On the Parallelepiped Method and Higher Order Methods

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Simulation of dynamical systems

Aims

- Given
  - A set of initial conditions $\mathbb{X}$
  - A function **f** (explicit expression, ODE solution operator, ...)
- Compute super sets of $\mathbf{f}(\mathbb{X})$, $\mathbf{f}(\mathbf{f}(\mathbb{X}))$, ...

Issues

- Choose a class $\mathcal{S}$ of sets (boxes, union of boxes, parallelepipeds, zonotopes, ellipsoids, ...)
- Design an interval method which can deal with this class of sets
  - Given $\mathbb{X} \in \mathcal{S}$
  - Find $\mathbb{Y} \in \mathcal{S}$
  - Such that $\mathbb{Y} \supseteq \mathbf{f}(\mathbb{X})$

Outline

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1. Naive methods
   - Box enclosures
   - Union of boxes
2. Parallelepiped Methods
3. Higher order methods
4. Conclusion

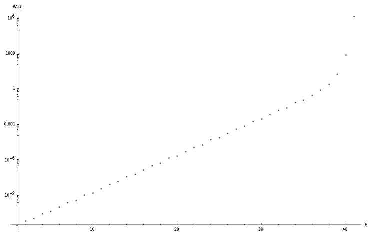
Box enclosures of sets

The class of sets

- n-dimensional boxes ($\mathbb{IR}^n$)
- Compromise between
  - ⊕ Simplicity: $2n$ floating point numbers
  - ⊖ Expressiveness: Very strong *wrapping effect*
- Method: Just evaluate interval extensions

Test case: Henon map

- $\mathbf{f}(\mathbf{x}) = \begin{pmatrix} x_2 + 1 - a x_1^2 \\ b x_1 \end{pmatrix}$
- With $a = 2.4$ and $b = -1$
- $\mathbb{X} = (0.4, -0.4) \pm 10^{-12}$



Union of boxes

The class of sets

- Union of n-dimensional boxes
- Simplicity vs. expressiveness $\longrightarrow$ tuned as desired

Comparison w.r.t. boxes

- Naive algorithm: Very poor improvement
  $\longrightarrow$ Each box of the union grows exponentially
- Clever algorithm?
- **The computational cost is prohibitive!**

Outline

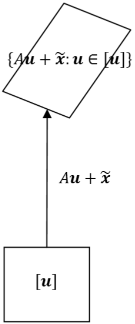
Parallelepipeds

Parallelepiped methods

- Working in an auxiliary basis (Moore, Kruckeberg, Lohner, Rhim, etc.)
- New method: similar but simpler (Goldsztejn and Hayes, SCAN 2006)

The class of sets

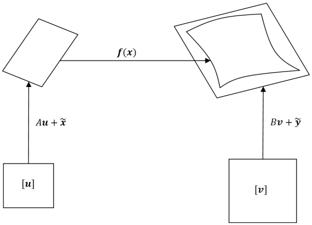
- *n*-dimensional parallelepipeds
  - Data: $A \in \mathbb{F}^{n\times n}$, $\tilde{\mathbf{x}} \in \mathbb{F}^n$ and $[\mathbf{u}] \in \mathbb{IF}^n$
  - Parallelepiped = $\{A\mathbf{u} + \tilde{\mathbf{x}} : \mathbf{u} \in [\mathbf{u}]\}$
- Compromise:
  - ⊕ Simplicity: $n^2 + 2n$ floating point numbers
  - ⊕ Expressiveness: wrapping effect much smaller *(especially for the image of very small parallelepipeds)*



The new parallelepipeds method (1/3)

Problem

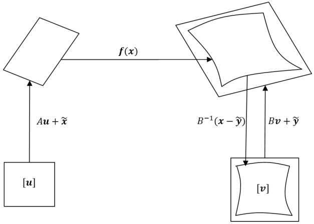
- Given $\mathbf{f}$ and $\langle A, [\mathbf{u}], \tilde{\mathbf{x}}\rangle$
- Find $\langle B, [\mathbf{v}], \tilde{\mathbf{y}}\rangle$
- Such that $\langle B, [\mathbf{v}], \tilde{\mathbf{y}}\rangle \supseteq \mathbf{f}\big(\langle A, [\mathbf{u}], \tilde{\mathbf{x}}\rangle\big)$



The new parallelepiped method (2/3)

Important remark

- Equivalently $[\mathbf{v}] \supseteq B^{-1}\big(\mathbf{f}\big(\langle A, [\mathbf{u}], \tilde{\mathbf{x}}\rangle\big) - \tilde{\mathbf{y}}\big)$
- Image of $[\mathbf{u}]$ by $B^{-1}\big(\mathbf{f}(A\mathbf{u} + \tilde{\mathbf{x}}) - \tilde{\mathbf{y}}\big)$



Suppose that B and $\tilde{\mathbf{y}}$ are found

- Simple solution: mean-value extension *(with correct factorization)*

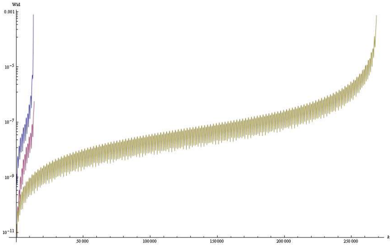
$$[\mathbf{v}] := \big(B^{-1}[J]A\big)[\mathbf{u}] + B^{-1}\big([\mathbf{f}](\tilde{\mathbf{x}}) - \tilde{\mathbf{y}}\big)$$

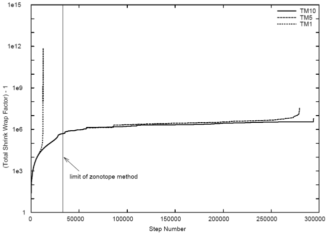
The new parallelepiped method (3/3)

How to find B and $\tilde{\mathbf{y}}$?

- Obviously, $\tilde{\mathbf{y}} \approx \mathbf{f}(\tilde{\mathbf{x}})$
- First choice: $B_{\text{par}} = \text{mid}[J]\,A$
  - If $\mathbf{f}(\mathbf{x}) = J(\mathbf{x} - \tilde{\mathbf{x}}) + \tilde{\mathbf{b}}$
  - Then $B_{\text{par}} = J\,A$ and $\tilde{\mathbf{y}} = \tilde{\mathbf{b}}$ is the exact image (up to rounding errors)
  - **Behaves poorly if B becomes close to singular**
- Second choice: $B_{\text{QR}} = \text{GramSchmidt}\big(\text{mid}[J]\,A\big)$ (idem QR-decomposition)
  - Behaves better than the first in average
- Third choice: mixed proposed by Nedialkov
- Fourth choice: new mixed
  - If $\kappa(B_{\text{par}}) < 100$ then $B_{\text{cond}} = B_{\text{par}}$ else $B_{\text{cond}} = B_{\text{QR}}$

Henon





Remark: Nedialkov's mixed method seems to have the same behavior as the first method ($B_{\mathrm{par}} = \mathrm{mid}[J]\,A$)

Outline

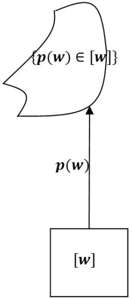
Taylor sets and the naive method (1/2)

Higher order sets

- Image of boxes through polynomial functions of arbitrary degree

$\longrightarrow$ *Taylor set*

- Used by Makino and Berz

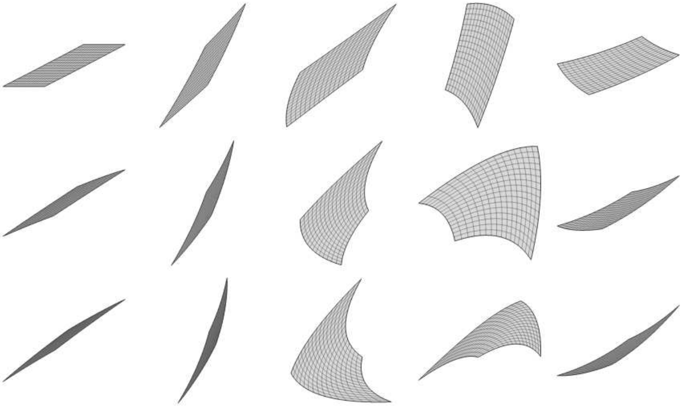


The naive method

- Find $\mathbf{q}$
- Such that $\{\mathbf{q}(\mathbf{w}) : \mathbf{w} \in [-1,1]^n\} \supseteq \{\mathbf{f}(\mathbf{p}(\mathbf{w})) : \mathbf{w} \in [-1,1]^n\}$

$\longrightarrow$ $\mathbf{q}(\mathbf{w}) = \mathbf{f}(\mathbf{p}(\mathbf{w}))$ (formal composition of polynomials)

Taylor sets and the naive method (2/2)



Last polynomial: degree 2^9

Parallelepiped-inflated Taylor sets (PITS)

Issues

- Limit the degree of the polynomial
- Deal rigorously with the truncation errors and the rounding errors

The class of sets

- PITS: Taylor set + parallelepiped
- Data: $\mathbf{p}$, A, $[\mathbf{u}]$
- Inflated Taylor set: $\{\mathbf{p}(\mathbf{w}) : \mathbf{w} \in [-1,1]^n\} + \{A\mathbf{u} : \mathbf{u} \in [\mathbf{u}]\}$

$$= \{\mathbf{p}(\mathbf{w}) + A\mathbf{u} : \mathbf{w} \in [-1,1]^n, \mathbf{u} \in [\mathbf{u}]\}$$

Enclosing the image of PITS

Problem

- Find $\mathbf{q}$ (with degree $\leq d_{\max}$), B and $[\mathbf{v}]$
- Such that $\{\mathbf{q}(\mathbf{w})+B\mathbf{v} : \mathbf{w} \in [-1,1]^n, \mathbf{v} \in [\mathbf{v}]\} \supseteq \{\mathbf{f}(\mathbf{p}(\mathbf{w})+A\mathbf{u}) : \mathbf{w} \in [-1,1]^n, \mathbf{u} \in [\mathbf{u}]\}$

$$
\begin{aligned}
& \{\mathbf{f}(\mathbf{p}(\mathbf{w}) + A\mathbf{u}) \ : \ \mathbf{w} \in [-1,1]^n, \mathbf{u} \in [\mathbf{u}]\} && (1)\\
\subseteq \ & \{\mathbf{f}(\mathbf{p}(\mathbf{w})) + JA\mathbf{u} \ : \ \mathbf{w} \in [-1,1]^n, \mathbf{u} \in [\mathbf{u}], J \in [J]\} && (2)\\
= \ & \{\mathbf{q}(\mathbf{w}) + (\mathbf{f}(\mathbf{p}(\mathbf{w})) - \mathbf{q}(\mathbf{w})) + JA\mathbf{u} \ : \ \mathbf{w} \in [-1,1]^n, \mathbf{u} \in [\mathbf{u}], J \in [J]\} && (3)\\
\subseteq \ & \{\mathbf{q}(\mathbf{w}) + \epsilon + JA\mathbf{u} \ : \ \mathbf{w} \in [-1,1]^n, \mathbf{u} \in [\mathbf{u}], J \in [J], \epsilon \in [\epsilon]\} && (4)
\end{aligned}
$$

Problem

- Find B and $[\mathbf{v}]$
- Such that $\{B\mathbf{v} : \mathbf{v} \in [\mathbf{v}]\} \supseteq \{\epsilon + JA\mathbf{u} : \mathbf{u} \in [\mathbf{u}], \epsilon \in [\epsilon]\}$

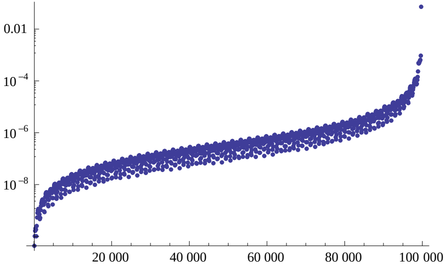
$\longrightarrow$ Similar parallelepiped method: $\mathbf{v} = B^{-1}\epsilon + (B^{-1}[J]A)[\mathbf{v}]$

Henon

Settings

- $\mathbb{X} = (0.4, -0.4) \pm 10^{-3}$
- $d_{\max} = 10$

$\rightarrow$ $||\epsilon|| \leq 10^{-14}$



(foreseen result, implementation not finished)

Conclusion

Summary

- New parallelepiped method
  - Simpler than existing methods
  - More efficient (potentially much more)
- New higher order method
  - Simpler than Makino and Berz's method
  - Good efficiency to be confirmed

Research directions

- Parallelepiped-inflated Taylor set $\longrightarrow$ Taylor-set-inflated Taylor set?