Interval unions on rigorous optimization

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Why interval unions?

- Let $f : \mathbf{R} \to \mathbf{R}$ be a differentiable function and $\mathbf{x}_0$ an interval where we are looking for x^* such that $f(x^*) = 0$.
- Interval Newton method encloses all roots of f.

$$\mathbf{x}^{(k+1)} := N(\mathbf{x}^k) \cap \mathbf{x}^k, \quad N(\mathbf{x}) = \check{\mathbf{x}} - \frac{f(\check{\mathbf{x}})}{\mathbf{f}'(\mathbf{x})}, \quad k = 0, 1, 2, \ldots.$$

- What if $0 \in \mathbf{f}'(\mathbf{x})$? Apply the extended division!

Why interval unions?

Let $\mathbf{a} = [\underline{a}, \overline{a}]$ and $\mathbf{b} = [\underline{b}, \overline{b}]$. The extended division is given by

$$\mathbf{a}/\mathbf{b} := \begin{cases} \mathbf{a} \cdot [1/\overline{b}, 1/\underline{b}] & \text{if } 0 \notin \mathbf{b}, \\ (-\infty, +\infty) & \text{if } 0 \in \mathbf{a} \wedge 0 \in \mathbf{b}, \\ [\overline{a}/\underline{b}, +\infty) & \text{if } \overline{a} < 0 \wedge \underline{b} < \overline{b} = 0, \\ (-\infty, \overline{a}/\overline{b}] \cup [\overline{a}/\underline{b}, +\infty) & \text{if } \overline{a} < 0 \wedge \underline{b} < 0 < \overline{b}, * \\ (-\infty, \overline{a}/\overline{b}] & \text{if } \overline{a} < 0 \wedge 0 = \underline{b} < \overline{b}, \\ (-\infty, \underline{a}/\underline{b}] & \text{if } 0 < \underline{a} \wedge \underline{b} < \overline{b} = 0, \\ (-\infty, \underline{a}/\underline{b}] \cup [\underline{a}/\overline{b}, +\infty) & \text{if } 0 < \underline{a} \wedge \underline{b} < 0 < \overline{b}, * \\ [\underline{a}/\overline{b}, +\infty) & \text{if } 0 < \underline{a} \wedge 0 = \underline{b} < \overline{b}, \\ \emptyset & \text{if } 0 \notin \mathbf{a} \wedge \underline{b} = \overline{b} = 0. \end{cases}$$

Why interval unions?

- Division by intervals containing zero is problematic. For example, if $\mathbf{a} = [2, 3]$ and $\mathbf{b} = [-1, 1]$ then

$$\mathbf{x} = \frac{[2, 3]}{[-1, 1]} = (-\infty, -2] \cup [2, \infty).$$

- $\mathbf{x}$ is not an interval.
- Extended division requires special treatment from a computational point of view.

What is an interval union?

- An interval union is a finite set of disjoint intervals:

$$\boldsymbol{u} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k) \quad \text{with} \quad \begin{array}{ll} \boldsymbol{u}_i \in \overline{\mathbb{IR}} & \forall\ i = 1, \ldots, k, \\ \overline{\boldsymbol{u}}_i < \underline{\boldsymbol{u}}_{i+1} & \forall\ i = 1, \ldots, k-1. \end{array}$$

where

$$\overline{\mathbb{IR}} := \{[\underline{a}, \overline{a}] \cap \mathbb{R} \mid \underline{a} \leq \overline{a},\ \underline{a}, \overline{a} \in \mathbb{R} \cup \{-\infty, \infty\}\}.$$

For example:

$$\boldsymbol{u} = \{[-1, 0], [2, 3]\}$$

$$\boldsymbol{v} = \{(-\infty, -1], [1, \infty)\}$$

$$\boldsymbol{w} = \{[2, 2], [3, 3]\}$$

Interval union arithmetic

- Let $\boldsymbol{u} = \{[-1, 1], [2, 3]\}$ and $\boldsymbol{v} = \{[-3, -2], [5, 6]\}$

$$\boldsymbol{u} + \boldsymbol{v} = \{[-4, 1], [4, 9]\}$$

$$\boldsymbol{u} - \boldsymbol{v} = \{[-7, -2], [1, 6]\}$$

$$\boldsymbol{u} * \boldsymbol{v} = \{[-9, 6], [10, 18]\}.$$

$$\boldsymbol{v}/\boldsymbol{u} = \{(-\infty, -2], [-1.5, -0.6666], [1.6666, \infty)\}.$$

What holds

- Magnitude: $|\boldsymbol{u}| := \max(|\mathbf{u}_1|, \ldots, |\mathbf{u}_k|) = \max(|\underline{\mathbf{u}}_1|, |\overline{\mathbf{u}}_k|)$,
- Mignitude: $\langle \boldsymbol{u} \rangle := \min(\langle \mathbf{u}_1 \rangle, \ldots, \langle \mathbf{u}_k \rangle)$,
- Max and Min: $\max(\boldsymbol{u}) := \overline{\mathbf{u}}_k$, $\min(\boldsymbol{u}) := \underline{\mathbf{u}}_1$,
- Inclusion isotonicity:

$$\boldsymbol{v}' \subseteq \boldsymbol{v}, \boldsymbol{u}' \subseteq \boldsymbol{u} \Rightarrow \boldsymbol{v}' \circ \boldsymbol{u}' \subseteq \boldsymbol{v} \circ \boldsymbol{u} \text{ for all } \{+, -, /, *\},$$

- Fundamental Theorem: If $\mathbf{f}$ is inclusion isotonic and the interval union extension of $f : \mathbb{R}^n \to \mathbb{R}$ then $f_{rg}(\boldsymbol{u}) \subseteq \mathbf{f}(\boldsymbol{u})$.

What does not

- Taylor expansion: Let $f : \mathbb{R}^n \to \mathbb{R}$ be a differentiable function defined in a box $\mathbf{x} \subset \mathbb{R}^n$. If $z \in \mathbf{x}$, $\mathbf{f}$ is an interval extension of f and $\mathbf{g}$ the interval extension of ∇f then

$$f(x) \in \mathbf{f}(z) + \mathbf{g}(\mathbf{x})^T (x - z), \quad \forall x \in \mathbf{x}.$$

- Let $f(x) = x^2$ and $\boldsymbol{u} = \{[-3, 1], [1, 3]\}$. Take $x = -2 \in [-3, -1]$ and $z = 2 \in [1, 3]$. There is not $\xi \in \boldsymbol{u}$ such that

$$4 = 4 - 8\xi.$$

Interval union matrices and vectors

$$\mathcal{A} = \begin{pmatrix} \{[-5,-3],[4,5]\} & \{[0.5,1.0],[2,3]\} \\ \{[0.5,1.0],[2,3]\} & \{[-3,-2],[2,3]\} \end{pmatrix}$$

$$\mathcal{b} = (\{[-1,1],[1.5,2],[3,4]\}, \{[-1,0],[1,3],[5,7]\})^T$$

- Regularity, $M-$matrices and $H-$matrices are well defined.
- $\mathcal{A}$ represents 16 interval matrices(with only 8 intervals) and $\mathcal{b}$ 9 boxes(6 intervals).

Interval union matrices and vectors

- An interval union linear system is the family of equations

$$Ax = b \ \ (A \in \mathcal{A}, b \in \mathcal{b}).$$

- The solution set is defined by

$$\Sigma(\mathcal{A}, \mathcal{b}) := \{x \in \mathbb{R}^n \mid Ax = b \text{ for some } A \in \mathcal{A}, b \in \mathcal{b}\}.$$

- Let $\mathcal{B}(\mathfrak{v}) := \mathfrak{v}_1 \otimes \mathfrak{v}_2 \otimes, \ldots \otimes \mathfrak{v}_n$, $\mathcal{A} \in \mathcal{U}^{n \times n}$ and $\mathcal{b} \in \mathcal{U}^n$. Then

$$\bigcup_{\substack{\mathbf{A}_i \in \mathcal{B}(\mathcal{A}) \\ \mathbf{b}_j \in \mathcal{B}(\mathcal{b})}} \Sigma(\mathbf{A}_i, \mathbf{b}_j) \equiv \Sigma(\mathcal{A}, \mathcal{b}).$$

Interval union matrices and vectors

- Let S be a finite set of intervals, the **union creator** $\mathcal{U}(S)$ is the smallest $\boldsymbol{u}$ that satisfies $\mathbf{a} \subseteq \boldsymbol{u}$ for all $\mathbf{a} \in S$.
- Finding $\mathcal{U}(\Sigma(\boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{b}}))$ is $NP-$Hard.
- In general, we look for $\boldsymbol{x}$ such that

$$\mathcal{U}(\Sigma(\boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{b}})) \subseteq \boldsymbol{x}.$$

- If $\boldsymbol{\mathcal{A}}$ is an $M-$matrix and $\boldsymbol{\mathcal{b}}$ is degenerate then

$$\mathcal{U}(\Sigma(\boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{b}})) = \bigcup_{\substack{\mathbf{A}_i \in \mathcal{B}(\boldsymbol{\mathcal{A}}) \\ \mathbf{b}_j \in \mathcal{B}(\boldsymbol{\mathcal{b}})}} [\underline{\mathbf{A}}_i, \overline{\mathbf{A}}_i]\mathbf{b}_j.$$

An interval linear system

- Let

$$\mathbf{A} = \begin{pmatrix} [3.5, 4.5] & [1.0, 2.0] \\ [1.0, 2.0] & [-0.5, 0.5] \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} [1.0, 2.0] \\ [1.5, 2.0] \end{pmatrix}$$

- Interval union Gaussian elimination(without pivoting)

$$\boldsymbol{q} = \frac{-\boldsymbol{a}_{21}}{\boldsymbol{a}_{11}},\ \boldsymbol{x}_2 = \frac{\boldsymbol{b}_2 + \boldsymbol{b}_1\boldsymbol{q}}{\boldsymbol{a}_{22} + \boldsymbol{a}_{12}\boldsymbol{q}},\quad \boldsymbol{x}_1 = \frac{\boldsymbol{b}_1 - \boldsymbol{a}_{12}\boldsymbol{x}_2}{\boldsymbol{a}_{11}}.$$

An interval linear system

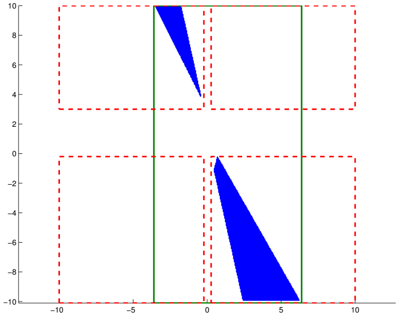

Figure : The solution obtained by the interval Gauss-Seidel is given in the solid box. The solution obtained by the interval union Gaussian elimination is given by dashed boxes.

An interval union linear system

- Let

$$\mathcal{A} = \begin{pmatrix} \{[-5,-3],[4,5]\} & \{[0.5,1.0]\} \\ \{[0.5,1.0]\} & \{[-3,-2],[2,3]\} \end{pmatrix}$$

and

$$\mathbf{b} = \{[1.0,2.0],[1.5,2.0]\}^T.$$

- We solve only one interval union linear system instead of 4 interval linear systems.

An interval union linear system

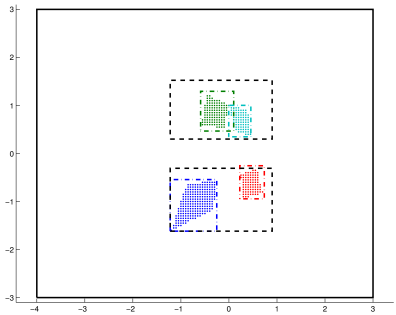

Figure : Interval Gauss-Seidel solution is given in the outer solid box, interval union Gaussian elimination is represented by dashed boxes. The solution set of each interval system and its interval hull in colored solid boxes.

Interval union Gauss-Seidel

Input: $\mathcal{A}$, $\mathcal{b}$ and $\boldsymbol{x}$

Output: $\boldsymbol{y}$ such that $\Sigma(\mathcal{A}, \mathcal{b}) \cap \boldsymbol{x} \subseteq \boldsymbol{y} \subseteq \boldsymbol{x}$.

```
for i = 1, ..., n do
    s ← b_i − Σ_{j=1}^{i−1} A_ij y_j − Σ_{j=i+1}^{n} A_ij x_j
    if 0 ∉ s − A_ii x_i then
        return ∅;
    end if
    if 0 ∈ s, 0 ∈ A_ii then
        y_i ← x_i;
        continue;
    end if
    y_i ← x_i ∩ (s / A_ii)
    if y_i == ∅ then
        return ∅;
    end if
end for
return y;
```

Example 1 revisited

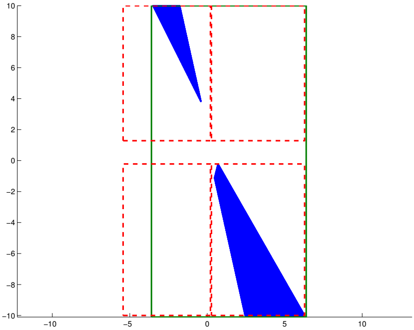

Figure : The solution obtained by the interval Gauss-Seidel is given in the solid box. The solution obtained by the interval union Gauss-Seidel procedure is given by dashed boxes.

Example 1 revisited - Complete Gauss-Seidel

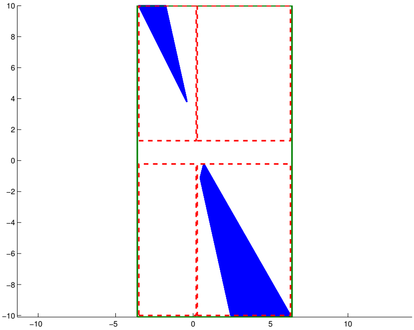

Figure : The solution obtained by the complete interval Gauss-Seidel is given in the solid box. The solution obtained by the complete interval union Gauss Seidel procedure is given by dashed boxes.

Interval union Gauss-Seidel

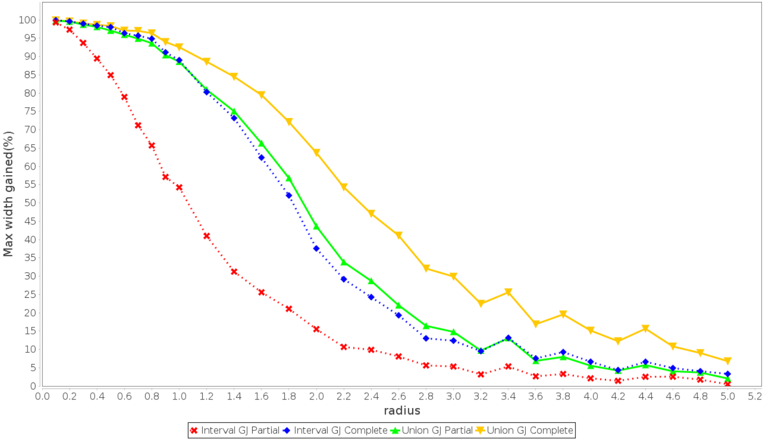

Figure : Width reduction(in average) obtained by interval and interval union Gauss-Seidel in random matrices of size $N = \{2, 5, 10, 15\}$. We perform 1000 experiments for each N.

The interval union Newton operator

- Let $f : \mathbf{R}^n \to \mathbf{R}^n$ be a differentiable function and $\boldsymbol{x}_0$ an interval union box.

$$f(x^*) = 0, \quad x^* \in \boldsymbol{x}_0.$$

- The interval union Newton operator is

$$\boldsymbol{x}_i^{k+1} = \boldsymbol{x}_i^k \cap \boldsymbol{y}_i, \quad i = 1 \ldots n, k \geq 0$$

where

$$\boldsymbol{y}_i = \check{\boldsymbol{x}}_i + \frac{\mathbf{r}_i(\boldsymbol{x})}{\mathcal{J}_{ii}(\boldsymbol{x})}, \quad \mathbf{r}_i = f_i(\check{\boldsymbol{x}}) - \sum_{\substack{j=1 \\ j \neq i}}^{n} \mathcal{J}_{ij}(\boldsymbol{x})(\boldsymbol{x}_j -_c \check{\boldsymbol{x}}_j).$$

The interval union Newton operator

- We want to enclose the solution set of

$$x_1^2 + x_2^2 - 1 = 0, \quad x_1^2 - x_2 = 0$$

on $\mathbf{x} = ([0, 0.9482],\ [-1.2502, 0])^T$.

- Interval Newton reduces the volume in 45%:

$$x \in \mathbf{x}' = ([0, 0.9482],\ [-1.2502, -0.8486])^T$$

and

$$x \in \mathbf{x}'' = ([0, 0.9482],\ [-0.2896, 0.0000])^T.$$

- Interval union Newton reduces the volume in 81%:

$$\boldsymbol{x}^* = \begin{pmatrix} \{[0, 0.1933], [0.825, 0.9482]\} \\ \{[-1.2502, -0.8486], [-0.2896, 0]\} \end{pmatrix}$$

The interval union Newton operator

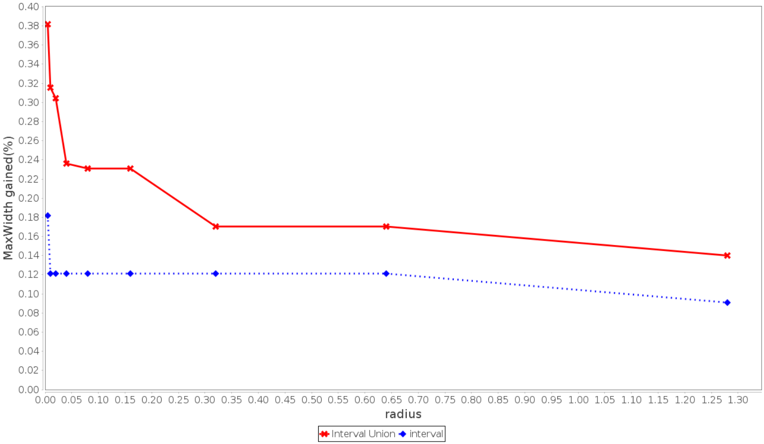

Figure : Width reduction(in average) obtained by interval and union Newton operators. Experiment performed on 102 multivariate problems taking a symmetric box around a known solution.

Unidimensional interval union Newton

Input: The interval union $\boldsymbol{u}_0$ and the narrow component tolerance $\epsilon > 0$.
Output: The interval union $\boldsymbol{s} = (\mathbf{x}_i)$ with $\mathrm{wid}(\mathbf{x}_i) < \epsilon$ and the guarantee that for all $y \in \boldsymbol{u}_0$ with $f(y) = 0$ there exist an $\mathbf{x}_i$ such that $y \in \mathbf{x}_i$.

```
u ← u_0;
while u ≠ ∅ do
    u ← u ∩ N(u);                                   ▷ Newton operator
    x ← ∅;
    for x_i ∈ u do
        if 0 ∉ f(x_i) then                          ▷ Elimination test
            if wid(x_i) < ε then                    ▷ Solution test
                S ← x_i;
            else
                x ← checkAndRemove(x_i, ε, f);
            end if
        end if
    end for
    u ← x;
end while
return S;
```

Unidimensional interval union Newton

fun	INewton			IUNewton			fun	INewton			IUNewton		
	Sol	FunEv	Wid	Sol	FunEv	Wid		Sol	FunEv	Wid	Sol	FunEv	Wid
f_1	3212	6424	10.0	410	6883	1E-7	f_2	3	164	1E-7	1	39	1E-7
f_3	3454	6916	10.0	6367	82782	1E-7	f_4	2	97	1E-7	1	37	1E-7
f_5	23832	95393	1E-2	3	59629	1E-2	f_6	2	38	1E-7	2	39	1E-7
f_7	14673	38638	0.1	7	367	1E-7	f_8	11521	96463	1	32	1931	1E-7
f_9	2	67	1E-7	2	50	1E-7	f_{10}	778	1569	10.0	63	893	1E-7
f_{11}	8082	22861	0.1	0	227	1E-7	f_{12}	5397	63841	1E-7	15	213	1E-7
f_{13}	0	1	1E-7	0	2	1E-7	f_{14}	0	1	1E-7	0	3	1E-7
f_{15}	15306	31865	1	15712	57924	1E-3	f_{16}	786	10218	1E-7	10	175	1E-7
f_{17}	0	1	1E-7	0	3	1E-7	f_{18}	0	1	1E-7	0	3	1E-7
f_{19}	1150	3319	1	8	339	1E-7	f_{20}	15772	73030	0.1	0	105	1E-7
f_{21}	0	28	1E-7	0	13	1E-7	f_{22}	1	123	1E-7	1	101	1E-7
f_{23}	3071	6340	10.0	3187	43862	1E-7	f_{24}	13362	30544	1	254	3757	1E-7
f_{25}	379	777	1	7011	77237	1E-7	f_{26}	0	1	1E-7	0	3	1E-7
f_{27}	3656	7312	10.0	20093	70984	1E-2	f_{28}	373	776	1	7011	72631	1E-7
f_{29}	15966	32320	1	17992	65801	1E-3	f_{30}	0	2	1E-7	0	1	1E-7
f_{31}	8	131	1E-7	7	117	1E-7	f_{32}	6	91	1E-7	6	109	1E-7

Table : Comparison between the interval and the interval union Newton methods. The number of solutions obtained with each method is given in `Sol`, the number of function evaluations in `FunEv` and the final tolerance is given in column `Wid`.

Conclusions

Thank You for your attention!

If you have question about interval unions please contact me during SWIM or send me an e-mail to: `demoraismt79@univie.ac.at`

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