Interval Methods and Taylor Model Methods for ODEs

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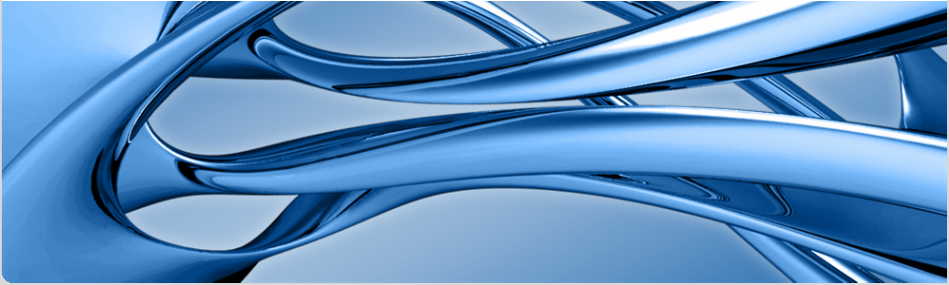

Validated Methods

- Also called: Verified Methods, Rigorous Methods, Guaranteed Methods, Enclosure Methods, . . .
- Aim: Compute guaranteed bounds for the solution of a problem, including
  - Discretization errors (ODEs, PDEs, optimization)
  - Truncation errors (Newton's method, summation)
  - Roundoff errors
- Used for
  - Modelling of uncertain data
  - Bounding of roundoff errors

Outline

1. Interval arithmetic
2. Interval methods for ODEs
3. Taylor model methods for ODEs

Interval Arithmetic

Interval Arithmetic

Compact real intervals:

$$\mathbb{IR} = \{\boldsymbol{x} = [\underline{x}, \overline{x}] \mid \underline{x} \leq \overline{x}\} \quad (\underline{x}, \overline{x} \in \mathbb{R}).$$

Basic arithmetic operations:

$$\boldsymbol{x} \circ \boldsymbol{y} := \{x \circ y \mid x \in \boldsymbol{x},\, y \in \boldsymbol{y}\}, \quad \circ \in \{+, -, *, /\} \qquad (0 \notin \boldsymbol{y} \text{ for } /)$$

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

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$$\begin{aligned}
\boldsymbol{x} + \boldsymbol{y} &= [\underline{x} + \underline{y}, \overline{x} + \overline{y}] && \text{FPIA}: [\underline{x} \triangledown \underline{y}, \overline{x} \triangle \overline{y}] \\
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\end{aligned}$$

Ranges and Inclusion Functions

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- **Range** of $f : D \to E$: $\quad \mathrm{Rg}\,(f, D) := \{f(x) \mid x \in D\}$
- **Inclusion function** $F : \mathbb{IR} \to \mathbb{IR}$ of $f : D \subseteq \mathbb{R} \to \mathbb{R}$:

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

- Examples:
  - $\dfrac{\boldsymbol{x}}{1+\boldsymbol{x}}, \quad 1 - \dfrac{1}{1+\boldsymbol{x}}, \quad$ are inclusion functions for

$$f(x) = \frac{x}{1+x} = 1 - \frac{1}{1+x}$$

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

IA: Dependency

- $f(x) = \frac{x}{1+x} = 1 - \frac{1}{1+x}, \;\; \boldsymbol{x} = [1,2]$:

- $\frac{\boldsymbol{x}}{1+\boldsymbol{x}} = \frac{[1,2]}{[2,3]} = [\frac{1}{3}, 1]$

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

- Reduced overestimation: centered forms, etc.

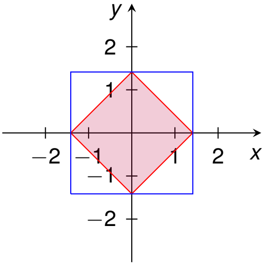
  Mean value form: $\mathrm{Rg}\,(f, \boldsymbol{x}) \subseteq f(c) + F'(\boldsymbol{x})(\boldsymbol{x} - c), \;\; c = m(\boldsymbol{x})$.

IA: 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 $\boldsymbol{x} = ([-1, 1], [-1, 1])$:



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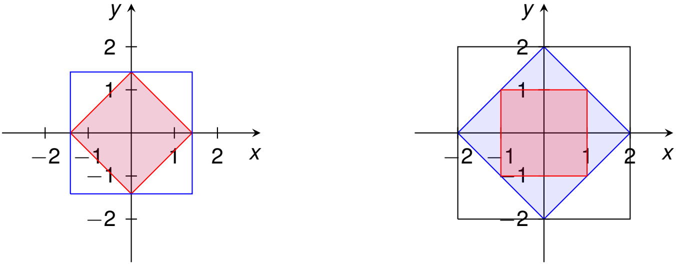

Interval Methods for ODEs

Validated Integration of ODEs

Interval IVP:

$$u' = f(t,u), \quad u(t_0) = u_0 \in \boldsymbol{u}_0, \quad t \in \boldsymbol{t} = [t_0, t_{\text{end}}]$$

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

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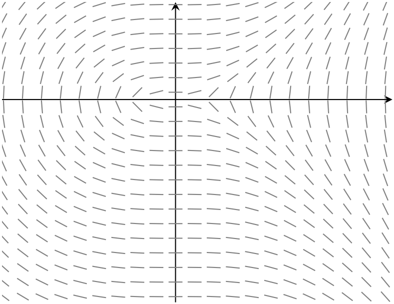

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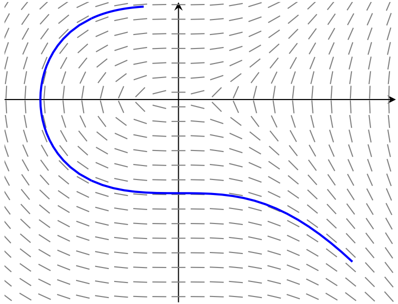

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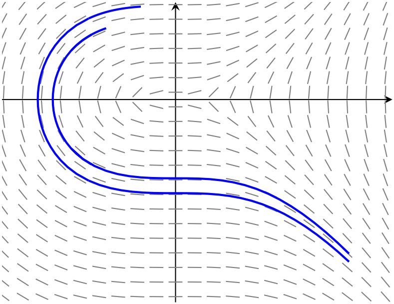

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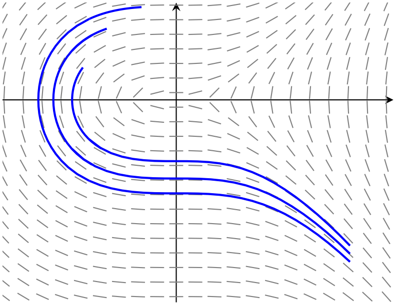

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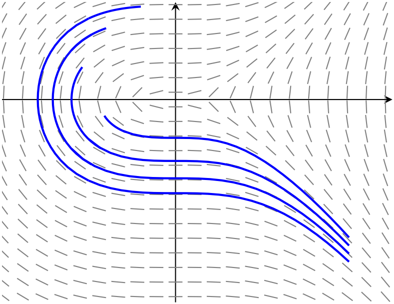

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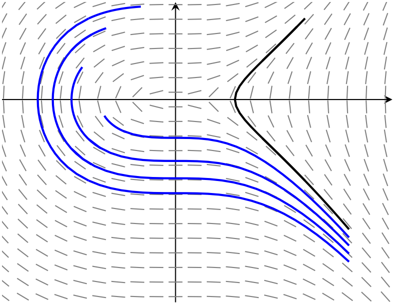

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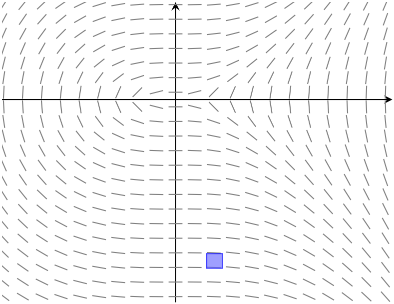

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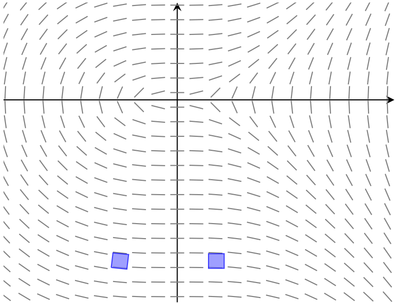

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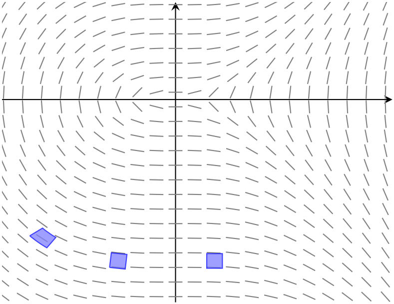

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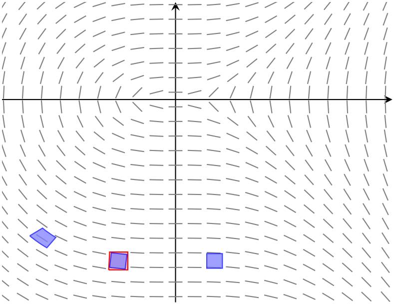

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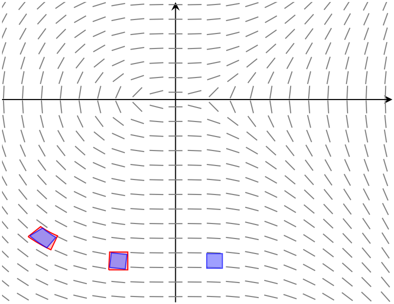

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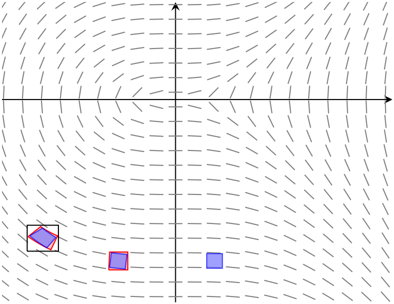


Autonomous Interval IVP

$$u' = f(u), \quad u(t_0) = u_0 \in \boldsymbol{u}_0, \ \ t \in \boldsymbol{t} = [t_0, t_{\text{end}}],$$

where $D \subset \mathbb{R}^m$, $f \in C^n(D)$, $f : D \rightarrow \mathbb{R}^m$, $\boldsymbol{u}_0 \in \mathbb{IR}^m$.

Moore's enclosure method:

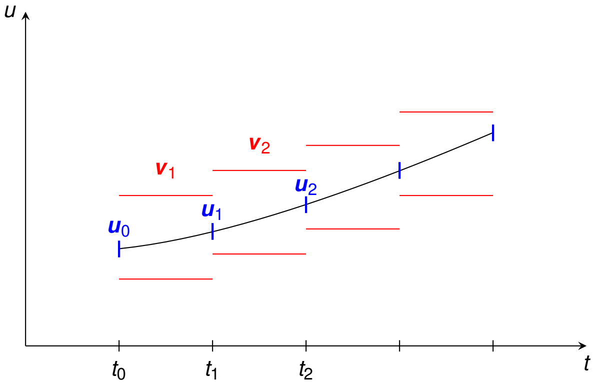
- Automatic computation of Taylor coefficients
- Interval iteration: For $j = 1, 2, \ldots$:

A priori enclosure: $\boldsymbol{v}_j \supseteq u(t)$ for all $t \in [t_{j-1}, t_j]$ ("Alg. I").

Truncation error: $\boldsymbol{z}_j := \dfrac{h_j^{n+1}}{(n+1)!} f^{(n)}(\boldsymbol{v}_j)$.

$$u(t_j) \in \boldsymbol{u}_j := \boldsymbol{u}_{j-1} + \sum_{k=1}^{n} \frac{h_j^k}{k!} f^{(k-1)}(\boldsymbol{u}_{j-1}) + \boldsymbol{z}_j \qquad \text{("Algorithm II")}.$$

Piecewise Constant A Priori Enclosure



A Priori Enclosures

- Picard iteration: find h_j, $\boldsymbol{v}_j$ such that

$$\boldsymbol{u}_{j-1} + [0, h_j] f(\boldsymbol{v}_j) \subseteq \boldsymbol{v}_j$$

- Step size restrictions: Explicit Euler steps
- Improvements: Lohner 1988, Corliss & Rihm 1996, Makino 1998, Nedialkov & Jackson 2001
- Alternatives: Neumaier 1994, N. 1999, N. 2007, Delanoue & Jaulin 2010, Kin, Kim & Nakao 2011

Modifications of Algorithm II

- Reduction of wrapping effect: Moore, Eijgenraam, Lohner, Rihm, Kuehn, Nedialkov & Jackson, . . .
- Nedialkov & Jackson: Hermite-Obreshkov-Method
- Rihm: Implicit methods
- Petras & Hartmann, Bouissou: Runge-Kutta-Methods
- Berz & Makino: Taylor models

  Taylor expansion of solution w.r.t. time and initial values

Direct Interval Method

Direct method (Moore 1965): Apply mean value form to $f^{(k)}$:

$$f^{[0]}(u) = u, \quad f^{[k]}(u) = \frac{1}{k}\left(\frac{\partial f^{[k-1]}}{\partial u} f\right)(u) \ \text{ for } \ k \geq 1.$$

Let

$$\boldsymbol{S}_{j-1} = I + \sum_{k=1}^{n} h_0^k J\big(f^{[k]}(\boldsymbol{u}_{j-1})\big), \quad \boldsymbol{z}_j = h_0^{n+1} f^{[n]}(\boldsymbol{v}_j),$$

(I: identity matrix, $J\big(f^{[k]}\big)$: Jacobian of $f^{[i]}$), then for some $\widehat{u}_{j-1} \in \boldsymbol{u}_{j-1}$

$$u(t_j; u_0) \in \boldsymbol{u}_j = \widehat{u}_{j-1} + \sum_{k=1}^{n-1} h_j^k f^{[k]}(\widehat{u}_{j-1}) + \boldsymbol{z}_j + \boldsymbol{S}_{j-1}(\boldsymbol{u}_{j-1} - \widehat{u}_{j-1}).$$

Global Error Propagation

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Wrapping effect: $\boldsymbol{S}_{j-1}(\boldsymbol{u}_{j-1} - \widehat{u}_{j-1})$ may overestimate

$$\mathcal{S} = \{S_{j-1}(u_{j-1} - \widehat{u}_{j-1}) \mid S_{j-1} \in \boldsymbol{S}_{j-1},\ u_{j-1} \in \boldsymbol{u}_{j-1}\}$$

$\rightarrow$ propagate $\mathcal{S}$ as a parallelepiped.

$\widehat{u}_0 := \mathrm{m}(\boldsymbol{u}_0)$, $\boldsymbol{r}_0 = \boldsymbol{u}_0 - \widehat{u}_0$, $B_0 = I$; for some nonsingular B_{j-1}:

$$\left.\begin{aligned} \widehat{u}_j &= \widehat{u}_{j-1} + \sum_{k=1}^{n-1} h_{j-1}^k f^{[k]}(\widehat{u}_{j-1}) + \mathrm{m}(\boldsymbol{z}_j), \\ \boldsymbol{u}_j &= \widehat{u}_{j-1} + \sum_{k=1}^{n-1} h_{j-1}^k f^{[k]}(\widehat{u}_{j-1}) + \boldsymbol{z}_j + (\boldsymbol{S}_{j-1} B_{j-1}) \boldsymbol{r}_{j-1}, \end{aligned}\right\}$$

$\widehat{u}_j$: approximate point solution for the central IVP

$\boldsymbol{z}_j$: local error; $\boldsymbol{r}_j$: global error

Global Error Propagation

Global error propagation:

$$\boldsymbol{r}_j = \left(B_j^{-1}(\boldsymbol{S}_{j-1}B_{j-1})\right)\boldsymbol{r}_{j-1} + B_j^{-1}(\boldsymbol{z}_j - \mathrm{m}(\boldsymbol{z}_j))$$

- Moore's direct method: $B_j = I$
- Pep method (Eijgenraam, Lohner): $B_j = \mathrm{m}(\boldsymbol{S}_{j-1}B_{j-1})$
- QR method (Lohner): $\mathrm{m}(\boldsymbol{S}_{j-1}B_{j-1}) = QR,\ B_j := Q$
- Blunting method (Berz, Makino): modify B_j in the pep method such that condition numbers remain small

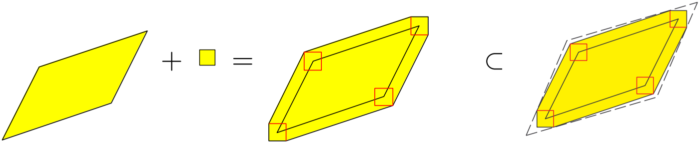
Autonomous Linear ODE

Autonomous linear system ($A \in \mathbb{R}^{m \times m}$):

$$u' = A\,u, \quad u(0) \in \boldsymbol{u}_0.$$

Propagation of the Global Error

$$\boldsymbol{r}_j = (B_j^{-1} T B_{j-1})\boldsymbol{r}_{j-1} + B_j^{-1}(\boldsymbol{z}_j - \mathrm{m}(\boldsymbol{z}_j)), \qquad T = \sum_{\nu=0}^{n-1} \frac{(hA)^\nu}{\nu!}.$$



Interval Methods for Linear ODEs

Direct method: $\boldsymbol{r}_j = T\boldsymbol{r}_{j-1} + \boldsymbol{z}_j - \mathrm{m}(\boldsymbol{z}_j)$.

- Optimal for local error, bad for global error (rotation)

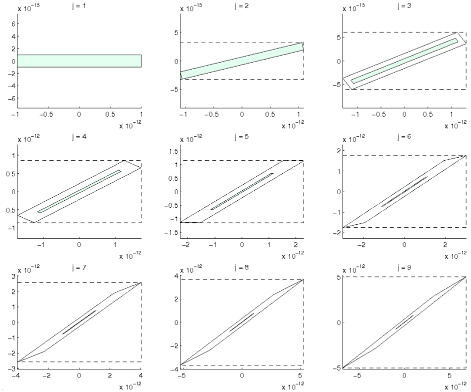
Parallelepiped method: $\boldsymbol{r}_j = \boldsymbol{r}_{j-1} + (T^{-j})(\boldsymbol{z}_j - (m(\boldsymbol{z}_j))$.

- Optimal for global error; suitable for local error, if cond(T^j) is small
- Bad for local error in presence of shear

QR method: $\boldsymbol{r}_j = R_j\boldsymbol{r}_{j-1} + Q_j^T\big(\boldsymbol{z}_j - \mathrm{m}(\boldsymbol{z}_j)\big), \quad j = 1, 2, \ldots.$

- Handles rotation, contraction, shear

Wrapping Effect: Direct Interval Method

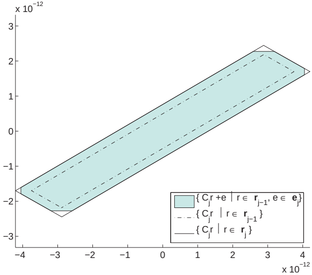


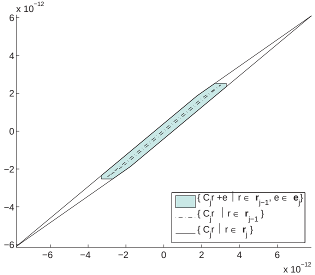
(Plots by Ned Nedialkov)

Huge overestimations in general

Wrapping Effect: Parallelepiped Method

$$B_j = TB_{j-1}$$

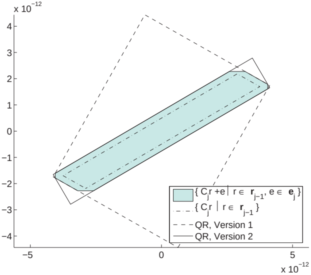


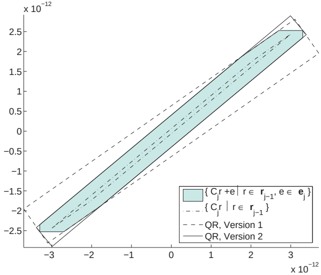


B_j often ill-conditioned, large overestimations

Wrapping Effect: QR Method

$$B_j = Q_j, \quad Q_j R_j = TB_{j-1}$$





Overestimation depends on column permutations of B_{j-1}

Taylor Model Methods for ODEs

Taylor Models (I)

- $\boldsymbol{x} \subset \mathbb{R}^m, \quad f : \boldsymbol{x} \to \mathbb{R}, \quad f \in C^{n+1}, \quad x_0 \in \boldsymbol{x};$

  $f(x) = p_{n,f}(x - x_0) + R_{n,f}(x - x_0), \ x \in \boldsymbol{x}$

  ($p_{n,f}$ Taylor polynomial, $R_{n,f}$ remainder term)

- **Interval remainder bound** of order n of f on $\boldsymbol{x}$:

  $$\forall x \in \boldsymbol{x} : \ R_{n,f}(x - x_0) \in \boldsymbol{i}_{n,f}$$

- **Taylor model** $T_{n,f} = (p_{n,f}, \boldsymbol{i}_{n,f})$ of order n of f:

  $$\forall x \in \boldsymbol{x}: \ f(x) \in p_{n,f}(x - x_0) + \boldsymbol{i}_{n,f}$$

Taylor Models (II)

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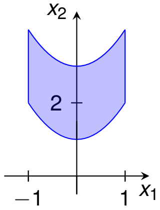
Taylor model: $\mathcal{U} := p_n(x) + \boldsymbol{i}, \quad x \in \boldsymbol{x},\ \boldsymbol{x} \in \mathbb{IR}^m,\ \boldsymbol{i} \in \mathbb{IR}^m$
(p_n: vector of m-variate polynomials of order n)

Function set: $\mathcal{U} = \{ f \in C^0(\boldsymbol{x}) : f(x) \in p_n(x) + \boldsymbol{i} \text{ for all } x \in \boldsymbol{x} \}$

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

Ex.: $\mathcal{U} := \begin{pmatrix} x_1 \\ 2 + x_1^2 + x_2 \end{pmatrix}, \quad x_1, x_2 \in [-1, 1]$

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



TM Arithmetic

Paradigm for TMA:

- $p_{n,f}$ is processed symbolically to order n
- Higher order terms are enclosed into the remainder interval of the result

Taylor Model Methods for ODEs

- Taylor expansion of solution w.r.t. time and initial values
- Computation of Taylor coefficients by Picard iteration: Parameters describing initial set treated symbolically
- Interval remainder bounds by fixed point iteration (Makino, 1998)

Example: Quadratic Problem

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

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

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

3rd order TM Method: Enclosure of the Flow

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$h = 0.1$, flow for $\tau \in [0, 0.1]$:

$$\widetilde{\mathcal{U}}_1(\tau, a, b) \quad := \quad 1 + a - \tau + b\tau + \tfrac{1}{2}\tau^2 + a\tau^2 - \tfrac{1}{3}\tau^3 + \boldsymbol{i}_0,$$

$$\widetilde{\mathcal{V}}_1(\tau, a, b) \quad := \quad -1 + b + \tau + 2a\tau - \tau^2 + a^2\tau - a\tau^2 + b\tau^2 + \tfrac{2}{3}\tau^3 + \boldsymbol{j}_0.$$

Flow at $t_1 = 0.1$:

$$\mathcal{U}_1(a, b) \quad := \quad \widetilde{\mathcal{U}}_1(0.1, a, b) = 0.905 + 1.01a + 0.1b + \boldsymbol{i}_0,$$

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

(nonlinear boundary).

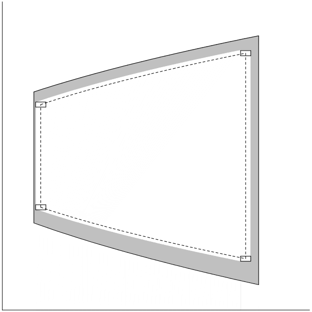
Naive TM Method

- Interval remainder terms accumulate
- Linear ODEs:

  Naive TM method performs similarly to the direct interval method
- $\longrightarrow$ Shrink wrapping, preconditioned TM methods

Shrink Wrapping

Absorb interval term into polynomial part (Makino and Berz 2002):



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

Linear ODEs: Shrink wrapping performs similarly to the pep method.

Integration with Preconditioned Taylor Models

Preconditioned integration: flow at t_j:

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

Purpose: stabilize integration as in the 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.

Preconditioned TMM for linear ODE

Global error:

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

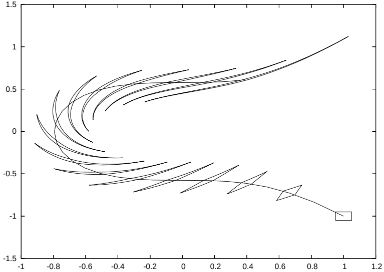
$C_{l,j+1} = TC_{l,j}$: parallelepiped preconditioning

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

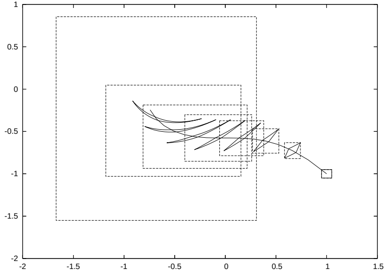
Other choices: curvilinear coordinates, blunting (Makino and Berz 2004)

Integration of Quadratic Problem

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



COSY Infinity



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Summary

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- Interval arithmetic
- Interval methods for ODEs
- Taylor model methods for ODEs

Open problems

- Treatment of high-dimensional problems
- Validated implicit methods