On Existence and Uniqueness Verification for Non-Smooth Functions

by

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- We will show actual computations, to illustrate the relationship between traditional interval Newton methods and degree theory.
- We will illustrate how the computations can succeed or break down in non-smooth problems.

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The General Question

Let $F(x) = 0$ represent a system of n equations in n unknowns, and suppose $\check{x}$ is a numerical approximation to a solution x^*, $F(x^*) = 0$. We wish to compute bounds

$$\begin{aligned} \boldsymbol{x} &= (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n) \\ &= ([\underline{x}_1, \overline{x}_1], [\underline{x}_2, \overline{x}_2], \ldots, [\underline{x}_n, \overline{x}_n], \end{aligned}$$

such that $\check{x}$ is the center of $\boldsymbol{x}$, and such that $\boldsymbol{x}$ is guaranteed to contain a solution x^* to $F(x) = 0$. That is,

> Given $F : \boldsymbol{x} \to \mathbb{R}^n$, where $\boldsymbol{x} \in \mathbb{IR}^n$, *rigorously* verify:
>
> - there exists a $x^* \in \boldsymbol{x}$ such that $F(x^*) = 0$.

(1)

Here, $\mathbb{IR}^n$ represents the set of interval n-vectors.

Interval Newton Methods

The Traditional Setting

If the Jacobi matrix $F'(x^*)$ is non-singular and continuous in $\boldsymbol{x}$, then we can use an interval Newton method:

$$\tilde{\boldsymbol{x}} = \boldsymbol{N}(F; \boldsymbol{x}, \check{x}) = \check{x} + \boldsymbol{v},$$

where

$$\Sigma(\boldsymbol{A}, -F(\check{x})) \subset \boldsymbol{v},$$

where $\boldsymbol{A}$ is a Lipschitz matrix for F over $\boldsymbol{x}$,

and where $\Sigma(\boldsymbol{A}, -F(\check{x}))$
$= \left\{x \in \mathbb{R}^n \mid \exists A \in \boldsymbol{A} \text{ with } AX = -F(\check{x})\right\}.$

We have:

Theorem 1 *(see Neumaier's book) Suppose $\tilde{\boldsymbol{x}} = \boldsymbol{N}(F; \boldsymbol{x}, \check{x})$ is the image of $\boldsymbol{x}$ and $\check{x}$ under an interval Newton method. If $\tilde{\boldsymbol{x}} \subseteq \boldsymbol{x}$, it follows that there exists a unique solution of $F(x) = 0$ within $\boldsymbol{x}$.*

Modifications for Singular / Non-Smooth Systems

The Topological Degree

- We can verify existence of solutions to $F(x) = 0$ within $\boldsymbol{x}$, even when $\det(F'(x^*)) = 0$.
- We do this with the *topological degree* $\mathrm{d}(F, \boldsymbol{x}, 0)$ of F over $\boldsymbol{x}$.
- If $\det(F'(x)) \neq 0$ when $F(x) = 0$, then

$$\mathrm{d}(F, \boldsymbol{x}, 0) = \sum_{\substack{x \in \mathrm{int}(\boldsymbol{x}),\\ F(x)=0}} \mathrm{sgn}(\det(F'(x))).$$

- The integer $\mathrm{d}(F, \boldsymbol{x}, 0)$ is continuous in F and depends only on values of F on the boundary $\partial\boldsymbol{x}$, so F' may be singular or non-smooth in the interior $\mathrm{int}(\boldsymbol{x})$.
- $\mathrm{d}(F, \boldsymbol{x}, 0) \neq 0 \Rightarrow F(x) = 0$ has a solution in $x^* \in \boldsymbol{x}$.

Modifications for Singular / Non-Smooth Systems

The Theorem Used in the Algorithms

- The boundary of $\boldsymbol{x}$ consists of:

$$\boldsymbol{x}_{\underline{k}} \equiv (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{k-1}, \underline{x}_k, \boldsymbol{x}_{k+1}, \ldots, \boldsymbol{x}_n)^T,$$
$$\boldsymbol{x}_{\overline{k}} \equiv (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{k-1}, \overline{x}_k, \boldsymbol{x}_{k+1}, \ldots, \boldsymbol{x}_n)^T,$$

  where $k = 1, \ldots, n$.

- For fixed ℓ, $1 \leq \ell \leq n$, define $F_{\neg\ell}(x) = (f_1(x), \ldots, f_{\ell-1}(x), f_{\ell+1}(x), \ldots, f_n(x))^T$.

- For this ℓ, define $\underline{K_0(s)}$ as that subset of $\{k | k \in \{1, \ldots, n\}\}$ such that $F_{\neg\ell} = 0$ has solutions on $\boldsymbol{x}_{\underline{k}}$ and $\mathrm{sgn}(f_\ell) = s$ at these solutions; similarly define $\overline{K_0(s)}$ such that $F_{\neg\ell} = 0$ has solutions on $\boldsymbol{x}_{\overline{k}}$ and $\mathrm{sgn}(f_\ell) = s$ at these solutions, where $s \in \{-1, +1\}$.

The Theorem Used in the Algorithms (continued)

Theorem 2 *If F is continuous, $F \neq 0$ on $\partial \boldsymbol{x}$, and there is an ℓ, $1 \leq \ell \leq n$, such that:*
(1) $F_{\neg\ell} \neq 0$ on $\partial \boldsymbol{x}_{\underline{k}}$ or $\partial \boldsymbol{x}_{\overline{k}}$, $k = 1, \ldots, n$;
(2) $\det(F'_{\neg\ell}) \neq 0$ whenever $F_{\neg\ell} = 0$ on $\partial \boldsymbol{x}$.
Then

$$
\begin{aligned}
\mathrm{d}(F, \boldsymbol{x}, 0) = (-1)^{\ell-1} s \\
\cdot \Bigg\{ \sum_{k \in \underline{K_0(s)}} (-1)^k \\
\sum_{\substack{x \in \boldsymbol{x}_{\underline{k}} \\ F_{\neg\ell}(x)=0}} \operatorname{sgn} \left| \frac{\partial F_{\neg\ell}}{\partial x_1 x_2 \ldots x_{k-1} x_{k+1} \ldots x_n}(x) \right| \\
+ \sum_{k \in \overline{K_0(s)}} (-1)^{k+1} \\
\sum_{\substack{x \in \boldsymbol{x}_{\overline{k}} \\ F_{\neg\ell}(x)=0}} \operatorname{sgn} \left| \frac{\partial F_{\neg\ell}}{\partial x_1 x_2 \ldots x_{k-1} x_{k+1} \ldots x_n}(x) \right| \Bigg\}.
\end{aligned}
$$

Simplifications to Make It Practical

In our methods, we

1. precondition F;
2. choose the coordinate widths $\mathrm{w}(\boldsymbol{x}_k)$, $1 \le k \le n$ to have $\boldsymbol{F}_{\neg\ell}(\boldsymbol{x}_{\underline{k}}) \neq 0$ and $\boldsymbol{F}_{\neg\ell}(\boldsymbol{x}_{\overline{k}}) \neq 0$ for all k except $k = n - p$ to $k = n$, where p is the dimension of the null space. This eliminates most terms in Theorem 2.
3. We then use a p-dimensional search on the remaining several faces of $\boldsymbol{x}$ to find the solutions of $F_{\neg\ell} = 0$.
4. In certain instances, we use a heuristic to guess the value of $\mathrm{d}(F, \boldsymbol{x}, 0)$.

Simplifications to Make It Practical

The Preconditioner

We use incomplete LU factorization (with full pivoting) to put the Jacobi matrix into the form

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

(for the case where the rank defect is 1).

An Example

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

with

$$\boldsymbol{x} = ([-0.02, 0.02], [-0.01, 0.01], [-0.01, 0.01])^T.$$

$$\boldsymbol{F}'(\boldsymbol{x}) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & [0, .0003] \\ 0 & 1 & [0, .0003] \end{pmatrix}, Y = \begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

We thus have

$$Y\boldsymbol{F}'(\boldsymbol{x}) = \begin{pmatrix} 1 & 0 & [0.9997, 1] \\ 0 & 1 & [-0.0003, 0] \\ 0 & 0 & [0, 0.0006] \end{pmatrix},$$

$$YF(x) \approx \begin{pmatrix} x_1 + x_3 - x_3^3 \\ x_2 - x_3^3 \\ 2x_3^3 \end{pmatrix}.$$

An Example (continued)

- We will find solutions to $F_{\neg 3} = 0$ on the boundary of $\boldsymbol{x}$ at which $\mathrm{sgn}(f_3) = +1$.
- We choose the widths of $\boldsymbol{x}$ appropriately, then we use mean value extensions to show
  - $f_1 \neq 0$ on $\boldsymbol{x}_{\underline{1}}$ and $\boldsymbol{x}_{\overline{1}}$ and
  - $f_2 \neq 0$ on $\boldsymbol{x}_{\underline{2}}$ and $\boldsymbol{x}_{\overline{2}}$.
- We then proceed with the interval Gauss–Seidel method on $\boldsymbol{x}_{\underline{3}}$ and $\boldsymbol{x}_{\overline{3}}$.

An Example (continued)

- No solutions on $\boldsymbol{x}_{\underline{1}}$:

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

- Similarly, on $\boldsymbol{x}_{\overline{1}}$: $(Yf)_1(\boldsymbol{x}_{\overline{1}}) \subseteq [.01, .03]$.

- We thus have verified $(YF)_{\neg 3} \neq 0$ on $\boldsymbol{x}_{\underline{1}} = (-0.02, [-0.01, 0.01], [-0.01, 0.01])^T$ and $\boldsymbol{x}_{\overline{1}} = (+0.002, [-0.01, 0.01], [-0.01, 0.01])^T$.

- Similarly, we use mean value extensions for $(Yf)_2$ on $\boldsymbol{x}_{\underline{2}}$ and $\boldsymbol{x}_{\overline{2}}$ to verify that $(YF)_{\neg 3} \neq 0$ on $\boldsymbol{x}_{\underline{2}}$ and $\boldsymbol{x}_{\overline{2}}$.

An Example (continued)

Verifying solutions on $\boldsymbol{x}_{\underline{3}}$ and $\boldsymbol{x}_{\overline{3}}$

<u>For $\boldsymbol{x}_{\underline{3}}$:</u>

- Plug in $x_3 = -0.01$ and apply the interval Gauss–Seidel method. Setting

  $$\{\text{Mean Value Extension for } (YF)_1\} = 0$$

  gives

  $$\begin{aligned}(YF)_1(0,0,-.01) \;&+\; 1\cdot(x_1-0)\\ &+\; 0\cdot x_2\\ &+\; [0.9997,1](0) = 0;\end{aligned}$$

  solving this for x_1 gives

  $$\begin{aligned}x_1 \;&\in\; 0-\{(YF)_1(0,0,-0.01)\\ &\qquad -([-0.01,-0.009997]\cdot 0)\}/1\\ &=\; 0.009999.\end{aligned}$$

- Similarly, $x_2 \in [-10^{-6}, -10^{-6}]$.

An Example (continued)

Verifying solutions on $\boldsymbol{x}_{\underline{3}}$ and $\boldsymbol{x}_{\overline{3}}$

- Thus,

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

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

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

- Since $(YF)_3 < 0$, this solution can be ignored.

- Similar computations on $\boldsymbol{x}_{\overline{3}}$ give a single point $\boldsymbol{x}^{(\overline{1})}$ at which $(YF)_3(\boldsymbol{x}^{(\overline{1})}) > 0$ and at which which

$$\det\left(\frac{\partial (YF)_{\neg 3}}{\partial x_1 \partial x_2}(\boldsymbol{x}^{\overline{1}})\right) > 0$$

- Combining these facts into the sum in the theorem gives a topological degree $\mathrm{d}(YF, \boldsymbol{x}, 0) = 1$.

An Example (continued)

Summary

- $\mathrm{d}(YF, \boldsymbol{x}, 0) = 1$ proves existence of a solution in $\boldsymbol{x}$.
- This result has been proven with $2 * (n-1)$ mean-value-extension evaluations of $(n-1)$ components of F and with two incomplete Gauss–Seidel sweeps.
- Can the same process succeed when the components of F are non-smooth?

The Principles Behind Our Degree Computation

- For the interval Gauss–Seidel method, we "solve" the preconditioned variable for the i-th variable in the i-th equation.
- Success depends on the magnitude of the off-diagonal elements being larger than the mignitude of the diagonal elements of $Y\boldsymbol{F}'(\boldsymbol{x})$.
- In degree computation, we fix the last variables, eliminating the uncontrolled widths in the last column of $Y\boldsymbol{F}'(\boldsymbol{x})$.

A Non-Smooth Example

Define

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

and take

$$\boldsymbol{x} = ([-0.02, 0.02], [-0.01, 0.01], [-0.01, 0.01])^T.$$

Then

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

- In this case, the off-diagonal entries of $Y\boldsymbol{F}'$ (excluding the last column) are sufficiently small and narrow to allow the verification process to succeed: $\mathrm{d}(YF, \boldsymbol{x}, 0) = 1$.

A Second Non-Smooth Example

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

In this case,

$$Y\boldsymbol{F}'(\boldsymbol{x}) = \begin{pmatrix} 1 & [-8.16\overline{6}, 8.16\overline{6}] & [1.0000, 1.00055] \\ 0 & [0.33\overline{3}, 1.66\overline{6}] & [-0.0001, 0] \\ 0 & [-0.81\overline{6}, 0.81\overline{6}] & [0, 0.000355] \end{pmatrix},$$

and the off-diagonal entries (excluding the last column) are <u>not</u> sufficiently small and narrow to allow the verification process to succeed.

- Details of these two examples can be found in
  `http://interval.louisiana.edu/preprints/nonsmooth_degree.pdf`

Additional Thoughts

- In these algorithms, the effect of the lack of smoothness is similar to the effect of non-smoothness on traditional interval Gauss–Seidel methods for verification of non-singular zeros.
- The degree $\mathrm{d}(F, \boldsymbol{x}, 0)$ depends only on the values F on the boundary of $\boldsymbol{x}$.
  - The formula in the theorem also only involves values on the boundary.
  - In principle, there is no problem applying the theorem for successful verification, as long as F is smooth on the boundary.

Additional Thoughts (continued)

- In practice, non-smoothness inside $\boldsymbol{x}$ makes simplifications as we have illustrated impossible in general.
- Direct application of the theorem involves $(2n)$ global optimization problems.
- For details, see `http://interval.louisiana.edu/preprints/nonsmooth_degree.pdf`
- Our fast method may work anyway (as illustrated with our first non-smooth example).
- There may be other simplifications, for particular non-smooth cases, that we haven't yet discovered.

These transparencies will be available from `http://interval.louisiana.edu/preprints.html`