On Taylor Model Based Integration of ODEs

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Outline

Why Interval Computations?

- Inclusion of discretization or truncation errors in numerical algorithms
  - Newton's method
  - Global optimization
  - Numerical integration
  - ...
- Modeling of uncertain data
- Bounding of roundoff errors
- Moore (1966):

  Matrix computations, ranges of functions, root-finding algorithms, integrals, initial value problems for ODEs.

Interval Arithmetic

Set of compact real intervals:

$$\mathbb{IR} = \{\mathbf{x} = [\underline{x}, \overline{x}] \mid \underline{x}, \overline{x} \in \mathbb{R},\ \underline{x} \leq \overline{x}\}.$$

Basic arithmetic operations:

$$\mathbf{x} \star \mathbf{y} \ := \ \{x \star y \mid x \in \mathbf{x},\, y \in \mathbf{y}\}, \quad \star \in \{+, -, \cdot, /\} \qquad (0 \notin \mathbf{y} \text{ for } /).$$

$$\begin{aligned}
\mathbf{x} + \mathbf{y} &= [\underline{x} + \underline{y}, \overline{x} + \overline{y}], \\
\mathbf{x} - \mathbf{y} &= [\underline{x} - \overline{y}, \overline{x} - \underline{y}], \\
\mathbf{x} \cdot \mathbf{y} &= [\min\{\underline{x}\underline{y}, \underline{x}\overline{y}, \overline{x}\underline{y}, \overline{x}\overline{y}, \}, \max\{\underline{x}\underline{y}, \underline{x}\overline{y}, \overline{x}\underline{y}, \overline{x}\overline{y}, \}], \\
\mathbf{x} \,/\, \mathbf{y} &= \mathbf{x} \cdot [1 \,/\, \overline{y}, 1 \,/\, \underline{y}].
\end{aligned}$$

Ranges and Inclusion Functions

1. **Range** of $f : D \to E$: $\mathrm{Rg}\,(f, D) := \{f(x) \mid x \in D\}$.
2. Let $f : D \subseteq \mathbb{R} \to \mathbb{R}$ be a continuous function. An **inclusion function** F of f is an interval function $F : \mathbb{IR} \to \mathbb{IR}$ which encloses the range of f for every compact interval $\mathbf{x} \subseteq D$:

$$F(\mathbf{x}) \supseteq \mathrm{Rg}\,(f, \mathbf{x}) \quad \text{for all} \quad \mathbf{x} \subseteq D.$$

3. Examples
   - $\mathbf{x} \cdot \mathbf{x} - 2 \cdot \mathbf{x}, \quad \mathbf{x} \cdot (\mathbf{x} - 2), \quad (\mathbf{x} - 1)^2 - 1$

     are inclusion functions for

     $$f(x) = x^2 - 2x = x(x-2) = (x-1)^2 - 1.$$

   - $e^{\mathbf{x}} := [e^{\underline{x}}, e^{\overline{x}}]$ is an inclusion function for exp.

Dependency Problem

- Interval-arithmetic evaluation of $f(x) := \dfrac{x}{1+x}$ on $\mathbf{x} = [1,2]$:

$$\frac{\mathbf{x}}{1+\mathbf{x}} = \frac{[1,2]}{[2,3]} = [\frac{1}{3}, 1].$$

- Interval-arithmetic evaluation of $g(x) := 1 - \dfrac{1}{1+x}$, $x \in \mathbf{x}$:

$$1 - \frac{1}{1+\mathbf{x}} = 1 - \frac{1}{[2,3]} = 1 - [\frac{1}{3}, \frac{1}{2}] = [\frac{1}{2}, \frac{2}{3}] = \mathrm{Rg}\,(f, \mathbf{x})\,.$$

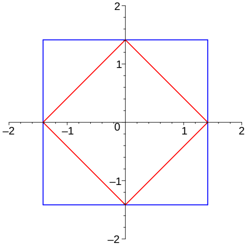
- Reduced overestimation: centered forms, etc.

Wrapping Effect

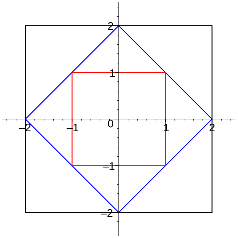
Overestimation: Enclose non-interval shaped sets by intervals.

Example: $f : (x, y) \to \frac{\sqrt{2}}{2}(x + y, y - x)$ (Rotation).

Interval evaluation of f on $\mathbf{x} = ([-1, 1], [-1, 1])$:



$\mathrm{Rg}\,(f, \mathbf{x}),\ F(\mathbf{x})$



$\mathrm{Rg}\,(f^2, \mathbf{x}),\ \mathrm{Rg}\,(f, F(\mathbf{x})),\ F(F(\mathbf{x}))$

Taylor Models

Taylor model: $\mathcal{U} := p_n(x) + \mathbf{i}, \quad x \in \mathbf{x},\ \mathbf{x} \in \mathbb{IR}^m,\ \mathbf{i} \in \mathbb{IR}$
(p_n: m-variate polynomial of order n).

Function set: $\mathcal{U} = \{f \in C_0(\mathbf{x}) : f(x) \in p_n(x) + \mathbf{i} \text{ for all } x \in \mathbf{x}\}$.

Range of a TM: $\mathrm{Rg}\,(\mathcal{U}) = \{z = p(x) + \xi \mid x \in \mathbf{x}, \xi \in \mathbf{i}\}$.

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Range of a TM: $\mathrm{Rg}\,(\mathcal{U}) = \{ z = p(x) + \xi \mid x \in \mathbf{x}, \xi \in \mathbf{i} \} \subset \mathbb{R}^m$.

Ex. 1: $$\mathcal{U} := \begin{pmatrix} 1 \\ 5 \end{pmatrix} + \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 + 2x \\ 5 + y \end{pmatrix}, \quad x, y \in [-1, 1].$$

$$\mathrm{Rg}\,(\mathcal{U}) = \begin{pmatrix} 1 \\ 5 \end{pmatrix} + \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} [-1, 1] \\ [-1, 1] \end{pmatrix} = \begin{pmatrix} [-1, 3] \\ [4, 6] \end{pmatrix}.$$

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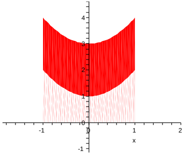
Ex. 2: $\mathcal{U} := \begin{pmatrix} x \\ 2 + x^2 + y \end{pmatrix}, \quad x,\ y \in [-1, 1]$

$\mathrm{Rg}\,(\mathcal{U})$:



Taylor Model Arithmetic

Multiplication:

$$(1 + x + \mathbf{i}_1) \cdot (2 - x + \mathbf{i}_2) := 2 + x$$
$$+\mathrm{Rg}\left(-x^2\right) + \mathrm{Rg}\,(1 + x) \cdot \mathbf{i}_2 + \mathrm{Rg}\,(2 - x) \cdot \mathbf{i}_1 + \mathbf{i}_1 \cdot \mathbf{i}_2.$$

Composition:

$$\mathcal{U}_1(x) := 3 + 2x^2 + \mathbf{i}_1, \quad \mathcal{U}_2(x) := \tfrac{1}{2}x - x^2 + \mathbf{i}_2, \qquad x \in \mathbf{x},$$

$$\mathcal{U}_1(x) \circ \mathcal{U}_2(x) \subseteq 3 + 2(\tfrac{1}{2}x - x^2 + \mathbf{i}_2)^2 + \mathbf{i}_1.$$

Taylor Model Arithmetic: Composition

For $x \in \mathbf{x} = [-\frac{1}{2}, \frac{1}{2}]$:

$$\begin{aligned} e^x &\in \mathcal{U}_1(x) := 1 + x + \tfrac{1}{2}x^2 + [-0.035, 0.035], \\ \cos x &\in \mathcal{U}_2(x) := 1 - \tfrac{1}{2}x^2 + [-0.010, 0.010]. \end{aligned}$$

Composition:

$$\begin{aligned} \mathcal{U}_1 \circ \mathcal{U}_2 &\subseteq 1 + (1 - \tfrac{1}{2}x^2 + \mathbf{i}_1) + \tfrac{1}{2}(1 - \tfrac{1}{2}x^2 + \mathbf{i}_1)^2 + \mathbf{i}_2 \\ &\subseteq \tfrac{5}{2} - x^2 + [-0.058, 0.066]. \end{aligned}$$

Taylor Model Arithmetic: Composition

Warning: $\mathcal{U}_1 \circ \mathcal{U}_2$ is **not** a valid enclosure of $e^{\cos x}$, $x \in \mathbf{x}$,

because the range of $\mathcal{U}_2$ is not contained in x.

For example,

$$(\mathcal{U}_1 \circ \mathcal{U}_2)(0) = [2.442, 2.566] \not\ni e = e^{\cos 0}.$$

Compositions of Taylor models are computed as above, but

the interval term of $\mathcal{U}_1$ must fit the range of $\mathcal{U}_2$.

Valid $\mathbf{i}_1$ for e^x, $x \in [-1, 1]$: $[-0.454, 0.454]$:

$$(\mathcal{U}_1 \circ \mathcal{U}_2)(x) := \frac{5}{2} - x^2 + [-0.477, 0.485], \quad x \in \mathbf{x}.$$

IA vs. TMA: Dependency Problem

- Example: $f(x) = x^2 + \cos x + \sin x - e^x, \quad x \in \mathbf{x} = [0,1].$
- Direct IA:

$$f(x) \in F(\mathbf{x}) = \mathbf{x}^2 + \cos \mathbf{x} + \sin \mathbf{x} - e^{\mathbf{x}}$$
$$= [0,1] + [\cos 1, 1] + [0, \sin 1] - [1, e] \approx [-2.178, 1.842].$$

- Mean Value Form:

$$f(x) \in f(\tfrac{1}{2}) + F'(\mathbf{x}) \cdot (\mathbf{x} - \tfrac{1}{2})$$
$$= f(\tfrac{1}{2}) + (2 \cdot \mathbf{x} - \sin \mathbf{x} + \cos \mathbf{x} - e^{\mathbf{x}}) \cdot [-\tfrac{1}{2}, \tfrac{1}{2}]$$
$$\subseteq [-0.042, -0.041] + [-3.020, 0] \cdot [-0.5, 0.5] = [-1.552, 1.469].$$

IA vs. TMA: Dependency Problem

- TMA (Taylor models of order 3):

$$\begin{aligned} f(x) &= x^2 + \cos x + \sin x - e^x \\ &= x^2 + 1 - \frac{x^2}{2} + I_1 + x - \frac{x^3}{6} + I_2 - 1 - x - \frac{x^2}{2} - \frac{x^3}{6} - I_3 \\ &= -\frac{x^3}{3} + I_1 + I_2 + I_3 \\ &\in [-0.334, 0] + 2 * [0, 0.042] - [0, 0.114] = [-0.448, 0.082]. \end{aligned}$$

- Range: $\mathrm{Rg}\,(f, \mathbf{x}) = [1 + \cos 1 + \sin 1 - e, 0] \subset [-0.337, 0]$.

Verified Integration of ODEs

Interval IVP:

$$u' = f(t, u), \quad u(t_0) \in \mathbf{u}_0, \quad t \in \mathbf{t} = [t_0, t_{\mathrm{end}}]$$

$f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ sufficiently smooth, $\mathbf{u}_0 \in \mathbb{IR}^m$, $t_{\mathrm{end}} > t_0$.

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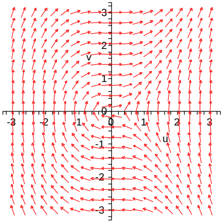

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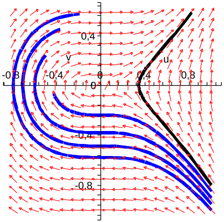

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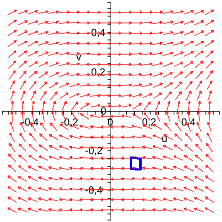

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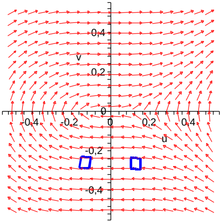

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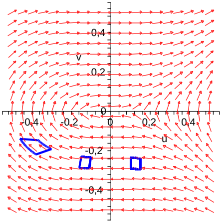

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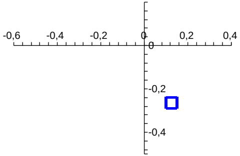

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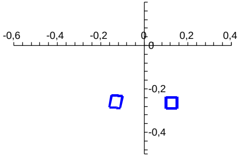

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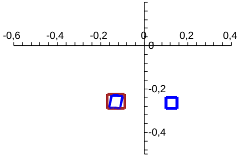

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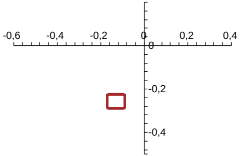

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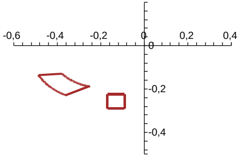

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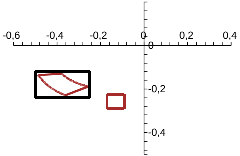

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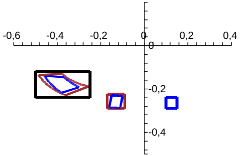


Interval Methods for ODEs

Sets used to enclose the flow:

Moore (1965):	Intervals
Eijgenraam (1981), Lohner (1987):	Parallelepipeds
Kühn (1998):	Zonotopes

Enclosure sets are convex.

Quadratic Model Problem

$$\begin{aligned} u' &= v, & u(0) &\in [0.95, 1.05], \\ v' &= u^2, & v(0) &\in [-1.05, -0.95]. \end{aligned}$$

Taylor model method: initial set described by parameters a and b:

$$\begin{aligned} u_0(a,b) &:= 1 + a, & a \in \mathbf{a} &:= [-0.05, 0.05], \\ v_0(a,b) &:= -1 + b, & b \in \mathbf{b} &:= [-0.05, 0.05]. \end{aligned}$$

Naive Taylor Model Method

Picard iteration ($n = 3,\ h = 0.1$):

$$u^{(0)}(\tau, a, b) = 1 + a, \quad v^{(0)}(\tau, a, b) = -1 + b,$$

$$u^{(1)}(\tau, a, b) = u_0(a, b) + \int_0^\tau v^{(0)}(s, a, b)\, ds$$

$$v^{(1)}(\tau, a, b) = v_0(a, b) + \int_0^\tau \left(u^{(0)}(s, a, b)\right)^2\, ds$$

$$u^{(3)}(\tau, a, b) = 1 + a - \tau + b\tau + \tfrac{1}{2}\tau^2 + a\tau^2 - \tfrac{1}{3}\tau^3,$$

$$v^{(3)}(\tau, a, b) = -1 + b + \tau + 2a\tau - \tau^2 + a^2\tau - a\tau^2 + b\tau^2 + \tfrac{2}{3}\tau^3.$$

Naive Taylor Model Method: Remainder Bounds

Remainder bounds by fixed point iteration (Makino, 1998):

Find $\mathbf{i}_0$ and $\mathbf{j}_0$ s.t.

$$u_0 + \int_0^\tau \left(v^{(3)}(s,a,b) + \mathbf{j}_0 \right) \, ds \subseteq u^{(3)}(\tau,a,b) + \mathbf{i}_0,$$

$$v_0 + \int_0^\tau \left(u^{(3)}(s,a,b) + \mathbf{i}_0 \right)^2 \, ds \subseteq v^{(3)}(\tau,a,b) + \mathbf{j}_0$$

for all $a \in \mathbf{a}$, $b \in \mathbf{b}$, $\tau \in [0, 0.1]$.

Naive Taylor Model Method: Enclosure of the Flow

Flow for $\tau \in [0, 0.1]$:

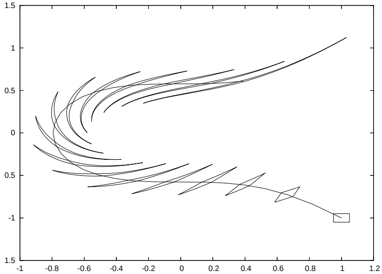
$$\widetilde{\mathcal{U}}_1(\tau, a, b) := u^{(3)}(\tau, a, b) + \mathbf{i}_0,$$
$$\widetilde{\mathcal{V}}_1(\tau, a, b) := v^{(3)}(\tau, a, b) + \mathbf{j}_0.$$

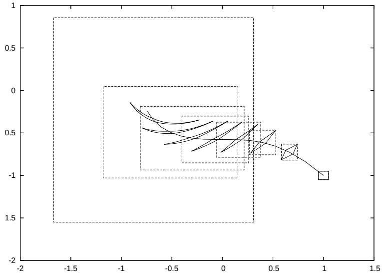
Flow at $t_1 = 0.1$:

$$\mathcal{U}_1(a, b) := \widetilde{\mathcal{U}}_1(0.1, a, b) = 0.905 + 1.01a + 0.1b + \mathbf{i}_0,$$
$$\mathcal{V}_1(a, b) := \widetilde{\mathcal{V}}_1(0.1, a, b) = -0.909 + 0.19a + 1.01b + 0.1a^2 + \mathbf{j}_0$$

(nonlinear boundary).

Integration of Model Problem with COSY Infinity and AWA





Naive Taylor Model Method: Second Integration Step

Find $\mathbf{i}_1$ and $\mathbf{j}_1$ s.t.

$$\mathcal{U}_1(a,b) + \int_0^\tau \left(v^{(3)}(s,a,b) + \mathbf{j}_1\right)\, ds \subseteq u^{(3)}(\tau,a,b) + \mathbf{i}_1,$$

$$\mathcal{V}_1(a,b) + \int_0^\tau \left(u^{(3)}(s,a,b) + \mathbf{i}_1\right)^2\, ds \subseteq v^{(3)}(\tau,a,b) + \mathbf{j}_1$$

for all $a,\ b \in [-0.05, 0.05]$ and for all $\tau \in [0, 0.1]$.

Naive Taylor Model Method: Second Integration Step

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for all $a,\ b \in [-0.05, 0.05]$ and for all $\tau \in [0, 0.1]$.

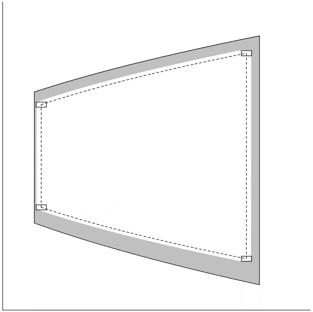
Since $\mathbf{i}_0$ and $\mathbf{j}_0$ are contained in $\mathcal{U}_1$ and $\mathcal{V}_1$, diameters of interval terms are nondecreasing!

Shrink Wrapping

Absorb interval term into polynomial part via shrink wrap factor q (Makino and Berz 2002):

$$\left.\begin{aligned}
\mathcal{U}(a,b) &:= 2 + 4a + \tfrac{1}{2}a^2 + [-0.2, 0.2],\\
\mathcal{V}(a,b) &:= 1 + 3b + 1ab + [-0.1, 0.1],\\
\mathcal{U}_{\mathrm{sw}}(a,b) &:= 2 + \frac{89}{20}a + \frac{89}{160}a^2,\\
\mathcal{V}_{\mathrm{sw}}(a,b) &:= 1 + \frac{287}{80}b + \frac{89}{80}ab.
\end{aligned}\right\} \quad \begin{aligned} &a,\ b \in [-1,1],\\ &\left(q = \frac{89}{80}\right).\end{aligned}$$

Shrink Wrapping



$\begin{pmatrix} \mathcal{U} \\ \mathcal{V} \end{pmatrix}$ *(white)* vs. $\begin{pmatrix} \mathcal{U}_{\text{sw}} \\ \mathcal{V}_{\text{sw}} \end{pmatrix}$.

Integration with Preconditioned Taylor Models

Preconditioned integration: flow at t_j:

$$\mathcal{U}_j = \mathcal{U}_{l,j} \circ \mathcal{U}_{r,j} = (p_{l,j} + \mathbf{i}_{l,j}) \circ (p_{r,j} + \mathbf{i}_{r,j}).$$

Purpose: stabilize integration similar to QR interval method.

Theorem (Makino and Berz 2004)

If the initial set of an IVP is given by a preconditioned Taylor model, then integrating the flow of the ODE only acts on the left Taylor model.

Linear ODE: Naive TMM

Linear autonomous system ($B \in \mathbb{R}^{m \times m}$):

$$u' = B\,u, \quad u(0) = \mathbf{u}_0 = \mathcal{U}_0.$$

Direct interval method ($\mathbf{z}_j$: local error, $T := \sum_{k=0}^{n} \frac{(hB)^k}{k!}$):

$$\mathbf{u}_j := T\,\mathbf{u}_{j-1} + \mathbf{z}_j, \quad j = 1, 2, \ldots .$$

Naive Taylor model method:

$$\mathcal{U}_j = T^j\,\mathcal{U}_0 + \sum_{k=1}^{j} (T\circ)^{j-k}\mathbf{i}_k, \quad j = 1, 2, \ldots,$$

where $(T\circ)^0\mathbf{x} := \mathbf{x}, \quad (T\circ)^k\mathbf{x} := T \cdot \big((T\circ)^{k-1}\mathbf{x}\big), \quad k \in \mathbb{N}.$

Linear ODE: Naive TMM with Shrink Wrapping

Linear autonomous system ($B \in \mathbb{R}^{m \times m}$):

$$u' = B\,u, \quad u(0) = \mathbf{u}_0 = \mathcal{U}_0.$$

Parallelepiped method ($\mathbf{z}_j$: local error, $\mathbf{r}_0 := \mathbf{u}_0 - m(\mathbf{u}_0)$):

$$\mathbf{r}_j := \mathbf{r}_{j-1} + (T^{j-1})^{-1}(\mathbf{z}_j - (m(\mathbf{z}_j)), \quad j = 1, 2, \ldots.$$

Naive Taylor model method with shrink wrapping:

$$d_j := \|\mathrm{w}((T^j)^{-1}\mathbf{i}_j)\|_\infty\,, \quad q_j := 1+d_j/2, \quad \widetilde{p}_{sw,j} := \left(\prod_{k=1}^{j} q_j\right) \widetilde{p}_0(x).$$

Preconditioned Taylor Model Method

Initial set: $p_{l,0}(x) = c_0 + C_0 x, \quad p_{r,0}(x) = x, \quad \mathbf{i}_{l,0} = \mathbf{i}_{r,0} = 0.$

jth initial set: $\mathcal{U}_j = (c_{l,j} + C_{l,j}\, x + \mathbf{i}_{l,j}) \circ (c_{r,j} + C_{r,j}\, x + \mathbf{i}_{r,j}),$

$$c_{l,j},\ c_{r,j} \in \mathbb{R}^m,\ \ C_{l,j},\ C_{r,j} \in \mathbb{R}^{m \times m}.$$

Integrated flow: $\widetilde{\mathcal{U}}_j := (Tc_{l,j} + TC_{l,j}\, x + \mathbf{i}_{l,j+1}) \circ (p_{r,j} + \mathbf{i}_{r,j}).$

Preconditioned Taylor Model Method

$C_{l,j+1}$ nonsingular: $\widetilde{\mathcal{U}}_j = (Tc_{l,j} + C_{l,j+1}\,x + [0,0])$

$$\circ \left\{ C_{l,j+1}^{-1}\,TC_{l,j}\,c_{r,j} + C_{l,j+1}^{-1}\,TC_{l,j}\,C_{r,j}\,x + C_{l,j+1}^{-1}\,TC_{l,j}\,\mathbf{i}_{r,j} + C_{l,j+1}^{-1}\mathbf{i}_{l,j+1} \right\}$$

$$=: (c_{l,j+1} + C_{l,j+1}\,x + [0,0]) \circ (c_{r,j+1} + C_{r,j+1}\,x + \mathbf{i}_{r,j+1}) =: \mathcal{U}_{j+1}$$

Global error:

$$\mathbf{i}_{r,j+1} := C_{l,j+1}^{-1}\,TC_{l,j}\,\mathbf{i}_{r,j} + C_{l,j+1}^{-1}\mathbf{i}_{l,j+1}, \quad j = 0, 1, \ldots .$$

$C_{l,j+1} = TC_{l,j}$: parallelepiped preconditioning

$C_{l,j+1} = Q_j$: QR preconditioning

Other choices: curvilinear coordinates, blunting (Makino and Berz 2004)

Example 1: Pure Contraction

$$B = \begin{pmatrix} -0.4375 & 0.0625 & -0.2652 \\ 0.0625 & -0.4375 & -0.2652 \\ -0.2652 & -0.2652 & -0.375 \end{pmatrix} \approx \begin{pmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{3}{4} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Method	Steps	$y_1(100)$	
AWA iv	216	1.4^{7301}_{5593}E-001	√
AWA pe	131	abort at $t = 52.6$	fail
AWA QR	216	1.4^{7301}_{5593}E-001	√
TM na	391	[−2.4E+26, 2.4E+26]	fail
TM sw	272	[−2.3E+112, 2.3E+112]	fail
TM QR	122	1.4^{7301}_{5593}E-001	√

$$(\mathbf{u}_0 = [0.999, 1.001] \cdot (1 \quad 1 \quad 1)^T)$$

Example 2: Pure Rotation

$$B = \begin{pmatrix} 0 & -0.7071 & -0.5 \\ 0.7071 & 0 & 0.5 \\ 0.5 & -0.5 & 0 \end{pmatrix} \approx \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Method	Steps	$y_1(100)$	
AWA iv	393	abort at $t = 76.5$	fail
AWA pe	449	1.49^{522}_{222}E+000	$\surd$
AWA QR	449	1.49^{522}_{222}E+000	$\surd$
TM na	396	[−1.6E+45, 1.6E+45]	fail
TM sw	343	1.49^{522}_{222}E+000	$\surd$
TM QR	343	1.49^{522}_{222}E+000	$\surd$

Example 3: Contraction and Rotation

$$B = \begin{pmatrix} -0.125 & -0.8321 & -0.3232 \\ 0.5821 & -0.125 & 0.6768 \\ 0.6768 & -0.3232 & -0.25 \end{pmatrix} \approx \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix}$$

Method	Steps	$y_1(100)$	
AWA iv	507	abort at $t = 85.5$	fail
AWA pe	404	abort at $t = 75.2$	fail
AWA QR	516	1.34^{862}_{592}E+000	√
TM na	397	[−1.7E+55, 1.7E+55]	fail
TM sw	357	[−3.6E+106, 3.6E+106]	fail
TM QR	362	1.34^{862}_{592}E+000	√

Summary

- Verified integration methods
- Interval methods vs. TM methods
- Performance for linear ODEs
- Future work: Analysis of TM methods for nonlinear ODEs