On the Blunting Method in Verified Integration of ODEs

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(joint work with Ken Jackson and Ned Nedialkov)

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Outline

Verified Integration of IVPs

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, $\quad \mathbf{u}_0 \in \mathbb{IR}^m, \quad t_{\mathrm{end}} > t_0.$

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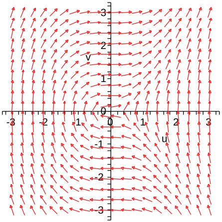

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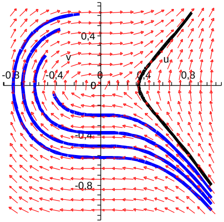

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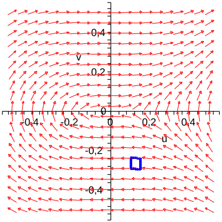

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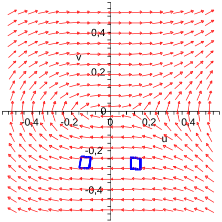

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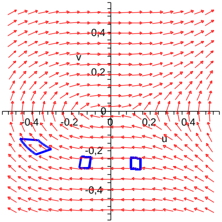

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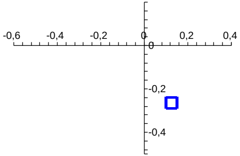

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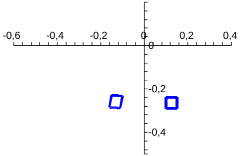

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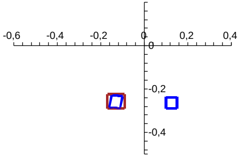

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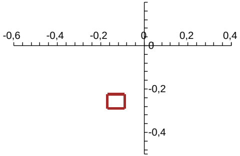

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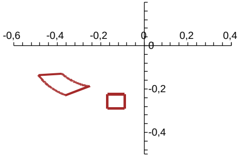

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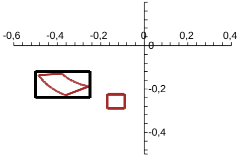

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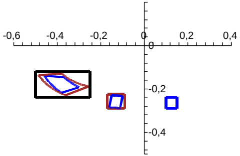

Enclosure Methods for ODEs

Convex sets used to enclose the flow:

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

Non-convex sets:

Berz & Makino (1996-):	Taylor models

Interval Methods: Enclosure Representation

$$\begin{aligned} u(t_j; \mathbf{u}_0) &= \{u(t_j; u_0) \mid u_0 \in \mathbf{u}_0\} \\ &\subseteq \{u_j + S_j w + B_j r \mid w \in \mathbf{u}_0 - \mathrm{m}(\mathbf{u}_0),\ r \in \mathbf{r}_j\}, \end{aligned}$$

where

- $u_j, w, r \in \mathbb{R}^m,\ \mathbf{r}_j \in \mathbb{IR}^m,$
- $S_j, B_j \in \mathbb{R}^{m \times m}, \quad B_j$ nonsingular,
- $\{u_j + S_j w \mid w \in \mathbf{u}_0 - \mathrm{m}(\mathbf{u}_0)\}$: approximation to $u(t_j; \mathbf{u}_0)$,
- $\{B_j r \mid r \in \mathbf{r}_j\}$: bound on global error.

$j = 0$: $\quad u_0 = \mathrm{m}(\mathbf{u}_0), \quad \mathbf{r}_0 = 0, \quad S_0 = B_0 = I.$

Taylor Method for Model Problem

Model problem:

$$u' = Au, \qquad (A \in \mathbb{R}^{m\times m},\ m \geq 2)$$

$$u(0) = u_0 \in \mathbf{u}_0.$$

Taylor method (constant order n, stepsize h):

$$u_j := Tu_{j-1} \quad , \quad j = 1, 2, \ldots.$$

$$\left(T = T_{n-1}(hA) = \sum_{\nu=0}^{n-1} \frac{(hA)^\nu}{\nu!} \right)$$

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Interval Taylor method (constant order n, stepsize h):

$$u_j := Tu_{j-1} + z_j, \quad j = 1, 2, \ldots.$$

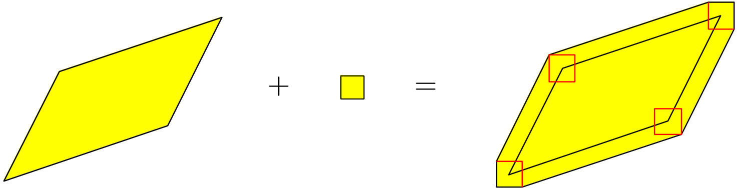
$$\left(T = T_{n-1}(hA) = \sum_{\nu=0}^{n-1} \frac{(hA)^\nu}{\nu!}; \quad z_j : \text{ local error} \right)$$

Propagation of the Global Error

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

Required: B_j for tight enclosure:

$$\{ T B_{j-1} r + z \mid r \in \mathbf{r}_{j-1},\ z \in \mathbf{z}_j - \mathrm{m}(\mathbf{z}_j) \} \subseteq \{ B_j r \mid r \in \mathbf{r}_j \}.$$



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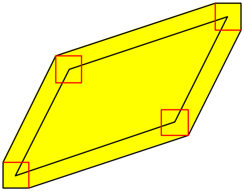

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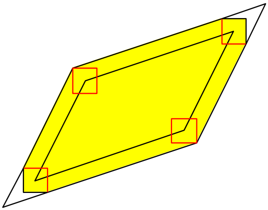

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- Direct method: $B_j = I$.
- Parallelepiped (P) method: $B_j = T B_{j-1}$.
- QR method: $B_j = Q_j$, $Q_j R_j = T B_{j-1}$.
- Blunting (B) method: $B_j = T B_{j-1} + \varepsilon Q_j$, $\varepsilon > 0$.

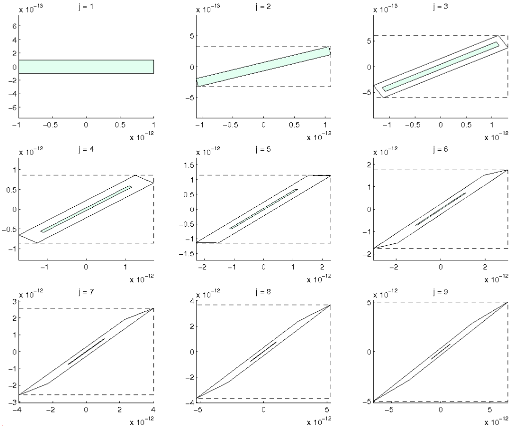
Wrapping Effect: Direct Method

$$\mathbf{r}_j = (B_j^{-1} T B_{j-1}) \mathbf{r}_{j-1} + B_j^{-1} (\mathbf{z}_j - \mathrm{m}(\mathbf{z}_j)), \quad B_j = I:$$

$$\mathbf{r}_j = T \mathbf{r}_{j-1} + \mathbf{z}_j - \mathrm{m}(\mathbf{z}_j).$$

- Optimal coordinates for local error.
- Bad coordinates for global error (rotation).

Wrapping Effect: Direct Method



Huge overestimations in general.

Wrapping Effect: P Method

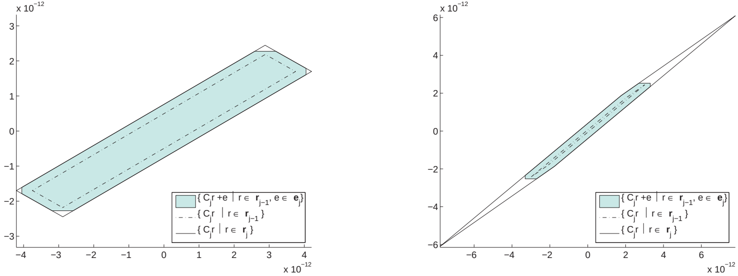
$$\mathbf{r}_j = (B_j^{-1} T B_{j-1})\mathbf{r}_{j-1} + B_j^{-1}\big(\mathbf{z}_j - \mathrm{m}(\mathbf{z}_j)\big), \quad B_j = TB_{j-1}:$$

$$\mathbf{r}_j = \mathbf{r}_{j-1} + T^{-j}\big(\mathbf{z}_j - \mathrm{m}(\mathbf{z}_j)\big).$$

- Optimal coordinates for global error.
- Suitable coordinates for local error, if cond(T^j) is small.
- Bad coordinates for local error in presence of shear (T^j becomes singular for $j \to \infty$).

Wrapping Effect: P Method

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



B_j often ill-conditioned, large overestimations.

Wrapping Effect: QR Method

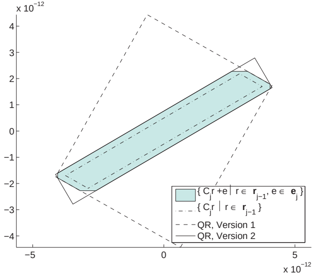
$$\mathbf{r}_j = (B_j^{-1} T B_{j-1})\mathbf{r}_{j-1} + B_j^{-1}\big(\mathbf{z}_j - \mathrm{m}(\mathbf{z}_j)\big), \quad B_j = Q_j,\ Q_j R_j = T B_{j-1} :$$

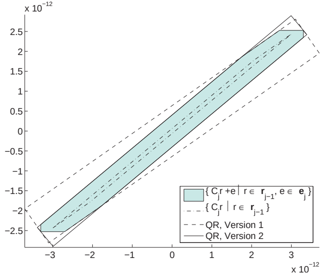
$$\mathbf{r}_j = R_j \mathbf{r}_{j-1} + Q_j^T \big(\mathbf{z}_j - \mathrm{m}(\mathbf{z}_j)\big).$$

- Suitable, but not optimal coordinates for global error.
- Kühn: Numerical example for exponential overestimation.
- Good coordinates for local error.
- Handles rotation, contraction, shear.

Wrapping Effect: QR Method

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





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

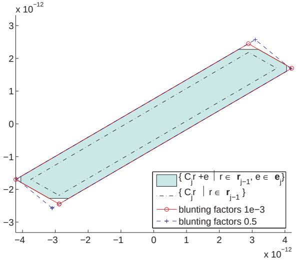
Wrapping Effect: B Method

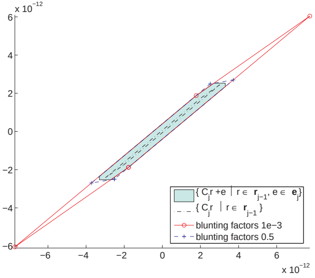
$$\mathbf{r}_j = (B_j^{-1} T B_{j-1})\mathbf{r}_{j-1} + B_j^{-1}\big(\mathbf{z}_j - \mathrm{m}(\mathbf{z}_j)\big), \quad B_j = T B_{j-1} + \varepsilon Q_j.$$

- Coordinates for global error sometimes better than QR.
- Sometimes worse?
- Suitable coordinates for local error.
- Handles rotation, contraction, shear.

Wrapping Effect: B Method

$$B_j = TB_{j-1} + \varepsilon Q_j,\ \varepsilon > 0.$$





Overestimation depends on blunting factors.

Propagation of the Global Error

Global error:

$$\mathbf{r}_j = (B_j^{-1} T B_{j-1})\mathbf{r}_{j-1} + B_j^{-1}\big(\mathbf{z}_j - \mathrm{m}(\mathbf{z}_j)\big),$$

$$\mathrm{w}(\mathbf{r}_j) = |B_j^{-1} T B_{j-1}|\mathrm{w}(\mathbf{r}_{j-1}) + |B_j^{-1}|\mathrm{w}(\mathbf{z}_j).$$

QR method (Nedialkov & Jackson 2001): Error propagation depends on spectral radius of

$$H_j = |Q_j^{-1} T Q_{j-1}|\,|Q_{j-1}^{-1} T Q_{j-2}| \cdots |Q_2^{-1} T Q_1|.$$

B method: Error propagation depends on spectral radius of

$$P_j = |B_j^{-1} T B_{j-1}|\,|B_{j-1}^{-1} T B_{j-2}| \cdots |B_2^{-1} T B_1|.$$

Propagation of the Global Error

Assume: T has eigenvalues λ_i of distinct magnitudes:

$$|\lambda_1| > |\lambda_2| > \cdots |\lambda_n| > 0.$$

QR method: $\operatorname{diag}(H_j) \to \left(|\lambda_1|^j, |\lambda_2|^j, \dots, |\lambda_n|^j \right). \qquad (j \to \infty)$

B method: $\operatorname{diag}(P_j) \to \left(|\lambda_1|^j, \alpha_2|\lambda_2|^j, \dots, \alpha_n|\lambda_n|^j \right),$

where

$$\frac{\varepsilon}{1+\varepsilon} \le \alpha_k \le 1 + \frac{1}{\varepsilon}.$$

$\varepsilon = 10^{-3}$: $$10^{-3} \approx \frac{10^{-3}}{1+10^{-3}} \le \alpha_k \le 1001.$$

$\varepsilon = 1$: $$0.5 \le \alpha_k \le 2.$$

Similar error propagation if $|\alpha_k| \approx 1$ for $k = 2, \dots, n$.

Condition number of B_j

B method: $B_j = Q_j V_j$, Q_j orthogonal:

$$\left\| V_j^{-1} \right\|_{1,\infty} \leq \frac{(1 + 1/\varepsilon)^{n-1}}{\varepsilon}.$$

$\varepsilon = 10^{-3}$:

$$\left\| V_j^{-1} \right\|_{1,\infty} \leq 10^3 (10^3 + 1)^{n-1}.$$

$\varepsilon = 1$:

$$\left\| V_j^{-1} \right\|_{1,\infty} \leq 2^{n-1}.$$

Open Problems

- Optimal choice of blunting factors $\left(D_j = \mathrm{diag}(\varepsilon_1, \ldots, \varepsilon_n)\right)$.
- Quality of upper bounds for cond(B_j).
- T with eigenvalues of same magnitude.
- Column permutations of B_j.

Thank you.

Questions or Remarks?