# Existence and Uniqueness Verification for Singular Zeros of Nonlinear Systems

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# The General Question

$$\boxed{\begin{array}{l}\text{Given } F : \mathbf{x} \to \mathbb{R}^n \text{ and } \mathbf{x} \in \mathbb{IR}^n, \\ \textit{rigorously} \text{ verify:} \\ \quad \bullet \text{ there exists a unique } x^* \in \mathbf{x} \text{ such} \\ \quad\ \ \text{that } F(x^*) = 0,\end{array}} \tag{1}$$

Computer arithmetic can be used to verify the assertion in Problem (1), with the aid of interval extensions and *computational fixed point theorems*.

# The General Question

*Uses*

- Producing rigorous bounds on approximate solutions to linear and nonlinear systems (The approximate solutions can be computed with traditional techniques.)
  - in analysis of stability of structures, where one wants to prove that all eigenvalues have negative real parts
  - in robust computational geometry (surface intersection problems, etc.)
- As a tool in branch and bound algorithms in global optimization.
- As a tool in the verification that *all* zeros of a nonlinear system have been found in a region of $\mathbb{R}^n$.

# The Nonsingular Case

*Traditional Interval Newton Methods*

*Assumptions (roughly stated):*

1. The Jacobi matrix $F'(x^*)$ is nonsingular.
2. $x^*$ is near the center of $\mathbf{x}$.
3. The component widths of $\mathbf{x}$ are small.
4. $\mathbf{N}(F; \mathbf{x}, \check{x})$ is the image of $\mathbf{x}$ under an appropriate, preconditioned interval Newton method, with $\check{x}$ the center of $\mathbf{x}$.

*Then:*

1. The preconditioned $F'(\mathbf{x})$ is approximately the identity matrix.
2. Thus, $\mathbf{N}(F; \mathbf{x}, \check{x}) \subset \mathbf{x}$. This proves that there is a unique solution of $F(x) = 0$ in $\mathbf{x}$.

# The Nonsingular Case

## *An Example*

**Example 1** *Take*

$$\begin{aligned} f_1(x_1, x_2) &= x_1^2 - x_2, \\ f_2(x_1, x_2) &= x_1 - x_2^2, \end{aligned}$$

*and*
$\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)^T = ([-0.1, 0.1], [-0.1, 0.3])^T.$

Take $\check{x} = (0, 0.1)^T$, so
$F(\check{x}) = (-0.1, -0.01)^T$, and an interval extension of the Jacobi matrix is

$$\mathbf{F}'(\mathbf{x}) = \begin{pmatrix} 2\mathbf{x}_1 & -1 \\ 1 & -2\mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} [-.2, .2] & -1 \\ 1 & [-0.6, 0.2] \end{pmatrix}.$$

Precondition by the inverse of the midpoint matrix

$$Y = \{\mathrm{m}(\mathbf{F}'(\mathbf{X}))\}^{-1} = \begin{pmatrix} -0.2 & 1 \\ -1 & 0 \end{pmatrix},$$

# The Nonsingular Case

*An Example (continued)*

so the corresponding linear interval system is

$$Y\mathbf{F}'(\mathbf{x})(\mathbf{x} - \check{x}) = -YF(\check{x}),$$

i.e.,

$$\begin{pmatrix} [0.96, 1.04] & [-0.4, 0.4] \\ [-0.2, 0.2] & 1 \end{pmatrix} (\mathbf{x} - \check{x}) = \begin{pmatrix} -0.01 \\ -0.1 \end{pmatrix}.$$

The interval Gauss–Seidel method applied to this system proves a unique solution in $\mathbf{x}$:

$$\begin{aligned} \tilde{\mathbf{x}}_1 &= 0 - \frac{-0.01 + [-0.4, 0.4][-0.2, 0.2]}{[0.96, 1.04]} \\ &\subseteq [-0.094, 0.073] \subset \mathrm{int}([-0.1, 0.1]). \end{aligned}$$

Similarly, $\tilde{\mathbf{x}}_2 \subset \mathrm{int}(\mathbf{x}_2)$.

# Singularities

When the Jacobi matrix $F'(x^*)$ is singular, computations as above cannot possibly prove existence and uniqueness.

**Example 2** *Take*

$$\begin{aligned} f_1(x_1, x_2) &= x_1^2 - x_2, \\ f_2(x_1, x_2) &= x_1^2 + x_2, \end{aligned}$$

*and*

$\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)^T = ([-0.1, 0.1], [-0.1, 0.3])^T.$

For such systems, the best that a preconditioner can do is reduce the Jacobi matrix to approximately the form

$$\begin{pmatrix} * & 0 & \ldots & 0 & \overbrace{* \ldots *}^{n\text{ - rank}} \\ 0 & * & 0 \ldots & 0 & * \ldots * \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \ldots & 0 & * & * \ldots * \\ 0 & \ldots & 0 & 0 & 0 \ldots 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \ldots & 0 & 0 & 0 \ldots 0 \end{pmatrix}.$$

# Singularities

*Philosophical Considerations*

Uniqueness verification within the original $\mathbf{x}$ is not possible. Alternatives are:

1. (Easy but perhaps not always adequate) *Verify the system has an $\epsilon$–approximate solution within $\mathbf{x}$.*

2. (Only possible in special cases) *Verify the system has at least one solution in $\mathbf{x}$.*

3. (More difficult computationally) *Verify the system has an exact number of solutions, counting multiplicities, in a complex extension of $\mathbf{x}$.*

Which alternative is appropriate in particular contexts?

# Singularities

*$\epsilon$–Approximate Solution*

1. Simply evaluate the interval extension $\mathbf{F}(\mathbf{x})$.
2. If $\|\mathbf{F}(\mathbf{x})\| < \epsilon$, then each component of $\mathbf{F}$ is less than $\epsilon$ everywhere within $\mathbf{x}$. (But all components of $\mathbf{f}$ may not simultaneously vanish.)
3. This technique can be used, along with scaling, etc., to handle non-isolated solutions in branch and bound algorithms.

# Singularities

*Verification of at Least One Solution*

1. The *topological degree* (to be explained shortly) may be computed over $\mathbf{x}$.
2. If the topological degree is non-zero, there is at least one solution of $F(x) = 0$ in $\mathbf{x}$.
3. No conclusion can be reached if the topological degree is zero.

# Singularities

*Verification of the Exact Multiplicity*

1. If $F : \mathbb{C}^n \to \mathbb{C}^n$, then the topological degree of $F$ over $\mathbf{x}$ gives the exact number of solutions, counting multiplicities.

2. If $F : \mathbb{R}^n \to \mathbb{R}^n$, and $F$ can be extended analytically into $\mathbb{C}^n$, then computations can verify existence of an exact solution or solutions (with multiplicity computed by the algorithm) within a small region of complex space containing $\mathbf{x}$.

3. Sometimes the value of the topological degree (i.e. the multiplicity of the solution) is of interest beyond the existence/uniqueness question.

# The Topological Degree

*What is it?*

- If $F : \mathbf{x} \subset \mathbb{R}^n \to \mathbb{R}^n$, $F'(x^*) \neq 0$ wherever $F(x^*) = 0$, $x^* \in \mathbf{x}$, and $F(x) \neq 0$ when $x \in \partial\mathbf{x}$, then the degree $\mathrm{d}(F, \mathbf{x}, 0)$ is the number of $x^* \in \mathbf{x}$, $F(x^*) = 0$ with $\det(F'(x^*)) > 0$, minus the number of such $x^* \in \mathbf{x}$ with $\det(F'(x^*)) < 0$.
- $\mathrm{d}(F, \mathbf{x}, 0)$ is a continuous function of $F$, and is defined even if $\det(F'(x^*)) = 0$, as long as there are no solutions to $F(x) = 0$ on $\partial\mathbf{x}$.
- If $F$ is extended to $\mathbb{C}^n$ and is thought of as mapping $\mathbb{R}^{2n}$ to $\mathbb{R}^{2n}$, and $\mathbf{x}$ is embedded in a box $\mathbf{z} \in \mathbb{C}^{2n}$, then $\mathrm{d}(F, \mathbf{z}, 0)$ is equal to the exact number of $z \in \mathbf{z}$, $F(z) = 0$, counting multiplicities.

# The Topological Degree

*An Example*

- If

$$\begin{aligned} f_1(x,y) &= x^2 - y^2 - \epsilon^2 \\ f_2(x,y) &= 2xy, \end{aligned}$$

  If $\epsilon \neq 0$, then $F$ has solutions at $(x,y) = (\epsilon, 0)$ and $(x,y) = (-\epsilon, 0)$. Since $\det(F'(x)) = 4(x^2 + y^2) = 4\epsilon^2$ at each of these solutions, $\mathrm{d}(F, \mathbf{z}, 0) = 2$, where

$$\mathbf{z} = \{(x,y) \mid x \in [-0.1, 0.1], y \in [-\delta, \delta]\}$$

  for any $\delta > 0$.

- If $\epsilon = 0$, then $\mathrm{d}(F, \mathbf{z}, 0)$ is still equal to 2, even though the Jacobi matrix vanishes at the only solution $(x,y) = (0,0)$.

# The Topological Degree

*How is it Computed?*

- $\mathrm{d}(F, \mathbf{x}, 0)$ depends only on values of $F$ on $\partial\mathbf{x}$.
- Define

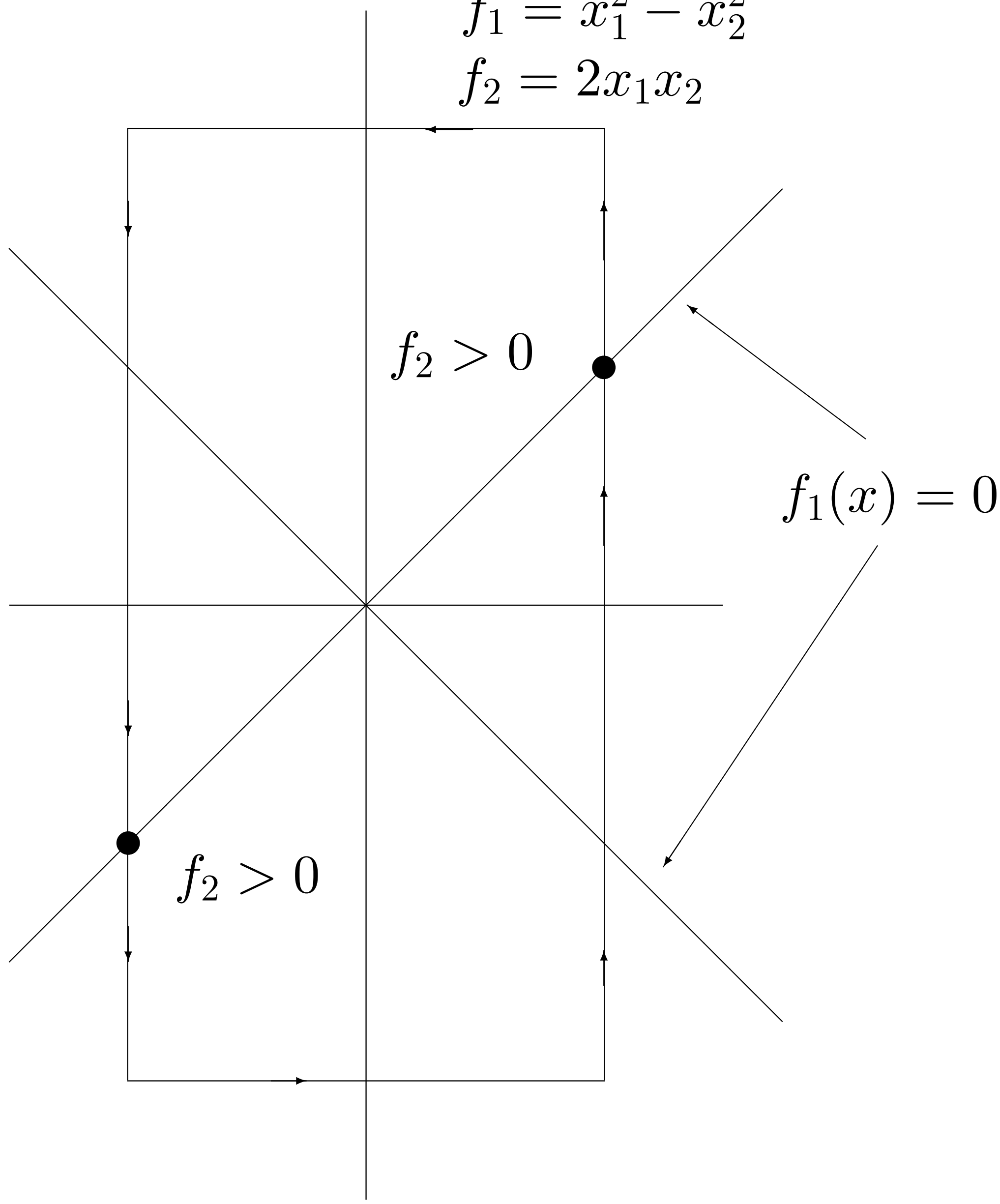
$$
\begin{aligned}
F_{\neg k}(\mathbf{x}) \;=\; & (f_1(\mathbf{x}), \ldots, f_{k-1}(\mathbf{x}), \\
& \quad f_{k+1}(\mathbf{x}), \ldots, f_n(\mathbf{x})),
\end{aligned}
$$

  and select $s \in \{-1, 1\}$. Then $\mathrm{d}(F, \mathbf{x}, 0)$ is equal to the number of zeros of $F_{\neg k}$ on $\partial\mathbf{x}$ with positive orientation at which $\mathrm{sgn}(f_k) = s$, minus the number of zeros of $F_{\neg k}$ on $\partial\mathbf{x}$ with negative orientation at which $\mathrm{sgn}(f_k) = s$.
- The orientation is computed by computing the sign of the determinant of the Jacobian of $F_{\neg k}$ and by taking account of which face.

# Computation of the Degree

$f_1 = x_1^2 - x_2^2$

$f_2 = 2x_1x_2$



# Computation of the Degree

*Computational Cost*

1. Directly finding all zeros of $F_{\neg k}$ on $\partial\mathbf{x}$ can be done in a straightforward branch and bound algorithm. However, that is perhaps too expensive for mere verification purposes.

2. The structure of the preconditioned system can be used to greatly simplify the computations.

3. The widths of the box $\mathbf{x}$ constructed about the approximate solution can be chosen so that only several one-dimensional searches need be done to compute $\mathrm{d}(F, \mathbf{z}, 0)$, where $F : \mathbb{C}^n \rightarrow \mathbb{C}^n$.

# Computation of the Degree

*Notation and Assumptions*

- For $F : \mathbb{R}^n \to \mathbb{R}^n$, extend $F$ to complex space: $z = x + iy$, $u_k(x, y) = \Re(f_k(z))$ and $v_k(x, y) = \Im(f_k(z))$.
- Define $\tilde{F}(x, y) = (u_1(x, y), v_1(x, y), \ldots, u_n(x, y), v_n(x, y)) : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$.
- Assume $F(x^*) \approx 0$.
- Assume $F$ has been preconditioned (say, through an incomplete LU factorization). Also assume $F'(x^*)$ has null space of dimension 1, so

$$f_k(x) \approx (x_k - {x^*}_k) + \frac{\partial f_k}{\partial x_n}(x^*)(x_n - {x^*}_n)$$

  for $1 \le k \le n - 1$.

# Structure of the System

*One-Dimensional Null Space*

For $1 \le k \le (n-1)$,

$$\begin{aligned} u_k(x,y) &= (x_k - \check{x}_k) + \frac{\partial f_k}{\partial x_n}(\check{x})(x_n - \check{x}_n) \\ &\quad + \mathcal{O}\left(\|(x-\check{x},y)\|^2\right) \\ v_k(x,y) &= y_k + \frac{\partial f_k}{\partial x_n}(\check{x})y_n \\ &\quad + \mathcal{O}\left(\|(x-\check{x},y)\|^2\right), \end{aligned}$$

and

$$\begin{aligned} u_n(x,y) &= \mathcal{O}\left(\|(x-\check{x},y)\|^2\right), \\ v_n(x,y) &= \mathcal{O}\left(\|(x-\check{x},y)\|^2\right). \end{aligned}$$

# Structure of the System

*Consequences*

1. Mean-value interval extensions $\mathbf{u}_k$ and $\mathbf{v}_k$ can be formed, $1 \le k \le n-1$.
2. If $x_n$ is known precisely, formally solving $\mathbf{u}_k(\mathbf{x}, \mathbf{y}) = 0$ for $x_k$ gives $\mathbf{x}_k$ with $\mathrm{w}(\mathbf{x}_k) = \mathcal{O}\left(\|(\mathbf{x} - \check{x}, \mathbf{y})\|^2\right)$, $1 \le k \le n-1$.
3. If $y_n$ is known precisely, formally solving $\mathbf{v}_k(\mathbf{x}, \mathbf{y}) = 0$ for $y_k$ gives $\mathbf{y}_k$ with $\mathrm{w}(\mathbf{y}_k) = \mathcal{O}\left(\|(\mathbf{x} - \check{x}, \mathbf{y})\|^2\right)$, $1 \le k \le n-1$.

# A Degree-Computation Algorithm

*Construction of the Box* $\mathbf{z}$

1. Define $\mathbf{x} = ([\underline{x}_1, \overline{x}_1], \ldots, [\underline{x}_n, \overline{x}_n])$ and
$$\mathbf{y} = ([\underline{y}_1, \overline{y}_1], \ldots, [\underline{y}_n, \overline{y}_n]).$$
2. Define $\mathbf{x}_{\underline{k}}$ as $(\mathbf{x}, \mathbf{y})$ with $[\underline{x}_k, \overline{x}_k]$ replaced by $\underline{x}_k$, and define $\mathbf{x}_{\overline{k}}$ as $(\mathbf{x}, \mathbf{y})$ with $[\underline{x}_k, \overline{x}_k]$ replaced by $\overline{x}_k$. Similarly define $\mathbf{y}_{\underline{k}}$ and $\mathbf{y}_{\overline{k}}$.
3. $u_k(x, y) = 0$ on $\mathbf{x}_{\underline{k}}$, $1 \le k \le n-1$, at approximately
$$x_n = \check{x}_n + \frac{\check{x}_k - \underline{x}_k}{\partial f_k / \partial x_n(\check{x})},$$
$u_k(x, y) = 0$ on $\mathbf{x}_{\overline{k}}$, $1 \le k \le n-1$, at approximately
$$x_n = \check{x}_n + \frac{\check{x}_k - \overline{x}_k}{\partial f_k / \partial x_n(\check{x})}.$$

# A Degree-Computation Algorithm

*Construction of* $\mathbf{z}$ *(continued)*

4. Similarly, $v_k(x, y) = 0$ on $\mathbf{y}_{\underline{k}}$, $1 \le k \le n-1$, at approximately $y_n = \frac{-\underline{y}_k}{\partial f_k / \partial x_n(\check{x})}$, and $v_k(x, y) = 0$ on $\mathbf{y}_{\overline{k}}$, $1 \le k \le n-1$, at approximately $y_n = \frac{-\overline{y}_k}{\partial f_k / \partial x_n(\check{x})}$.
5. Thus, if $\mathbf{x}_n$ is chosen so
$$\mathrm{w}(\mathbf{x}_n) \le \frac{1}{2} \min_{1 \le k \le n-1} \left\{ \frac{\mathrm{w}(\mathbf{x}_k)}{|\partial f_k / \partial x_n(\check{x})|} \right\},$$
then it is unlikely that $u_k(x, y) = 0$ on either $\mathbf{x}_{\underline{k}}$ or $\mathbf{x}_{\overline{k}}$.
6. Similarly, if $\mathbf{y}_n$ is chosen so that
$$\mathrm{w}(\mathbf{y}_n) \le \frac{1}{2} \min_{1 \le k \le n-1} \left\{ \frac{\mathrm{w}(\mathbf{y}_k)}{|\partial f_k / \partial x_n(\check{x})|} \right\},$$
then it is unlikely that $v_k(x, y) = 0$ on either $\mathbf{y}_{\underline{k}}$ or $\mathbf{y}_{\overline{k}}$.

# Degree Computation

*An Actual Algorithm*

1. For $k = 1$ to $n - 1$:
   (a) Do mean-value interval evaluations of $u_k(x, y)$ over $\mathbf{x}_{\underline{k}}$ and $\mathbf{x}_{\overline{k}}$ to show that $u_k(x, y) \neq 0$ on these faces of $\mathbf{z}$.
   (b) Similarly do second-order interval evaluations of $v_k(x, y)$ over $\mathbf{y}_{\underline{k}}$ and $\mathbf{y}_{\overline{k}}$ to show that $v_k(x, y) \neq 0$ on these faces of $\mathbf{z}$.
2. On $\mathbf{x}_{\underline{n}}$ and $\mathbf{x}_{\overline{n}}$:
   (a) Use mean-value extensions $\mathbf{u}_k(\mathbf{x}, \mathbf{y}) = 0$ to solve for $\mathbf{x}_k$ with width $\mathcal{O}\left(\|(\mathbf{x} - \check{x}, \mathbf{y})\|^2\right)$, $1 \leq k \leq n - 1$.
   (b) Perform a binary search on $\mathbf{y}_{\underline{n}}$ to find verified intervals where $\tilde{F}_{\neg v_n} = 0$ and $v_n(x, y) > 0$.

# A Degree Computation Algorithm

*(continued)*

3. On $\mathbf{y}_{\underline{n}}$ and $\mathbf{y}_{\overline{n}}$ (similar to Step 2):
   (a) Use mean-value extensions $\mathbf{v}_k(\mathbf{x}, \mathbf{y}) = 0$ to solve for $\mathbf{x}_k$ with width $\mathcal{O}\left(\|(\mathbf{x} - \check{x}, \mathbf{y})\|^2\right)$, $1 \le k \le n-1$.
   (b) Perform a binary search on $\mathbf{x}_n$ to find verified intervals where $\tilde{F}_{\neg v_n} = 0$ and $v_n(x, y) > 0$.
4. For each solution to $F_{\neg v_n} = 0$ found in Steps 2b and 3b, compute an orientation, to sum to find the degree.

# The Degree Computation Algorithm

*Some Notes*

- For each interval on $y_n$ produced in the search in Step 2b, narrower intervals on $y_k$ can be produced with a mean-value extension $\mathbf{v}_k(x) = 0$, $1 \le k \le n-1$.
- Similarly, for each interval on $x_n$ produced in the search in Step 3b, narrower intervals on $x_k$ can be produced with a mean-value extension $\mathbf{u}_k(x) = 0$, $1 \le k \le n-1$.
- An interval Newton method can be set up for $\tilde{F}_{\neg v_n}$ to verify existence and uniqueness.