

On Existence and Uniqueness Verification for Non-Smooth Functions

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Abstract. Given an approximate solution to a nonlinear system of equations at which the Jacobi matrix is nonsingular, and given that the Jacobi matrix is continuous in a region about this approximate solution, a small box can be constructed about the approximate solution in which interval Newton methods can verify existence and uniqueness of an actual solution. Recently, we have shown how to verify existence and uniqueness, up to multiplicity, for solutions at which the Jacobi matrix is singular. We do this by efficient computation of the topological index over a small box containing the approximate solution. Since the topological index is defined and computable when the Jacobi matrix is not even defined at the solution, one may speculate that efficient algorithms can be devised for verification in this case, too. In this note, however, we discuss, through examples, key techniques in underlying our simplification of the calculations that cannot necessarily be used when the function is non-smooth. We also present those parts of the theory that are valid in the non-smooth case, and suggest when degree computations involving non-smooth functions may be practical.

As a bonus, the examples lead to additional understanding of previously published work on verification involving the topological degree.

Keywords: singular nonlinear algebraic systems, existence verification, interval computations, Brouwer degree

1. Introduction

Given a system of nonlinear equations $F(x) = 0$, numerical methods produce an approximation \tilde{x} to a solution x^* . It is then sometimes desirable to compute bounds

$$\begin{aligned} \mathbf{x} &= (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) \\ &= ([\underline{x}_1, \bar{x}_1], [\underline{x}_2, \bar{x}_2], \dots, [\underline{x}_n, \bar{x}_n]), \end{aligned}$$

such that \tilde{x} is the center of \mathbf{x} , and such that \mathbf{x} is guaranteed to contain a solution x^* to $F(x) = 0$. This leads to the problem

Given $F : \mathbf{x} \rightarrow \mathbb{R}^n$, where $\mathbf{x} \in \mathbb{IR}^n$, <i>rigorously</i> verify: <ul style="list-style-type: none">• there exists a $x^* \in \mathbf{x}$ such that $F(x^*) = 0$.	(1)
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Here, \mathbb{IR}^n represents the set of n -dimensional vectors, as \mathbf{x} , whose components are intervals.

In this introduction, we give a brief overview of our approaches to (1). For a fuller understanding of the theory and techniques, see the references cited here.

If the Jacobi matrix $F'(x^*)$ is non-singular and continuous in \mathbf{x} , then it has been well-known for some time that we can construct an algorithm, based on an interval Newton method, that verifies existence and uniqueness; see [6, Chapter 8], [8, pp. 219–223], and the references therein. Such interval Newton methods are of the form

$$\tilde{\mathbf{x}} = \mathbf{N}(F; \mathbf{x}, \tilde{\mathbf{x}}) = \tilde{\mathbf{x}} + \mathbf{v}, \quad (2)$$

where

$$\Sigma(\mathbf{A}, -F(\tilde{\mathbf{x}})) \subset \mathbf{v}, \quad (3)$$

where \mathbf{A} is a Lipschitz matrix for F over \mathbf{x} , and where

$$\Sigma(\mathbf{A}, -F(\tilde{\mathbf{x}})) = \{x \in \mathbb{R}^n \mid \exists A \in \mathbf{A} \text{ with } AX = -F(\tilde{\mathbf{x}})\}. \quad (4)$$

Here $\tilde{\mathbf{x}}$ is some point in \mathbf{x} (often taken to be its midpoint) that, in the context of this paper, we consider to be an approximate solution.

THEOREM 1 ([8, Theorem 1.19, p. 62], originally from [12]) *Suppose $\tilde{\mathbf{x}} = \mathbf{N}(F; \mathbf{x}, \tilde{\mathbf{x}})$ is the image of \mathbf{x} and $\tilde{\mathbf{x}}$ under an interval Newton method. If $\tilde{\mathbf{x}} \subseteq \mathbf{x}$, it follows that there exists a unique solution of $F(x) = 0$ within \mathbf{x} .*

Combined with good heuristics for setting the widths of the box \mathbf{x} , such interval Newton methods reliably verify existence and uniqueness, provided we use at least an order-one interval extension of the Jacobi matrix for the matrix \mathbf{A} ; see [8, pp. 219–223] for a simple analysis of this. However, if \mathbf{A} contains a singular matrix (which *must* be true if an interval extension of the Jacobi matrix is used and the Jacobi matrix is singular at some point within \mathbf{x}), then the solution set $\Sigma(\mathbf{A}, -F(\tilde{\mathbf{x}}))$ in (4) must be unbounded, and existence / uniqueness verification as in Theorem 1 cannot occur¹.

Recently, we have developed techniques that can verify existence of solutions to $F(x) = 0$ within \mathbf{x} , even when $F'(x) = 0$ for some $x \in \mathbf{x}$. These techniques are based on computing the *topological degree* $d(F, \mathbf{x}, 0)$ of F over \mathbf{x} . If every $x \in \mathbf{x}$ where $F(x) = 0$ has the Jacobi matrix $F'(x)$ nonsingular, then $d(F, \mathbf{x}, 0)$ is equal to the number of solutions of $F(x) = 0$ in \mathbf{x} at which the determinant of $F'(x)$ is positive, minus the number of solutions of $F(x) = 0$ in \mathbf{x} at which the determinant is negative. However, the integer $d(F, \mathbf{x}, 0)$ depends only on values of F on the boundary $\partial\mathbf{x}$, so F' may be singular, and indeed, even non-smooth, in the interior $\text{int}(\mathbf{x})$.

In particular, in our efficient methods for existence and uniqueness verification, we have utilized a derivation from a known formula relating the degree $d(F, \mathbf{x}, 0)$ to zeros of components of F on the boundary $\partial\mathbf{x}$. Namely, the boundary $\partial\mathbf{x}$ of \mathbf{x} consists of $2n(n-1)$ -dimensional boxes

$$\begin{aligned} \mathbf{x}_{\underline{k}} &\equiv (\mathbf{x}_1, \dots, \mathbf{x}_{k-1}, \underline{x}_k, \mathbf{x}_{k+1}, \dots, \mathbf{x}_n)^T \quad \text{and} \\ \mathbf{x}_{\bar{k}} &\equiv (\mathbf{x}_1, \dots, \mathbf{x}_{k-1}, \bar{x}_k, \mathbf{x}_{k+1}, \dots, \mathbf{x}_n)^T, \end{aligned}$$

where $k = 1, \dots, n$. The oriented boundary $\partial \mathbf{x}$ can be divided into $\mathbf{x}_{\underline{k}}$ and $\mathbf{x}_{\overline{k}}$, $k = 1, \dots, n$, with the associated orientations. Furthermore, fix a ℓ between 1 and n and define

$$F_{-\ell}(x) = (f_1(x), f_2(x), \dots, f_{\ell-1}(x), f_{\ell+1}(x), \dots, f_n(x))^T.$$

For this fixed ℓ , let $\underline{K}_0(s)$ denote the subset of the integers $k \in \{1, \dots, n\}$ such that $F_{-\ell} = 0$ has solutions on $\mathbf{x}_{\underline{k}}$ and $\text{sgn}(f_\ell) = s$ at these solutions, and let $\overline{K}_0(s)$ denote the subset of the integers $k \in \{1, \dots, n\}$ such that $F_{-\ell} = 0$ has solutions on $\mathbf{x}_{\overline{k}}$ and $\text{sgn}(f_\ell) = s$ at these solutions, where $s \in \{-1, +1\}$. We then have

THEOREM 2 (See [11].) *Suppose F is continuous, $F \neq 0$ on $\partial \mathbf{x}$, and suppose there is an ℓ , $1 \leq \ell \leq n$, such that:*

1. $F_{-\ell} \neq 0$ on $\partial \mathbf{x}_{\underline{k}}$ or $\partial \mathbf{x}_{\overline{k}}$, $k = 1, \dots, n$; and
2. the Jacobi matrices of $F_{-\ell}$ are non-singular at all solutions of $F_{-\ell} = 0$ on $\partial \mathbf{x}$.

Then

$$\begin{aligned} d(F, \mathbf{x}, 0) = & (-1)^{\ell-1} s \\ & \cdot \left\{ \sum_{k \in \underline{K}_0(s)} (-1)^k \sum_{\substack{x \in \mathbf{x}_{\underline{k}} \\ F_{-\ell}(x)=0}} \text{sgn} \left| \frac{\partial F_{-\ell}}{\partial x_1 x_2 \dots x_{k-1} x_{k+1} \dots x_n}(x) \right| \right. \\ & \left. + \sum_{k \in \overline{K}_0(s)} (-1)^{k+1} \sum_{\substack{x \in \mathbf{x}_{\overline{k}} \\ F_{-\ell}(x)=0}} \text{sgn} \left| \frac{\partial F_{-\ell}}{\partial x_1 x_2 \dots x_{k-1} x_{k+1} \dots x_n}(x) \right| \right\}. \end{aligned}$$

In our methods, we precondition F , then arrange the coordinate widths of \mathbf{x} about our approximate solution \tilde{x} so that we can verify, with a single interval evaluation of a component of F per face $\mathbf{x}_{\underline{k}}$ or $\mathbf{x}_{\overline{k}}$ eliminated, that there are only several terms in the sum in Theorem 2. We then use a very low-dimensional search on the remaining several faces of \mathbf{x} to find the solutions of $F_{-\ell} = 0$. In certain instances, we have used a heuristic to guess the value of $d(F, \mathbf{x}, 0)$. In [11], we assumed that the rank defect of the Jacobi matrix at the solution x^* , $F(x^*) = 0$ was 1, and that quadratic terms of the “singular” component in the preconditioned function did not vanish. We also reposed the verification task in complex n -space, necessary to verify even-multiplicity solutions. (See [11, §4].) Under these assumptions, we can verify that $d(F, \mathbf{x}, 0) = 2$, and hence, there exists precisely either a singular solution of multiplicity 2 or two nonsingular solutions in \mathbb{C}^n near \tilde{x} . Our verification process proceeds with $2n - 2$ interval evaluations of a component of F and 2 one-dimensional searches for solutions of a single nonlinear equation. Furthermore, the one-dimensional searches are particularly efficient, since the solution locations can be accurately predicted from a local model. Our analysis indicated the verification

proceeded in $\mathcal{O}(n^3)$; this order was verified experimentally with solutions to finite discretizations of a model problem with n up to 320.

In [9], we continued to consider the rank-defect-one case, but we no longer assumed the quadratic terms did not vanish. If terms of the Taylor series up to degree d vanish, but not all degree d terms vanish, then, in [9], we show how to construct \mathbf{x} about \tilde{x} (in complex n -space) to easily verify that $d(F, \mathbf{x}, 0) = d$. This algorithm is a straightforward generalization of the degree-2 algorithm in [11], and also runs in $\mathcal{O}(n^3)$ time, both according to our analysis and according to experiments done with finite-difference discretizations of degree 2 and 3, up to $n = 160$. Also in [9], we present a heuristic that guesses the degree d before the verification proceeds; knowing d beforehand allows us to structure the two one-dimensional searches efficiently.

In [10], we first provide a general introduction and brief review of our techniques, then speculate on the applicability of our techniques for rank defect higher than 1. In particular, we showed that, if the rank defect is p and the first terms in the multivariate Taylor expansions that do not vanish are of order d , then verification of the degree reduces, not to 2 one-dimensional searches for zeros of a single function, but to $4p$ $2p-1$ -dimensional searches (over boxes in \mathbb{R}^{2p}) for solutions of a system of $2p-1$ equations in $2p-1$ variables. Furthermore, contrary to when $p = 1$, predicting where the solutions to this system lie would, in general, involve finding the solutions (in projective space) to an arbitrary system of p d -homogeneous polynomials in p unknowns. Thus, verification appears significantly more costly in this case.

In theoretical developments of the topological degree as in [2] or [3], the degree is defined for merely continuous, and not-necessarily differentiable F , and the degree depends only on values of the components of F on the boundary $\partial\mathbf{x}$; the dependence on the boundary only is exemplified in the formula in Theorem 2. In other words, the degree $d(F, \mathbf{x}, 0)$ (and hence the existence of solutions within \mathbf{x} , is invariant under continuous deformations of the graph of F in the interior of \mathbf{x} , with values on the boundary $\partial\mathbf{x}$ held constant. This fact has led people to propose degree computation as a way of verifying solutions to nonlinear systems of equations $F(x) = 0$ where the components of F are defined in a piecewise fashion, such as if these components are piecewise linear. (In fact, these considerations led us to entitle [5] “Existence Verification for Singular and Non-Smooth Zeros of Real Nonlinear Systems”.) The purpose of this paper is to clarify the possibilities of applying our techniques in to non-smooth problems.

2. Are Degree Techniques Efficient to Verify Solutions for Nonsmooth Functions?

Theorem 2 is related to a class of methods of computation of the topological degree, derived from formulas first proposed by Stenger [14]. The first computational techniques considered the computation as a global problem, in contrast to the local problem of verifying existence within a small region around an approximate solution. In contrast to the verification techniques we developed, an exhaustive search is done on the boundary of the region, without shortcuts. In [7] and [15], the degree

was computed over an n -simplex, while the degree was computed over an n -box in [16]. In all three of these developments, only the algebraic signs of the components of F needed to be correct; however, the three methods used only heuristics to determine when the boundary was sufficiently subdivided, and could thus produce incorrect values, without an indication that the result is incorrect. In [1], Aberth proposed a method based on interval evaluations on the boundary of a (relatively large box) \mathbf{x} ; this method could never give an incorrect value of $d(F, \mathbf{x}, 0)$.

In contrast, in our work in [4], [11], [9], [10], and [5], we are not given a large box \mathbf{x} , but we construct \mathbf{x} sufficiently small to allow us to use a local model of F to both reduce the dimension of the search on the boundary and to greatly speed the resulting low-dimensional search. The question we ask here is: “Can we do similar simplifications if F is defined in a piecewise fashion, or is otherwise non-smooth?” Such simplifications include

1. preconditioning the system,
2. applying a local model to the preconditioned system to reduce the dimension, and
3. using a local model to predict where the solutions to $F_{-\ell} = 0$ are on $\partial\mathbf{x}$, as in Theorem 2.

Can our algorithms succeed, even when, strictly speaking, the local models that justify the algorithms are not valid, because the components of F are non-smooth? We consider several examples.

2.1. Degree Verification: Some Examples

In the work for [11], [9], and [5], we assumed a singular solution x^* near our approximate solution \tilde{x} such that the rank of the Jacobi matrix $F'(x^*)$ is $n - 1$. (In [9], we assumed rank $n - p$, and proceeded similarly, but we consider $p = 1$ here for simplicity.) We implicitly assumed local linearity, and we preconditioned the system with an incomplete LU-factorization to eliminate (approximately) all but the last variable from the first $n - 1$ functions. In other words, we replaced f_k , $1 \leq k \leq n$ by linear combinations

$$f_k \leftarrow \sum_{j=1}^n y_{k,j} f_j,$$

such that the all of the order 1 terms in the multivariate Taylor series for f_k $1 \leq k \leq n - 1$ vanished except for $\frac{\partial f_k}{\partial x_k} = 1$ and $\frac{\partial f_k}{\partial x_n}$, and such that all first order terms in f_n vanished. In other words, the preconditioned Jacobi matrix is of the form

$$YF'(x^*) \approx \begin{pmatrix} 1 & 0 & \dots & 0 & * \\ 0 & 1 & 0 \dots & 0 & * \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & 1 & * \\ 0 & \dots & 0 & 0 & 0 \end{pmatrix}. \quad (5)$$

To precondition in such a way, we take an incomplete LU-factorization of the Jacobi matrix $F'(\check{x})$ at the approximate solution \check{x} .

EXAMPLE: Define

$$\begin{aligned} f_1(x) &= x_1 + x_2 + x_3, \\ f_2(x) &= -x_2 + x_3^3, \\ f_3(x) &= x_2 + x_3^3, \end{aligned} \tag{6}$$

□

In this example, $F(x) = 0$ at $x = (0, 0, 0)^T$, and

$$F'(0) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

If we choose $\mathbf{x} = ([-0.02, 0.02], [-0.01, 0.01], [-0.01, 0.01])^T$, then an interval Jacobi matrix is

$$\mathbf{F}'(\mathbf{x}) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & [0, 0.0003] \\ 0 & 1 & [0, 0.0003] \end{pmatrix}.$$

Let Y represent a nonsingular matrix corresponding to the incomplete preconditioning. We can obtain such a matrix by replacing the last column of U by the corresponding column of the identity matrix, to form \tilde{U} ; we then set $Y = \tilde{U}^{-1}L^{-1}$. Then

$$Y\mathbf{F}'(\mathbf{x}) = \begin{pmatrix} 1 & 0 & [0.9997, 1] \\ 0 & 1 & [-0.0003, 0] \\ 0 & 0 & [0, 0.0006] \end{pmatrix}, \quad \text{and } YF(x) \approx \begin{pmatrix} x_1 + x_3 - x_3^3 \\ x_2 - x_3^3 \\ 2x_3^3 \end{pmatrix},$$

where

$$Y = \begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

Our simplification techniques in [11], [9], and [5] rely on numerically “solving” for x_k in terms of x_n in the k -th equation, $1 \leq k \leq n - 1$, using interval techniques to take account of the fact that the form in (5) is only approximate. To illustrate, we follow the general procedure in [11]. In Theorem 2, we will choose $\ell = 3$ and $s = +1$. First, we see that the relative widths of the coordinates of \mathbf{x} follow [11, (5.1)], so we would expect there to be no solutions of $f_1 = 0$, and hence, no solutions of $F_{-\ell} = 0$, on $\mathbf{x}_{\underline{1}}$ and $\mathbf{x}_{\overline{1}}$. We verify this by evaluating $f_1(\mathbf{x}_{\underline{1}})$ and $f_1(\mathbf{x}_{\overline{1}})$ with mean value extensions:

$$\begin{aligned} (YF)_1(\mathbf{x}_{\underline{1}}) &\subseteq (YF)_1(0, 0, 0) + 1 \cdot (-0.02) + [0.9997, 1] \cdot [-0.01, 0.01] \\ &\subseteq [-0.03, -0.01], \end{aligned}$$

so we have verified that $0 \notin (Yf)_1(\mathbf{x}_1)$. Similarly, $(Yf)_1(\mathbf{x}_1) \subseteq [.01, .03]$, and we have verified that $(YF)_{-3} \neq 0$ on $\mathbf{x}_1 = (-0.02, [-0.01, 0.01], [-0.01, 0.01])^T$ and $\mathbf{x}_1 = (+0.002, [-0.01, 0.01], [-0.01, 0.01])^T$. Similarly, we use mean value extensions for $(Yf)_2$ on \mathbf{x}_2 and \mathbf{x}_2 to verify that $(YF)_{-3} \neq 0$ on \mathbf{x}_2 and \mathbf{x}_2 .

Now, we proceed as in the search phase of [5, Algorithm 1], to find the solutions of $(YF)_{-3} = 0$ on \mathbf{x}_3 and \mathbf{x}_3 . The search proceeds by “substitution” of the bound for x_3 into the mean value extensions for $(YF)_1$ and $(YF)_2$, to determine bounds on \mathbf{x}_1 and \mathbf{x}_2 where $F_{-3} = 0$. It is necessary here to use mean value extensions based at the midpoint vector of the face. For example, on \mathbf{x}_3 , $x_3 = -0.01$. Plugging into $(YF)_1 = 0$ gives

$$\begin{aligned} & (YF)_1(0, 0, -0.01) + (x_1 - 0) + 0 \cdot x_2 + [0.9997, 1](0) = 0 \\ \Rightarrow x_1 \in & 0 - \frac{(YF)_1(0, 0, -0.01) - ([-0.01, -0.009997] \cdot 0)}{1} = 0.009999. \end{aligned}$$

Similarly, we obtain $x_2 \in [-10^{-6}, -10^{-6}]$. (Note that this is simply the same as applying two of the three steps of a Gauss–Seidel sweep to the preconditioned system YF ; this can be considered as an *incomplete Gauss–Seidel sweep*.) We thus obtain that the solution of $(YF)_{-3} = 0$ on \mathbf{x}_3 must be at

$$x \in ([0.009999], [-10^{-6}], [-0.01])^T = \mathbf{x}^{(1)}.$$

An interval evaluation of $F(\mathbf{x}^{(1)})$ gives

$$YF(x) \in ([0, 0], [0, 0], [-2 \times 10^{-6}, -2 \times 10^{-6}])^T,$$

thus showing that $(YF)_3 < 0$ at the unique solution of $(YF)_{-3} = 0$ on \mathbf{x}_3 . (On an actual computer, there would be some roundout error in the above, although it would not be significant here.) Since $(YF)_3(\mathbf{x}^{(2)}) < 0$ and we have chosen $s = 1$, this solution of $(YF)_{-3} = 0$ on $\partial \mathbf{x}$ does not occur in the sum in Theorem 2. However, we do a similar computation on \mathbf{x}_3 , to obtain a point $\mathbf{x}^{(\bar{1})} \in \mathbf{x}_3$ with

$$\mathbf{x}^{(\bar{1})} = \begin{pmatrix} -0.009999 \\ +10^{-6} \\ +0.01 \end{pmatrix}, \quad YF(\mathbf{x}^{(\bar{1})}) = \begin{pmatrix} 0 \\ 0 \\ +2 \times 10^{-6} \end{pmatrix}.$$

Since $(YF)_{-3}(\mathbf{x}^{(\bar{1})}) > 0$, $\mathbf{x}^{(\bar{1})}$ figures into the sum in Theorem 2. At $\mathbf{x}^{(\bar{1})}$, we have

$$\frac{\partial(YF)_{-3}}{\partial x_1 \partial x_2}(\mathbf{x}^{(\bar{1})}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \det \left(\frac{\partial(YF)_{-3}}{\partial x_1 \partial x_2}(\mathbf{x}^{(\bar{1})}) \right) > 0.$$

Finally, since $k = 3$ for the sum in Theorem 2 and since the upper faces correspond to the second summation in Theorem 2, the contribution of $\mathbf{x}^{(\bar{1})}$ to this sum is $+1$.

Since the entire process above has exhaustively and rigorously searched all of $\partial \mathbf{x}$, we have verified that $d(YF, \mathbf{x}, 0) = +1$, and hence, there exists a solution of $F(x) = 0$ in \mathbf{x} . Note that we have done this with $2 * (n - 1)$ mean-value-extension evaluations of $(n - 1)$ components of F and with two incomplete Gauss–Seidel sweeps².

Can we do a similar computation when when the components of F are non-smooth? Consider

EXAMPLE: Define

$$\begin{aligned} f_1(x) &= x_1 + x_2 + x_3, \\ f_2(x) &= \begin{cases} -x_2 + x_3^3 & \text{if } x_2 \geq 0, \\ -5x_2 + x_3^3 & \text{if } x_2 < 0, \end{cases} \\ f_3(x) &= \begin{cases} x_2 + x_3^3 & \text{if } x_2 \geq 0, \\ 0.1x_2 + x_3^3 & \text{if } x_2 < 0. \end{cases} \end{aligned} \quad (7)$$

□

This example is similar to the previous example, except that the Jacobi matrix F' is not defined at the solution $x^* = (0, 0, 0)^T$. However, we may possibly use techniques for non-smooth extensions as described in [8, Ch. 5]³. In short, to evaluate $F'(\mathbf{x})$ for use in mean-value extensions, etc., we simply take the interval hull of the range of F' over all $x \in \mathbf{x}$ for which $F'(x)$ is defined. If we take $\mathbf{x} = ([-0.02, 0.02], [-0.01, 0.01], [-0.01, 0.01])^T$, we obtain

$$F'(\mathbf{x}) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & [-5, -1] & [0, 0.0003] \\ 0 & [0.1, 1] & [0, 0.0003] \end{pmatrix}.$$

We can try preconditioning using the matrix of midpoints of $F'(\mathbf{x})$:

$$m(F'(\mathbf{x})) = \begin{pmatrix} 1 & 1.00 & 1.00000 \\ 0 & -3.00 & 0.00015 \\ 0 & 0.55 & 0.00015 \end{pmatrix}.$$

Although $m(F'(\mathbf{x}))$ is non-singular, $F'(\mathbf{x})$ contains singular matrices, and, in this case, the midpoint matrix is approximately singular. We may still do an incomplete LU-factorization for $m(F'(\mathbf{x}))$ (stopping at the small pivot element) to obtain:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.18\bar{3} & 1 \end{pmatrix}, \quad \tilde{U} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad Y = \tilde{U}^{-1}L^{-1} = \begin{pmatrix} 1 & 0.33\bar{3} & 0 \\ 0 & -0.33\bar{3} & 0 \\ 0 & 0.18\bar{3} & 1 \end{pmatrix},$$

and

$$YF'(\mathbf{x}) = \begin{pmatrix} 1 & [-0.66\bar{6}, 0.66\bar{6}] & [1.0000, 1.0001] \\ 0 & [0.33\bar{3}, 1.66\bar{6}] & [-0.0001, 0] \\ 0 & [-0.81\bar{6}, 0.81\bar{6}] & [0, 0.000355] \end{pmatrix}.$$

We will now attempt to proceed as in the previous example. We observe that the main difference in this example is that the entries in the preconditioned Jacobi matrix are wider, and, in contrast to the previous example, cannot be made narrower by decreasing the coordinate widths of \mathbf{x} . Proceeding with the verification that $(YF)_{-3} \neq 0$ on \mathbf{x}_1 , \mathbf{x}_1 , \mathbf{x}_2 , and \mathbf{x}_2 , we obtain:

$$\begin{aligned} (YF)_1(\mathbf{x}_1) &\subseteq (YF)_1(0, 0, 0) + 1 \cdot (-0.02) + [-0.66\bar{6}, 0.66\bar{6}] \cdot [-0.01, 0.01] \\ &\quad + [1, 1.0001] \cdot [-0.01, 0.01] \\ &\subseteq [-0.037, -0.002], \end{aligned}$$

and the verification that $0 \notin (YF)_1(\mathbf{x}_1)$ succeeds in this case. However, extra width is introduced due to the off-diagonal entries of the preconditioned Jacobi matrix; these off-diagonal entries cannot be made small by making the box widths small, and could cause a problem in this step of the verification process, in other non-smooth examples. Nonetheless, in this case, we can also verify $0 \notin (YF)_1(\mathbf{x}_1)$, $0 \notin (YF)_2(\mathbf{x}_2)$, and $0 \notin (YF)_2(\mathbf{x}_2)$ with corresponding mean value extensions.

Proceeding to the incomplete Gauss–Seidel sweep,

$$(YF)(\check{x}) = (YF)(0, 0, -0.01) = \begin{pmatrix} -0.010000\bar{3} \\ 0.000000\bar{3} \\ -0.000000118\bar{3} \end{pmatrix},$$

and the incomplete Gauss–Seidel sweep gives, for the solution to $(YF)_{-3} = 0$ on \mathbf{x}_3 ,

$$x \in ([0.003333\bar{6}, 0.016667], [-1.0 \times 10^{-6}, -0.2 \times 10^{-6}], [-0.01, -0.01])^T = \mathbf{x}^{(1)}.$$

Continuing, an interval evaluation of $F(\mathbf{x}^{(1)})$ gives

$$YF(x) \in \begin{pmatrix} [-0.006667\bar{3}, 0.0066681\bar{3}] \\ [-0.000001\bar{3}, 0.0000000] \\ [-0.0000011, -0.00000028\bar{6}] \end{pmatrix}.$$

The above computation shows that $(YF)_3 < 0$ at any points on \mathbf{x}_3 where $(YF)_{-3}(x) = 0$; since we have chosen $s = 1$, such points do not enter into the sum in Theorem 2. However, proceeding similarly with \mathbf{x}_3 gives

$$\mathbf{x}^{(\bar{1})} = \begin{pmatrix} [-0.016667, -0.003333\bar{6}] \\ [+0.0000002, +0.000001] \\ 0.01 \end{pmatrix}, (YF)(\mathbf{x}^{(\bar{1})}) = \begin{pmatrix} [-0.0066668, 0.0066676] \\ [-0.0000002\bar{6}, 0] \\ [0.0000012, 0.00000214\bar{6}] \end{pmatrix}.$$

Furthermore, over $\mathbf{x}^{(\bar{1})}$,

$$\frac{\partial(YF)_{-3}}{\partial x_1 \partial x_2}(\mathbf{x}^{(\bar{1})}) = \begin{pmatrix} 1 & 0.\bar{6} \\ 0 & 0.\bar{3} \end{pmatrix}, \quad \det \left(\frac{\partial(YF)_{-3}}{\partial x_1 \partial x_2}(\mathbf{x}^{(\bar{1})}) \right) > 0.$$

Thus, as in the previous, smooth example, we have shown that $d(YF, \mathbf{x}, 0) = 1$, and, therefore, since Y is non-singular, we have verified existence of a solution of $F(x) = 0$ within \mathbf{x} . (Note that, since $\det(Y) = -0.\bar{3} < 0$ here, $d(F, \mathbf{x}, 0) = -1$.)

Although the computations succeeded with this second, non-smooth, example, we see that the extra widths (that cannot be reduced by making the coordinate widths of \mathbf{x} smaller) could cause either failure to verify $F_{-n} \neq 0$ on \mathbf{x}_k or \mathbf{x}_k^- for some k between 1 and $n - 1$, or else these excess widths may cause failure to obtain sufficiently tight bounds to the solutions to $F_{-n} = 0$ on \mathbf{x}_n and \mathbf{x}_n^- to rigorously determine $\text{sgn}(f_n)$ at these solutions. Such excessive overestimation seems more likely when $n > 3$; nonetheless, the following modification to Example (7) exhibits such excess.

EXAMPLE: Define

$$\begin{aligned} f_1(x) &= \begin{cases} x_1 + x_2 + x_3 & \text{if } x_2 \geq 0, \\ x_1 + 10x_2^2 + x_3 & \text{if } x_2 < 0, \end{cases} \\ f_2(x) &= \text{same as in Example (7),} \\ f_3(x) &= \text{same as in Example (7).} \end{aligned} \tag{8}$$

□

Again taking $\mathbf{x} = ([-0.02, 0.02], [-0.01, 0.01], [-0.01, 0.01])^T$, we obtain

$$\mathbf{F}'(\mathbf{x}) = \begin{pmatrix} 1 & [1, 10] & 1 \\ 0 & [-5, -1] & [0, 0.0003] \\ 0 & [0.1, 1] & [0, 0.0003] \end{pmatrix}, \quad \mathbf{m}(\mathbf{F}'(\mathbf{x})) = \begin{pmatrix} 1 & 5.50 & 1.00000 \\ 0 & -3.00 & 0.00015 \\ 0 & 0.55 & 0.00015 \end{pmatrix}.$$

Computing the incomplete LU-factorization as before now gives

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.18\bar{3} & 1 \end{pmatrix}, \quad \tilde{U} = \begin{pmatrix} 1 & 5.5 & 0 \\ 0 & -3.0 & 0 \\ 0 & 0.0 & 1 \end{pmatrix}, \quad Y = \tilde{U}^{-1}L^{-1} = \begin{pmatrix} 1 & 1.83\bar{3} & 0 \\ 0 & -0.33\bar{3} & 0 \\ 0 & 0.18\bar{3} & 1 \end{pmatrix},$$

and

$$YF'(\mathbf{x}) = \begin{pmatrix} 1 & [-8.16\bar{6}, 8.16\bar{6}] & [1.0000, 1.00055] \\ 0 & [0.33\bar{3}, 1.66\bar{6}] & [-0.0001, 0] \\ 0 & [-0.81\bar{6}, 0.81\bar{6}] & [0, 0.000355] \end{pmatrix}.$$

Trying, as before, to verify $(YF)_{-3} \neq 0$ on \mathbf{x}_1 , we obtain:

$$\begin{aligned} (YF)_1(\mathbf{x}_1) &\subseteq (YF)_1(0, 0, 0) + 1 \cdot (-0.02) + [-8.16\bar{6}, 8.16\bar{6}] \cdot [-0.01, 0.01] \\ &\quad + [1, 1.00055] \cdot [-0.01, 0.01] \\ &\subset [-0.116721\bar{6}, +0.071621\bar{6}], \end{aligned}$$

and we cannot conclude that $0 \notin (YF)_1$. In fact, for this particular example, we can compute the sharp range of $(YF)_1$ over \mathbf{x}_1 . We have

$$\begin{aligned} (YF)_1(x) &= f_1(x) + 1.8\bar{3}f_2(x) \\ &= \begin{cases} x_1 - 0.8\bar{3}x_2 + x_3 + x_3^3 & \text{if } x_2 \geq 0 \\ x_1 - 4.8\bar{3}x_2 + x_3 + x_3^3 & \text{if } x_2 < 0, \end{cases} \end{aligned}$$

from which it follows that the range of $(YF)_1$ over \mathbf{x}_1 must be equal to

$$\begin{aligned} &\underbrace{\mathbf{x}_1}_{-0.02} + \underbrace{\text{range of } x_2 \text{ terms}}_{[-0.008\bar{3}, +0.048\bar{3}]} + \underbrace{\text{range of } x_3 \text{ terms}}_{[-0.010001, +0.010001]} \\ &= [-0.038334\bar{3}, +0.038334\bar{3}]. \end{aligned} \tag{9}$$

Our construction of the box as in [11, (5.1)] fails in Example (8) to arrange that $(YF)_{-3}$ is non-zero on \mathbf{x}_1 . The reason is that the heuristic presented in [11, (5.1)] to select the ratio of coordinate widths to force $0 \notin (YF)_1(\mathbf{x}_1)$ assumes that the

off-diagonal entries of $Y\mathbf{F}'(\mathbf{x})$, except in the last column, are approximately zero, and that $(YF)_k$, $1 \leq k \leq n-1$ is thus approximately a linear function of x_1 and x_n . If the components of F have continuous second derivatives and if usual interval extensions are employed to obtain the entries in $\mathbf{F}'(\mathbf{x})$, then this assumption becomes valid if the coordinate widths of \mathbf{x} are all sufficiently small. However, in Example (8), one of the off-diagonal entries is large, no matter how small we make the widths of the box \mathbf{x} . To see this, observe that each of the three terms in (9) is approximately linear, so, if the ratios of the widths of \mathbf{x} remain the same, the range will be an interval that is approximately symmetric around zero, no matter how small we make \mathbf{x} , as long as \mathbf{x} is centered on the solution $x^* = (0, 0, 0)^T$.

2.2. The Degree Prediction Heuristic: Examples

To verify existence, we verify that the topological degree is a particular non-zero value. To efficiently prove that the degree is a certain value, we first conjecture what that value is. For example, we do not need to extend to complex space to verify existence if the degree is odd (as in the examples above), and verification of the degree in complex space (corresponding to solutions of even degree) as described in [11] and [9] is efficient only if we first correctly conjecture the value of $d(F, \mathbf{x}, 0)$. We presented a heuristic for guessing the value of $d(F, \mathbf{x}, 0)$ in [9, §5] as follows:

1. Assume we have an accurate approximate solution \check{x} to $F(x) = 0$, and assume that F' has been preconditioned so $YF'(\check{x}) \approx YF'(x^*)$ is roughly of the form (5).
2. In view of the form (5), define

$$\begin{aligned} g(x_n - \check{x}_n) &= (YF)_n(t_1, \dots, t_n), \quad \text{where } t_n = x_n \text{ and} \\ t_k &= \check{x}_k - \frac{\partial(YF)_k}{\partial x_n}(\check{x})(x_n - \check{x}_n), \quad 1 \leq k \leq n-1, \\ K(r, x_n - \check{x}_n) &\equiv \frac{g(x_n - \check{x}_n)}{(x_n - \check{x}_n)^r}, \quad \text{and} \\ R(r) &= \frac{K(r, \delta(x_n - \check{x}_n))}{K(r, x_n - \check{x}_n)} = \frac{g(\delta(x_n - \check{x}_n))}{g(x_n - \check{x}_n)} \delta^{-r}, \end{aligned} \tag{10}$$

for integers r and a heuristic parameter δ .

Then, as was shown in [9, §5], $R(r)$ is approximately equal to δ^{d-r} , provided F (and hence YF) can be represented as a multivariate Taylor polynomial of degree at least d about $x^* \approx \check{x}$. Thus, if we chose, say, $\delta = 100$, then we could compute $R(r)$ for different values of r , until we found an r_0 for which $0.01 < R(r_0) < 100$; $d(F, \mathbf{z}, 0)$ is then probably equal to r_0 , where \mathbf{z} is a small box in complex n -space containing the real point \check{x} . For example, in Example 6, suppose we have found the solution $\check{x} = x^* = (0, 0, 0)^T$ exactly. Then we may choose $x_n - \check{x}_n = 0.01$. Then,

since

$$YF'(\tilde{x}) = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$t_1 = -1 \cdot (0.01) = -0.01$ and $t_2 = 0$, $F(t_1, t_2, x_3) = (0, 10^{-6}, 10^{-6})$, and $g(x_n - \tilde{x}_n) = (YF)_3(t_1, t_2, x_3) = 2 \times 10^{-6}$. Similarly, $g(\delta(x_n - \tilde{x}_n)) = 2$, so

$$R(r) = \frac{g(\delta(x_n - \tilde{x}_n))}{g(x_n - \tilde{x}_n)} \cdot \delta^{-r} = \frac{2}{2 \times 10^{-6}} \cdot 100^{-r} = 10^{6-2r}$$

Since $R(r)$ is between 0.01 and 100 when $r = 3$, this heuristic provides the guess that $d(F, \mathbf{z}, 0) = 3$. In fact, the heuristic happens to also give the correct $d(F, \mathbf{z}, 0)$ for Example 7 and Example 8, since if either $YF'(0, 0, 0)$ or $m(YF'(\mathbf{x}))$ is used, the heuristic gives $t_2 > 0$. However, consider

EXAMPLE: Define

$$\begin{aligned} f_1(x) &= x_1 + x_2 + x_3, \\ f_2(x) &= \begin{cases} -x_2 + x_3^2 & \text{if } x_3 \geq 0, \\ -x_2 + x_3^3 & \text{if } x_3 < 0, \end{cases} \\ f_3(x) &= \begin{cases} x_2 + x_3^2 & \text{if } x_3 \geq 0, \\ x_2 + x_3^3 & \text{if } x_3 < 0. \end{cases} \end{aligned} \tag{11}$$

□

Again taking $\mathbf{x} = ([-0.02, 0.02], [-0.01, 0.01], [-0.01, 0.01])^T$, we obtain

$$\begin{aligned} \mathbf{F}'(\mathbf{x}) &= \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & [-3 \times 10^{-4}, 2 \times 10^{-2}] \\ 0 & 1 & [-3 \times 10^{-4}, 2 \times 10^{-2}] \end{pmatrix}, \quad m(\mathbf{F}'(\mathbf{x})) = \begin{pmatrix} 1 & 1 & 1.00000 \\ 0 & -1 & 0.00985 \\ 0 & 1 & 0.000985 \end{pmatrix}, \\ Y &= \begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}, \quad \text{and } YF'(\mathbf{x}) = \begin{pmatrix} 1 & 0 & [0.9997, 1.02] \\ 0 & 1 & [-0.02, 0.0003] \\ 0 & 1 & [-0.0006, 0.04] \end{pmatrix}. \end{aligned}$$

The degree verification process now proceeds very similarly to Example (6): After verifying no solutions of $(YF)_{-3}$ on \mathbf{x}_1 , \mathbf{x}_1 , \mathbf{x}_2 , and \mathbf{x}_2 , we verify that $(YF)_3 < 0$ at the solution of $(YF)_{-3} = 0$ on \mathbf{x}_3 . On \mathbf{x}_3 , we obtain the solution

$$\mathbf{x}^{(\bar{1})} = \begin{pmatrix} -1.01 \times 10^{-2} \\ 1.00 \times 10^{-4} \\ 1.00 \times 10^{-2} \end{pmatrix}, \quad (YF)_3(\mathbf{x}^{(\bar{1})}) = 2 \times 10^{-3}.$$

Computations similar to those for Example (6) then verify that the contribution of $\mathbf{x}^{(\bar{1})}$ to the sum in Theorem 2 is +1. Furthermore, since F is smooth at $\mathbf{x}^{(\bar{1})}$, this successfully verifies that $d(YF, \mathbf{x}, 0) = 1$. (See §3 below for comments on why the theory is still valid.)

However, let us attempt to apply the heuristic (10) to Example 11. Using $x_n - \check{x}_n = x_3 = 0.01$, we obtain $t_1 = 1.00985 \times 10^{-2}$, $t_2 = 9.85^{-5}$, and $g(x_n - \check{x}_n) = (YF)_3(t_1, t_2, x_3) = 0.0002$. Similarly, with $\delta = 100$, we obtain $g(\delta(x_n - \check{x}_n)) = 2$. Thus,

$$R(r) = \frac{2}{2 \times 10^{-4}} \cdot 100^{-r} = 10^{2-r},$$

and the heuristic predicts that $d(F, \mathbf{z}, 0) = 2$. In fact, the actual degree of the complex extension must be odd, since the degree in real space is non-zero.

2.3. Summary: What do These Examples Illustrate?

The topological-degree-based algorithms we introduced in [11], [9], and [5] depend on being able to reduce the system, with preconditioning, to a form in which the off-diagonal elements of the interval Jacobi matrix (except for the last rows, corresponding to the singular part) are intervals that approximately contain zero. For systems with continuous derivatives of at least 2, it can always be arranged so that the off-diagonal elements are sufficiently small by making the approximate solution sufficiently accurate and making the box \mathbf{x} , centered on the approximate solution, sufficiently small. In the non-smooth case, depending on particulars of the system, it may not be possible to precondition the system such that, for small boxes \mathbf{x} , the off-diagonal elements corresponding to the non-singular part of the preconditioned interval Jacobi matrix are sufficiently small.

Second, the verification procedure works with a heuristic that determines a probable topological index. In the smooth case, subject to a size being chosen reasonably, this heuristic can be expected to usually work. Examples have shown that the underlying assumption upon which this heuristic is based (that is, that the system can be reduced to an equation that behaves like a power of one of the variables) no longer holds for non-smooth problems, and that the heuristic actually fails for such cases.

Finally⁴, in the complex case (corresponding to solutions of even degree) described in [11] and [9], an exhaustive one-dimensional search is made more efficient by predicting locations of the solutions of $F_{-n} = 0$ on the boundary $\partial\mathbf{x}$. The predicted locations are based on a quadratic model (when the degree is suspected to be 2) or on a higher-order model (when the degree is suspected to equal some number higher than 2). In the non-smooth case, such predictions make no sense, and the solutions may appear anywhere.

3. Theoretical Considerations

The theoretical grounding of the index verification procedure consists of Theorem 2, combined with the preconditioning, interval evaluations, and incomplete Gauss-Seidel steps illustrated in §2.1. Both Theorem 2 and the procedures illustrated in §2.1 are valid when F is non-smooth, for the following reasons.

3.1. *Why Theorem 2 is true for non-smooth functions*

The topological degree depends only on values on the boundary, and, furthermore, the topological degree is a continuous function of F . (See [2],[3], [13], etc.) Finally, it is well known that any continuous function $F : \mathbf{x} \rightarrow \mathbb{R}^n$ can be approximated arbitrarily closely by a differentiable function. These facts, combined with the proof of Theorem 2 in [11], show that Theorem 2 is valid even for F nonsmooth.

3.2. *Why the elimination and incomplete Gauss–Seidel procedure are valid for non-smooth functions*

Verification that the faces $\mathbf{x}_{\underline{k}}$ and $\mathbf{x}_{\bar{k}}$ do not contain solutions of $F_{\neg n} = 0$, for $1 \leq k \leq n - 1$, depends only on interval evaluations. Thus, whether or not F is smooth, the conclusions will be correct provided the interval extensions are correct. Similarly, the incomplete Gauss–Seidel procedure involves only interval arithmetic (on possibly non-smooth expressions), and hence always gives correct results.

3.3. *Consequences*

Thus, regardless of whether or not F is smooth at solutions of $F = 0$, the verification procedure will never incorrectly verify existence. However, for the procedure to actually assert existence, certain widths need to be sufficiently small. In our previous analyses, the conditions we used to argue that those widths could be made small depended strongly on F having a Taylor approximation of an appropriate order. As a consequence, the verification is more likely to fail, if applied naively for non-smooth F .

Nonetheless, since Theorem 2 is true for continuous functions, as long as the determinants in the statement of the theorem are defined and non-zero, Theorem 2 can still be used in a generalized verification procedure for non-smooth functions. However, without elimination and incomplete Gauss–Seidel procedures, direct application of Theorem 2 requires an exhaustive search of $2n(n - 1)$ -dimensional hypercubes, a prohibitive amount of work when n is large.

4. Conclusions

The procedures we have previously proposed for verifying existence of solutions of nonlinear systems at which the Jacobi matrix is singular are also applicable when the system is non-smooth at the solutions. However, these procedures are less likely to produce a positive result. The underlying theorem is still valid, but acceleration procedures may not work. The underlying theorem can be applied directly, without the acceleration procedures, but then, the amount of computation would increase exponentially (rather than cubically) with the number of variables. Nonetheless, as our examples have hinted, it may be possible to arrange computations to avoid excessive computational expense in specific non-smooth cases.

Notes

1. If \mathbf{A} is a slope matrix for F over \mathbf{x} and centered at some point $\tilde{x} \in \mathbf{x}$, then it is possible that \mathbf{A} contains no singular matrices, even though the Jacobi matrix $F'(x)$ is singular at some $x \in \mathbf{x}$. However, it is happenstance when this occurs, and may not be easy to purposefully arrange.
2. We have shown that $d(YF, \mathbf{x}, 0) = 1$. However, $d(F, \mathbf{x}, 0) = \det(Y) \cdot d(F, \mathbf{x}, 0)$. If we verify that $\det(Y) = -1$, we will have shown that $d(F, \mathbf{x}, 0) = -1$.
3. The theory underlying such non-smooth extensions is covered by *cset theory*, developed in [17].
4. Examples of the complex case have not been given here; such examples, fully worked out, have significantly more computation, and require two one-dimensional searches.

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