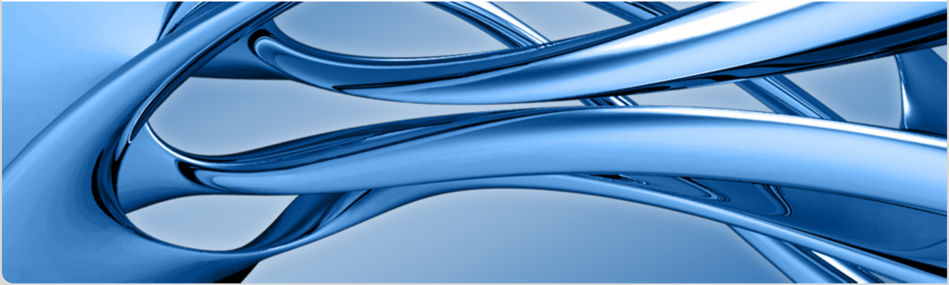
Verified Integration of ODEs with Taylor Models

Markus Neher, Dept. of Mathematics

KARLSRUHE INSTITUTE OF TECHNOLOGY (KIT)



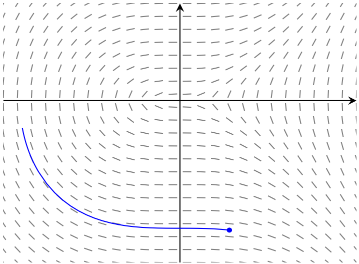
Introduction

Initial Value Problem

IVP:

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

$f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ sufficiently smooth, $\quad u_0 \in \mathbb{R}^m, \quad t_{\mathrm{end}} > t_0$



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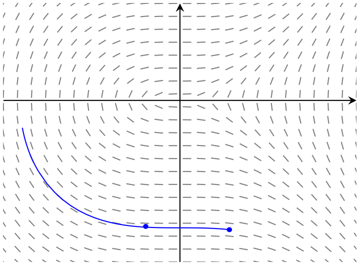

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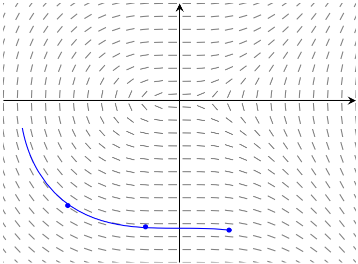

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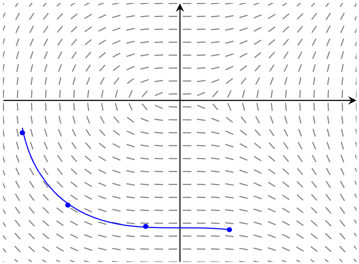

Verified Initial Value Problem I

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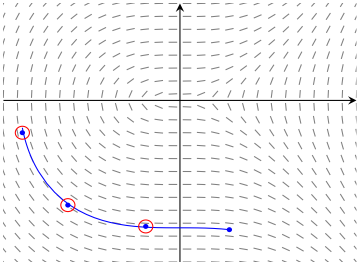

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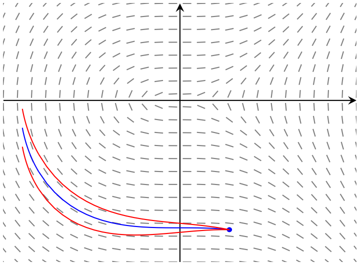

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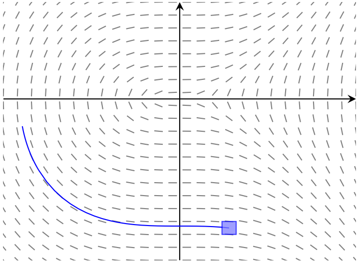

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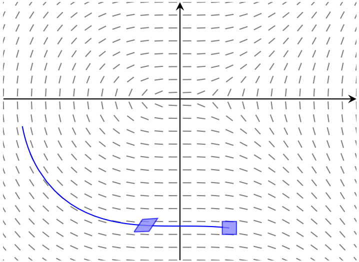

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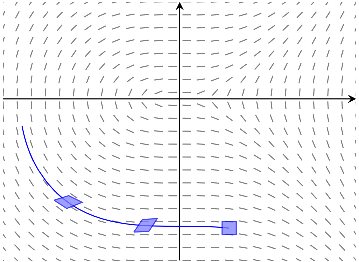

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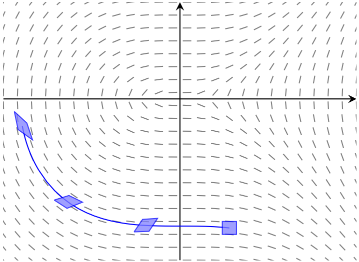

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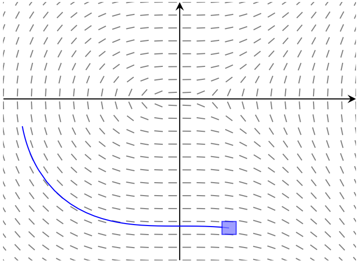

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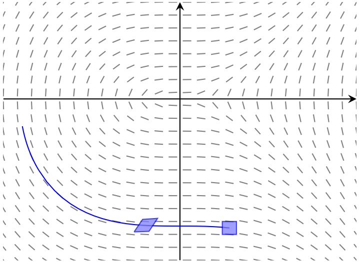

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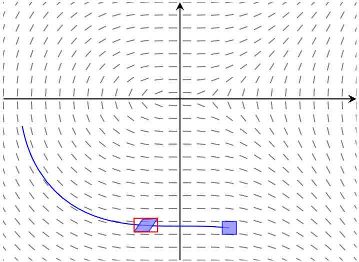

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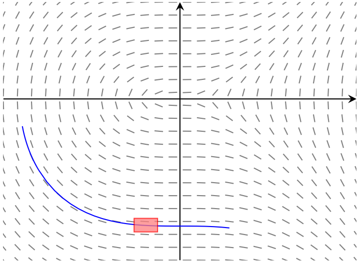

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Karlsruhe Institute of Technology

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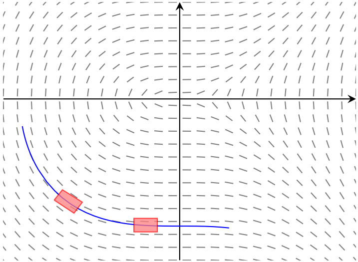

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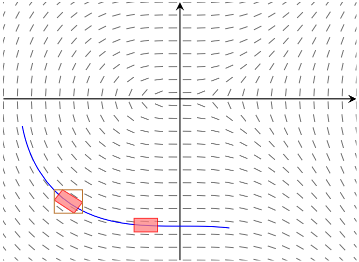

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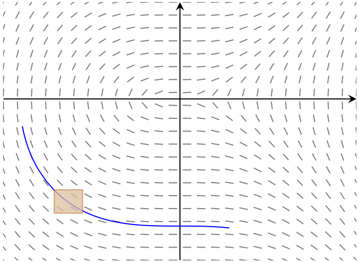

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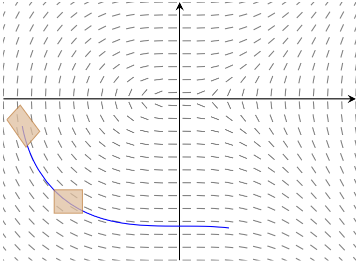

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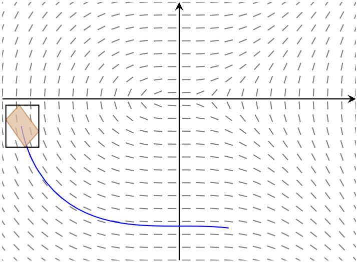

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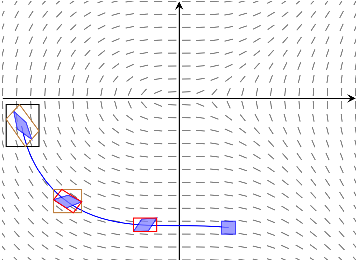

Initial Value Problem with Uncertainty II

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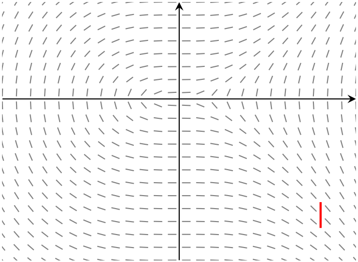

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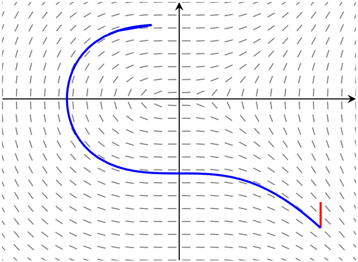

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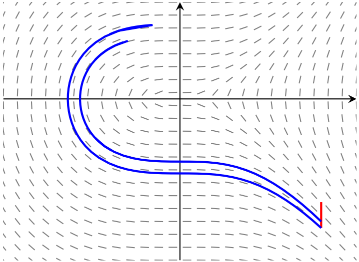

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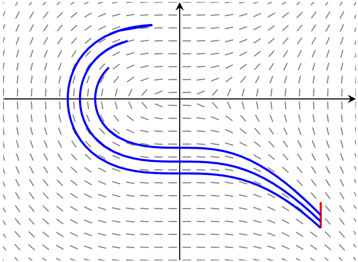

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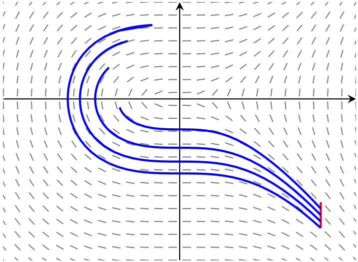

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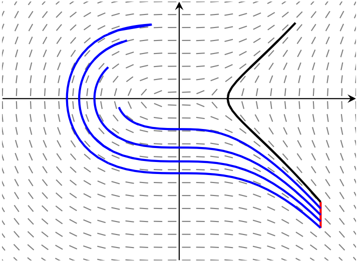

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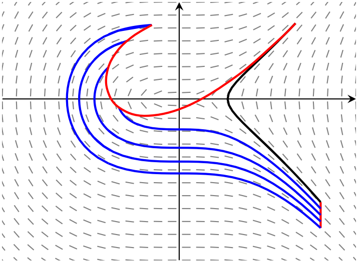


Outline

Interval Methods for ODEs

Taylor Models

Taylor Model Methods for ODEs

Interval Methods for ODEs

Taylor Method for IVPs

Autonomous IVP:

$$u' = f(u), \quad u(t_0) = u_0,$$

where $f : D \subset \mathbb{R}^m \to \mathbb{R}^m$, $f \in C^n(D)$, $u_0 \in D$

- Taylor method: $$u(t) = \sum_{k=0}^{n} \frac{(t-t_0)^k}{k!} u^{(k)}(t_0) + R_n$$
- Automatic (recursive) computation of Taylor coefficients:

$$u^{(0)} = f^{[0]}(u) = u, \quad u^{(1)} = f^{[1]}(u) = f(u),$$

$$\frac{1}{k!} u^{(k)} = f^{[k]}(u) = \frac{1}{k} \left(\frac{\partial f^{[k-1]}}{\partial u} f \right)(u) \;\text{ for }\; k \geq 2$$

Moore's enclosure method

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

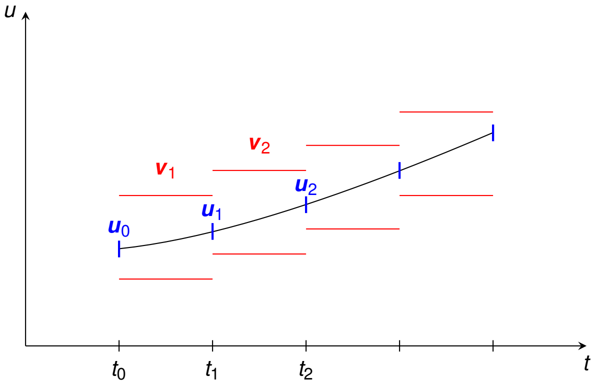
- Interval iteration: For $j = 1, 2, \ldots$:

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

  Truncation error: $\boldsymbol{z}_j := h_j^{n+1} f^{[n+1]}(\boldsymbol{v}_j), \quad h_j = t_j - t_{j-1}$

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

Predictor-Corrector Scheme



A Priori Enclosures

- Constant a priori enclosure by 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

- A priori enclosures using Picard iterations:
  - Interval polynomials: Lohner 1988, Corliss & Rihm 1996, Makino 1998, Nedialkov & Jackson 2001
  - Arbitrary interval functions: Rauh, Auer & Hofer 2005

- Alternative a priori bounds: Neumaier 1994, N. 1999, N. 2007

Refinement step

The iteration

$$\boldsymbol{u}_j = \boldsymbol{u}_{j-1} + \sum_{k=1}^{n} h_j^k f^{[k]}(\boldsymbol{u}_{j-1}) + \boldsymbol{z}_j$$

is width increasing:

$$w(\boldsymbol{u}_j) = w(\boldsymbol{u}_{j-1}) + \sum_{k=1}^{n} h_j^k w\big(f^{[k]}(\boldsymbol{u}_{j-1})\big) + w(\boldsymbol{z}_j)$$

$\rightarrow$ Reduce overestimation by improved evaluation of rhs

Modifications of Algorithm II

- Moore, Eijgenraam, Lohner: Local coordinate systems
- Kühn: Zonotopes
- Nedialkov & Jackson: Hermite-Obreshkov-Method
- Rihm: Implicit methods
- Petras & Hartmann, Bouissou & Martel: Runge-Kutta-Methods

Dependency Reduction: Direct Interval Method

Apply mean value form to $f^{[k]}(\boldsymbol{u}_{j-1})$: For fixed $\widehat{u}_{j-1} \in \boldsymbol{u}_{j-1}$,

$$\left\{\, f^{[k]}(u_{j-1}) \mid u_{j-1} \in \boldsymbol{u}_{j-1} \,\right\} \subseteq f^{[k]}(\widehat{u}_{j-1}) + J\big(f^{[k]}(\boldsymbol{u}_{j-1})\big)(\boldsymbol{u}_{j-1} - \widehat{u}_{j-1}),$$

where $J\big(f^{[k]}\big)$ is the Jacobian of $f^{[k]}$

Let I denote the identity matrix and let

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

Then

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

Wrapping Effect in Global Error Propagation

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

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

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

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

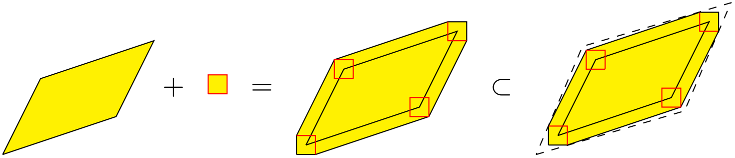
$\boldsymbol{z}_j$: local error; $\boldsymbol{r}_j$: global error

Global Error Propagation

Global error:

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

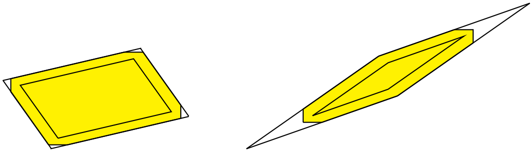
- Direct method: $B_j = I$
- Pep method (Eijgenraam, Lohner): $B_j = \mathrm{m}(\mathbf{S}_{j-1}B_{j-1})$
- QR method (Lohner): $\mathrm{m}(\mathbf{S}_{j-1}B_{j-1}) = QR,\ \ B_j := Q$
- Blunting method (Berz, Makino): $B_j = \mathrm{m}(\mathbf{S}_{j-1}B_{j-1}) + \varepsilon Q_j,\ \ \varepsilon > 0$



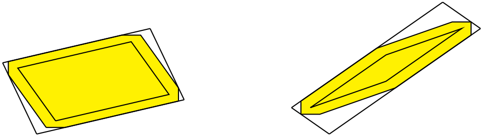
Wrapping Effect

Direct method:

Pep method:



QR method:



Taylor Models

Symbolic Enhancements of IA

- Ultra-arithmetic (arbitrary basis functions; Kaucher & Miranker, 1980s)
- Boundary Arithmetic (multivariate Taylor forms; Lanford, Eckmann, Koch & Wittwer, 1980s)
- Taylor models (Berz & Makino, 1990s–today)

Taylor Models of Type 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;
  in the following: $x_0 = 0$)

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

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

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

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

Taylor Models: Example

$\boldsymbol{x} = [-\frac{1}{2}, \frac{1}{2}], \quad x \in \boldsymbol{x}$:

$$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 e^{\xi}, \quad x, \xi \in \boldsymbol{x},$$

$$\cos x = 1 - \frac{1}{2}x^2 + \frac{1}{6}x^3 \sin\xi, \quad x, \xi \in \boldsymbol{x},$$

$$T_{2,e^x} = 1 + x + \tfrac{1}{2}x^2 + [-0.035, 0.035], \quad x \in \boldsymbol{x},$$

$$T_{2,\cos x} = 1 - \tfrac{1}{2}x^2 + [-0.010, 0.010], \quad x \in \boldsymbol{x}$$

TM Arithmetic

Paradigm for TM Arithmetic:

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

TMA: Addition and Multiplication

- $T_{n,f\pm g} := T_{n,f} \pm T_{n,g} := (p_{n,f} \pm p_{n,g}, \boldsymbol{i}_{n,f} \pm \boldsymbol{i}_{n,g})$,
- $T_{n,\alpha\cdot f} := \alpha \cdot T_{n,f} := (\alpha \cdot p_{n,f}, \alpha \cdot \boldsymbol{i}_{n,f}) \quad (\alpha \in \mathbb{R})$,
- $T_{n,f\cdot g} := T_{n,f} \cdot T_{n,g} := (p_{n,f\cdot g}, \boldsymbol{i}_{n,f\cdot g})$,

  where

  - $p_{n,f}(x) \cdot p_{n,g}(x) = p_{n,f\cdot g}(x) + p_e(x)$,
  - $\mathrm{Rg}\,(p_e) \subseteq \boldsymbol{i}_{p_e}, \quad \mathrm{Rg}\,(p_{n,f}) \subseteq \boldsymbol{i}_{p_{n,f}}, \quad \mathrm{Rg}\,(p_{n,g}) \subseteq \boldsymbol{i}_{p_{n,g}}$,
  - $f(x) \cdot g(x) \in p_{n,f\cdot g}(x) + \underbrace{\boldsymbol{i}_{p_e} + \boldsymbol{i}_{p_{n,f}} \boldsymbol{i}_{n,g} + \boldsymbol{i}_{n,f} \left(\boldsymbol{i}_{p_{n,g}} + \boldsymbol{i}_{n,g}\right)}_{=:\boldsymbol{i}_{n,f\cdot g}}$

Numerical Example

Multiplication: $\boldsymbol{x} = [-\frac{1}{2}, \frac{1}{2}]$, $x \in \boldsymbol{x}$:

$$T_{2,e^x} \cdot T_{2,\cos x} \subseteq (1 + x + \tfrac{1}{2}x^2)(1 - \tfrac{1}{2}x^2) + \mathrm{Rg}\left(1 + x + \tfrac{1}{2}x^2\right)[-0.010, 0.010]$$

$$+[-0.035, 0.035]\left(\mathrm{Rg}\left(1 - \tfrac{1}{2}x^2\right) + [-0.010, 0.010]\right)$$

$$\subseteq (1 + x) + \mathrm{Rg}\left(-\tfrac{1}{2}x^3 - \tfrac{1}{4}x^4\right) + [-0.218, 0.218]$$

$$\subseteq 1 + x + [-0.281, 0.281]$$

TMA: Polynomials, Standard Functions

- If $T_{n,f} = (p_{n,f}, \boldsymbol{i}_{n,f})$ is a Taylor model for f, then $T_{n,\sum a_\nu f^\nu}$ is a Taylor model for $\sum a_\nu f^\nu$

- Standard functions: $\varphi \in \{\exp, \ln, \sin, \cos, \ldots\}$
  Taylor model for $\varphi(f) = \varphi(p_{n,f} + \boldsymbol{i}_{n,f})$:
  - Special treatment of the constant part in $p_{n,f}$
  - Evaluate $p_{n,\varphi}$ for the non-constant part of $p_{n,f}$

Taylor Model for Exponential Function

$x \in \boldsymbol{x}, \quad c := f(0), \quad h(x) := f(x) - c$:

$$p_{n,f}(x) = p_{n,h}(x) + c, \quad \boldsymbol{i}_{n,h} = \boldsymbol{i}_{n,f}$$

$$\exp\left(f(x)\right) = \exp\left(c + h(x)\right) = \exp(c) \cdot \exp\left(h(x)\right)$$

$$= \exp(c) \cdot \left\{1 + h(x) + \frac{1}{2}\left(h(x)\right)^2 + \ldots + \frac{1}{n!}\left(h(x)\right)^n\right\}$$

$$+ \exp(c) \cdot \frac{1}{(n+1)!} \underbrace{\left(h(x)\right)^{n+1} \exp\left(\theta \cdot h(x)\right)}, \quad 0 < \theta < 1$$

$$\subseteq \left(\mathrm{Rg}\,(h) + \boldsymbol{i}\right)^{n+1} \exp\left([0,1] \cdot \left(\mathrm{Rg}\,(h) + \boldsymbol{i}\right)\right)$$

Taylor Model for Exponential Function

Numerical example: TM for $e^{\cos x}$, $x \in \boldsymbol{x} = [-\frac{1}{2}, \frac{1}{2}]$,

$$\cos x \in p_{2,\cos}(x) + \boldsymbol{i} = 1 - \frac{1}{2}x^2 + [-0.010, 0.010]$$

We have $c = 1$, $h(x) = -\frac{1}{2}x^2$, $\mathrm{Rg}\,(h) + \boldsymbol{i} = [-0.135, 0.10] =: \boldsymbol{j}$

$$\begin{aligned} e^{\cos x} &\in e\left\{1 + h + \boldsymbol{i} + \frac{1}{2}(h + \boldsymbol{i})^2\right\} + \frac{e}{6}\boldsymbol{j}^3 \exp([0,1] \cdot \boldsymbol{j}) \\ &\subseteq e\left\{1 - \tfrac{1}{2}x^2\right\} + e\,\boldsymbol{i} + \frac{e}{2}\boldsymbol{j}^2 + \frac{e}{6}\boldsymbol{j}^3 \exp([0,1] \cdot \boldsymbol{j}) \\ &= e\left\{1 - \tfrac{1}{2}x^2\right\} + [-0.031, 0.053] \end{aligned}$$

Taylor Models of Type II

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

Taylor Models of Type II

Taylor model: $\mathcal{U} := p_n(x) + \boldsymbol{i}, \quad x \in \boldsymbol{x},\ \boldsymbol{x} \in \mathbb{IR}^m,\ \boldsymbol{i} \in \mathbb{IR}^m$
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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. 1: $\mathcal{U} := \begin{pmatrix} 1 \\ 5 \end{pmatrix} + \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 + 2x_1 \\ 5 + x_2 \end{pmatrix}, \quad x_1, x_2 \in [-1, 1]$

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

Taylor Models of Type II

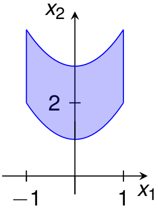
Taylor model: $\mathcal{U} := p_n(x) + \boldsymbol{i}, \quad x \in \boldsymbol{x},\ \boldsymbol{x} \in \mathbb{IR}^m,\ \boldsymbol{i} \in \mathbb{IR}^m$
(p_n: vector of m-variate polynomials of order n)

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

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



TM Arithmetic: Composition

Example: $\boldsymbol{x} = [-\frac{1}{2}, \frac{1}{2}], \quad x \in \boldsymbol{x}$:

$$\mathcal{U}_1 = 1 + x + \tfrac{1}{2}x^2 + [-0.035, 0.035], \quad x \in \boldsymbol{x},$$

$$\mathcal{U}_2 = 1 - \tfrac{1}{2}x^2 + [-0.010, 0.010], \quad x \in \boldsymbol{x}$$

$$\begin{aligned} \mathcal{U}_1 \circ \mathcal{U}_2 \quad &\subseteq \quad 1 + (1 - \tfrac{1}{2}x^2 + \boldsymbol{i}_2) + \tfrac{1}{2}(1 - \tfrac{1}{2}x^2 + \boldsymbol{i}_2)^2 + \boldsymbol{i}_1 \\ &\subseteq \quad \tfrac{5}{2} - x^2 + [-0.048, 0.056] \end{aligned}$$

TM Arithmetic: Composition

Observation: For $x \in \boldsymbol{x} = [-\frac{1}{2}, \frac{1}{2}]$, we have

$$e^x \in \mathcal{U}_1 = 1 + x + \tfrac{1}{2}x^2 + [-0.035, 0.035],$$

$$\cos x \in \mathcal{U}_2 = 1 - \tfrac{1}{2}x^2 + [-0.010, 0.010],$$

but

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

For example,

$$(\mathcal{U}_1 \circ \mathcal{U}_2)(0) = [2.452, 2.556] \not\ni e = e^{\cos 0}$$

TM Arithmetic: Composition

Analysis: $\mathcal{U}_1$ is only a TM for e^x, $x \in \boldsymbol{i} = [-\frac{1}{2}, \frac{1}{2}]$. However, in

$$e^{\cos x}, \quad x \in \boldsymbol{i},$$

we have $\cos x \notin \boldsymbol{i}$.

When evaluating $\mathcal{U}_1 \circ \mathcal{U}_2$

the interval term of $\mathcal{U}_1$ must fit $\square\big(\mathrm{Rg}\,(\mathcal{U}_2) \cup \{x_0\}\big)$.

Valid $\boldsymbol{i}_1$ for e^x, $x \in \square\big(\mathrm{Rg}\,(\mathcal{U}_2) \cup \{0\}\big)$: $[0.106, 0.472]$

$$\Rightarrow \; e^{\cos x} \in (\mathcal{U}_1 \circ \mathcal{U}_2)(x) \subseteq \frac{5}{2} - x^2 + [0.093, 0.493], \quad x \in \boldsymbol{x}$$

Taylor Model Methods for ODEs

Taylor Model Methods for ODEs

- Taylor expansion of solution w.r.t. time and initial values
  $\rightarrow$ reduced dependency problem

- Computation of Taylor coefficients by Picard iteration:
  Parameters describing initial set treated symbolically

- Interval remainder bounds by fixed point iteration (Makino, 1998)

- Enclosure sets for flow can be non-convex
  $\rightarrow$ reduced wrapping effect

Example: Quadratic Problem

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

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

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

Naive TM Method of Order 3

Picard iteration:

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

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

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

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

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

Naive TM Method: Remainder Bounds

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

For some $h > 0$, find $\boldsymbol{i}_0$ and $\boldsymbol{j}_0$ s.t.

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

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

for all $a \in \boldsymbol{a}$, $b \in \boldsymbol{b}$, $\tau \in [0, h]$

3rd order TM Method: Enclosure of the Flow

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

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

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

Flow at $t_1 = 0.1$:

$$\mathcal{U}_1(a, b) \;:=\; \overline{\mathcal{U}}_1(0.1, a, b) = \underbrace{0.905 + 1.01a + 0.1b}_{=:u_1(a,b)} + \boldsymbol{i}_0$$

$$\mathcal{V}_1(a, b) \;:=\; \overline{\mathcal{V}}_1(0.1, a, b) = \underbrace{-0.909 + 0.19a + 1.01b + 0.1a^2b}_{=:v_1(a,b)} + \boldsymbol{j}_0$$

(nonlinear boundary)

Naive TM Method: 2nd Integration Step

From u_1, v_1, compute new $u^{(3)}$, $v^{(3)}$ by Picard iteration

Then find $\boldsymbol{i}_1$ and $\boldsymbol{j}_1$ s.t.

$$\begin{aligned}
\mathcal{U}_1(a,b) + \int_0^\tau \left(v^{(3)}(s,a,b) + \boldsymbol{j}_1\right) ds &\subseteq u^{(3)}(\tau,a,b) + \boldsymbol{i}_1, \\
\mathcal{V}_1(a,b) + \int_0^\tau \left(u^{(3)}(s,a,b) + \boldsymbol{i}_1\right)^2 ds &\subseteq v^{(3)}(\tau,a,b) + \boldsymbol{j}_1
\end{aligned}$$

for all $a,\ b \in [-0.05, 0.05]$ and for all $\tau \in [0, h_2]$

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

Naive TM Method

Karlsruhe Institute of Technology

- Interval remainder terms accumulate
- Linear ODEs:

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

Shrink Wrapping

Idea: Absorb the interval part of the TM into the polynomial part by increasing the polynomial coefficients

Example:

$$\left\{\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} + \begin{pmatrix} [-1,1] \\ [-3,3] \end{pmatrix} \mid a, b \in [-1,1]\right\}$$

$$= \left\{\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} \mid a, b \in [-1,1]\right\} = \begin{pmatrix} [-2,4] \\ [-8,8] \end{pmatrix}$$

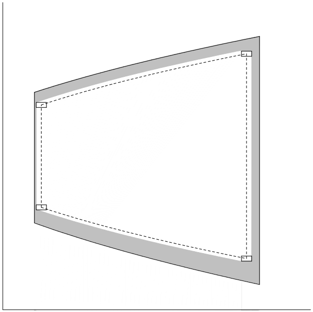
Shrink Wrapping

General case: Multiply all polynomial coeffs except for the constant part by suitable shrink factor q (Berz & Makino 2002, 2005)

Example:

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

Shrink Wrapping



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

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

Integration with Preconditioned Taylor Models

Preconditioned integration: represent flow at t_j as

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

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.

Integration with Preconditioned Taylor Models

"Proof" of the theorem: If

$$\int f(x,t)\,dt = F(x,t) \quad \text{and} \quad x = g(u),$$

then

$$\int f\big(g(u),t\big)\,dt = F\big(g(u),t\big).$$

Application: After each integration step, modify $\mathcal{U}_{l,j}\,\mathcal{U}_{r,j}$ such that the initial set $\mathcal{U}_{l,j}$ for the next integration step is well-conditioned.

Preconditioned TMM for linear ODE

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

$$u' = A\,u, \quad u(0) \in \boldsymbol{u}_0 = \mathcal{U}_0, \quad T = \sum_{\nu=0}^{n} \frac{(hA)^\nu}{\nu!}$$

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

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

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

Integrated flow:

$$\widetilde{\mathcal{U}}_j := (Tc_{l,j} + TC_{l,j}\,x + \boldsymbol{i}_{l,j+1}) \circ (c_{r,j} + C_{r,j}\,x + \boldsymbol{i}_{r,j})$$

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

Preconditioned TMM for linear ODE

Global error:

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

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

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

Integration with Preconditioned Taylor Models

Preconditioned integration: flow at t_j:

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

Note that the polynomial part of $\widetilde{\mathcal{U}}_j$ is independent of $\mathcal{U}_{r,j}$,

but the interval remainder bound depends on the range of $\mathcal{U}_{r,j}$ **!**

Scaling:

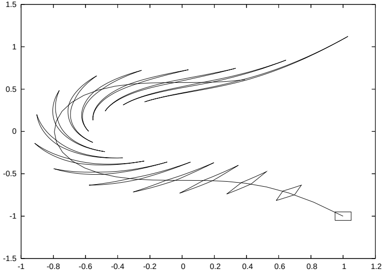
$$\mathcal{U}_j = (\widehat{\mathcal{U}}_{l,j} \circ S_j) \circ (S_j^{-1} \circ \widehat{\mathcal{U}}_{r,j}) \qquad S_j : \text{ scaling matrix}$$

such that

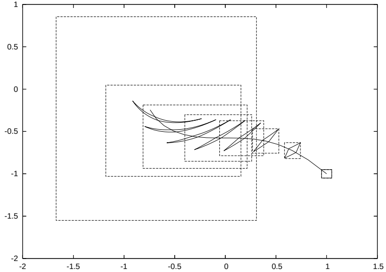
$$\mathrm{Rg}\left(S_j^{-1} \circ \widehat{\mathcal{U}}_{r,j}\right) \approx [-1, 1]^m$$

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



AWA

Enhancements

- Taylor expansion with respect to reference trajectory
  (defect correction, order k/n in space/time) (Berz & Makino)
- Adaptive domain splitting (Berz & Makino)
- Taylor models with pep; parametric ODEs (Lin & Stadtherr)
- Consistency testing by backward integration (Rauh, Auer & Hofer)
- Exponential enclosure techniques (Rauh & Auer)

Applications

- Solar system dynamics, orbits of NEOs (Berz et al.)
- Space flight simulation (Armellin & Di Lizia)
- Parametric ODEs in chemistry, biology, engineering (Stadtherr, Lin & Enszer)
- Control problems in engineering (Rauh, Auer et al.)

Software

- AWA (Lohner 1987; IA; free)
- COSY Infinity, COSY-VI (Berz 1990s, Makino 1998; TMs; restricted)
- VNODE/VNODE-LP (Nedialkov 1999/2010; IA; free)
- ValEncIA-IVP (Rauh, Auer & Hofer, 2005; IA; upon request)
- VSPODE (Lin & Stadtherr, 2006; IA, TMs; upon request)
- RiOT (Eble 2006; TMs; free)

Summary / To Do

+ For nonlinear ODEs, Taylor models benefit from reduced dependency problem and reduced wrapping effect (non-convex enclosure sets).

– Free general purpose state-of-the-art TM software

– Analysis of TM methods for nonlinear ODEs

– Dimensionality curse: No. of coeffs of m-variate TMs of order n:

$N(m,n)$	N(4,10)	N(4,20)	N(6,10)	N(6,20)	N(20,10)
$\binom{m+n}{m}$	1,001	10,626	8,008	230,230	30,045,015

– Verified implicit methods

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