) \in \Xi | v(x, y) = g(x, y) \text{ on } \partial\Omega\}$ and Ξ is the set of admissible functions defined in Ω.

We study two examples with $\Omega = [0, 1] \times [0, 1]$, $f(x, y) = 0$ in Ω and

$$g(x, y) = \left\{ \begin{array}{ll} 1 - (2x - 1)^2, & \text{if} \quad y = 0, 1 \\ 0 & \text{otherwise} \end{array} \right.$$

The obstacles for the first problem are given by

$$\psi_1(x, y) = \left\{ \begin{array}{ll} 1 & \text{if} \quad \left|x - \frac{1}{2}\right| \leq \frac{1}{4}, \left|y - \frac{1}{2}\right| \leq \frac{1}{4}, \\ 0 & \text{otherwise} \end{array} \right.$$

and for the second one:

$$\psi_2(x, y) = \left\{ \begin{array}{l} 400 \left(x - \frac{1}{4}\right)\left(x - \frac{3}{4}\right)\left(y - \frac{1}{4}\right)\left(y - \frac{3}{4}\right) \\ \text{if} \quad \left|x - \frac{1}{2}\right| \leq \frac{1}{4}, \left|y - \frac{1}{2}\right| \leq \frac{1}{4} \\ 0, \text{ otherwise} \end{array} \right.$$

A central finite differences numerical model is employed. The mesh is regular and several cases are studied changing the discretization.

Tables 7 and 8 describe the iterations required to solve the membrane problem for different meshes. The dimension of the problem, n, is equal to the number of internal nodes, since the nodal displacements on the boundary are prescribed.

Figures 2 and 3 show the vertical displacements of the membrane for a mesh with 52x52 nodes, for the obstacles ψ_1 and ψ_2 respectively.

7.3 The dike problem with vertical walls

We consider now the classical problem of seepage through a porous dam studied by several authors, (Baiocchi and Capelo 1984; Kinderlehrer and Stampacchia 1980; Crank 1984; Leontiev and Huacasi 2001).

Let be a dam of rectangular cross section made of porous material with permeable vertical walls and impermeable horizontal base, separating two reservoirs of levels H and h, represented by Fig. 4. Assuming that the dam is long, the problem can be represented in a bi-dimensional domain, defined in the rectangle $\Omega = [0, a] \times [0, H]$, which corresponds to the cross section of the dam. The wet area is

$$\Omega^w = \{(x, y) \in \Omega\,;\; 0 \leq y \leq \phi(x)\},$$

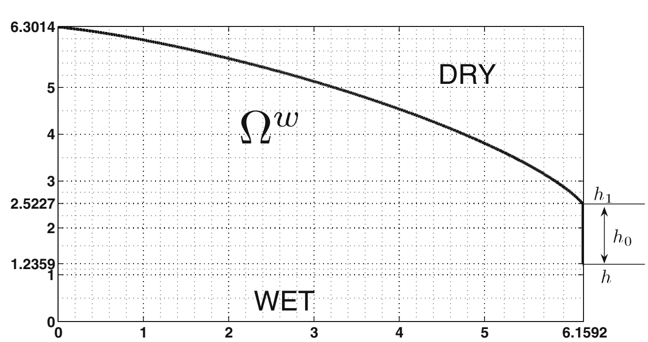

Fig. 5 Dike problem - wet domain for a 700 × 700 mesh

Table 9 Iterations for the dike problem

Alg	NCP-FDA				FB	
β	1.1		2		-	
n	Iter	Iter LS	Iter	Iter LS	Iter	Iter LS
10000	27	15	27	24	104	791
40000	27	21	27	28	188	2939
90000	27	22	27	30	331	6064
160000	28	26	27	33	492	9822
250000	28	22	27	78⋆	*	*
360000	28	29	27	101⋆	*	*
490000	28	30	27	155⋆	*	*

where $y = \phi(x)$ satisfies $\phi(0) = H$ and $\phi(a) \geq h$. This is a free boundary problem that consists on determining the wet domain Ω^w and the flow velocity potential, $\varphi(x, y)$ in Ω^w.

We solve this problem employing a formulation proposed in Baiocchi and Capelo (1984). This formulation, as well as a complete description of the physical model, are described in Crank (1984).

Let us consider the transformed of Baiocchi, defined as follows:

$$\psi(x, y) = \int_y^{\phi(x)} [\varphi(x, t) - t]dt \ , \ (x, y) \in \Omega^w. \qquad (26)$$

The mentioned formulation for the Dike Problem solves a Complementarity Problem in Ω (Table 9):

Find $\psi(x, y)$ such that:

$$\begin{cases} \psi(x, y) \geq 0 \\ 1 - \Delta\psi(x, y) \geq 0 \\ \psi(x, y)[1 - \Delta\psi(x, y)] = 0 \end{cases} \qquad (27)$$

in Ω, with $\psi(x, y) = g(x, y)$ on $\partial\Omega$, where

$$g(x, y) = \begin{cases} \frac{1}{2}(H-y)^2 + \frac{x}{2a}[(h-y)^2 - (H-y)^2] & \text{for } 0 \leq y \leq h \\ \frac{1}{2}(H-y)^2 - \frac{x}{2a}(H-y)^2 & \text{for } h \leq y \leq H \end{cases}$$

The wet domain is given by the set of points (x, y) such that $\psi(x, y) > 0$. It follows from (26) that

$$\varphi(x, y) = y - \frac{\partial\psi(x, y)}{\partial y} \text{ in } \Omega^w.$$

To solve the problem with NCP-FDA, we define a regular mesh and compute derivatives by central finite differences. We take $H = 6.3014$, $h = 1.2359$ and $a = 6.1592$. The wet domain is represented in Fig. 5.

The present algorithm solves all the tests with a similar number of main and line search iterations, even for very large size problems. Minimization of Fischer-Burmeister NCP function with Newton's method fails for large values of n.

8 Conclusions

In this paper a new feasible points algorithm for NCP is presented. Global convergence is proved and two theoretical results about the asymptotic convergence are obtained. Taking $\beta \in (1, 2)$, a strong prove of superlinear convergence is presented. When $\beta = 2$, a weaker proof of quadratic convergence is also obtained.

The performance of the present algorithm in the numerical examples is very good, even in the cases when the solution is degenerate. The number of iterations remains almost unchanged when n is increased.

The present technique is simple and also robust, since there are not significant parameters to be adjusted and all the test problems were solved with the same set of parameters.

We also remark that conditioning of the linear system (7) is improved by the fact that all the iterates are strictly feasible.

Even if Maratos effect is rarely observed, including a line search along an arc should improve the efficiency and robustness of the present method in a similar way as in Herskovits et al. (2005) and Herskovits and Santos (1998).

Our results can also be extended to other problems, like mixed complementarity or optimization problems with complementarity constraints.

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