Relaxed method to certify a linear system

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Problem

Objective:

1. Solve a linear system
   - $A \in \mathbb{R}^{n \times n}$
   - $b \in \mathbb{R}^{n}$
   - Calculate an approximation $\widetilde{x} \in \mathbb{R}^n$ of the exact solution x^* to a linear system $A * x = b$
2. Simultaneously bound the error upon this approximation using interval arithmetic
   - $\Delta x = x^* - \widetilde{x}$
   - Calculate a small interval **e** containing Δx.

Classical iterative refinements

Wilkinson, Li & Demmel, Higham, ...

Algorithm 1 (Classical methods of iterative refinement)

Input: $A \in \mathbb{F}^{n \times n}, b \in \mathbb{F}^n$
$\widetilde{x} = A \setminus b;$
while(not converged)
    $\widetilde{r} = b - A * \widetilde{x};$
    $\widetilde{e} = A \setminus \widetilde{r};$
    $\widetilde{x} = \widetilde{x} + \widetilde{e};$
end

Iterative refinement: switch to interval arithmetic

Notations: x^* exact solution, $\widetilde{x}$ floating point approximation, $\mathbf{x}$ an interval containing the exact solution

Algorithm 2 (Interval iterative refinement)

Input: $A \in \mathbb{F}^{n \times n}, b \in \mathbb{F}^n$
$\widetilde{x} = A \setminus b;$
while(not converged)
    $\mathbf{r} = [b - A * \widetilde{x}];$ % $A * (x^* - \widetilde{x}) \in \mathbf{r}$
    $\mathbf{e} = A \setminus \mathbf{r};$ % $x^* - \widetilde{x} \in \mathbf{e}$
    $\widetilde{x} = \widetilde{x} + mid(\mathbf{e});$
end

Residual system

$$A * \mathbf{e} = \mathbf{r}$$

Principle: precondition the system by an approximative inverse R of A.

$$\mathbf{K} = [R * A] \qquad \mathbf{z} = R * \mathbf{r}$$

$$\mathbf{K} * \mathbf{e} = \mathbf{z}$$

Method: Interval iterative improvement

- do not solve directly the interval system.
- consider it as constraints to improve the error bound

$$\begin{aligned} \mathbf{e'} &= \mathbf{e} \cap (\mathbf{K} \setminus \mathbf{z}) \\ &= \{\widetilde{e} \in \mathbf{e} \quad | \quad \exists \widetilde{K} \in \mathbf{K}, \quad \exists \widetilde{z} \in \mathbf{z} : \quad \widetilde{K} * \widetilde{e} = \widetilde{z}\} \end{aligned}$$

Residual system (2)

Rough initial solution by **Simplified Neumaier proposition** (CUP 1990) [1]:

If $\langle \mathbf{K} \rangle u \geq v > 0$ for $u \geq 0$ then

$$\mathbf{K}^{-1}\mathbf{z} \subseteq \|\mathbf{z}\|_v * [-u, u].$$

Where

- $\langle \mathbf{K} \rangle$ is the comparison matrix of $\mathbf{K}$:

$$\begin{aligned} \langle \mathbf{K} \rangle_{i,i} &= \min(|\mathbf{K}_{i,i}|) \\ \langle \mathbf{K} \rangle_{i,j \neq i} &= -\max(|\mathbf{K}_{i,j}|) \end{aligned}$$

- $\|\mathbf{z}\|_v = \max_i(|\mathbf{z}_i|/|v_i|)$

[1] page 121, Arnold Neumaier, *Interval Methods for Systems of Equations*

Interval Gauss-Seidel iterations

$$(\mathbf{K} \setminus \mathbf{z}) \cap \mathbf{e} = \{\widetilde{e} \in \mathbf{e} \quad | \quad \exists \widetilde{K} \in \mathbf{K}, \exists \widetilde{z} \in \mathbf{z} : \quad \widetilde{K} * \widetilde{e} = \widetilde{z}\}$$

$$\widetilde{K}_{i,1}\widetilde{e}_1 + \ldots + \widetilde{K}_{i,i-1}\widetilde{e}_{i-1} + \widetilde{K}_{i,i}\widetilde{e}_i + \widetilde{K}_{i,i+1}\widetilde{e}_{i+1} + \ldots + \widetilde{K}_{i,n}\widetilde{e}_n = z_i$$

$$\widetilde{e}_i = \left(\widetilde{z}_i - \sum_{j=1}^{i-1} \widetilde{K}_{i,j}\widetilde{e}_j - \sum_{j=i+1}^{n} \widetilde{K}_{i,j}\widetilde{e}_j\right) \Big/ \widetilde{K}_{i,i}$$

$$\mathbf{e}'_i \subseteq \left(\mathbf{z}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j}\mathbf{e}'_j - \sum_{j=i+1}^{n} \mathbf{K}_{i,j}\mathbf{e}_j\right) \Big/ \mathbf{K}_{i,i} \quad \cap \mathbf{e}_i$$

Interval Gauss-Seidel iterations

$$(\mathbf{K} \setminus \mathbf{z}) \cap \mathbf{e} = \{\widetilde{e} \in \mathbf{e} \quad | \quad \exists \widetilde{K} \in \mathbf{K}, \exists \widetilde{z} \in \mathbf{z} : \quad \widetilde{K} * \widetilde{e} = \widetilde{z}\}$$

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Detailed method

Algorithm 3 (Interval iterative refinement)

Input: $A \in \mathbb{F}^{n \times n}, b \in \mathbb{F}^n$

$\widetilde{x} = A \setminus b;$

$R = inv(A);$

$K = [R * A];$

$z = R * [b - A * \widetilde{x}];$

Calculate an initial solution to $K * e = z$;

while(not converged)

  Apply at most 5 interval Gauss-Seidel iterations on $K * e = z$;

  $\widetilde{x} = \widetilde{x} + \texttt{mid}(e); \quad e = e - \texttt{mid}(e)$ % $\widetilde{x} + e \ni x^*$

  $z = R * [b - A * \widetilde{x}];$

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 $\widetilde{x} = \widetilde{x} + \mathtt{mid}(e); \quad e = e - \mathtt{mid}(e) \qquad \% \quad \widetilde{x} + e \ni x^*$
 $z = R * [b - A * \widetilde{x}];$
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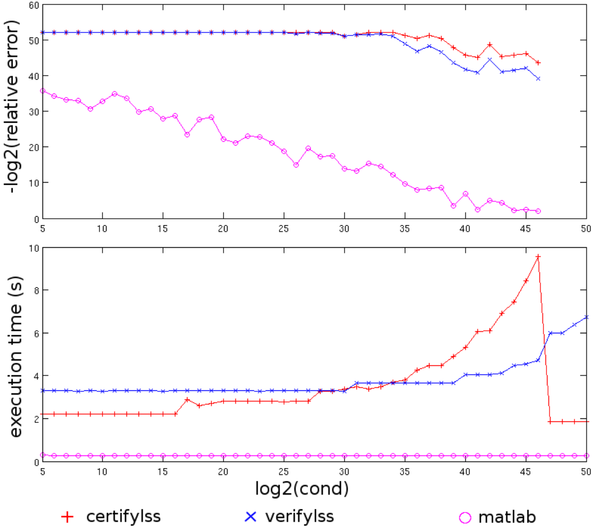
  Apply at most 5 interval Gauss-Seidel iterations on $\mathbf{K} * \mathbf{e} = \mathbf{z}$;
  $\widetilde{x} = \widetilde{x} + \mathtt{mid}(\mathbf{e});$ $\mathbf{e} = \mathbf{e} - \mathtt{mid}(\mathbf{e})$ % $\widetilde{x} + \mathbf{e} \ni x^*$
  $\mathbf{z} = R * [b - A * \widetilde{x}];$
end

Experimental Results

System rank: 1000 $b = [1, \ldots, 1]^T$



Performance Problem

Problem: Each Gauss-Seidel/Gauss refinement costs $\mathcal{O}(n^2)$ interval operations $\longrightarrow$ execution time increases rapidly when number of iterations increases.

Example using Intlab (INTerval LABoratory)
iA interval matrix of size 1000x1000, **ib**: interval vector of size 1000.

$$tic; A * A; toc \quad \longrightarrow 0.550s$$

$$tic; A * b; toc \quad \longrightarrow 0.004s$$

$$tic; iA * ib; toc \quad \longrightarrow 0.14s$$

$$\Rightarrow factor > 30$$

Special cases of interval calculations

Let $\mathbf{x}$, $\mathbf{y}$ and $\mathbf{z}$ be three intervals and $\mathbf{y}, \mathbf{z}$ are centered by zero
$\rightarrow \underline{\mathbf{y}} = -\overline{\mathbf{y}}, \underline{\mathbf{z}} = -\overline{\mathbf{z}}$,

Addition:

$$
\begin{aligned}
tmp &\triangleq \overline{\mathbf{y}} + \overline{\mathbf{z}} \\
\mathbf{y} + \mathbf{z} &= \mathtt{infsup}(-tmp, tmp)
\end{aligned}
$$

Multiplication:

$$
\begin{aligned}
tmp &\triangleq \overline{\mathbf{y}} * \mathtt{mag}(\mathbf{x}) \\
\mathbf{x} * \mathbf{y} &= \mathtt{infsup}(-tmp, tmp)
\end{aligned}
$$

Fused Multiplier-Adder

$$
\begin{aligned}
tmp &\triangleq \overline{\mathbf{y}} * \mathtt{mag}(\mathbf{x}) + \overline{\mathbf{z}} \\
\mathbf{x} * \mathbf{y} + \mathbf{z} &= \mathtt{infsup}(-tmp, tmp)
\end{aligned}
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Special cases of interval calculations

Let x, y and z be three intervals and y, z are centered by zero $\rightarrow \underline{y} = -\overline{y}, \underline{z} = -\overline{z}$,

Addition:

$$tmp \triangleq \overline{y} + \overline{z}$$
$$y + z = \texttt{infsup}(-tmp, tmp)$$

Multiplication:

$$tmp \triangleq \overline{y} * \texttt{mag}(x)$$
$$x * y = \texttt{infsup}(-tmp, tmp)$$

Fused Multiplier-Adder

$$tmp \triangleq \overline{y} * \texttt{mag}(x) + \overline{z}$$
$$x * y + z = \texttt{infsup}(-tmp, tmp)$$

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Addition:

$$\begin{aligned} \mathbf{y} + \mathbf{z} &= \mathtt{infsup}(\underline{\mathbf{y}} + \underline{\mathbf{z}}, \overline{\mathbf{y}} + \overline{\mathbf{z}}) \\ &= \mathtt{infsup}(-(\overline{\mathbf{y}} + \overline{\mathbf{z}}), \overline{\mathbf{y}} + \overline{\mathbf{z}}) \end{aligned}$$

$$\begin{aligned} tmp &\triangleq \overline{\mathbf{y}} + \overline{\mathbf{z}} \\ \mathbf{y} + \mathbf{z} &= \mathtt{infsup}(-tmp, tmp) \end{aligned}$$

Multiplication:

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tmp &\triangleq \overline{\mathbf{y}} + \overline{\mathbf{z}} \\
\mathbf{y} + \mathbf{z} &= \mathtt{infsup}(-tmp, tmp)
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Multiplication:

$$
\begin{aligned}
\underline{\mathbf{x*y}} &= \mathtt{min}(\underline{\mathbf{x}} * \underline{\mathbf{y}}, \underline{\mathbf{x}} * \overline{\mathbf{y}}, \overline{\mathbf{x}} * \underline{\mathbf{y}}, \overline{\mathbf{x}} * \overline{\mathbf{y}}) \\
\overline{\mathbf{x*y}} &= \mathtt{max}(\underline{\mathbf{x}} * \underline{\mathbf{y}}, \underline{\mathbf{x}} * \overline{\mathbf{y}}, \overline{\mathbf{x}} * \underline{\mathbf{y}}, \overline{\mathbf{x}} * \overline{\mathbf{y}})
\end{aligned}
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tmp &\triangleq \overline{\mathbf{y}} * \mathtt{mag}(\mathbf{x}) \\
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Fused Multiplier-Adder

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tmp \triangleq \overline{\mathbf{y}} * \mathtt{mag}(\mathbf{x}) + \overline{\mathbf{z}}
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Special cases of interval calculations

Let x, y and z be three intervals and y, z are centered by zero
$\rightarrow \underline{y} = -\overline{y}, \underline{z} = -\overline{z}$,

Addition:

$$\begin{aligned} tmp &\triangleq \overline{y} + \overline{z} \\ y + z &= \mathtt{infsup}(-tmp, tmp) \end{aligned}$$

Multiplication:

$$\begin{aligned} \underline{x*y} &= \mathtt{min}(-\overline{y} * |\underline{x}|, -\overline{y} * |\overline{x}|) \\ \overline{x*y} &= \mathtt{max}(\overline{y} * |\underline{x}|, \overline{y} * |\overline{x}|) \end{aligned}$$

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Multiplication:

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Let **x**, **y** and **z** be three intervals and **y**, **z** are centered by zero
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$$

Multiplication:

$$
\begin{aligned}
\underline{\mathbf{x*y}} &= -\overline{\mathbf{y}} * \mathtt{mag}(\mathbf{x}) \\
\overline{\mathbf{x*y}} &= \overline{\mathbf{y}} * \mathtt{mag}(\mathbf{x})
\end{aligned}
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$$
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tmp &\triangleq \overline{\mathbf{y}} * \mathtt{mag}(\mathbf{x}) \\
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Special cases: matrix calculations

Let $\mathbf{b}$ be an interval vector.

If $\mathbf{a}$ is an interval vector centered by zero

$$\begin{aligned} tmp &\triangleq \overline{\mathbf{a}} \circ \mathtt{mag}(\mathbf{b}) \\ \mathbf{a} \circ \mathbf{b} &= \mathtt{infsup}(-tmp, tmp) \end{aligned}$$

If $\mathbf{A}$ is a interval matrix centered by zero

$$\begin{aligned} tmp &\triangleq \overline{\mathbf{A}} * \mathtt{mag}(\mathbf{b}) \\ \mathbf{A} * \mathbf{b} &= \mathtt{infsup}(-tmp, tmp) \end{aligned}$$

Relaxed Gauss-Seidel iterations

Calculate a truncated solution to $\mathbf{Ke} = \mathbf{z}$.

Let $\mathbf{D}, \mathbf{L}, \mathbf{U}$ be the diagonal, lower part and upper part of $\mathbf{K}$.

Jacobi: $\mathbf{D} * \mathbf{e'} = \mathbf{z} - \mathbf{U} * \mathbf{e} - \mathbf{L} * \mathbf{e}$
Gauss-Seidel: $\mathbf{D} * \mathbf{e'} = \mathbf{z} - \mathbf{U} * \mathbf{e} - \mathbf{L} * \mathbf{e'}$

$\mathbf{L}, \mathbf{U}$ are close to zero $\Rightarrow$ Inflate $\mathbf{L}$ and $\mathbf{U}$ so that they are centered by zero:

$$\begin{aligned} \mathbf{Ui} &= \mathtt{infsup}(-\mathtt{mag}(\mathbf{U}), \mathtt{mag}(\mathbf{U})) \\ \mathbf{Li} &= \mathtt{infsup}(-\mathtt{mag}(\mathbf{L}), \mathtt{mag}(\mathbf{L})) \end{aligned}$$

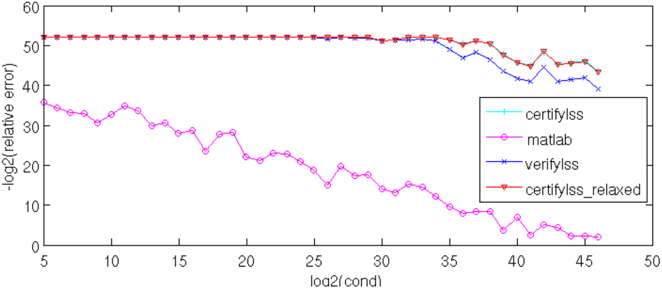
$\Rightarrow \mathbf{U} \subseteq \mathbf{Ui}, \mathbf{L} \subseteq \mathbf{Li}$

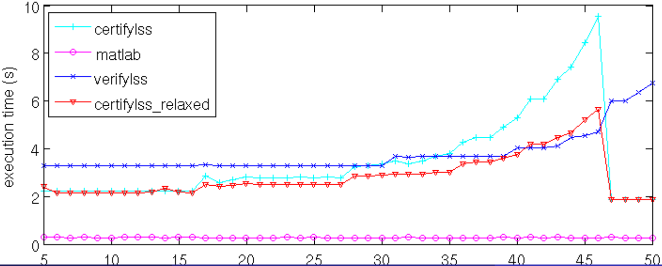
Relaxed Gauss-Seidel iteration

$$\begin{aligned} \mathbf{D} * \mathbf{e''} &= \mathbf{z} - \mathbf{Ui} * \mathbf{e} - \mathbf{Li} * \mathbf{e''} \\ \mathbf{e'} &\subseteq \mathbf{e''} \end{aligned}$$

Relaxed method: Results

System rank: 1000 $b = [1, \ldots, 1]^T$





Conclusions

- Combining the floating-point refinement and the interval iterations, our method provides accurate results when the condition number of the coefficient matrix is much smaller than 2^p (p is the working precision).
- With the proposed relaxation technique, we managed to reduce alot the execution time of interval refinement part.

Perspectives

In the future: Expand to the other problems

- Linear system of inequalities
- Nonlinear system
- Numerical constraint system, using the techniques of constraint propagation

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