Verification of Multiple Roots: An Interval Arithmetic Approach

1 Conditioning: Well-Conditioned vs. Ill-Conditioned Problems

Definition 1 (Condition Number)**.** *The **condition number** of a problem measures how sensitive the output is to small perturbations in the input. For a problem computing $y = f(x)$, the relative condition number is:*

$$\kappa = \left| \frac{x \cdot f'(x)}{f(x)} \right|$$

Interpretation

- **Well-conditioned** (κ small): Small changes in input produce small changes in output. The problem is numerically stable.
- **Ill-conditioned** (κ large): Small changes in input can produce large changes in output. The problem is numerically unstable.

Example 1 (Simple vs. Ill-Conditioned Systems)**.**

1. ***Well-conditioned**: Solving $Ax = b$ where A has condition number $\kappa(A) \approx 10$.*

   $$\text{If } \|A\| \approx 10, \quad \|A^{-1}\| \approx 1 \quad \Rightarrow \quad \kappa(A) = \|A\| \cdot \|A^{-1}\| \approx 10$$

   Small errors in b produce small errors in x.

2. ***Ill-conditioned**: Near-singular matrix with $\kappa(A) \approx 10^{10}$.*

   $$\text{If } \|A\| \approx 1, \quad \|A^{-1}\| \approx 10^{10} \quad \Rightarrow \quad \kappa(A) \approx 10^{10}$$

   Tiny errors in b produce huge errors in x.

2 The Problem with Multiple Roots

Definition 2 (Multiple Root)**.** *A point $\hat{x}$ is a **multiple root of multiplicity** m of $f(x)$ if:*

$$f(\hat{x}) = f'(\hat{x}) = f''(\hat{x}) = \cdots = f^{(m-1)}(\hat{x}) = 0, \quad \text{but} \quad f^{(m)}(\hat{x}) \neq 0$$

*For a **double root** ($m = 2$): $f(\hat{x}) = f'(\hat{x}) = 0$ and $f''(\hat{x}) \neq 0$.*

Example 2 (Polynomial with Multiple Roots). *Consider:*

$$f(x) = 18x^7 - 183x^6 + 764x^5 - 1675x^4 + 2040x^3 - 1336x^2 + 416x - 48$$

which factors as:

$$f(x) = (3x - 1)^2(2x - 3)(x - 2)^4$$

This has:

- *A* ***double root*** *at* $x_1 = 1/3$ *(multiplicity 2)*
- *A* ***simple root*** *at* $x_2 = 3/2$ *(multiplicity 1)*
- *A* ***quadruple root*** *at* $x_3 = 2$ *(multiplicity 4)*

2.1 Why Multiple Roots Are Ill-Conditioned

Theorem 1 (Perturbation Analysis). *For a root* $\hat{x}$ *of multiplicity* m*, if we perturb the polynomial by a small amount* ε *(i.e., consider* $\tilde{f}(x) = f(x) - \varepsilon$*), the perturbed root* $\hat{x}(\varepsilon)$ *satisfies:*

$$\hat{x}(\varepsilon) - \hat{x} = \varepsilon^{1/m}\left(-\frac{m!\, a_i \hat{x}^i}{f^{(m)}(\hat{x})}\right)^{1/m} + O(\varepsilon^{2/m})$$

Key Consequence for Double Roots

For a **double root** ($m = 2$), we have:

$$|\hat{x}(\varepsilon) - \hat{x}| \approx \sqrt{\varepsilon} \cdot \sqrt{\frac{2}{|f''(\hat{x})|}}$$

This means:

- With machine precision $\varepsilon \approx 10^{-16}$
- The root error is $\approx \sqrt{10^{-16}} = 10^{-8}$
- **We lose half the digits of precision!**

For a quadruple root ($m = 4$): error $\approx \varepsilon^{1/4} \approx 10^{-4}$ (lose 75% of precision!)

2.2 Numerical Evidence

Using INTLAB's `verifypoly` on our example polynomial:

```
>> X1 = verifypoly(f, 1.3)  % Simple root
intval X1 = [1.49999999999904, 1.50000000000078]
             ~~~~~~~~~~~~~~~~~~ ~~~~~~~~~~~~~~~~~~
             15 correct digits
```

```
>> X2 = verifypoly(f, 0.3)  % Double root
intval X2 = [0.33333316656015, 0.33333343640539]
             ~~~~~~~~~~~~~~~~~~ ~~~~~~~~~~~~~~~~~~
             Only 7 correct digits!

>> X3 = verifypoly(f, 2.1)  % Quadruple root
intval X3 = [1.99741678159164, 2.00363593397305]
             ~~~~~~~~~~~~~~~~~~ ~~~~~~~~~~~~~~~~~~
             Only 3 correct digits!
```

Observation: The width of the interval grows dramatically as multiplicity increases, reflecting the ill-conditioning.

3 The Verification Approach: Reformulation

3.1 The Naive Approach (Fails)

Simply trying to solve $f(x) = 0$ near a double root is ill-conditioned because:

- The condition number $\kappa \approx 1/|f'(\hat{x})| = \infty$ (since $f'(\hat{x}) = 0$)
- Newton's method: $x_{k+1} = x_k - f(x_k)/f'(x_k)$ fails when $f'(x_k) \approx 0$

3.2 The Clever Reformulation (Succeeds)

Key Idea: Instead of computing the exact root (impossible with finite precision), we compute:

1. An interval X guaranteed to contain the true root
2. An interval E containing the perturbation

Such that $\exists \hat{x} \in X$ and $\exists \hat{\varepsilon} \in E$ where $\hat{x}$ is a double root of $\tilde{f}(x) := f(x) - \hat{\varepsilon}$.

Mathematical Formulation

We solve the **2D nonlinear system**:

$$G(x, \varepsilon) = \begin{pmatrix} f(x) - \varepsilon \\ f'(x) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

This system has unknowns $(x, \varepsilon) \in \mathbb{R}^2$ and seeks a point where:

- $f(x) - \varepsilon = 0$ (the function value equals the perturbation)
- $f'(x) = 0$ (the derivative vanishes, ensuring multiplicity ≥ 2)

3.3 Why This Works: The Jacobian

The Jacobian of $G(x, \varepsilon)$ is:

$$J_G(x, \varepsilon) = \begin{pmatrix} \frac{\partial}{\partial x}(f(x) - \varepsilon) & \frac{\partial}{\partial \varepsilon}(f(x) - \varepsilon) \\ \frac{\partial}{\partial x} f'(x) & \frac{\partial}{\partial \varepsilon} f'(x) \end{pmatrix} = \begin{pmatrix} f'(x) & -1 \\ f''(x) & 0 \end{pmatrix}$$

Why This Is Well-Conditioned

At a double root $\hat{x}$ where $f(\hat{x}) = f'(\hat{x}) = 0$ but $f''(\hat{x}) \neq 0$:

$$J_G(\hat{x}, \hat{\varepsilon}) = \begin{pmatrix} 0 & -1 \\ f''(\hat{x}) & 0 \end{pmatrix}$$

The determinant is:

$$\det(J_G) = 0 \cdot 0 - (-1) \cdot f''(\hat{x}) = f''(\hat{x}) \neq 0$$

Conclusion: J_G is **nonsingular**, so the system is well-conditioned!
The condition number $\kappa(J_G)$ is bounded, typically $O(1)$ or $O(10)$, not $O(10^8)$ as in the original problem.

4 Interval Newton Method for the Reformulated System

To solve $G(x, \varepsilon) = 0$ with guaranteed bounds, we use the **Interval Newton method**:

Theorem 2 (Interval Newton for Nonlinear Systems)**.** *Let $G : \mathbb{R}^n \to \mathbb{R}^n$ be differentiable, $\tilde{z} \in \mathbb{R}^n$ an approximate solution, and $Z \in \mathbb{IR}^n$ an interval vector with $0 \in Z$.*

Let $M \in \mathbb{IR}^{n \times n}$ be an interval matrix such that:

$$\nabla G_i(\zeta) \in M_{i,:} \quad \forall \zeta \in \tilde{z} + Z, \ \forall i$$

If $R \in \mathbb{R}^{n \times n}$ satisfies $\det(R) \neq 0$ and:

$$N(\tilde{z}, Z) := -RG(\tilde{z}) + (I - RM)Z \subseteq int(Z)$$

Then:

1. *$\exists! \hat{z} \in \tilde{z} + Z$ such that $G(\hat{z}) = 0$*
2. *Every matrix $\tilde{M} \in M$ is nonsingular*
3. *In particular, $\nabla G(\hat{z})$ is nonsingular*

4.1 Application to Our Problem

For $G(x, \varepsilon) = (f(x) - \varepsilon,\ f'(x))^T$:

1. Compute approximate solution $(\tilde{x}, \tilde{\varepsilon})$ using standard floating-point Newton
2. Choose interval box $[X, E]$ around $(\tilde{x}, \tilde{\varepsilon})$
3. Compute interval extension of Jacobian J_G over $[X, E]$
4. Compute $R \approx J_G(\tilde{x}, \tilde{\varepsilon})^{-1}$
5. Verify $-RG(\tilde{x}, \tilde{\varepsilon}) + (I - RM)[X, E] \subseteq \mathrm{int}([X, E])$

If verification succeeds, we have **mathematical proof** that a solution exists in $[X, E]$.

5 Numerical Results

Using INTLAB's `verifynlss` (verified nonlinear system solver):

```
>> Y2 = verifynlss(G, [0.3; 0])
intval Y2 =
[ 3.333333333333328e-001, 3.333333333333337e-001]
[ -2.131628207280424e-014, 2.131628207280420e-014]
```

Interpretation

This proves rigorously that:

$$\exists \hat{x} \in [0.333333333333328, 0.333333333333337]$$

$$\exists \hat{\varepsilon} \in [-2.13 \times 10^{-14}, 2.13 \times 10^{-14}]$$

such that $\hat{x}$ is a **double root** of $\tilde{f}(x) = f(x) - \hat{\varepsilon}$.
Key observations:

- The interval for x has width $\approx 10^{-15}$ (almost full double precision!)
- The perturbation $|\hat{\varepsilon}| \leq 2.13 \times 10^{-14}$ is tiny
- We have a **mathematical guarantee**, not just a numerical approximation

6 Summary: Ill-Conditioned vs. Well-Conditioned

Original Problem (Ill-Conditioned)	**Reformulated Problem (Well-Conditioned)**
Solve $f(x) = 0$ for double root	Solve $G(x, \varepsilon) = \begin{pmatrix} f(x) - \varepsilon \\ f'(x) \end{pmatrix} = 0$
$f'(\hat{x}) = 0 \Rightarrow$ singular Jacobian	$J_G = \begin{pmatrix} 0 & -1 \\ f''(\hat{x}) & 0 \end{pmatrix}$ nonsingular
Condition number $\kappa \to \infty$	Condition number $\kappa = O(1)$
Error $\approx \sqrt{\varepsilon} \approx 10^{-8}$	Error $\approx \varepsilon \approx 10^{-16}$
Lose half the digits	Keep (almost) all digits
Only approximation possible	Rigorous verification possible