

Numerical validation of solutions of complementarity problems: The nonlinear case

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Summary. This paper proposes a validation method for solutions of nonlinear complementarity problems. The validation procedure performs a computational test. If the result of the test is positive, then it is guaranteed that a given multi-dimensional interval either includes a solution or excludes all solutions of the nonlinear complementarity problem.

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1 Introduction

Let $f : R^n \rightarrow R^n$ be a continuous function. The nonlinear complementarity problem (NCP) consists in finding a vector $x \in R^n$ such that

$$x \geq 0, \quad f(x) \geq 0, \quad x^T f(x) = 0.$$

The NCP models many important problems in engineering and economy. Moreover, the NCP is a fundamental problem for optimization theory, since the first order necessary condition for optimality can be formulated as an NCP. Although there are some general results about the existence of solutions for some classes of NCPs, it is rather difficult to verify that a particular

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NCP has a solution. It is even more difficult to verify that an NCP has a solution in a particular region. A comparison of some codes for solving NCPs developed prior to 1995 is given in [7]. Since then new efficient methods for solving NCPs have been developed based either on interior point methods [5, 6, 25, 30, 31], or Newton-like methods applied to (non-smooth) reformulations of NCPs [9, 15, 24]. Under certain conditions, for example if the NCP is monotone and satisfies a scaled Lipschitz condition [25, 31] then for any strictly feasible starting point the interior point method will produce a sequence that converges to a solution of the problem. However, in practice it is extremely difficult to find a strictly feasible point. Typically, a primal-dual interior point method uses a positive starting vector ($x^0 > 0, s^0 > 0$) with a residual $r^0 = s^0 - f(x^0)$ and stops when a point (x, s) is obtained such that

$$(1.1) \quad x > 0, s > 0, \|s - f(x)\| < \varepsilon, x^T s < \varepsilon,$$

for a given $\varepsilon > 0$. Even if ε is very small this does not guarantee that the NCP has a solution. In case the NCP has a solution it is very difficult to obtain reliable bounds on the distance between a solution of the NCP and a point satisfying (1.1).

In [2, 10] the special case of the so-called linear complementarity problem (LCP) was considered. In this case the mapping f has the special form $f(x) = Mx + q$ where $M \in R^{n \times n}$ and $q \in R^n$ are given. The general case of a nonaffine f is much more difficult to handle than the linear case.

The present paper describes a computational test that guarantees that a given multi-dimensional interval contains a solution of the NCP. Our test also applies for algorithms which have stopping criteria different from (1.1). The idea is to choose a relatively small multidimensional interval around a point (x, s) (presumably an approximate solution of the problem) and to test computationally if a certain inclusion holds. If the result of the test is positive, then the given interval is guaranteed to contain a solution of the NCP. It is notable that the involved function f is not necessarily differentiable for the validation. In Sect. 2, we describe a slope for the numerical validation of the solution of an NCP. In Sect. 3 we give an interval arithmetic evaluation of the slope. In Sect. 4 we propose an algorithm for testing the existence of solutions, and report numerical results to illustrate the robustness of the new method. In what follows we denote an interval by $[x] = \{x \in R^n, \underline{x} \leq x \leq \bar{x}\}$. The nonnegative orthant of R^n is denoted by R_+^n .

2 The slope of a NCP

It is well known and easy to verify that the NCP is equivalent to the following system of nonlinear equations

$$(2.1) \quad F(x) := \min(f(x), x) = 0,$$

where the “min” operator denotes the componentwise minimum of two vectors. For the case f is differentiable, the function F is not necessarily differentiable at x if $f(x) = x$. F is differentiable on an interval $[x]$ if $f(x) > x$ for all $x \in [x]$ or $f(x) < x$ for all $x \in [x]$. Many existing algorithms for validation of solutions of a system $F(x) = 0$ of nonlinear equations assume that the involved function is continuously differentiable. Such algorithms are based on the mean value theorem for differentiable functions and an interval extension of the derivative. For instance, if F is differentiable on $[x]$, then

$$(2.2) \quad F(x) - F(y) \in F'([x])(x - y), \quad \text{for all } x, y \in [x],$$

where $F'([x])$ is an interval evaluation of the Fréchet derivative. The Krawczyk operator is defined by

$$K(x, A, [x]) = x - A^{-1}F(x) + (I - A^{-1}F'([x]))([x] - x),$$

where A is an $n \times n$ nonsingular matrix. If $[x]$ is a multi-dimensional interval such that $K(x, A, [x]) \subset [x]$ then it is guaranteed that there is an $x^* \in [x]$ such that $F(x^*) = 0$. For details see [2]. Since the function F defined in (2.1) is in general nondifferentiable, the above validation algorithm does not apply to our problem. Recently, some methods have been proposed for general nondifferentiable equations [8,27]. In this paper we give a sharp and computable interval operator for the special nondifferentiable system (2.1). Using this interval operator, we can numerically verify the existence of solutions of the NCP. The first step is to define a slope for F , which is a mapping $\delta F : [x] \times [x] \rightarrow R^{n \times n}$ such that for a fixed $x \in [x]$

$$(2.3) \quad F(x) - F(y) = \delta F(x, y)(x - y), \quad \text{for all } y \in [x].$$

We assume that f has a slope $\delta f : [x] \times [x] \rightarrow R^{n \times n}$ such that for a fixed $x \in [x]$

$$(2.4) \quad f(x) - f(y) = \delta f(x, y)(x - y), \quad \text{for all } y \in [x].$$

Let us use the following notations

$$S_i^+ = \{x \in [x] \mid f_i(x) > x_i\}$$

$$S_i^- = \{x \in [x] \mid f_i(x) < x_i\}$$

$$S_i^0 = \{x \in [x] \mid f_i(x) = x_i\}$$

$$N = \{1, 2, \dots, n\}.$$

For a vector $x \in [x]$ and an $i \in N$, x is in one of the three sets. Hence for any two vectors $x, y \in [x]$ and an $i \in N$ we define $\delta F_i(x, y)$ as shown in Table 1.

Lemma 2.1 *Let the i th row of $\delta F(x, y)$ be defined by Table 1. Then for every two vectors $x, y \in [x]$,*

$$F(x) - F(y) = \delta F(x, y)(x - y).$$

Proof. Let $i \in N$ be fixed. Since δf_i is a slope of f_i , we have

$$f_i(x) - f_i(y) = \delta f_i(x, y)(x - y).$$

If $x \in S_i^+ \cup S_i^0$ and $y \in S_i^+ \cup S_i^0$, then

$$F_i(x) - F_i(y) = x_i - y_i = e_i^T(x - y).$$

If $x \in S_i^-$ and $y \in S_i^0 \cup S_i^-$, or $y \in S_i^-$ and $x \in S_i^0$, then

$$F_i(x) - F_i(y) = f_i(x) - f_i(y) = \delta f_i(x, y)(x - y).$$

If $x \in S_i^-$ and $y \in S_i^+$, then

$$(\delta f_i(x, y) - e^T)(x - y) = f_i(x) - x_i + y_i - f_i(y) < 0$$

and

$$\begin{aligned} F_i(x) - F_i(y) &= f_i(x) - y_i \\ &= f_i(x) - x_i + e_i^T(x - y) \\ &= \frac{(f_i(x) - x_i)(\delta f_i(x, y) - e_i^T)(x - y)}{(\delta f_i(x, y) - e_i^T)(x - y)} + e_i^T(x - y) \\ &= \left(\frac{f_i(x) - x_i}{(f(x) - f(y) - x + y)_i} (\delta f_i(x, y) - e_i^T) + e_i^T \right) \\ &\quad \times (x - y) \\ &= (\beta_i(\delta f_i(x, y) - e_i^T) + e_i^T)(x - y). \end{aligned}$$

Finally, if $x \in S_i^+$ and $y \in S_i^-$ then

$$(\delta f_i(x, y) - e^T)(x - y) = f_i(x) - x_i + y_i - f_i(y) > 0$$

and

$$\begin{aligned} F_i(x) - F_i(y) &= x_i - f_i(y) \\ &= y_i - f_i(y) + e_i^T(x - y) \\ &= \frac{(y_i - f_i(y))(\delta f_i(x, y) - e_i^T)(x - y)}{(\delta f_i(x, y) - e_i^T)(x - y)} + e_i^T(x - y) \\ &= \left(\frac{y_i - f_i(y)}{(f(x) - f(y) - x + y)_i} (\delta f_i(x, y) - e_i^T) + e_i^T \right) \\ &\quad \times (x - y) \\ &= (\alpha_i(\delta f_i(x, y) - e_i^T) + e_i^T)(x - y). \end{aligned}$$

□

Lemma 2.2 *The numbers α_i and β_i defined in Table 1 satisfy the following relations*

$$\alpha_i \in (0, 1) \quad \text{and} \quad \beta_i \in (0, 1).$$

Proof. Notice that α_i is used when $x \in S_i^+$ and $y_i \in S_i^-$. Then from $y_i - f_i(y) > 0$ and $f_i(x) - x_i > 0$, we have

$$\alpha_i = \frac{y_i - f_i(y)}{(y_i - f_i(y)) + (f_i(x) - x_i)} \in (0, 1).$$

Since β_i is used when $x \in S_i^-$ and $y_i \in S_i^+$, we have $f_i(x) - x_i < 0$ and $y_i - f_i(y) < 0$, so that

$$\beta_i = \frac{f_i(x) - x_i}{(f_i(x) - x_i) + (y_i - f_i(y))} \in (0, 1). \quad \square$$

We now discuss the nonsingularity of $\delta F(x, y)$. The nonsingularity of $\delta F(x, y)$ depends on the properties of $\delta f(x, y)$. An $n \times n$ matrix A is called a P_0 matrix if all principal minors of A are nonnegative. A matrix A is called a P matrix if all its principal minors are positive [13]. Using some results from Gabriel and Moré [15] we obtain the following proposition.

Proposition 2.1 *1. If $\delta f(x, y)$ is a P matrix, then $\delta F(x, y)$ is nonsingular.
2. If $\delta f(x, y)$ is a P_0 matrix and S_i^+ contains x or y for every $i \in N$, then $\delta F(x, y)$ is nonsingular.*

Proof. 1. By Lemma 2.1 and Lemma 2.2, $\delta F(x, y)$ can be written as

$$\delta F(x, y) = I + D(\delta f(x, y) - I),$$

where $D = \text{diag}(d_i)$ is a diagonal matrix with $0 \leq d_i \leq 1$. Hence by Theorem 4.4 in [15], $\delta F(x, y)$ is nonsingular.

2. If S_i^+ contains x or y for every $i \in N$, then

$$\delta F(x, y) = I + D(\delta f(x, y) - I),$$

where $D = \text{diag}(d_i)$ is a diagonal matrix with $0 \leq d_i < 1$. Hence by Theorem 4.3 in [15], $\delta F(x, y)$ is nonsingular. \square

Table 1. Slope of the function F

| $\delta F_i(x, y)$ | | y | | |
|--------------------|---------|---|--|--------------------|
| | | S_i^+ | S_i^- | S_i^0 |
| | S_i^+ | e_i^T | $\alpha_i(\delta f_i(x, y) - e_i^T) + e_i^T$ | e_i^T |
| x | S_i^- | $\beta_i(\delta f_i(x, y) - e_i^T) + e_i^T$ | $\delta f_i(x, y)$ | $\delta f_i(x, y)$ |
| | S_i^0 | e_i^T | $\delta f_i(x, y)$ | e_i^T |

$$\alpha_i = \frac{(y - f(y))_i}{(f(x) - f(y) - x + y)_i}, \quad \beta_i = \frac{(f(x) - x)_i}{(f(x) - x + y - f(y))_i}.$$

If f is an affine function, say $f(x) = Ax + c$, then $A = \delta f(x, y)$. If A is a P_0 matrix and we choose $x \in S_i^+$, then according to Proposition 2.1 $\delta F(x, y)$ is nonsingular for all $y \in R^n$.

Definition 2.1 A mapping f from an interval $[x]$ in R^n into R^n is said to be

1. a P_0 function on $[x]$ if for all $x, y \in [x]$ with $x \neq y$, there is an index i such that

$$x_i \neq y_i \quad \text{and} \quad (f_i(x) - f_i(y))(x_i - y_i) \geq 0;$$

2. a P function on $[x]$ if for all $x, y \in [x]$ with $x \neq y$, there is an index i such that

$$x_i \neq y_i \quad \text{and} \quad (f_i(x) - f_i(y))(x_i - y_i) > 0;$$

3. a uniform P function on $[x]$ if for some $\gamma > 0$

$$\max_{i \in N} (f_i(x) - f_i(y))(x_i - y_i) \geq \gamma \|x - y\| \quad \text{for all } x, y \in [x];$$

4. a monotone function on $[x]$ if for all $x, y \in [x]$,

$$(f(x) - f(y))^T (x - y) \geq 0;$$

5. a strictly monotone function on $[x]$ if for all $x, y \in [x]$,

$$(f(x) - f(y))^T (x - y) > 0;$$

6. a strongly monotone function if for some $\gamma > 0$

$$(f(x) - f(y))^T (x - y) \geq \gamma \|x - y\| \quad \text{for all } x, y \in [x].$$

It is easy to verify that every monotone function is a P_0 function, every strictly monotone function is a P function, and every strongly monotone function is a uniform P function. For a Fréchet differentiable function f , the following results are known [16, 23]:

1. If $f'(x)$ is a P matrix for all $x \in [x]$, then f is a P function on $[x]$;
2. If f is a uniform P function on $[x]$, then $f'(x)$ is a P matrix for all $x \in [x]$;
3. f is a P_0 function on $[x]$ if and only if $f'(x)$ is a P_0 matrix for all $x \in [x]$.

For a semismooth locally Lipschitzian function f , Song, Gowda and Ravindran [29] showed that f is a P_0 function on $[x]$ if and only if the Bouligand subdifferential $\partial_B f(x)$ consists of P_0 matrices at all $x \in [x]$. Notice that the mean value theorem does not hold for $\partial_B f$. Moreover, for a P_0 function, the Clarke generalized Jacobian $\partial f(x) = \text{co } \partial_B f(x)$ may consist of a matrix which is not P_0 . Hence we consider that f is a monotone function in the following theorem.

Theorem 2.1 *Suppose that f is a locally Lipschitzian function. Then there is a $\delta f(x, y) \in \text{co}\partial f(\overline{xy})$.*

1. *If f is a strongly monotone function, then for any $\delta f(x, y) \in \text{co}\partial f(\overline{xy})$, $\delta F(x, y)$ is nonsingular.*
2. *If f is a monotone function and S_i^+ contains x or y for every $i \in N$, then for any $\delta f(x, y) \in \text{co}\partial f(\overline{xy})$, $\delta F(x, y)$ is nonsingular.*

Here $\text{co}\partial f(\overline{xy})$ denotes the convex hull of all points $Z \in \partial F(u)$ for $u \in \overline{xy}$, and \overline{xy} denotes the line segment between x and y .

Proof. According to Proposition 2.6.5 in [11], there is a matrix $\delta f(x, y) \in \text{co}\partial f(\overline{xy})$ such that

$$f(x) - f(y) = \delta f(x, y)(x - y).$$

1) Since f is a locally Lipschitzian function, f is differentiable almost everywhere. Moreover at a point $z \in [x]$ where f is differentiable, $f'(z)$ is a strongly monotone matrix. By definition, the Clarke generalized Jacobian at y is defined by

$$\partial f(y) = \text{co}\left\{ \lim_{k \rightarrow \infty} f'(z^k) : z^k \rightarrow y, f \text{ is differentiable at } z^k \right\}.$$

Since $f'(z^k)$ is a strongly monotone matrix, the limit $\lim_{z^k \rightarrow y} f'(z^k)$ is a strongly monotone matrix. Moreover, the convex combination of strongly monotone matrices is still a strongly monotone matrix. A strongly monotone matrix is a P matrix, so that by using Proposition 2.1, we deduce that $\delta F(x, y)$ is nonsingular. The proof for Part 2 is similar. \square

3 Interval evaluation

We assume that f has an interval arithmetic evaluation of the slope $\delta f(x, [x])$ for fixed $x \in [x]$ and all $y \in [x]$, i.e., $\delta f(x, [x])$ is an $n \times n$ -matrix with interval entries such that $\delta f(x, y) \in \delta f(x, [x])$, for all $y \in [x]$. For different aspects relating to the notion of an arithmetic evaluation of a slope of a nonlinear map see [19]. To define an interval arithmetic evaluation for δF , we consider the following nonlinear programming problems

$$(3.1) \quad \begin{array}{ll} \min & y_i - f_i(y) \\ \text{s.t.} & y \in [x] \end{array}$$

and

$$(3.2) \quad \begin{array}{ll} \max & y_i - f_i(y) \\ \text{s.t.} & y \in [x]. \end{array}$$

Let $y^{i,1}$ and $y^{i,2}$ be solutions of the nonlinear programming problems (3.1) and (3.2), respectively (see Remark 3.1). For a fixed $x \in [x]$, let

$$\alpha_i = \frac{(y^{i,2} - f(y^{i,2}))_i}{(f(x) - x + y^{i,2} - f(y^{i,2}))_i} \text{ if } (f(x) - x + y^{i,2} - f(y^{i,2}))_i \neq 0$$

and

$$\beta_i = \frac{(f(x) - x)_i}{(f(x) - x + y^{i,1} - f(y^{i,1}))_i} \text{ if } (f(x) - x + y^{i,1} - f(y^{i,1}))_i \neq 0.$$

Then we can define the following interval arithmetic evaluation:

$$\begin{aligned} \delta F_i(x, [x]) \\ = \begin{cases} e_i^T, & y^{i,2} \in S_i^+ \cup S_i^0 \\ \delta f_i(x, [x]), & y^{i,1} \in S_i^- \cup S_i^0 \\ [0, \alpha_i](\delta f_i(x, [x]) - e_i^T) + e_i^T, & x \in S_i^+ \cup S_i^0, y^{i,2} \in S_i^- \\ [\beta_i, 1](\delta f_i(x, [x]) - e_i^T) + e_i^T, & x \in S_i^-, y^{i,1} \in S_i^+. \end{cases} \end{aligned}$$

Theorem 3.1 For a fixed $x \in [x]$, we have

$$F(x) - F(y) \in \delta F(x, [x])(x - y), \quad \text{for all } y \in [x].$$

Proof. 1) First we suppose $y^{i,2} \in S_i^+ \cup S_i^0$. Then for all $y \in [x]$,

$$y_i - f_i(y) \leq y_i^{i,2} - f_i(y^{i,2}) \leq 0.$$

That is, $y \in S_i^+ \cup S_i^0$ for all $y \in [x]$. In particular $x \in S_i^+ \cup S_i^0$. Hence

$$F_i(x) - F_i(y) = x_i - y_i = e_i^T(x - y) = \delta F_i(x, [x])(x - y).$$

2) Now we suppose $y^{i,1} \in S_i^- \cup S_i^0$. Then for all $y \in [x]$,

$$y_i - f_i(y) \geq y_i^{i,1} - f_i(y^{i,1}) \geq 0.$$

It follows that $y \in S_i^- \cup S_i^0$ for all $y \in [x]$. In particular we have $x \in S_i^- \cup S_i^0$. Hence

$$\begin{aligned} F_i(x) - F_i(y) &= f_i(x) - f_i(y) \\ &= \delta f_i(x, y)(x - y) \\ &\in \delta f_i(x, [x])(x - y) \\ &= \delta F_i(x, [x])(x - y). \end{aligned}$$

3) Finally we suppose that $y^{i,2} \in S_i^-$ and $x \in S_i^+ \cup S_i^0$. Let $y \in [x]$. If $y \in S_i^+ \cup S_i^0$, then

$$\begin{aligned} F_i(x) - F_i(y) &= e_i^T(x - y) \\ &\in ([0, \alpha_i](\delta f_i(x, [x]) - e_i^T) + e_i^T)(x - y) \\ &= \delta F_i(x, [x])(x - y), \end{aligned}$$

where we use the fact that $0 < \alpha_i \leq 1$. If $y \in S_i^-$, then by Lemma 2.1, we have

$$F_i(x) - F_i(y) = \left(\frac{y_i - f_i(y)}{(f(x) - f(y) - x + y)_i} (\delta f_i(x, y) - e_i^T) + e_i^T \right) (x - y).$$

Since $y^{i,2}$ is an optimal solution of (3.2), we have

$$0 < \frac{y_i - f_i(y)}{(f(x) - f(y) - x + y)_i} \leq \frac{y_i^{i,2} - f_i(y^{i,2})}{(f(x) - f(y^{i,2}) - x + y^{i,2})_i} = \alpha_i \leq 1.$$

Therefore,

$$F_i(x) - F_i(y) \in ([0, \alpha_i](\delta f_i(x, [x]) - e_i^T) + e_i^T)(x - y) = \delta F_i(x, [x])(x - y).$$

4) The case $x \in S_i^-$, $y_i^{i,1} \in S_i^+$ can be treated in a similar fashion.

Remark 3.1 In general it is a non-trivial problem to find solutions $y^{i,1}$ and $y^{i,2}$ of (3.1) and (3.2), respectively. However, in some practical important examples $y^{i,1}$ and $y^{i,2}$ can easily be found. See Example 1 of this paper, e.g.

Furthermore the following interval arithmetic evaluation can be considered as a simple but overestimated interval arithmetic evaluation:

$$\hat{G}(x, [x]) = [0, 1](\delta f(x, [x]) - I) + I.$$

Following the discussion above, we can show that

$$\delta F(x, [x]) \subseteq \hat{G}(x, [x])$$

and

$$F(x) - F(y) \in \hat{G}(x, [x])(x - y) \quad \text{for all } x, y \in [x].$$

Proposition 3.1 1. If $\delta f(x, [x])$ consists of P matrices at all $y \in [x]$, then every element in $\hat{G}(x, [x])$ is nonsingular.

2. If $\delta f(x, [x])$ consists of P_0 matrices at all $y \in [x]$ and $x \in S_i^+$ for all $i \in N$, then every element in $\delta F(x, [x])$ is nonsingular.

Proof. The proof for the part 1 is similar to the proof of part 1 of Proposition 2.1. For part 2, by Theorem 4.3 in [15], we only need to show $\delta f_i(x, [x])$ is not in $\delta F_i(x, [x])$ for every $i \in N$. Since $x \in S_i^+$ and

$$y_i^{i,1} - f_i(y^{i,1}) \leq x_i - f_i(x) < 0,$$

we have $y^{i,1} \in S_i^+$. Hence

$$\delta F_i(x, [x]) \neq \delta f_i(x, [x])$$

and

$$\delta F_i(x, [x]) \neq [\beta_i, 1](\delta f_i(x, [x]) - e_i^T) + e_i^T.$$

This implies that

$$\delta F_i(x, [x]) = [0, \alpha_i](\delta f_i(x, [x]) - e_i^T) + e_i^T,$$

where α_i is a number between 0 and 1. Now we show that $\alpha_i \neq 1$. If $y^{i,2} \in S_i^+ \cup S_i^0$, then $\alpha_i = 0$; If $y^{i,2} \in S_i^-$, then from $x \in S_i^+$, we have

$$f_i(x) - x_i > 0$$

and

$$0 < \alpha_i = \frac{y_i^{i,2} - f_i(y^{i,2})}{(f(x) - f(y^{i,2}) - x + y^{i,2})_i} < 1.$$

The proof is complete. \square

4 Algorithm and numerical tests

Based on the results in [3, 8], we propose the following validation method.

Algorithm 1 Let $r > 0$ be a given tolerance and let $x > 0$ be an approximate solution of the system (2.1). Calculate

$$(4.1) \quad [x] = x + r[-e, e]$$

where $e = [1, \dots, 1]^T$ and choose a nonsingular matrix A . Compute

$$(4.2) \quad L(x, A, [x]) = x - A^{-1}F(x) + (I - A^{-1}\delta F(x, [x]))([x] - x).$$

– If

$$(4.3) \quad L(x, A, [x]) \subseteq [x],$$

then there is a solution $x^* \in [x]$ of (2.1).

– If

$$(4.4) \quad L(x, A, [x]) \cap [x] = \emptyset,$$

then the interval $[x]$ contains no solution of (2.1).

The algorithm is tested using the following two examples.

Example. Consider the following equilibrium problem for an unknown function $u(y, z)$ [20]:

$$(4.5) \quad \begin{cases} u = [u + \Delta u - \phi(u) - q(y, z)]_+, & (y, z) \in \Omega = (0, 1) \times (0, 1) \\ u = 0, & (y, z) \in \partial\Omega, \end{cases}$$

where ϕ is a monotone function and q is a given function.

Applying the centered five point difference approximation to (4.5), we obtain a system of nonlinear equations

$$(4.6) \quad x = (x - Mx - g(x) - c)_+$$

which is equivalent to

$$F(x) = x - \max(0, x - Mx - g(x) - c) = \min(x, Mx + g(x) + c) = 0.$$

In particular, for $\phi(u) = e^u$, we have

$$M = \frac{1}{h^2} \begin{pmatrix} H & -I & & & \\ -I & H & \ddots & & \\ & \ddots & \ddots & -I & \\ & & & -I & H \end{pmatrix} \in R^{n \times n},$$

$$H = \begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & & -1 & 4 \end{pmatrix} \in R^{\sqrt{n} \times \sqrt{n}}$$

and

$$g(x) = (e^{x_1}, e^{x_2}, \dots, e^{x_n})^T.$$

Let

$$f(x) = Mx + g(x) + c.$$

Then

$$f'(x) = M + \text{diag}(e^{x_i}).$$

Define $h(x) = x - f(x)$. Then it is easy to see that for $x \in R_+^n$ and $1 \leq i \leq n$ it holds

$$\frac{\partial h_i}{\partial x_i} = 1 - \frac{4}{h^2} - e^{x_i} < 0,$$

$$\frac{\partial h_i}{\partial x_j} \in \{0, \frac{1}{h^2}\}, i \neq j; \text{ hence } \frac{\partial h_i}{\partial x_j} \geq 0, i \neq j.$$

From this it follows that we can define the global optimal solutions of (3.1) and (3.2) as follows:

$$y_j^{i,1} = \begin{cases} \bar{x}_j & \text{if } i = j \\ \underline{x}_j & \text{otherwise} \end{cases},$$

and

$$y_j^{i,2} = \begin{cases} \underline{x}_j & \text{if } i = j \\ \bar{x}_j & \text{otherwise} \end{cases}.$$

We have chosen

$$x^* = (0, 1, 0, 1, \dots, 1)^T$$

Table 2. Numerical results for Example 1, $x^* \in [x]$

| α | | $n = 9$ | $n = 25$ | $n = 36$ | $n = 64$ | $n = 100$ |
|----------|-----------------|------------|------------|------------|------------|------------|
| -0.75 | \bar{r} | 10^{-2} | 10^{-3} | 10^{-3} | 10^{-3} | 10^{-4} |
| | \underline{r} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} |
| -0.5 | \bar{r} | 10^{-1} | 10^{-2} | 10^{-4} | 10^{-3} | 10^{-3} |
| | \underline{r} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} |
| -0.25 | \bar{r} | 10^{-2} | 10^{-3} | 10^{-2} | 10^{-4} | 10^{-3} |
| | \underline{r} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} |
| 0 | \bar{r} | 10^{-1} | 10^{-2} | 10^{-4} | 10^{-4} | 10^{-4} |
| | \underline{r} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} |
| 0.25 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-3} |
| | \underline{r} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} |
| 0.5 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-2} | 10^{-4} |
| | \underline{r} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} |
| 0.75 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-2} | 10^{-3} |
| | \underline{r} | 10^{-16} | 10^{-14} | 10^{-16} | 10^{-15} | 10^{-16} |

and

$$c_i = - \begin{cases} (Mx^*)_i + g_i(x^*) & \text{if } x_i^* > 0 \\ (Mx^*)_i + g_i(x^*) - \xi_i & \text{otherwise} \end{cases},$$

where ξ_i is a random nonnegative number. Obviously, x^* is a solution of (4.6). Moreover, F is not differentiable at x^* if there is an i such that $\xi_i = 0$. \square

Example 2 (U. Schäfer, Karlsruhe) Let

$$f(x) = Mx + q + s(x),$$

where

$$M = \begin{pmatrix} 1 & 2 & 2 & \cdots & 2 \\ 0 & 1 & 2 & \cdots & 2 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 2 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix},$$

and $s(x) = \text{diag}(s_i(x_i))$ with $s_i(x_i) = (x_i + 1)^3 - i$, $i = 1, \dots, n$;

q is chosen such that $x^* = (x_1^*, x_2^*, \dots, x_n^*)^T$ with

$$x_i^* = \begin{cases} 0 & \text{if } i \bmod 7 = 0 \\ i & \text{otherwise} \end{cases}$$

is an exact solution of (2.1).

In our numerical experiment, we choose

$$q_i := \begin{cases} i - (Mx^* + s(x^*))_i & \text{if } i \bmod 7 = 0 \\ -(Mx^* + s(x^*))_i & \text{otherwise.} \end{cases}$$

Table 3. Numerical results for Example 2, $x^* \in [x]$

| α | | $n = 5$ | $n = 10$ | $n = 20$ | $n = 50$ | $n = 100$ |
|----------|-----------------|------------|------------|------------|------------|------------|
| -0.75 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-3} | 10^{-3} |
| | \underline{r} | 10^{-14} | 10^{-14} | 10^{-13} | 10^{-12} | 10^{-12} |
| -0.5 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-3} | 10^{-3} |
| | \underline{r} | 10^{-14} | 10^{-14} | 10^{-13} | 10^{-13} | 10^{-12} |
| -0.25 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-3} |
| | \underline{r} | 10^{-14} | 10^{-14} | 10^{-14} | 10^{-13} | 10^{-12} |
| 0 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-3} |
| | \underline{r} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} | 10^{-16} |
| 0.25 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-2} | 10^{-3} | 10^{-3} |
| | \underline{r} | 10^{-14} | 10^{-14} | 10^{-14} | 10^{-13} | 10^{-12} |
| 0.5 | \bar{r} | 10^{-2} | 10^{-2} | 10^{-2} | 10^{-2} | 10^{-3} |
| | \underline{r} | 10^{-14} | 10^{-14} | 10^{-14} | 10^{-13} | 10^{-12} |
| 0.75 | \bar{r} | 10^{-1} | 10^{-1} | 10^{-2} | 10^{-2} | 10^{-2} |
| | \underline{r} | 10^{-14} | 10^{-14} | 10^{-13} | 10^{-12} | 10^{-12} |

Of course, there are also other choices possible for q_i . Note that M is a P matrix and $s'(x) = \text{diag}(3(x_i + 1)^2)$. Hence it is easy to see that f is a uniform P function for any choice of q . It is known that an NCP with a uniform P function always has a solution which is unique in R^n . \square

Let x^* be an exact solution. We choose as an approximation

$$x = x^* - r\alpha e,$$

where $\alpha \in (-1, 1)$ and $r > 0$.

As a test interval for Algorithm 1 we try

$$[x] = x + [-r, r]e,$$

where $e = (1, \dots, 1)^T$. This choice of $[x]$ guarantees that for all $\alpha \in (-1, 1)$ and $r > 0$ the inclusion

$$x^* \in [x]$$

holds. Varying α and r shows how sensitive our algorithm is with respect to these parameters. If $|\alpha| > 1$ then $[x]$ does not contain x^* for any $r > 0$. For $|\alpha| > 1$ we keep αr (and therefore the center x of the test interval $[x]$) constant. Therefore by enlarging $|\alpha|$ we have to diminish the half width r of the components of the diameter of $[x]$. Table 2 (for Example 1) and Table 3 (for Example 2) contain the numerical results for the case that $x^* \in [x]$ (that is for $\alpha \in (-1, 1)$). \bar{r} denotes the largest $r \leq 10^{-1}$ for which the validation (4.3) was performed successfully.

\underline{r} denotes the smallest $r \geq 10^{-16}$ for which the validation (4.3) was performed successfully. In our numerical experiments we have tested the

Table 4. Numerical results for Example 1, $\alpha r = 5$

| r | $n = 9$ | $n = 25$ | $n = 36$ | $n = 64$ | $n = 100$ |
|-----|---------|----------|----------|----------|-----------|
| 0.5 | y | y | y | y | y |
| 1 | y | y | y | y | y |
| 1.5 | y | n | n | n | n |
| 2.0 | n | n | n | n | n |

Table 5. Numerical results for Example 2, $\alpha r = 5$

| r | $n = 5$ | $n = 10$ | $n = 20$ | $n = 50$ | $n = 100$ |
|-----|---------|----------|----------|----------|-----------|
| 1 | y | y | y | y | y |
| 2 | y | y | y | y | y |
| 3 | y | y | y | y | y |
| 3.5 | y | y | y | y | y |
| 3.6 | n | y | y | y | y |
| 3.7 | n | y | y | y | y |
| 3.8 | n | y | y | y | y |
| 3.9 | n | n | y | y | y |
| 4 | n | n | y | y | y |
| 4.7 | n | n | n | n | y |
| 4.8 | n | n | n | n | n |
| 4.9 | n | n | n | n | n |

algorithm starting with $r = \bar{r}$ and decreasing the radius r successively by multiplying it with 10^{-1} until we reached \underline{r} .

Table 4 (for Example 1) and Table 5 (for Example 2) contain the numerical results for the case that $x^* \notin [x]$ (that is for $|\alpha| > 1$). In these tables “y” means that the test (4.4) was successful, “n” means that it was not successful. We choose $\alpha r = 5$ and obtain the results in Table 4 and Table 5.

The above numerical results as well as other numerical experiments show that our validation algorithm is robust and can be used to prove numerically that a certain multidimensional interval centered at an approximate solution contains an exact solution of the NCP.

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