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Error bounds for complementarity problems with tridiagonal nonlinear functions ^{*}

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Abstract

In this paper we consider the complementarity problem $\text{NCP}(f)$ with $f(x) = Mx + \varphi(x)$, where $M \in \mathbf{R}^{n \times n}$ is a real matrix and φ is a so-called tridiagonal (nonlinear) mapping defined in the introduction (see (11) and (12)). This problem occurs, for example, if certain classes of free boundary problems are discretized. We compute error bounds for approximations \hat{x} to a solution x^* of the discretized problems. The error bounds are improved by an iterative method and can be made arbitrarily small. The ideas are illustrated by numerical experiments.

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Key words: complementarity, error bound, free boundary problem

1 Introduction

Let $f : \mathbf{R}^n \rightarrow \mathbf{R}^n$ be a given mapping. A nonlinear complementarity problem, denoted by $\text{NCP}(f)$, is to find a vector x^* such that

$$x^* \geq 0, \quad f(x^*) \geq 0, \quad x^{*T} f(x^*) = 0. \quad (1)$$

The inequalities are meant componentwise. $\text{NCP}(f)$ has many real world applications, in engineering, for example. We refer to [13] for source problems of it.

Assume that we have computed an approximation \hat{x} to a solution x^* of (1) by some numerical algorithm (see [11], e.g.). Then it is important to estimate the distance of \hat{x} to x^* . Without such an estimation the approximation \hat{x} is of doubtful utility.

This distance is usually measured by some norm or may be defined componentwise. Error estimation in this sense has been extensively studied up to now in the papers [8, 9, 12, 14, 15, 17] and the monograph [11]. In the papers [1, 3] a verification method for the existence of a solution of $\text{NCP}(f)$, defined in (1), was given. If the method is successful, error bounds are delivered automatically.

In [6, 7] we studied the complementarity problem $\text{NCP}(f)$ with the mapping f of the form

$$f(x) = Mx + \varphi(x), \quad (2)$$

where $M \in \mathbf{R}^{n \times n}$, and

$$\varphi(x) = (\varphi_i(x_i)). \quad (3)$$

φ is a so-called diagonal mapping. This problem comes, for example, by considering the following free boundary problems.

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Example 1.1. Let $g : [0, 1] \times \mathbf{R} \rightarrow \mathbf{R}$ be a given function, let $\alpha, \beta > 0$ be given constants. We consider finding a function $u : [0, 1] \rightarrow \mathbf{R}_+$ such that

$$\begin{cases} u''(t) &= g(t, u(t)) & t \in \mathbf{D}_+, \\ u(0) &= \alpha, \\ u(1) &= \beta, \end{cases} \quad (4)$$

where the set $\mathbf{D}_+ := \{t \in (0, 1) : u(t) > 0\}$ is unknown.

We can approximate $u(t)$ from Example 1.1 by a vector $x^* = (x_i^*) \in \mathbf{R}^n$, using the well-known second order approximation of the second order derivative. This gives us an NCP(f) of the form (2) and (3), where

$$M = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & & -1 & 2 \end{bmatrix} \quad (5)$$

and where $\varphi(x) = (\varphi_i(x_i))$ with

$$\begin{aligned} \varphi_i(x_i) &= h^2 g(t_i, x_i), \quad i = 1, 2, \dots, n, \\ x_0 &= \alpha, \quad x_{n+1} = \beta. \end{aligned}$$

Here $h = \frac{1}{n+1}$ is the stepsize, $t_i = ih$, $i = 1, \dots, n$, and $u(t_i) \approx x_i^*$.

However, using the so-called Mehrstellenverfahren (see [10], Table III, p.538, second to the last line) we can approximate the free boundary problem from Example 1.1 by (1), where

$$f(x) = Mx + \varphi(x). \quad (6)$$

M is the same matrix as in (5). The mapping $\varphi : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is now a so-called *tridiagonal (nonlinear) function*

$$\varphi(x) = (\varphi_i(x_{i-1}, x_i, x_{i+1})) \quad (7)$$

with

$$\varphi_i(x_{i-1}, x_i, x_{i+1}) = \frac{h^2}{12} (g(t_{i-1}, x_{i-1}) + 10g(t_i, x_i) + g(t_{i+1}, x_{i+1})), \quad (8)$$

$i = 1, 2, \dots, n$, where again $x_0 = \alpha$ and $x_{n+1} = \beta$.

Example 1.2. Let $g : [0, 1] \times \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R}$ be a given function, let $\alpha, \beta > 0$ be given constants. We consider finding a function $u : [0, 1] \rightarrow \mathbf{R}_+$ such that

$$\begin{cases} u''(t) &= g(t, u(t), u'(t)) & t \in \mathbf{D}_+, \\ u(0) &= \alpha, \\ u(1) &= \beta, \end{cases} \quad (9)$$

where the set $\mathbf{D}_+ := \{t \in (0, 1) : u(t) > 0\}$ is unknown.

This is also a free boundary problem. However, in contrast to Example 1.1, also the first order derivative occurs in the differential equation. We can approximate $u(t)$ from Example 1.2 by a vector $x^* = (x_i^*) \in \mathbf{R}^n$ using the well known second order approximations of the first and second order derivatives. This gives us an NCP(f), defined by (6), where M is defined by (5) and $\varphi(x)$ is again a *tridiagonal (nonlinear) function* $\varphi(x) = (\varphi_i(x_{i-1}, x_i, x_{i+1}))$, with

$$\varphi_i(x_{i-1}, x_i, x_{i+1}) = h^2 g(t_i, x_i, \frac{x_{i+1} - x_{i-1}}{2h}), \quad (10)$$

$i = 1, 2, \dots, n$. In φ_1 we have to set $x_0 = \alpha$ and correspondingly $x_{n+1} = \beta$ in φ_n .

In the present article we prove some general results on the existence of solutions and error bounds of $\text{NCP}(f)$ with

$$f(x) = Mx + \varphi(x) \quad (11)$$

where $M \in \mathbf{R}^{n \times n}$ is a given matrix and where

$$\varphi(x) = (\varphi_i(x_{i-1}, x_i, x_{i+1})) \quad (12)$$

is a *tridiagonal (nonlinear) function*. We focus on conditions on g from Example 1.1 and 1.2.

The paper is organized as follows. In Section 2 we introduce the notations and some frequently used results. In Section 3 we compute under certain conditions on the matrix M and the tridiagonal nonlinear function φ error bounds for an approximate solution of $\text{NCP}(f)$ defined by (11). In Section 4 we introduce and investigate an iterative method, which allows to improve the error bounds systematically. Finally, we present results from numerical experiments in Section 5.

2 Preliminaries

Let us make some theoretical preparation for the presentation of the results of this paper. Denote by \mathbf{R}_+^n the nonnegative orthant of \mathbf{R}^n . Denote by " \leq " the natural (or componentwise) partial ordering in \mathbf{R}^n . For any $x, y \in \mathbf{R}^n$ we denote by $\max\{x, y\}$ and $\min\{x, y\}$ the componentwise maximum and minimum of the two vectors, respectively.

Subsequently some basic facts from interval analysis are used. Let $\underline{A} = (\underline{a}_{ij}), \bar{A} = (\bar{a}_{ij}) \in \mathbf{R}^{n \times n}$ with $\underline{a}_{ij} \leq \bar{a}_{ij}$, $i = 1, \dots, n$, $j = 1, \dots, n$. We denote by $[A] = [\underline{A}, \bar{A}]$ an $n \times n$ interval matrix, which is a set

$$[A] := \{A = (a_{ij}) \in \mathbf{R}^{n \times n} : \underline{a}_{ij} \leq a_{ij} \leq \bar{a}_{ij}\}.$$

We denote by $\mathbf{IR}^{n \times n}$ the set of all $n \times n$ real interval matrices. The (i, j) -th element of $[A]$ is denoted by $[a_{ij}]$. Let $\underline{x}, \bar{x} \in \mathbf{R}^n$ with $\underline{x} \leq \bar{x}$. We denote by $[x] = [\underline{x}, \bar{x}]$ an interval vector, which is an $n \times 1$ real interval matrix. We denote by \mathbf{IR}^n the set of all real interval vectors with n components. The i -th component of $[x]$ is denoted by $[x_i]$. For an interval vector $[x] = [\underline{x}, \bar{x}]$ we denote the midpoint and the radius by $m([x])$ and $r([x])$, respectively. They are defined by

$$m([x]) := \frac{1}{2}(\underline{x} + \bar{x}), \quad r([x]) := \frac{1}{2}(\bar{x} - \underline{x}). \quad (13)$$

Let $[x], [y] \in \mathbf{IR}^n$ be given, it can be verified that

$$r([x] + [y]) = r([x]) + r([y]), \quad (14)$$

and if the intersection $[x] \cap [y]$ is not empty

$$r([x] \cap [y]) \leq \min\{r([x]), r([y])\} \quad (15)$$

We define the interval operator $\max\{0, [x]\}$ for an interval vector $[x] = [\underline{x}, \bar{x}]$ by

$$\max\{0, [x]\} = [\max\{0, \underline{x}\}, \max\{0, \bar{x}\}].$$

Notice that the operator is inclusion monotonic, i.e.,

$$[x] \subseteq [y] \Rightarrow \max\{0, [x]\} \subseteq \max\{0, [y]\}.$$

Furthermore,

$$r(\max\{0, [x]\}) \leq r([x]). \quad (16)$$

For an interval matrix $[A] \in \mathbf{IR}^{n \times n}$ we define the absolute value $\|[A]\| \in \mathbf{R}^{n \times n}$ by

$$\|[A]\| := (\max\{|\underline{a}_{ij}|, |\bar{a}_{ij}|\}).$$

For more details on interval analysis and computation we refer to [2] or [16], for example.

Let $A \in \mathbf{R}^{n \times n}$, denote by Λ and $-B$ the diagonal and off-diagonal part of A , respectively. A is called a Z-matrix if $B \geq 0$, that is each off-diagonal element of A is non-positive. A is called an M-matrix if it is a Z-matrix and has a nonnegative inverse, that is each element of A^{-1} is nonnegative. The diagonal elements of an M-matrix are positive. If A is an M-matrix and Δ is a nonnegative diagonal matrix, then $A + \Delta$ is also an M-matrix. A is called an H-matrix if the so-called comparison matrix

$$\langle A \rangle := |\Lambda| - |B|$$

is an M-matrix. The diagonal elements of an H-matrix are different from zero.

Let $f : \mathbf{R}^n \rightarrow \mathbf{R}^n$ be given, let $\hat{x} \in \mathbf{R}^n$ be arbitrary but fixed. A slope of f with respect to \hat{x} and $x \in \mathbf{R}^n$, denoted by $\delta f(\hat{x}, x)$, is an $n \times n$ matrix such that

$$f(x) - f(\hat{x}) = \delta f(\hat{x}, x)(x - \hat{x}).$$

We denote the i -th row of $\delta f(\hat{x}, x)$ by $\delta f_i(\hat{x}, x)$. Let $[x] \in \mathbf{IR}^n$ be given, let $\hat{x} \in [x]$ be fixed. An interval extension of the slope $\delta f(\hat{x}, x)$ over $[x]$, denoted by $\delta f(\hat{x}, [x])$, is an $n \times n$ interval matrix such that for any $x \in [x]$

$$f(x) - f(\hat{x}) \in \delta f(\hat{x}, [x])([x] - \hat{x}).$$

For slopes, its interval extension and their properties we refer to [2, 16], for example.

3 Error bounds for an approximate solution

In this section we study bounding a solution of $\text{NCP}(f)$ defined by (11), where $\varphi(x)$ is a tridiagonal nonlinear function. At first we give the following existence theorem, which holds for (1).

Theorem 3.1. *Let $[x] = ([x_i]) \in \mathbf{IR}^n$ be given and let $\hat{x} = (\hat{x}_i) \in [x]$ be chosen fixed. Let $D = \text{diag}(d_i) \in \mathbf{R}^{n \times n}$ be a given diagonal matrix with $d_i > 0$, $i = 1, \dots, n$. Denote by $\delta f(\hat{x}, [x]) \in \mathbf{IR}^{n \times n}$ an interval extension of the slope of f over the interval $[x]$. Define*

$$\Gamma(\hat{x}, [x], D) := \max\{0, \hat{x} - D f(\hat{x}) + (I - D \delta f(\hat{x}, [x]))([x] - \hat{x})\}. \quad (17)$$

(a) If

$$\Gamma(\hat{x}, [x], D) \subseteq [x], \quad (18)$$

then $\text{NCP}(f)$ has a solution $x^* \in \Gamma(\hat{x}, [x], D)$.

(b) If $\text{NCP}(f)$ has a solution $x^* \in [x]$, then $x^* \in \Gamma(\hat{x}, [x], D)$.

Proof The proof is omitted since it is very similar to that for Theorem 2.1 in [5]. □

We use Theorem 3.1 to construct an interval $[x]$ containing a solution of $\text{NCP}(f)$, defined by (11) and (12), that is, $f(x) = Mx + \varphi(x)$, where $M \in \mathbf{R}^{n \times n}$ is a given matrix, and $\varphi(x)$ is a given tridiagonal function. In the remainder of this paper we impose the following assumptions on the matrix M and the tridiagonal function φ .

Assumptions 3.2. Let $[z]$ be a given interval vector and let $\hat{x} = (\hat{x}_i) \in [z]$ be arbitrary but fixed. Assume that

- there exist nonnegative constants $\gamma_{i,i-1}$, $i = 2, \dots, n$, such that for $x = (x_i) \in [z]$

$$|\varphi_i(x_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, x_{i+1})| \leq \gamma_{i,i-1} |x_{i-1} - \hat{x}_{i-1}|; \quad (19)$$

- there exist nonnegative constants $\gamma_{i,i+1}$, $i = 1, \dots, n-1$, such that for $x = (x_i) \in [z]$

$$|\varphi_i(\hat{x}_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1})| \leq \gamma_{i,i+1} |x_{i+1} - \hat{x}_{i+1}|; \quad (20)$$

- there exist nonnegative constants γ_{ii} , $i = 1, \dots, n$, such that for $x = (x_i) \in [z]$ with $x_i \neq \hat{x}_i$, $i = 1, \dots, n$

$$\frac{\varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1})}{x_i - \hat{x}_i} \geq \gamma_{ii}; \quad (21)$$

- the matrix $\tilde{M} = (\tilde{m}_{ij}) \in \mathbf{R}^{n \times n}$ is an M-matrix, where \tilde{m}_{ij} is defined using $M = (m_{ij}) \in \mathbf{R}^{n \times n}$ by

$$\tilde{m}_{ij} = \begin{cases} -\gamma_{i,i+1} - |m_{i,i+1}| & \text{if } j = i + 1, \\ \gamma_{ii} + m_{ii} & \text{if } j = i, \\ -\gamma_{i,i-1} - |m_{i,i-1}| & \text{if } j = i - 1, \\ -|m_{ij}| & \text{otherwise,} \end{cases} \quad (22)$$

$i = 1, \dots, n$.

- there exist nonnegative constants γ'_{ii} , $i = 1, \dots, n$, such that for $x = (x_i) \in [z]$ with $x_i \neq \hat{x}_i$, $i = 1, \dots, n$

$$\frac{\varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1})}{x_i - \hat{x}_i} \leq \gamma'_{ii}. \quad (23)$$

Now we are going to find an interval vector $[x]$ such that the inclusion (18) holds, and as a result of Theorem 3.1, this interval vector $[x]$ contains a solution of the complementarity problem NCP(f) defined by (11) with a tridiagonal nonlinear function.

Theorem 3.3. *Let Assumptions 3.2 be fulfilled for an interval vector $[z]$, let $\tilde{M} = (\tilde{m}_{ij}) \in \mathbf{R}^{n \times n}$, be defined by (22). Let $\hat{x} = (\hat{x}_i) \in [z]$ be a given vector with $\hat{x} \geq 0$. Let $r = \tilde{M}^{-1}|M\hat{x} + \varphi(\hat{x})|$ and suppose that $[x]^0 = [\hat{x} - r, \hat{x} + r] \subseteq [z]$. Then NCP(f), defined by (11) with the tridiagonal nonlinear function φ , has a solution $x^* \in [x]^0$.*

Remark 3.4. *Since in Assumptions 3.2 it is assumed that the matrix \tilde{M} is an M-matrix, we have $\tilde{M}^{-1} \geq 0$, and therefore $r = \tilde{M}^{-1}|M\hat{x} + \varphi(\hat{x})| \geq 0$, and the interval vector $[x]^0$ in Theorem 3.3 is well defined.*

Proof. We write

$$\begin{aligned} \varphi_i(x_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1}) &= \varphi_i(x_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, x_{i+1}) \\ &\quad + \varphi_i(\hat{x}_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) \\ &\quad + \varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1}). \end{aligned}$$

Assumptions 3.2 give an interval extension of the slope $\delta\varphi(\hat{x}, x)$ of $\varphi(x)$ over $[x]^0$:

$$[\delta\varphi_1(\hat{x}, [x]^0)]_j = \begin{cases} [\gamma_{11}, \gamma'_{11}] & \text{if } j = 1, \\ [-\gamma_{12}, \gamma_{12}] & \text{if } j = 2, \\ 0 & \text{if } j > 2; \end{cases}$$

$$[\delta\varphi_i(\hat{x}, [x]^0)]_j = \begin{cases} [-\gamma_{i,i-1}, \gamma_{i,i-1}] & \text{if } j = i - 1, \\ [\gamma_{ii}, \gamma'_{ii}] & \text{if } j = i, \\ [-\gamma_{i,i+1}, \gamma_{i,i+1}] & \text{if } j = i + 1, \\ 0 & \text{otherwise,} \end{cases}$$

where $i = 2, \dots, n - 1$;

$$[\delta\varphi_n(\hat{x}, [x]^0)]_j = \begin{cases} 0 & \text{if } j < n - 1, \\ [-\gamma_{n,n-1}, \gamma_{n,n-1}] & \text{if } j = n - 1, \\ [\gamma_{nn}, \gamma'_{nn}] & \text{if } j = n. \end{cases}$$

From this we obtain an interval extension $\delta f(\hat{x}, [x]^0)$ of the slope of $f(x)$ over $[x]^0$:

$$[\delta f_1(\hat{x}, [x]^0)]_j = \begin{cases} m_{11} + [\gamma_{11}, \gamma'_{11}] & \text{if } j = 1, \\ m_{12} + [-\gamma_{12}, \gamma_{12}] & \text{if } j = 2, \\ m_{1j} & \text{otherwise,} \end{cases}$$

$$[\delta f_i(\hat{x}, [x]^0)]_j = \begin{cases} m_{i,i-1} + [-\gamma_{i,i-1}, \gamma_{i,i-1}] & \text{if } j = i-1, \\ m_{ii} + [\gamma_{ii}, \gamma'_{ii}] & \text{if } j = i, \\ m_{i,i+1} + [-\gamma_{i,i+1}, \gamma_{i,i+1}] & \text{if } j = i+1, \\ m_{ij} & \text{otherwise,} \end{cases}$$

for $i = 2, \dots, n-1$;

$$[\delta f_n(\hat{x}, [x]^0)]_j = \begin{cases} m_{n,n-1} + [-\gamma_{n,n-1}, \gamma_{n,n-1}] & \text{if } j = n-1, \\ m_{nn} + [\gamma_{nn}, \gamma'_{nn}] & \text{if } j = n, \\ m_{nj} & \text{otherwise.} \end{cases}$$

For later use we set

$$[\Delta]^0 = [\underline{\Delta}^0, \overline{\Delta}^0] = \delta f(\hat{x}, [x]^0). \quad (24)$$

Set $D = \text{diag}((m_{ii} + \gamma'_{ii})^{-1})$, $i = 1, \dots, n$. Then we have

$$|I - D \delta f(\hat{x}, [x]^0)|_{1j} = \begin{cases} 1 - d_1(m_{11} + \gamma_{11}) & \text{if } j = 1, \\ d_1(|m_{12}| + \gamma_{12}) & \text{if } j = 2, \\ d_1|m_{1j}| & \text{otherwise;} \end{cases}$$

$$|I - D \delta f(\hat{x}, [x]^0)|_{ij} = \begin{cases} d_i(|m_{i,i-1}| + \gamma_{i,i-1}) & \text{if } j = i-1, \\ 1 - d_i(m_{ii} + \gamma_{ii}) & \text{if } j = i, \\ d_i(|m_{i,i+1}| + \gamma_{i,i+1}) & \text{if } j = i+1, \\ d_i|m_{ij}| & \text{otherwise,} \end{cases}$$

for $i = 2, \dots, n-1$;

$$|I - D \delta f(\hat{x}, [x]^0)|_{nj} = \begin{cases} d_n(|m_{n,n-1}| + \gamma_{n,n-1}) & \text{if } j = n-1, \\ 1 - d_n(m_{nn} + \gamma_{nn}) & \text{if } j = n, \\ d_n|m_{nj}| & \text{otherwise.} \end{cases}$$

Now we have

$$|I - D \delta f(\hat{x}, [x]^0)| = |I - D \langle \delta f(\hat{x}, [x]^0) \rangle|.$$

From (22) we know that $\langle \delta f(\hat{x}, [x]^0) \rangle = \tilde{M}$, where $\underline{\delta f(\hat{x}, [x]^0)}$ denotes the lower bound of the interval matrix $\delta f(\hat{x}, [x]^0)$. Therefore we have

$$|I - D \delta f(\hat{x}, [x]^0)| = |I - D\tilde{M}| = D(D^{-1} - \tilde{M}).$$

We use this relation to verify the inclusion (18). Let

$$\Gamma(\hat{x}, [x]^0, D) = [\underline{\Gamma(\hat{x}, [x]^0, D)}, \overline{\Gamma(\hat{x}, [x]^0, D)}]$$

for (17). Then we have

$$\begin{aligned} \underline{\Gamma(\hat{x}, [x]^0, D)} &= \max\{0, \hat{x} - D(M\hat{x} + \varphi(\hat{x})) - |I - D\delta f(\hat{x}, [x]^0)|r\} \\ &= \max\{0, \hat{x} - D(M\hat{x} + \varphi(\hat{x})) - D(D^{-1} - \tilde{M})r\}, \\ \overline{\Gamma(\hat{x}, [x]^0, D)} &= \max\{0, \hat{x} - D(M\hat{x} + \varphi(\hat{x})) + |I - D\delta f(\hat{x}, [x]^0)|r\} \\ &= \max\{0, \hat{x} - D(M\hat{x} + \varphi(\hat{x})) + D(D^{-1} - \tilde{M})r\}. \end{aligned}$$

From $r = \tilde{M}^{-1}|M\hat{x} + \varphi(\hat{x})|$, we obtain $\tilde{M}r = |M\hat{x} + \varphi(\hat{x})|$, so $\tilde{M}r \geq M\hat{x} + \varphi(\hat{x})$, and so

$$-D(M\hat{x} + \varphi(\hat{x})) - D(D^{-1} - \tilde{M})r \geq -r.$$

From this we achieve

$$\hat{x} - D(M\hat{x} + \varphi(\hat{x})) - D(D^{-1} - \tilde{M})r \geq \hat{x} - r,$$

therefore

$$\begin{aligned} \underline{\Gamma(\hat{x}, [x]^0, D)} &= \max\{0, \hat{x} - D(M\hat{x} + \varphi(\hat{x})) - D(D^{-1} - \tilde{M})r\} \\ &\geq \hat{x} - D(M\hat{x} + \varphi(\hat{x})) - D(D^{-1} - \tilde{M})r \\ &\geq \hat{x} - r. \end{aligned}$$

In a similar way we can show that

$$\hat{x} - D(M\hat{x} + \varphi(\hat{x})) + D(D^{-1} - \tilde{M})r \leq \hat{x} + r,$$

which, together with the fact that $\hat{x} + r \geq 0$, yields

$$\begin{aligned} \overline{\Gamma(\hat{x}, [x]^0, D)} &= \max\{0, \hat{x} - D(M\hat{x} + \varphi(\hat{x})) + D(D^{-1} - \tilde{M})r\} \\ &\leq \hat{x} + r. \end{aligned}$$

Therefore $\Gamma(\hat{x}, [x]^0, D) \subseteq [x]^0 = [\hat{x} - r, \hat{x} + r]$. From Theorem 3.1 it follows that $\text{NCP}(f)$ has a solution x^* in $[x]^0$. \square

Remark 3.5. For the linear complementarity problem, that is, for the problem $\text{NCP}(f)$, where $f(x) = Mx + q$, $M \in \mathbf{R}^{n \times n}$ and $q \in \mathbf{R}^n$ is a constant vector, Assumptions 3.2 are fulfilled if M is an H -matrix with positive diagonal elements. Hence, Theorem 3.3 delivers for this problem the error estimation

$$|\hat{x} - x^*| \leq \langle M \rangle^{-1} |M\hat{x} + q|. \quad (25)$$

In [9] Chen and Xiang gave an error bound for this linear complementarity problem

$$\|\hat{x} - x^*\|_p \leq \|\max\{I, D\} \langle M \rangle^{-1}\|_p \|\min\{\hat{x}, M\hat{x} + q\}\|_p. \quad (26)$$

It is not easy to compare these bounds theoretically. On the other hand, it is clear that the right hand side of (26) approaches zero if \hat{x} approaches x^* , which is not the case for (25). However, note that (25) is a componentwise error bound, whereas in (26) the norm of $\hat{x} - x^*$ is bounded.

4 Improving the error bound

In this section we give an iterative method for improving the enclosure of x^* given by $[x]^0$ of Theorem 3.3.

Algorithm 4.1. Let f be defined by (11). Let $\hat{x} \geq 0$ be given. Let Assumptions 3.2 be fulfilled. Let \tilde{M} be defined by (22). Let $[x]^0 \in \mathbf{IR}^n$ be given by

$$[x]^0 := [\hat{x} - r, \hat{x} + r] \quad \text{with} \quad r = \tilde{M}^{-1} |M\hat{x} + \varphi(\hat{x})|.$$

Let $[\Delta]^0 = [\underline{\Delta}^0, \overline{\Delta}^0]$ be defined by (24) for the interval vector $[x]^0$, and set $k := 0$. Denote by $m([x]^k)$ the midpoint of the interval vector $[x]^k$, $k = 0, \dots$ (see (13)).

Step 1 Let $[\Delta]^k = [\underline{\Delta}^k, \overline{\Delta}^k]$ be defined analogously to (24) for the interval vector $[x]^k$;

Step 2 Set $D^k := \text{diag}(\frac{1}{\Delta_{11}^k}, \frac{1}{\Delta_{22}^k}, \dots, \frac{1}{\Delta_{nn}^k})$;

Step 3 Generate a sequence $\{[x]^k\}_{k=0}^\infty$ of interval vectors by the method

$$[x]^{k+1} := \Gamma(m([x]^k), [x]^k, D^k) \cap [x]^k, \quad (27)$$

where $\delta f(m([x]^k), [x]^k) = [\underline{\Delta}^k, \overline{\Delta}^k]$ and $\Gamma(m([x]^k), [x]^k, D^k)$ is defined by (17);

Step 4 Set $k := k + 1$ and go to Step 1.

Remark 4.2. Since the matrix \tilde{M} , defined by (22) is assumed to be an M -matrix, its diagonal elements are positive. Therefore also the diagonal elements of $\overline{\Delta}^k$ are positive, and Step 2 of Algorithm 4.1 is well defined.

Remark 4.3. Since $[x]^0$ contains a solution x^* of $\text{NCP}(f)$, from Theorem 3.1 it follows

$$[x]^{k+1} = \Gamma(m([x]^k), [x]^k, D^k) \cap [x]^k \neq \emptyset.$$

Theorem 4.4. *Let the assumptions of Theorem 3.3 be fulfilled. Let $\{[x]^k\}_{k=0}^\infty$ be the sequence generated by Algorithm 4.1. Assume that for the interval matrix $[\Delta]^k$ from Step 1 it holds*

$$[\Delta]^k \subseteq [\Omega] := [\underline{\Omega}, \overline{\Omega}], \quad k = 1, 2, \dots, \quad (28)$$

and assume that $\underline{\Omega}$ and $\overline{\Omega}$ are H-matrices, whose diagonal elements are all positive. Then

- (a) the problem $\text{NCP}(f)$ has a solution x^* which is contained in each $[x]^k$, $k = 0, 1, \dots$;
- (b) $\{[x]^k\}_{k=0}^\infty$ is nested, that is $[x]^0 \supseteq [x]^1 \supseteq \dots \supseteq [x]^k \supseteq \dots$;
- (c) $\{[x]^k\}_{k=0}^\infty \rightarrow x^*$;
- (d) for each $[x]^k$, we have for the approximate solution $x^k := m([x]^k)$ the error bound

$$|x^k - x^*| \leq r([x]^k).$$

Remark 4.5. *The relation (28) can be fulfilled if f' has an interval arithmetic evaluation over $[x]^0$.*

Proof. (a): Theorem 3.3 guarantees that the problem $\text{NCP}(f)$ has a solution x^* in $[x]^0$. From (b) of Theorem 3.1 it follows that for each $k = 0, 1, \dots$, we have $x^* \in [x]^k$.

(b): The result follows directly from the iterative formula (27) given in Algorithm 4.1.

(c): Denote by $r([x]^k)$ the radius of the interval vector $[x]^k$ (see (13)). From (14), (15), (16) and (17) we have

$$\begin{aligned} r([x]^{k+1}) &= r(\Gamma(m([x]^k), [x]^k, D^k) \cap [x]^k) \\ &\leq r(\Gamma(m([x]^k), [x]^k, D^k)) \\ &= r((I - D^k \delta f(m([x]^k), [x]^k))([x]^k - m([x]^k))) \\ &= r((I - D^k [\underline{\Delta}^k, \overline{\Delta}^k])([x]^k - m([x]^k))) \\ &\leq |I - D^k [\underline{\Delta}^k, \overline{\Delta}^k]| r([x]^k), \end{aligned}$$

where $\delta f(m([x]^k), [x]^k) = [\underline{\Delta}^k, \overline{\Delta}^k]$, D^k is the inverse of the diagonal part of $\overline{\Delta}^k$. From the assumptions of the theorem we have:

$$[\Delta]^k \subseteq [\Omega] := [\underline{\Omega}, \overline{\Omega}].$$

Denote by $[\tilde{D}] = \text{diag}([\overline{\Omega}_{ii}^{-1}, \underline{\Omega}_{ii}^{-1}])$. From the choice of D^k , we know $D^k \in [\tilde{D}]$. We obtain the relation

$$I - D^k [\underline{\Delta}^k, \overline{\Delta}^k] \subseteq I - [\tilde{D}][\Omega].$$

Therefore we have the further estimation of the radius $r([x]^{k+1})$:

$$\begin{aligned} r([x]^{k+1}) &\leq |I - D^k [\underline{\Delta}^k, \overline{\Delta}^k]| r([x]^k) \\ &\leq |I - [\tilde{D}][\Omega]| r([x]^k). \end{aligned}$$

From the assumptions of this theorem we know that each matrix in $[\Omega]$ is an H-matrix whose diagonal elements are positive. Hence, we have $\rho(|I - [\tilde{D}][\Omega]|) < 1$ (see [4]).

(d): The result is straightforward. \square

5 Application and numerical experiments

In this section we move on to application of Algorithm 4.1 to the complementarity problems $\text{NCP}(f)$, where $f(x) = Mx + \varphi(x)$, M is defined by (5), and $\varphi(x)$ is defined by (8) or by (10), respectively. This problem arises from approximating the solution of the free boundary problem given in Example 1.1 and Example 1.2, respectively.

5.1 Study of Example 1.1

For the free boundary problem formulated in Example 1.1 we make the following assumptions.

Assumptions 5.1. Assume that $\partial g_2(t, s)$ is continuous with respect to s , and assume that there exist nonnegative constants $\underline{\gamma}$ and $\overline{\gamma}$ such that

$$0 \leq \underline{\gamma} \leq \partial_2 g(t, s) \leq \overline{\gamma} \quad \text{for all } (t, s) \in [0, 1] \times \mathbf{R},$$

where $\partial_2 g(t, s)$ means the partial derivative with respect to the second variable.

Let the tridiagonal mapping $\varphi(x) = (\varphi_i(x_{i-1}, x_i, x_{i+1}))$ be defined by (8). From the mean value theorem and Assumption 5.1 we know that

- there are $\xi_{i-1} \in (\min\{\hat{x}_{i-1}, x_{i-1}\}, \max\{\hat{x}_{i-1}, x_{i-1}\})$, such that

$$\begin{aligned} & |\varphi_i(x_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, x_{i+1})| \\ &= \frac{1}{12}h^2|g(t_{i-1}, x_{i-1}) - g(t_{i-1}, \hat{x}_{i-1})| \\ &= \frac{1}{12}h^2|\partial g_2(t_{i-1}, \xi_{i-1})||x_{i-1} - \hat{x}_{i-1}| \leq \frac{1}{12}\bar{\gamma}h^2|x_{i-1} - \hat{x}_{i-1}|; \end{aligned}$$

- there are $\zeta_{i+1} \in (\min\{\hat{x}_{i+1}, x_{i+1}\}, \max\{\hat{x}_{i+1}, x_{i+1}\})$, such that

$$\begin{aligned} & |\varphi_i(\hat{x}_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1})| \\ &= \frac{1}{12}h^2|g(t_{i+1}, x_{i+1}) - g(t_{i+1}, \hat{x}_{i+1})| \\ &= \frac{1}{12}h^2|\partial g_2(t_{i+1}, \zeta_{i+1})||x_{i+1} - \hat{x}_{i+1}| \leq \frac{1}{12}\bar{\gamma}h^2|x_{i+1} - \hat{x}_{i+1}|; \end{aligned}$$

- there are $\varsigma_i \in (\min\{\hat{x}_i, x_i\}, \max\{\hat{x}_i, x_i\})$, such that

$$\begin{aligned} & \frac{\varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1})}{x_i - \hat{x}_i} \\ &= \frac{1}{12}h^2 \frac{10g(t_i, x_i) - 10g(t_i, \hat{x}_i)}{x_i - \hat{x}_i} = \frac{5}{6}h^2\partial g_2(t_i, \varsigma_i) \geq \frac{5}{6}\underline{\gamma}h^2; \end{aligned}$$

- and

$$\frac{\varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1})}{x_i - \hat{x}_i} = \frac{5}{6}h^2\partial g_2(t_i, \varsigma_i) \leq \frac{5}{6}\bar{\gamma}h^2.$$

That is, (19), (20), (21) and (23) are fulfilled with

$$\begin{aligned} \gamma_{i,i-1} &= \frac{1}{12}h^2\bar{\gamma}, & i &= 2, \dots, n \\ \gamma_{i,i+1} &= \frac{1}{12}h^2\bar{\gamma}, & i &= 1, \dots, n-1 \\ \gamma_{ii} &= \frac{5}{6}h^2\underline{\gamma} & i &= 1, \dots, n \\ \gamma'_{ii} &= \frac{5}{6}h^2\bar{\gamma} & i &= 1, \dots, n. \end{aligned}$$

Furthermore, the elements \tilde{m}_{ij} of the matrix $\tilde{M} = (\tilde{m}_{ij}) \in \mathbf{R}^{n \times n}$, defined by (22) have the following form

$$\tilde{m}_{ij} = \begin{cases} -\frac{1}{12}h^2\bar{\gamma} - 1 & \text{if } j = i + 1, \\ \frac{5}{6}h^2\underline{\gamma} + 2 & \text{if } j = i, \\ -\frac{1}{12}h^2\bar{\gamma} - 1 & \text{if } j = i - 1, \\ 0 & \text{otherwise,} \end{cases}$$

$i = 1, \dots, n$. \tilde{M} is a symmetric Z-matrix, therefore it is a Stieltjes matrix if it is positive definite. See Definition 3.4 in [19]. By Corollary 3. in Section 3.5 of [19] it then is an M-matrix. By Theorem 1.7 in [19], \tilde{M} is positive definite if

$$5\underline{\gamma} \geq \bar{\gamma}. \quad (29)$$

Therefore, Assumptions 3.2 hold under Assumptions 5.1 and under the conditions (29). Consequently, under Assumptions 5.1 and under the conditions (29), we can apply Algorithm 4.1 to problem NCP(f), defined by (6), (7) and (8), which comes from the free boundary problem (4). We illustrate this by the following problem.

Consider finding a function $u(t) : [0, 1] \rightarrow \mathbf{R}_+$ such that

$$\begin{cases} u''(t) &= \frac{1}{2} + \frac{3}{t+2} + \arctan(u(t)) + 2u(t) & t \in \mathbf{D}_+, \\ u(0) &= 0.35, \\ u(1) &= 0.15, \end{cases}$$

where the set $\mathbf{D}_+ := \{t \in (0, 1) : u(t) > 0\}$ is unknown.

It is clear that Assumptions 5.1 hold with $\underline{\gamma} = 2$ and $\bar{\gamma} = 3$. We choose $n = 99$, and so the condition (29) is fulfilled:

$$5\underline{\gamma} = 10 > 3 = \bar{\gamma}.$$

We can apply Theorem 3.3 and Algorithm 4.1 to the nonlinear complementarity problem NCP(f), where $f(x) = Mx + \varphi(x)$, $M \in \mathbf{R}^{99 \times 99}$ is defined by (5), and $\varphi(x) = (\varphi_i(x_{i-1}, x_i, x_{i+1}))$ is defined by

$$\begin{aligned} \varphi_i(x_{i-1}, x_i, x_{i+1}) &= \frac{1}{12} h^2 \left\{ \left(\frac{1}{2} + \frac{3}{t_{i-1} + 2} + \arctan(x_{i-1}) + 2x_{i-1} \right) \right. \\ &+ 10 \left(\frac{1}{2} + \frac{3}{t_i + 2} + \arctan(x_i) + 2x_i \right) \\ &\left. + \left(\frac{1}{2} + \frac{3}{t_{i+1} + 2} + \arctan(x_{i+1}) + 2x_{i+1} \right) \right\} \end{aligned}$$

$i = 1, \dots, 99$, with $x_0 = 0.35$, $x_{100} = 0.15$, $t_i = ih$. We code Algorithm 4.1 with Intlab 5.3 (see [18]) and terminate the algorithm when

$$\|r([x]^{k+1})\|_\infty \leq \epsilon \|r([x]^k)\|_\infty \quad \text{for } \epsilon = 10^{-5}. \quad (30)$$

We take the midpoint of $[x]^{k+1}$ as numerical approximation to x^* and plot it in Figure 1.

Figure 1

From Figure 1 we conclude that $\mathbf{D}_+ := \{t \in (0, 1) : u(t) > 0\} \approx (0, 0.35] \cup [0.7, 1)$. (Note, however, that we have not taken into account the discretization error.)

5.2 Study of Example 1.2

For the free boundary problem formulated in Example 1.2 we make the following assumptions.

Assumptions 5.2. Assume that $\partial g_2(t, s, \nu)$ is continuous with respect to s , and that there exist nonnegative constants $\underline{\gamma}$ and τ such that

$$\left. \begin{aligned} \partial_2 g(t, s, \nu) &\geq \underline{\gamma} \\ |\partial_3 g(t, s, \nu)| &\leq \tau \end{aligned} \right\} \quad \text{for all } (t, s, \nu) \in [0, 1] \times \mathbf{R} \times \mathbf{R},$$

where $\partial_2 g(t, s, \nu)$ and $\partial_3 g(t, s, \nu)$ mean the partial derivatives with respect to the second and the third variable, respectively.

Let the tridiagonal mapping $\varphi(x) = (\varphi_i(x_{i-1}, x_i, x_{i+1}))$ be defined by (10). From the mean value theorem and Assumptions 5.2 we know that:

- there are $\xi_{i-1} \in (\min\{\hat{x}_{i-1}, x_{i-1}\}, \max\{\hat{x}_{i-1}, x_{i-1}\})$, such that

$$\begin{aligned}
& |\varphi_i(x_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, x_{i+1})| \\
&= |h^2 g(t_i, x_i, \frac{x_{i+1} - x_{i-1}}{2h}) - h^2 g(t_i, x_i, \frac{x_{i+1} - \hat{x}_{i-1}}{2h})| \\
&= \frac{h}{2} |\partial g_3(t_i, x_i, \frac{x_{i+1} - \xi_{i-1}}{2h})| |x_{i-1} - \hat{x}_{i-1}| \\
&\leq \frac{h}{2} \tau |x_{i-1} - \hat{x}_{i-1}|;
\end{aligned}$$

- there are $\zeta_{i+1} \in (\min\{\hat{x}_{i+1}, x_{i+1}\}, \max\{\hat{x}_{i+1}, x_{i+1}\})$, such that

$$\begin{aligned}
& |\varphi_i(\hat{x}_{i-1}, x_i, x_{i+1}) - \varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1})| \\
&= |h^2 g(t_i, x_i, \frac{x_{i+1} - \hat{x}_{i-1}}{2h}) - h^2 g(t_i, x_i, \frac{\hat{x}_{i+1} - \hat{x}_{i-1}}{2h})| \\
&= \frac{h}{2} |\partial g_3(t_i, x_i, \frac{\zeta_{i+1} - \hat{x}_{i-1}}{2h})| |x_{i+1} - \hat{x}_{i+1}| \\
&\leq \frac{h}{2} \tau |x_{i+1} - \hat{x}_{i+1}|;
\end{aligned}$$

- and there are $\varsigma_i \in (\min\{\hat{x}_i, x_i\}, \max\{\hat{x}_i, x_i\})$, such that

$$\begin{aligned}
& \frac{\varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1})}{x_i - \hat{x}_i} \\
&= h^2 \frac{g(t_i, x_i, \frac{\hat{x}_{i+1} - \hat{x}_{i-1}}{2h}) - g(t_i, \hat{x}_i, \frac{\hat{x}_{i+1} - \hat{x}_{i-1}}{2h})}{x_i - \hat{x}_i} \\
&= h^2 \partial g_2(t_i, \varsigma_i, \frac{\hat{x}_{i+1} - \hat{x}_{i-1}}{2h}) \\
&\geq h^2 \underline{\gamma}.
\end{aligned}$$

That is, (19), (20) and (21) are fulfilled with

$$\begin{aligned}
\gamma_{i,i-1} &= \frac{1}{2} h \tau, & i = 2, \dots, n \\
\gamma_{i,i+1} &= \frac{1}{2} h \tau, & i = 1, \dots, n-1 \\
\gamma_{ii} &= h^2 \underline{\gamma} & i = 1, \dots, n.
\end{aligned}$$

In order to fulfill (23), we proceed as follows: we compute the vector $r = \tilde{M}^{-1} |M\hat{x} + \varphi(\hat{x})|$, and $[x]^0 = [\hat{x} - r, \hat{x} + r]$ from Theorem 3.3. Then we set $[z] = [x]^0$. Since $\partial g_2(t, s, \nu)$ is bounded by some nonnegative constant, say $\bar{\gamma}$ on a compact set, we obtain

$$\frac{\varphi_i(\hat{x}_{i-1}, x_i, \hat{x}_{i+1}) - \varphi_i(\hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1})}{x_i - \hat{x}_i} = h^2 \partial g_2(t_i, \varsigma_i, \frac{\hat{x}_{i+1} - \hat{x}_{i-1}}{2h}) \leq h^2 \bar{\gamma}.$$

Therefore we define $\gamma'_{ii} = h^2\bar{\gamma}$, $i = 1, \dots, n$, for this example and (23) holds.

Furthermore, the elements \tilde{m}_{ij} of the matrix $\tilde{M} = (\tilde{m}_{ij}) \in \mathbf{R}^{n \times n}$, defined by (22) have the following form

$$\tilde{m}_{ij} = \begin{cases} -\frac{1}{2}h\tau - 1 & \text{if } j = i + 1, \\ h^2\bar{\gamma} + 2 & \text{if } j = i, \\ -\frac{1}{2}h\tau - 1 & \text{if } j = i - 1, \\ 0 & \text{otherwise,} \end{cases}$$

$i = 1, \dots, n$. Again, if

$$\frac{\tau}{\bar{\gamma}} \leq h = \frac{1}{n+1}, \quad (31)$$

then \tilde{M} is an M-matrix. We apply Theorem 3.3 and Algorithm 4.1 to problem $\text{NCP}(f)$, defined by (6), (7) and (10), which comes from the free boundary problem (9).

Remark 5.3. *The stepsize limitation (31) is dependent on the constants τ and $\bar{\gamma}$. In the limiting case that the right hand side of the differential equation in Example 1.2 is independent on the derivative u' , there is no limitation with respect to h . Otherwise the lower bound for h is given by the relation of τ and $\bar{\gamma}$.*

To be specific, we consider finding a function $u(t) : [0, 1] \rightarrow \mathbf{R}_+$ such that

$$\begin{cases} u''(t) &= \frac{1}{2} + \frac{3}{t+2} + \frac{1}{2}u(t)^3 + 100u(t) + \frac{1}{10}u'(t) & t \in \mathbf{D}_+, \\ u(0) &= 0.3, \\ u(1) &= 0.6, \end{cases}$$

where the set $\mathbf{D}_+ := \{t \in (0, 1) : u(t) > 0\}$ is unknown.

It is clear that Assumptions 5.2 hold with $\bar{\gamma} = 100$ and $\tau = 0.1$. We choose $n = 99$, and so h satisfies the restrictions (31):

$$10^{-3} = \frac{\tau}{\bar{\gamma}} < h = \frac{1}{n+1} = \frac{1}{100}.$$

We apply Algorithm 4.1 to the nonlinear complementarity problem $\text{NCP}(f)$, where $f(x) = Mx + \varphi(x)$, $M \in \mathbf{R}^{99 \times 99}$ is defined by (5), and $\varphi(x) = (\varphi_i(x_{i-1}, x_i, x_{i+1}))$ is defined by

$$\varphi_i(x_{i-1}, x_i, x_{i+1}) = \frac{1}{2}h^2 + \frac{3}{t_i+2}h^2 + \frac{1}{2}h^2x_i^3 + 100h^2x_i + \frac{1}{20}h(x_{i+1} - x_{i-1}),$$

$i = 1, \dots, 99$, with $x_0 = 0.3$, $x_{100} = 0.6$, $t_i = ih$. We terminate the algorithm by criteria (30). We take the midpoint of $[x]^{k+1}$ as numerical approximation to x^* and plot it in Figure 2.

Figure 2

From Figure 2 we conclude that $\mathbf{D}_+ := \{t \in (0, 1) : u(t) > 0\} \approx (0, 0.32] \cup [0.6, 1)$.

6 Final remarks

The iterative method (27) may be considered to be a kind of Jacobi-method. It is also possible to use the idea of the so-called Gauss-Seidel-method. We omit the necessary details for the modification of Algorithm 4.1 and mention without proof that Theorem 4.4 holds also for the Gauss-Seidel modification (see [20] for the case of linear complementarity problems). From practical experience we can conclude that in general it delivers much tighter enclosures than the Jacobi-method if both are started with the same enclosure $[x]^0$. In our examples we had to perform approximately 50% steps less, compared with the total step method, if the same stopping criterion was used.

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