Verified Numerical Computation for Nonlinear Equations

Goetz Alefeld

University of Karlsruhe
Kaiserstrasse 12, 76131 Karlsruhe, Germany
E-mail: goetz.alefeld@math.uni-karlsruhe.de

> After the introduction basic properties of interval arithmetic are discussed and different approaches are repeated by which one can compute verified numerical approximations for a solution of a nonlinear equation.

> *Key words*: fixed point iteration, Newton-like methods, nonsmooth equation

1. Introduction

In this paper we give a survey of existing methods for the verified solution of nonlinear (systems) of equations. We start by explaining the fundamental ideas: If we use one of the well known iterative methods, like Newton's method, then we have to stop after a finite number of steps getting an approximation $\hat{x}$ to a solution x^* of the given system. Of course, without any further preinformation we have to decide whether there exists a solution x^* at all. Furthermore, $\hat{x}$ is in general without any value if we are not in the position to compute bounds for the distance between $\hat{x}$ and x^*. Since all computation is done on a computer, usually working in a floating point system, we have also to take into account rounding errors. Combining all the necessary steps for these ideas we arrive at what is nowadays called verified computation of solutions of (nonlinear) systems.

Subsequently, we present several different fundamental ideas, which have been developed in the past. Our methods are based on interval arithmetic tools. There exists a great variety of such methods (see [6], [13], e.g.). The purpose of this article consists in discussing the main principles of verifying methods for nonlinear systems. Therefore, we limit ourselves to only a few methods.

The paper is organized as follows: In the next section we introduce the notations and basic properties of interval arithmetic. Section 3 consists of three parts. In part 3.1 we consider the fixed point iteration and discuss some properties. Part 3.2 is concerned with Newton-like methods and their application to verifying solutions of nonlinear systems. In part 3.3 we do not assume differentiability of the mapping under consideration. Using the slope we can derive similar results as those obtained in part 3.2 for smooth mappings. We close with a final remark concerning the software needed for the verifying process.

Most parts of this paper contain well known results which have already been published in scientific journals or in other survey articles. Especially, we refer to the joint paper with G. Mayer [7].

2. Basics

We start by repeating some definitions, notations and basic facts.

Let $[a] = [\underline{a}, \overline{a}]$, $b = [\underline{b}, \overline{b}]$ be real compact intervals and $\circ$ one of the basic operations "addition," "subtraction," "multiplication" and "division," respectively, for real numbers, that is $\circ \in \{+, -, \cdot, /\}$. Then we define the corresponding operations for intervals $[a]$ and $[b]$ by

$$[a] \circ [b] = \{a \circ b \mid a \in [a], \ b \in [b]\}, \tag{1}$$

where we assume $0 \notin [b]$ in case of division.

It is easy to prove that the set $I(\mathbb{R})$ of real compact intervals is closed with respect to these operations. What is even more important is the fact that $[a] \circ [b]$ can be represented by using only the bounds of $[a]$ and $[b]$. The following rules hold:

$$\begin{aligned}
[a] + [b] &= [\underline{a} + \underline{b}, \overline{a} + \overline{b}], \\
[a] - [b] &= [\underline{a} - \overline{b}, \overline{a} - \underline{b}], \\
[a] \cdot [b] &= [\min\{\underline{a}\underline{b}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b}\}, \max\{\underline{a}\underline{b}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b}\}].
\end{aligned}$$

If we define

$$\frac{1}{[b]} = \left\{ \frac{1}{b} \ \middle| \ b \in [b] \right\}, \quad \text{if } 0 \notin [b],$$

then

$$[a]/[b] = [a] \cdot \frac{1}{[b]}.$$

If $\underline{a} = \overline{a}$, i.e., if $[a]$ consists only of the element a, then we identify the real number a with the degenerate interval $[a, a]$ keeping the real notation, i.e., $a \equiv [a, a]$. In this way one recovers at once the real numbers $\mathbb{R}$ and the corresponding real arithmetic when restricting $I(\mathbb{R})$ to the set of degenerate real intervals equipped with the arithmetic defined in (1). Unfortunately, $(I(\mathbb{R}), +, \cdot)$ is neither a field nor a ring. The structures $(I(\mathbb{R}), +)$ and $(I(\mathbb{R})/\{0\}, \cdot)$ are commutative semigroups with the neutral elements 0 and 1, respectively, but they are not groups. A nondegenerate interval $[a]$ has no inverse with respect to addition or multiplication. Even the distributive law has to be replaced by the so-called subdistributivity

$$[a]([b] + [c]) \subseteq [a][b] + [a][c]. \tag{2}$$

The simple example $[-1, 1](1 + (-1)) = 0 \subset [-1, 1] \cdot 1 + [-1, 1] \cdot (-1) = [-2, 2]$ illustrates (2) and shows that $-[-1, 1]$ is certainly not the inverse of $[-1, 1]$ with respect to $+$. It is worth noticing that equality holds in (2) in some important particular cases, for instance if $[a]$ is degenerate or if $[b]$ and $[c]$ lie on the same side with respect to 0.

From (1) it follows immediately that the introduced operations for intervals are inclusion monotone in the following sense:

$$[a] \subseteq [c], \ [b] \subseteq [d] \implies [a] \circ [b] \subseteq [c] \circ [d]. \tag{3}$$

Standard interval functions $\varphi \in F = \{\sin, \cos, \tan, \arctan, \exp, \ln, \mathrm{abs}, \mathrm{sqr}, \mathrm{sqrt}\}$ are defined via their range, i.e.,

$$\varphi([x]) = \{\varphi(x) \mid x \in [x]\}. \tag{4}$$

Apparently, they are extensions of the corresponding real functions. These real functions are continuous and piecewise monotone on any compact subinterval of their domain of definition. Therefore, the values $\varphi([x])$ can be computed directly from the values at the bounds of $[x]$ and from selected constants such as 0 in the case of the square, or -1, 1 in the case of sine and cosine. It is obvious that the standard interval functions are inclusion monotone, i.e., they satisfy

$$[x] \subseteq [y] \implies \varphi([x]) \subseteq \varphi([y]). \tag{5}$$

Let $f \colon D \subseteq \mathbb{R} \to \mathbb{R}$ be given by a mathematical expression $f(x)$ which is composed by finitely many elementary operations $+, -, \cdot, /$ and standard functions $\varphi \in F$. If one replaces the variable x by an interval $[x] \subseteq D$ and if one can evaluate the resulting interval expression following the rules in (1) and (4) then one gets again an interval. It is denoted by $f([x])$ and as usually called (an) interval arithmetic evaluation of f over $[x]$. For simplicity and without mentioning it separately we assume that $f([x])$ exists whenever it occurs in the paper. From (3) and (5) the interval arithmetic evaluation turns out to be inclusion monotone, i.e.,

$$[x] \subseteq [y] \implies f([x]) \subseteq f([y]) \tag{6}$$

holds. In particular, $f([x])$ exists whenever $f([y])$ does for $[y] \supseteq [x]$. From (6) we obtain

$$x \in [x] \implies f(x) \in f([x]), \tag{7}$$

whence

$$R(f \colon [x]) \subseteq f([x]). \tag{8}$$

Here $R(f \colon [x])$ denotes the range of f over $[x]$.

Relation (8) is the fundamental property on which nearly all applications of interval arithmetic are based. It is important to stress what (8) really is delivering: Without any further assumptions it is possible to compute lower and upper bounds for the range over an interval by using only the bounds of the given interval.

In order to measure the distance between two intervals we introduce the so-called Hausdorff distance $q(\,\cdot\,,\,\cdot\,)$ with which $I(\mathbb{R})$ is a complete metric space: Let $[a] = [\underline{a}, \overline{a}]$, $[b] = [\underline{b}, \overline{b}]$, then

$$q([a], [b]) = \max\{|\underline{a} - \underline{b}|, |\overline{a} - \overline{b}|\}. \tag{9}$$

Furthermore, we use

$$\check{a} = \frac{1}{2}(\underline{a} + \overline{a}),$$
$$d(a) = \overline{a} - \underline{a},$$
$$|[a]| = \max\{|a| \mid a \in [a]\} = \max\{|\underline{a}|, |\overline{a}|\}, \tag{10}$$
$$\langle[a]\rangle = \min\{|a| \mid a \in [a]\} = \begin{cases} 0, & \text{if } 0 \in [a], \\ \min\{|\underline{a}|, |\overline{a}|\}, & \text{if } 0 \notin [a] \end{cases}$$

and call $\check{a}$ center, $d[a]$ diameter and $|[a]|$ absolute value of $[a]$.

In order to consider multidimensional problems we introduce $m \times n$ interval matrices $[A] = ([a_{ij}])$ with entries $[a_{ij}]$, $i = 1, \ldots, m$, $j = 1, \ldots, n$ and interval vectors $[x] = ([x_i])$ with n components $[x_i]$, $i = 1, \ldots, n$. We denote the corresponding sets by $I(\mathbb{R}^{m \times n})$ and $I(\mathbb{R}^n)$, respectively. Trivially, $[A]$ coincides with the matrix interval $[\underline{A}, \overline{A}] = \{B \in \mathbb{R}^{m \times n} \mid \underline{A} \leq B \leq \overline{A}\}$ if $\underline{A} = (\underline{a}_{ij})$, $\overline{A} = (\overline{a}_{ij}) \in \mathbb{R}^{m \times n}$ and if $A = (a_{ij}) \leq B = (b_{ij})$ means $a_{ij} \leq b_{ij}$ for all i, j. Since interval vectors can be identified with $n \times 1$ matrices, a similar property holds for them. The null matrix O and the identity matrix I have the usual meaning, e denotes the vector $e = (1, 1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^n$. Operations between interval matrices and between interval vectors are defined in the usual manner. They satisfy an analogue of (6)–(8). For example,

$$\{Ax \mid A \in [A], \ x \in [x]\} \subseteq [A][x] = \left(\sum_{j=1}^{n} [a_{ij}][x_j]\right) \in I(\mathbb{R}^m) \tag{11}$$

if $[A] \in I(\mathbb{R}^{m \times n})$ and $[x] \in I(\mathbb{R}^n)$. It is easily seen that $[A][x]$ is the smallest vector which contains the left set in (11), but normally it does not coincide with it. An interval item which encloses some set S as tight as possible is called (interval) hull of S. The above-mentioned operations with two interval operands always yield to the hull of the corresponding underlying sets.

An interval matrix $[A] \in I(\mathbb{R}^{n \times n})$ is called nonsingular if it contains no singular real $n \times n$ matrix. The Hausdorff distance, the center, the diameter and the absolute value in (9), (10) can be generalized to interval matrices and interval vectors, respectively, by applying them entrywise. Note that the results are real matrices and vectors, respectively, as can be seen, e.g., for

$$q([A], [B]) = (q([a_{ij}], [b_{ij}])) \in \mathbb{R}^{m \times n}$$

if $[A], [B] \in I(\mathbb{R}^{m \times n})$. We also use the comparison matrix $\langle [A] \rangle = (c_{ij}) \in \mathbb{R}^{n \times n}$ which is defined for $[A] \in I(\mathbb{R}^{n \times n})$ by

$$
c_{ij} = \begin{cases} \langle [a_{ij}] \rangle, & \text{if } i = j, \\ -|[a_{ij}]|, & \text{if } i \neq j. \end{cases}
$$

By $\text{int}([x])$ we denote the interior of an interval vector $[x]$, by $\rho(A)$ the spectral radius of $A \in \mathbb{R}^{n \times n}$ and by $\| \cdot \|_\infty$ the usual maximum norm for vectors from $\mathbb{R}^n$ or the row sum norm for matrices from $\mathbb{R}^{m \times n}$. In addition, the Euclidean norm $\| \cdot \|_2$ in $\mathbb{R}^n$ will be used. We recall that $A \in \mathbb{R}^{n \times n}$ is an M matrix if $a_{ij} \leq 0$ for $i \neq j$ and if A^{-1} exists and is nonnegative, i.e., $A^{-1} \geq O$. If each matrix A from a given interval matrix $[A]$ is an M matrix then we call $[A]$ an M matrix, too.

Let each component f_i of $f \colon D \subseteq \mathbb{R}^m \to \mathbb{R}^n$ be given by an expression $f_i(x)$, $i = 1, \ldots, n$, and let $[x] \subseteq D$. Then the interval arithmetic evaluation $f([x])$ is defined analogously to the one-dimensional case.

In this paper we restrict ourselves to real compact intervals. However, complex intervals of the form $[z] = [a] + i[b]$ ($[a], [b] \in I(\mathbb{R})$) and $[z] = \langle \check{z}, r \rangle$ ($\check{z} \in \mathbb{C}$, $r \in \mathbb{R}$, $r \geq 0$) are also used in practice. In the first form $[z]$ is a rectangle in the complex plane, in the second form it means a disc with midpoint $\check{z}$ and radius r. In both cases a complex arithmetic can be defined and complex interval functions can be considered which extend the presented ones.

As a simple example for the demonstration how the ideas of interval arithmetic can be applied we consider the following problem: Let there be given a continuously differentiable function $f \colon D \subset \mathbb{R} \to \mathbb{R}$ and an interval $[x]^0 \subseteq D$ for which the interval arithmetic evaluation of the derivative exists and does not contain zero: $0 \notin f'([x]^0)$. We want to check whether there exists a zero x^* in $[x]^0$, and if it exists we want to compute it by producing a sequence of intervals containing x^* with the property that the lower and upper bounds are converging to x^*.

For $[x] \subseteq [x]^0$ we introduce the so-called interval Newton operator

$$
N[x] = m[x] - \frac{f(m[x])}{f'([x])}, \quad m[x] \in [x] \tag{12}
$$

and consider the following iteration method:

$$
[x]^{k+1} = N[x]^k \cap [x]^k, \quad k = 0, 1, 2, \ldots, \tag{13}
$$

which is called interval Newton method.

Properties of operator (12) and method (13) are described in the following result.

THEOREM 1. *Under the above assumptions the following holds for* (12) *and* (13):
(a) *If*

$$
N[x] \subseteq [x] \subseteq [x]^0, \tag{14}
$$

then f has a zero $x^* \in [x]$ which is unique in $[x]^0$.

(b)   *If f has a zero $x^* \in [x]^0$ then $\{[x]^k\}_{k=0}^\infty$ is well defined by (13), $x^* \in [x]^k$ and*
      $\lim_{k \to \infty}[x]^k = x^*$.
      If $df'([x]) \le cd[x]$, $[x] \subseteq [x]^0$, then $d[x]^{k+1} \le \gamma(d[x]^k)^2$.

(c)   *$N[x]^{k_0} \cap [x]^{k_0} = \emptyset$ (= empty set) for some $k_0 \ge 0$ if and only if $f(x) \ne 0$ for*
      all $x \in [x]^0$.

Theorem 1 delivers two strategies to study zeros in $[x]^0$. By the first it is *proved* that f *has* a unique zero x^* in $[x]^0$. It is based on (a) and can be realized by performing (13) and checking (14) with $[x] = [x]^k$. By the second—based on (c)—it is proved that f *has no* zero x^* in $[x]^0$. While the second strategy is always successful if $[x]^0$ contains no zero of f, the first one can fail as the simple example $f(x) = x^2 - 4$, $[x]^0 = [2,4]$ shows when choosing $m[x]^k > \underline{x}^k$. Here the iteratives have the form $[x]^k = [2, a_k]$ with appropriate $a_k > 2$ while $\underline{N[x]^k} < 2$. Hence (14) can never be fulfilled.

In case (b), the diameters are converging quadratically to zero. On the other hand, if method (13) breaks down because of empty intersection after a finite number of steps then from a practical point of view it would be interesting to have qualitative knowledge about the size of k_0 in this case. This will be discussed in the next section in a more general setting.

3.   Nonlinear equations

3.1.   Fixed point iteration

Assume, we have given a mapping

$$f: D \subseteq I(\mathbb{R}^n) \to I(\mathbb{R}^n). \tag{15}$$

We are considering the problem of looking for fixed points $[x]^*$ of f:

$$[x]^* = f([x]^*).$$

(Note, that a fixed point $[x]^*$ is a subset of D, in general.)

We first present some ideas concerning the existence of fixed points. Furthermore, we discuss the computation of fixed points. Finally, we give an interpretation of a fixed point related to (a special mapping) f.

For illustration we start with a simple class of mappings. Assume that we have given a real polynomial of degree m,

$$p(x) = a_0 + a_1 x + \cdots + a_m x^m.$$

Assume that the coefficients a_i, $i = 0, \ldots, m$, are not exactly known. Instead, we assume that they are known to vary in given intervals $[a_i]$, $i = 0, \ldots, m$. Define $f: I(\mathbb{R}) \to I(\mathbb{R})$ by

$$f([x]) := [a_0] + [a_1][x] + \cdots + [a_m][x]^m. \tag{16}$$

This mapping is called an interval polynomial. We will come back to this example later.

Of course, the mapping f defined by (16) is inclusion monotone and continuous on D (with respect to $[x]$).

Subsequently, we only consider mappings (15) which are inclusion monotone and continuous on D.

Assume now, that there is known an $[x]^0 \subseteq D$ such that

$$f([x]^0) \subseteq [x]^0. \tag{17}$$

Then, we consider the iteration method

$$[x]^{k+1} = f([x]^k), \quad k = 0, 1, 2, \ldots \tag{18}$$

Since f is inclusion monotone, we obtain a nested sequence

$$[x]^0 \supseteq [x]^1 \supseteq \cdots \supseteq [x]^k \supseteq [x]^{k+1} \cdots,$$

which has a limit $[x]^*$ in D. Since f is assumed to be continuous, it follows that $[x]^*$ is a fixed point of f. Summarizing, we obtain that (17) guarantees the existence and (18) gives a method for the approximation of a fixed point. In general, it is not easy or even impossible to find an $[x]^0$ such that (17) holds. However, since $I(\mathbb{R}^n)$ can be equipped with a metric, we could try to verify the assumption of the Banach fixed theorem on D. This has been worked out for a variety of mappings admitted in (15) in [6], e.g.. We mention just one result (see [6]).

THEOREM 2. *Let there be given an $n \times n$ interval matrix $[A] = ([a_{ij}])$ and an interval vector $[b]$. Assume that $\rho(|[A]|) < 1$, where $\rho(\cdot)$ denotes the spectral radius of a real matrix. Then*

$$[x]^{k+1} = f([x]^k) = [A][x]^k + [b], \quad k = 0, 1, \ldots, \tag{19}$$

in convergent for arbitrary $[x]^0 \in I(\mathbb{R}^n)$ to the unique fixed point $[x]^*$ of the mapping

$$f[x] = [A][x] + [b]. \tag{20}$$

If one has more general mappings f, which are for example, defined componentwise by polynomials of several variables, then one has to prove that D is mapped into itself and that f is a contraction on D.

Interpretation of a fixed point of f: In order that the presentation becomes not too overloaded we only consider mappings defined by (20). Assume that $\rho(|[A]|) < 1$. Then, by Theorem 2, f has exactly one fixed point $[x]^* \in I(\mathbb{R}^n)$. Consider a fixed, but arbitrary real matrix $A \in [A]$. Then $|A| \leq |[A]|$ and by the Perron–Frobenius theory on nonnegative matrices it follows that $\rho(A) \leq \rho(|A|) \leq \rho(|[A]|) < 1$. Therefore, for arbitrary $b \in [b]$, there exists a unique x^* such that

$$x^* = Ax^* + b \quad \text{or} \quad x^* = (I - A)^{-1}b.$$

Consider now the iteration method (19) with $[x]^0 := x^*$. Then

$$[x]^0 = x^* = Ax^* + b \in [A][x]^0 + [b] = [x]^1$$

and

$$x^* \in [x]^1 = [A]x^* + [b] \subseteq [A][x]^1 + [b] = [x]^2.$$

By mathematical induction we conclude $x^* \in [x]^k$, $k \geq 0$, and since f is continuous we have $x^* \in [x]^*$. Therefore, since $A \in [A]$ and $b \in [b]$ were chosen arbitrarily, the fixed point $[x]^*$ of f contains the set

$$\{(I - A)^{-1}b \mid A \in [A], \ b \in [b]\}$$

of all possible solutions.

A similar result holds for more general mappings, for example, if f is defined componentwise by polynomials in several variables. We mention without going into details that instead of (18), we can also consider the Gauss–Seidel method, which is in general faster convergent.

3.2. Newton-like methods

Let

$$\mathrm{IGA}([A], [b])$$

be the result of Gaussian algorithm applied formally to a nonsingular interval matrix $[A] \in I(\mathbb{R}^{n \times n})$ and an interval vector $[b] \in I(\mathbb{R}^n)$. Here we assumed that no division by an interval which contains zero occurs in the elimination process. It is easy to see that

$$S = \{x = A^{-1}b \mid A \in [A], \ b \in [b]\} \subseteq \mathrm{IGA}([A], [b]) \tag{21}$$

holds. By

$$\mathrm{IGA}([A])$$

we denote the interval matrix whose i-th column is obtained as $\mathrm{IGA}([A], e^i)$ where e^i is the i-th unit vector. In other words, $\mathrm{IGA}([A])$ is an enclosure for the inverses of all matrices $A \in [A]$. Now assume that

$$f : D \subset \mathbb{R}^n \to \mathbb{R}^n \tag{22}$$

is continuously differentiable, if $x, y \in [x] \subseteq D$ then

$$f(x) - f(y) = J(y, x)(x - y), \tag{23}$$

where

$$J(y, x) = \int_0^1 f'(y + t(x - y)) \, dt. \tag{24}$$

Note that J is a continuous mapping of x and y which satisfies $J(y,x) = J(x,y)$. Since $t \in [0,1]$ we have $y + t(x - y) \in [x]$ and therefore

$$J(y,x) \in f'([x]),\tag{25}$$

where $f'([x])$ denotes the interval arithmetic evaluation of the Jacobian of f. For fixed $y \in [x]$ we obtain from (23) and (25)

$$\begin{aligned}p(x) &= x - J^{-1}(y,x)f(x)\\ &= y - J^{-1}(y,x)f(y) \in y - \text{IGA}(f'([x]), f(y)).\end{aligned}\tag{26}$$

If $x \in [x]$ is a zero of f then (26) implies $x \in y - \text{IGA}(f'([x]), f(y))$. This leads to the following definition of the interval Newton operator $N[x]$ which we introduce in analogy to (13): suppose that $m[x] \in [x]$ is a real vector. Then

$$N[x] = m[x] - \text{IGA}(f'([x]), f(m[x])).\tag{27}$$

The interval Newton method is defined by

$$[x]^{k+1} = N[x]^k \cap [x]^k, \quad k = 0, 1, 2, \ldots\tag{28}$$

Analogously to Theorem 1 we have the following result.

THEOREM 3. *Let $F\colon D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable and assume that $\text{IGA}(f'([x]^0))$ exists for some interval vector $[x]^0 \subseteq D$. (This is identical to assuming that the Gaussian algorithm is feasible for $f'([x]^0)$. In particular, $f'([x]^0)$ is nonsingular in this case.)*
(a) *If*

$$N[x] \subseteq [x]$$

for some $[x] \subseteq [x]^0$ then f has a zero x^* in $[x]$ which is unique even in $[x]^0$. Assume that

$$\rho(A) < 1, \quad \text{where } A = |I - \text{IGA}(f'([x]^0))f'([x]^0)|.\tag{29}$$

(b) *If f has a zero x^* in $[x]^0$ then the sequence $\{[x]^k\}_{k=0}^{\infty}$ defined by (28) is well defined, $x^* \in [x]^k$ and $\lim_{k \to \infty}[x]^k = x^*$. In particular, $\{[x]^k\}_{k=0}^{\infty}$ is monotonically decreasing and x^* is unique in $[x]^0$.*
Moreover, if

$$df'([x])_{ij} \leq \alpha\|d[x]\|_{\infty}, \quad \alpha \geq 0,\ 1 \leq i,j \leq n\tag{30}$$

for all $[x] \subseteq [x]^0$ then

$$\|d[x]^{k+1}\|_{\infty} \leq \gamma\|d[x]^k\|_{\infty}^2, \quad \gamma \geq 0.\tag{31}$$

(c) *$N[x]^{k_0} \cap [x]^{k_0} = \emptyset$ for some $k_0 \geq 0$ if and only if $f(x) \neq 0$ for all $x \in [x]^0$.*

The proof of (a) can be quickly done by applying Brouwer's fixed point theorem to p of (26). The results of (b) and (c) can be found in [2].

Note that in contrast to the one-dimensional case we need condition (29) in cases (b) and (c). Because of continuity reasons this condition always holds if the diameter $d[x]^0$ of the given interval vector ("starting interval") is componentwise small enough (and if $f'([x]^0)$ contains no singular matrix) since we have $A = O$ in the limit case $d[x]^0 = 0$. Schwandt [14] has discussed a simple example in the case $\rho(A) \geq 1$ which shows that for a certain interval vector (28) is feasible, $x^* \in [x]^k$, but $\lim_{k \to \infty} [x]^k \neq x^*$.

In case (a) of the preceding theorem we have by (31) quadratic convergence of the diameters of the enclosing intervals to the zero vector. This is the same favorable behavior as it is well known for the usual Newton method. If there is no solution x^* of $f(x) = 0$ in $[x]^0$ this can be detected by applying (28) until the intersection becomes empty for some k_0. From a practical point of view it is important that k_0 is not big in general. Under natural conditions it can really be proved that k_0 is small if the diameter of $[x]^0$ is small: Let $N[x] = [\underline{n}, \overline{n}]$ for the interval Newton operator (27). It is easy to prove that

$$N[x] \cap [x] = \emptyset$$

if and only if for at least one component i_0 either

$$(\overline{n} - \underline{x})_{i_0} < 0 \tag{32}$$

or

$$(\overline{x} - \underline{n})_{i_0} < 0 \tag{33}$$

holds. Furthermore, it can be shown that

$$\overline{x} - \underline{n} \leq \mathrm{O}(\|d[x]\|_\infty^2)e + A^2 f(\overline{x}) \tag{34}$$

and

$$\overline{n} - \underline{x} \leq \mathrm{O}(\|d[x]\|_\infty^2)e - A^1 f(\underline{x}) \tag{35}$$

provided (30) holds. Here A^1 and A^2 are two real matrices contained in $\mathrm{IGA}(f'([x]^0))$. Furthermore, if $f(x) \neq 0$, $x \in [x]$, then for sufficiently small diameter $d[x]$ there is at least one $i_0 \in \{1, 2, \ldots, n\}$ such that

$$(A^1(\underline{x}))_{i_0} \neq 0 \tag{36}$$

and

$$\mathrm{sign}(A^1 f(\underline{x}))_{i_0} = \mathrm{sign}(A^2 f(\overline{x}))_{i_0}. \tag{37}$$

Assume now that $\text{sign}(A^1 f(\underline{x}))_{i_0} = 1$. Then for sufficiently small diameter $d[x]$ we have $(\overline{n} - \underline{x})_{i_0} < 0$ by (35) and by (32) the intersection becomes empty. If $\text{sign}(A^1 f(\underline{x}))_{i_0} = -1$ then by (34) we obtain $(\overline{x} - \underline{n})_{i_0} < 0$ for sufficiently small $d[x]$ and by (33) the intersection becomes again empty.

If $N[x]^{k_0} \cap [x]^{k_0} = \emptyset$ for some k_0 then the interval Newton method breaks down and we speak of divergence of this method. Because of the terms $O(\|d[x]\|^2_\infty)$ in (34) and (35) we can say that in the case $f(x) \neq 0$, $x \in [x]^0$, the interval Newton method is quadratically divergent.

We demonstrate this behavior by a simple one-dimensional example.

Example 1.   Consider the polynomial

$$f(x) = x^5 - x^4 - 11x^3 - 3x^2 + 18x,$$

which has only simple real zeros contained in the interval $[x]^0 = [-5, 6]$. Unfortunately, (13) cannot be performed since $0 \in f'([x]^0)$. Using a modification of the interval Newton method described already in [1] one can compute disjoint subintervals of $[x]^0$ for which the interval arithmetic evaluation of the derivative does not contain zero. Hence (13) can be performed for each of these intervals. If such a subinterval contains a zero (a) of Theorem 1 holds, otherwise (b) is true. Table 1 contains the intervals which are obtained by applying the above-mentioned modification of the interval Newton method until $0 \notin f'([x])$ for all computed subintervals of $[x]^0$ (for simplicity we only give three digits in the mantissa).

The subintervals which do not contain a zero of f are marked by a star in Table 2. The number in the second line exhibits the number of steps until the intersection becomes empty. For $n = 9$ we have a diameter of approximately 2.75, which is not small, and after only 3 steps the intersection becomes empty. The intervals with the numbers $n = 1, 2, 3, 6, 8$ each contain a zero of f. In the second line the number of steps are given which have to be performed until the lower and upper bound can be no longer improved on the computer. These numbers confirm the quadratic convergence of the diameters of the enclosing intervals. (For $n = 3$ the enclosed zero is $x^* = 0$ and we are in the underflow range.)

Table 1.   The modified interval Newton method applied to f from Example 1.

n	
1	$[-0.356 \cdot 10^1, -0.293 \cdot 10^1]$
2	$[-0.141 \cdot 10^1, -0.870 \cdot 10^0]$
3	$[-0.977 \cdot 10^0, -0.499 \cdot 10^0]$
4	$[0.501 \cdot 10^0, 0.633 \cdot 10^0]$
5	$[0.140 \cdot 10^1, 0.185 \cdot 10^1]$
6	$[0.188 \cdot 10^1, 0.212 \cdot 10^1]$
7	$[0.265 \cdot 10^1, 0.269 \cdot 10^1]$
8	$[0.297 \cdot 10^1, 0.325 \cdot 10^1]$
9	$[0.327 \cdot 10^1, 0.600 \cdot 10^1]$

Table 2.   The interval Newton method applied to f from Example 1.

n	1	2	3	4*	5*	6	7*	8	9*
	5	6	9	1	2	6	1	5	3

The interval Newton method has the big disadvantage that even if the interval arithmetic evaluation $f'([x]^0)$ of the Jacobian contains no singular matrix its feasibility is not guaranteed, $\mathrm{IGA}(f'([x]^0))f'(m[x]^0)$ can in general only be computed if $d[x]^0$ is sufficiently small. For this reason Krawczyk [12] had the idea to introduce a mapping which today is called the Krawczyk operator: Assume again that a mapping (22) with the corresponding properties is given. Then analogously to (27) we consider the so-called Krawczyk operator

$$K[x] = m[x] - Cf(m[x]) + (I - Cf'([x]))([x] - m[x]), \tag{38}$$

where C is a nonsingular real matrix and where $m[x] \in [x]$. For fixed C we define the so-called Krawczyk method by

$$[x]^{k+1} = K[x]^k \cap [x]^k, \quad k = 0, 1, 2, \ldots \tag{39}$$

For this method an analogous result holds as it was formulated for the interval Newton method in Theorem 3:

THEOREM 4.   *Let* $f \colon D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ *be continuously differentiable and assume that the interval arithmetic evaluation* $f'([x]^0)$ *of the Jacobian exists for some interval vector* $[x]^0 \subseteq D^0$.
(a)   *If*

$$K[x] \subseteq [x] \tag{40}$$

for some $[x] \subseteq [x]^0$ *then* f *has a zero* x^* *in* $[x]$.
If (40) *is slightly sharpened to*

$$(K[x])_i \subset [x_i] \subseteq [x_i]^0 \quad \text{for } i = 1, \ldots, n, \tag{41}$$

then $\rho(|I - Cf'([x])|) < 1$ *holds,* $f'([x])$ *is nonsingular and* x^* *is unique in* $[x]$. *Let* $m[x]$ *be the center of* $[x]$ *and assume that*

$$\rho(B) < 1, \quad \text{where } B = |I - Cf'([x]^0)|. \tag{42}$$

(b)   *If* f *has a zero* x^* *in* $[x]^0$ *then the sequence* $\{[x]^k\}_{k=0}^\infty$ *given by* (39) *is well defined,* $x^* \in [x]^k$ *and* $\lim_{k\to\infty}[x]^k = x^*$. *In particular,* $\{[x]^k\}_{k=0}^\infty$ *is monotonically decreasing and* x^* *is unique in* $[x]^0$. *Moreover, if* $C = C_k$ *varies with* k *such that it is the inverse of some matrix contained in* $f'([x]^k)$, *and if*

$$df'([x])_{ij} \leq \alpha \|d[x]\|_\infty, \quad \alpha \geq 0, \ 1 \leq i, j \leq n \tag{43}$$

for all $[x] \subseteq [x]^0$ *then*

$$\|d[x]^{k+1}\|_\infty \leq \gamma \|d[x]^k\|_\infty^2, \quad \gamma \geq 0. \tag{44}$$

(c) $K[x]^{k_0} \cap [x]^{k_0} = \emptyset$ for some $k_0 \geq 0$ if and only if $f(x) \neq 0$ for all $x \in [x]^0$.

Proof. (a)   Consider for the nonsingular matrix C in the definition of $K[x]$ the continuous mapping

$$g \colon D \subseteq \mathbb{R}^n \to \mathbb{R}^n$$

defined by

$$g(x) = x - Cf(x).$$

It follows, using (23) and the assumption,

$$
\begin{aligned}
g(x) &= x - Cf(x) \\
&= x - C(f(x) - f(m[x])) - Cf(m[x]) \\
&= m[x] + (x - m[x]) - CJ(m[x], x)(x - m[x]) - Cf(m[x]) \\
&\in m[x] - Cf(m[x]) + (I - Cf'([x]))([x] - m[x]) \\
&= K[x] \subseteq [x], \quad x \in [x].
\end{aligned}
$$

By Brouwer's fixed point theorem g has a fixed point $x^* \in [x]$. This fixed point is a zero of f.

If (40) is replaced by (41) then $|I - Cf'([x])|d[x] \leq dK[x] < d[x]$. Therefore,

$$\max_{j \leq i \leq n} \frac{\sum_{j=1}^n |I - Cf'([x])|_{ij} d[x_j]}{d[x_i]} < 1,$$

which is equivalent to

$$\left\| \hat{D}^{-1} |I - Cf'([x])| \hat{D} \right\|_\infty < 1.$$

Here, $\hat{D}$ is the diagonal matrix with $\hat{d}_{ii} = d[x_i]$, $i = 1, \ldots, n$. Therefore,

$$
\begin{aligned}
\rho(|I - Cf'([x])|) &= \rho(\hat{D}^{-1} |I - Cf'([x])| \hat{D}) \\
&\leq \left\| \hat{D}^{-1} |I - Cf'([x])| \hat{D} \right\|_\infty < 1.
\end{aligned}
$$

If $f'([x])$ contained a singular matrix A then $I - CA$ would have the eigenvalue 1 and we would get the contradiction

$$1 \leq \rho(I - CA) \leq \rho(|I - CA|) \leq \rho(|I - Cf'([x])|) < 1. \tag{45}$$

Therefore, $f'([x])$ is nonsingular. If f had two zeros $x^*, y^* \in [x]$ then (23) and (25) would imply $x^* = y^*$.

(b)   By (23) we have

$$f(x^*) - f(m[x]) = J(m[x], x^*)(x^* - m[x])$$

and since $f(x^*) = 0$ it follows

$$
\begin{aligned}
x^* &= m[x] - Cf(m[x]) + (I - CJ(m[x], x^*))(x^* - m[x]) \\
&\in m[x] - Cf(m[x]) + (I - CJ([x]))([x] - m[x]) \\
&= K[x].
\end{aligned}
$$

Hence, if $x^* \in [x]^0$ then $x^* \in K[x]^0$ and therefore $x^* \in K[x]^0 \cap [x]^0 = [x]^1$. Mathematical induction proves $x^* \in [x]^k$, $k \geq 0$.

For the diameters of the sequence $\{[x]^k\}_{k=0}^\infty$ we have $d[x]^{k+1} \leq dK[x]^k \leq Bd[x]^k$, where the last inequality holds because we assumed that $m[x]^k$ is the center of $[x]^k$. Since $\rho(B) < 1$ we have $\lim_{k\to\infty} d[x]^k = 0$, and from $x^* \in [x]^k$ it follows $\lim_{k\to\infty}[x]^k = x^*$. In particular, x^* is unique within $[x]^0$.

Analogously to (a) assumption (42) implies that $f'([x]^0)$ is nonsingular. Since it is compact and since the inverse of a matrix $M \in \mathbb{R}^{n\times n}$ depends continuously on the entries of M the set $\{|M^{-1}| \mid M \in f'([x]^0)\}$ is bounded by some matrix $\hat{C}$. The quadratic convergence behavior (44) follows now from

$$
\begin{aligned}
d[x]^{k+1} &\leq |I - C_k f'([x]^k)| d[x]^k \\
&\leq |C_k| \, |C_k^{-1} - f'([x]^k)| d[x]^k \\
&\leq \hat{C} |f'([x]^k) - f'([x]^k)| d[x]^k \\
&= \hat{C} d f'([x]^k) d[x]^k
\end{aligned}
$$

by using (43).

(c)   Assume now that $K[x]^{k_0} \cap [x]^{k_0} = \emptyset$ for some $k_0 \geq 0$. Then $f(x) \neq 0$ for $x \in [x]^0$ since if $f(x^*) = 0$ for some $x^* \in [x]^0$ then Krawczyk's method is well defined and $x^* \in [x]^k$, $k \geq 0$.

If on the other hand $f(x) \neq 0$ and $K[x]^k \cap [x]^k \neq \emptyset$ then $\{[x]^k\}$ is well defined. Because of $\rho(B) < 1$ we have $d[x]^k \to 0$ and since we have a nested sequence it follows $\lim_{k\to\infty}[x]^k = \hat{x} \in \mathbb{R}^n$. Since the Krawczyk operator is continuous and since the same holds for forming intersections we obtain by passing to infinity in (39)

$$\hat{x} = K\hat{x} \cap \hat{x} = K\hat{x} - Cf(\hat{x}).$$

From this it follows that $f(\hat{x}) = 0$ in contrast to the assumption that $f(x) \neq 0$ for $x \in [x]^0$.

This completes the proof of Theorem 4.   □

REMARKS.

(a) When we defined the Krawczyk operator in (38) we required C to be non-singular. We need not know this in advance if (40) or (42) holds since either of these two conditions implies the nonsingularity by an analogous argument as in the proof for (a).

(b) It is easy to see that in case (a) of the preceding theorem all the zeros x^* of f in $[x]$ are even in $K[x]$.

(c) If $m[x]$ is not the center of $[x]$ but still an element of it the assertions in (b), (c) remain true if (42) is replaced by $\rho(B) < \frac{1}{2}$.

(d) Assumption (42) certainly holds if (29) is true with $C \in \text{IGA}(f'([x]^0))$.

In case (c) of the Theorem 4, that is if $K[x]^{k_0} \cap [x]^{k_0} = \emptyset$ for some k_0, we speak again of divergence (of the Krawczyk method). Similar as for the interval Newton method k_0 is small if the diameter of $[x]^0$ is small. This will be demonstrated subsequently under the following assumptions:

(i) $f'([x]^0)$ is nonsingular,

(ii) (43) holds,

(iii) $C = C_k$ varies with k such that it is the inverse of some matrix from $f'([x]^k)$.

As for the interval Newton operator we write $K[x] = [\underline{k}, \overline{k}]$.

Now $K[x] \cap [x] = \emptyset$ if and only if

$$(\overline{x} - \underline{k})_{i_0} < 0 \tag{46}$$

or

$$(\overline{k} - \underline{x})_{i_0} < 0 \tag{47}$$

for at least one $i_0 \in \{1, 2, \ldots, n\}$. (Compare with (32) and (33).)

We first prove that for $K[x]$ defined by (38) we have the vector inequalities

$$\overline{x} - \underline{k} \le \text{O}(\|d[x]\|_\infty^2)e + Cf(\overline{x}) \tag{48}$$

and

$$\overline{k} - \underline{x} \le \text{O}(\|d[x]\|_\infty^2)e - Cf(\underline{x}), \tag{49}$$

where again $e = (1, 1, \ldots, 1)^{\text{T}} \in \mathbb{R}^n$.

We prove (49). For $[x] \subseteq [x]^0$ let $f'([x]) = [\underline{F}', \overline{F}']$ and set $C = \hat{M}^{-1}$ with some matrix $\hat{M} \in f'([x])$.

An easy computation shows that

$$I - Cf'([x]) = C[\hat{M} - \overline{F}', \hat{M} - \underline{F}']$$
$$\subseteq |C|[\underline{F}' - \overline{F}', \overline{F}' - \underline{F}'] \subseteq [-1, 1]\hat{C}df'([x]),$$

where $\hat{C}$ is any upper bound for the set $\{|M^{-1}| \mid M \in f'([x]^0)\}$. Therefore

$$K[x] \subseteq m[x] - Cf(m[x]) + [-1,1]\hat{C}df'([x]) \cdot |[x] - m[x]|.$$

Hence,

$$\overline{k} - \underline{x} \le m[x] - \underline{x} - Cf(m[x]) + \hat{C}df'([x])d[x]$$
$$\le \frac{1}{2}d[x] - Cf(m[x]) + \mathrm{O}(\|d[x]\|_\infty^2)e,$$

where we have used (43) and $m[x] \in [x]$. Choosing $x = m[x]$, $y = \underline{x}$ in (23) we obtain

$$f(m[x]) - f(\underline{x}) = J(\underline{x}, m[x])(m[x] - \underline{x}).$$

It follows that

$$\overline{k} - \underline{x} \le \frac{1}{2}d[x] - Cf(\underline{x}) - \frac{1}{2}CJ(\underline{x}, m[x])d[x] + \mathrm{O}(\|d[x]\|_\infty^2)e$$
$$= \frac{1}{2}(I - CJ(\underline{x}, m[x]))d[x] - Cf(\underline{x}) + \mathrm{O}(\|d[x]\|_\infty^2)e.$$

Since

$$I - CJ(\underline{x}, m[x]) = C(C^{-1} - J(\underline{x}, m[x]))$$
$$\in \hat{C}(f'([x]) - f'([x])) = \hat{C}df'([x]),$$

the assertion follows by applying (43).

The second inequality can be shown in the same manner, hence (48) and (49) are proved.

If $f(x) \neq 0$, $x \in [x]$ and $d[x]$ is sufficiently small, then there exists an $i_0 \in \{1, 2, \ldots, n\}$ such that

$$(Cf(\underline{x}))_{i_0} \neq 0 \tag{50}$$

and

$$\mathrm{sign}(Cf(\overline{x}))_{i_0} = \mathrm{sign}(Cf(\underline{x}))_{i_0}. \tag{51}$$

This can be seen as follows: Since $\underline{x} \in [x]$ we have $f(\underline{x}) \neq 0$ and since C is non-singular it follows that $Cf(\underline{x}) \neq 0$ and therefore $(Cf(\underline{x}))_{i_0} \neq 0$ for at least one $i_0 \in \{1, 2, \ldots, n\}$ which proves (50).

Using again (23) with $x = \overline{x}$, $y = \underline{x}$ we get

$$f(\overline{x}) - f(\underline{x}) = J(\underline{x}, \overline{x})(\overline{x} - \underline{x}).$$

It follows

$$Cf(\overline{x}) = Cf(\underline{x}) + CJ(\underline{x}, \overline{x})(\overline{x} - \underline{x}).$$

Since the second term on the right-hand side approaches zero if $d[x] \to 0$ we have (51) for sufficiently small diameter $d[x]$.

Using (48), (49) together with (50) and (51) we can now show that for sufficiently small diameters of $[x]$ the intersection $K[x] \cap [x]$ becomes empty. See the analogous conclusions for the interval Newton method using (36), (37) together with (34) and (35). By the same motivation as for the interval Newton method we denote this behavior as "quadratic divergence" of the Krawczyk method.

3.3. Nonsmooth equations

We continue our discussion by considering mappings $f\colon D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ which are not assumed to be differentiable everywhere in D. As a simple, but important problem, which leads to such an f, we consider the (nonlinear) complementarity problem $\mathrm{NCP}(F)$ defined as follows:

Let there be given a mapping $F\colon D \subseteq \mathbb{R}^n \to \mathbb{R}^n$. Then $\mathrm{NCP}(F)$ consists in looking for a vector $x^* \in \mathbb{R}^n$ such that x^* fulfills

$$x \geq 0, \quad F(x) \geq 0, \quad x^{\mathrm{T}} F(x) = 0, \tag{52}$$

where the inequalities are defined componentwise. It is easy to see, that (52) holds iff x^* is a solution of the nonlinear system $f(x) = 0$ where $f\colon D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ is defined by

$$f(x) = \min\{x, F(x)\} \tag{53}$$

and where the minimum is taken componentwise. Even if F is smooth, f is not differentiable everywhere in D. Therefore the ideas from Section 3.2 cannot be applied immediately. However, using the so-called slope of a mapping f (instead of the Jacobian) we can construct an operator which admits similar statements as in the Theorem 3 and 4 for the Newton and Krawczyk operator, respectively.

Assume that we have given a continuous mapping

$$f\colon D \subseteq \mathbb{R}^n \to \mathbb{R}^n$$

and an interval vector $[x] \subseteq D$. A mapping

$$\delta f\colon [x] \times [x] \to \mathbb{R}^{n \times n}$$

is called slope of f, if

$$f(x) - f(y) = \delta f(x, y)(x - y), \quad x, y \in [x] \tag{54}$$

holds. Assume now that there exists an interval matrix $\delta f(x, [x])$ such that

$$\delta f(x, y) \in \delta f(x, [x]) \tag{55}$$

for some fixed $x \in [x]$ and all $y \in [x]$. The interval matrix $\delta f(x, [x])$ is called slope extension.

Let A be a nonsingular matrix and define the interval operator $L: I(\mathbb{R}^n) \to I(\mathbb{R}^n)$ by

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

Then the following hold:

a)   If $L(x, A, [x]) \subseteq [x]$, then there exists an $x^* \in [x]$ such that $H(x^*) = 0$.

b)   If $L(x, A, [x]) \cap [x] = \emptyset$ (empty set), then $f(x) \neq 0$ for all $x \in [x]$.

    The proof can be performed by applying the Brouwer fixed point theorem.

    In [3], [4] explicit formulae were given for the slope (54) and its extension $\delta f(x, [x])$ if f is defined by (53). No special assumptions have been made about the mapping F. Numerical experiments are also contained in these papers.

    If the mapping F used in (53) has the special form

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

where $M \in \mathbb{R}^{n \times n}$ and $q \in \mathbb{R}^n$, then the complementarity problem (52) is called linear. It is then denoted by $\mathrm{LCP}(M, q)$. For this special case one can find verification methods in the papers [8], [9], [10], e.g.

    We demonstrate by a simple example that verification is a very important task also for complementarity problems. First we note that (52) can also be equivalently formulated as the following problem: Find $w, z \in \mathbb{R}^n$ such that

$$w \geq 0, \quad x \geq 0, \quad w = F(x), \quad x^{\mathrm{T}}w = 0. \tag{56}$$

Consider now

$$F(x) = Mx + q,$$

where

$$M = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ -1 & -1 & 0 \end{pmatrix} \quad \text{and} \quad q = \begin{pmatrix} 2 \\ 1 \\ -10^{-6} \end{pmatrix}.$$

For

$$x = \begin{pmatrix} 10^{-6} \\ 10^{-6} \\ 1 \end{pmatrix} \geq 0, \quad w = \begin{pmatrix} 3 \\ 2 \\ 10^{-6} \end{pmatrix} \geq 0$$

one obtains

$$\|F(x) - w\|_\infty = \|Mx + q - w\|_\infty = 4 \times 10^{-6}$$

and

$$x^{\mathrm{T}}w = 6 \times 10^{-6}.$$

Therefore, x, w may by considered as good approximations of the problem (56). In many iterative methods (e.g., for interior-point-methods) the condition

$$\max\{x^{\mathrm{T}}w, \|Mx + q - w\|_\infty\} \le \epsilon$$

is used as a stopping criteria for some fixed ϵ (for $x \ge 0$, $w \ge 0$). A pair $(x, w)^{\mathrm{T}}$ which fulfils this inequality is then called an ϵ-approximation solution. In this sense the given vectors x, w form a 6×10^{-6}-approximate solution. However, using the test b) from above it can be shown that there is no exact solution of the LCP(M, q) within an $\|\cdot\|_\infty$ distance of 0.25 from this ϵ-approximate solution with $\epsilon = 6 \times 10^{-6}$.

4. Final remarks

For performing the methods discussed in this paper one needs software realizing the interval arithmetic operations. Furthermore, if the computation is done on a computer using floating point representation of numbers, rounding errors have to be taken into account. For a discussion of existing software we refer to the last chapter of the paper [7] and to the references found there.

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