Introduction to Taylor Model Methods

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May 26, 2009

Outline

1. Interval Arithmetic
2. Taylor Models
3. Overestimation
4. Applications

Interval Arithmetic

Why Interval Computations?

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

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

Ranges and Inclusion Functions

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

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

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

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

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

Dependency

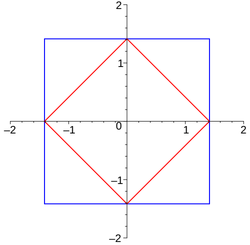
- $f(x) = \dfrac{x}{1+x} = 1 - \dfrac{1}{1+x}$, $\mathbf{x} = [1,2]$:
- $\dfrac{\mathbf{x}}{1+\mathbf{x}} = \dfrac{[1,2]}{[2,3]} = [\frac{1}{3}, 1]$
- $1 - \dfrac{1}{1+\mathbf{x}} = 1 - \dfrac{1}{[2,3]} = 1 - [\frac{1}{3}, \frac{1}{2}] = [\frac{1}{2}, \frac{2}{3}] = \mathrm{Rg}\,(f, \mathbf{x})$
- Reduced overestimation: centered forms, etc.

Wrapping Effect

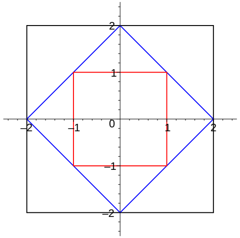
Overestimation: Enclose non-interval shaped sets by intervals

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

Symbolic Enhancements of IA

- Ultra-arithmetic (Kaucher & Miranker, 1984)
- Multivariate Taylor forms (Eckmann, Koch & Wittwer, 1984)
- Taylor models (Berz & Makino, 1990s–today)

Taylor Models of Type I

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

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

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

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

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

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

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

Taylor Models: Example

$\mathbf{x} = [-\frac{1}{2}, \frac{1}{2}], \quad x_0 = 0$:

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

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

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

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

TM Arithmetic

Paradigm for TMA:

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

Addition and Multiplication

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

  where

  - $p_{n,f}(x - x_0) \cdot p_{n,g}(x - x_0) = p_{n,f\cdot g}(x - x_0) + p_e(x - x_0)$,
  - $p_e(x - x_0) \in \mathbf{i}_{p_e}, \quad p_{n,f}(x - x_0) \in \mathbf{i}_{p_{n,f}}, \quad p_{n,g}(x - x_0) \in \mathbf{i}_{p_{n,g}}$,
  - $f(x) \cdot g(x) \in p_{n,f\cdot g}(x - x_0) + \underbrace{\mathbf{i}_{p_e} + \mathbf{i}_{p_{n,f}}\mathbf{i}_{n,g} + \mathbf{i}_{n,f}\left(\mathbf{i}_{p_{n,g}} + \mathbf{i}_{n,g}\right)}_{=:\mathbf{i}_{n,f\cdot g}}$

Numerical Example

Multiplication: $\mathbf{x} = [-\frac{1}{2}, \frac{1}{2}] \quad x_0 := 0, \quad x \in \mathbf{x}$:

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

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

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

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

TM Arithmetic: Polynomials, Standard Functions

- If $T_{n,f} = (p_{n,f}\,, \mathbf{i}_{n,f})$ 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 $\varphi(f)$:
  - Special treatment of the constant part in $p_{n,f}$
  - Evaluate $p_{n,\varphi}$ for the non-constant part of $T_{n,f}$

Taylor Model for Exponential Function

$x \in \mathbf{x}, \quad c := f(x_0), \quad h(x) := f(x) - c$:

$$p_{n,f}(x - x_0) = p_{n,h}(x - x_0) + c, \quad \mathbf{i}_{n,h} = \mathbf{i}_{n,f}$$

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

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

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

$$\subseteq (\mathrm{Rg}\,(h) + \mathbf{i})^{n+1} \; \exp\big([0,1] \cdot (\mathrm{Rg}\,(h) + \mathbf{i})\big)$$

Taylor Model for Exponential Function

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

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

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

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

Taylor Model for Other Standard Functions

$x \in \mathbf{x}, \quad c := f(x_0), \quad h(x) := f(x) - c:$

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

  $$= \ln c + \frac{1}{c}h(x) + \cdots + (-1)^{n+1}\frac{1}{n}(\frac{1}{c}h(x))^n$$

  $$+ (-1)^{n+2}\frac{1}{n+1}(\frac{1}{c}h(x))^{n+1}\frac{1}{(1+\theta h(x)/c)^{n+1}}, \quad 0 < \theta < 1$$

- $\frac{1}{f(x)} = \frac{1}{c}\frac{1}{1+h(x)/c} = \frac{1}{c}\left\{1 - \frac{h(x)}{c} + \cdots + (-1)^n\left(\frac{h(x)}{c}\right)^n\right\} + \mathbf{i}$
- $\cos(f(x)) = \cos c \; \cos(h(x)) - \sin c \; \sin(h(x))$
- ...

Overestimation

Overestimation

Sources of overestimation:

- data errors
- discretization or truncation erors
- dependency problem: lack of IA to identify different occurrences of the same variable
- wrapping effect: enclosure of intermediate results into intervals

IA vs. TMA: Dependency

- 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:

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

IA vs. TMA: Dependency

- TMA (Taylor models of order 3):

$$\begin{aligned} f(x) &= x^2 + \cos x + \sin x - e^x \\ &\in x^2 + 1 - \frac{x^2}{2} + \mathbf{i}_1 + x - \frac{x^3}{6} + \mathbf{i}_2 - 1 - x - \frac{x^2}{2} - \frac{x^3}{6} - \mathbf{i}_3 \\ &= -\frac{x^3}{3} + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3 \\ &\subseteq [-0.376, 0.082] \end{aligned}$$

- Range: $\mathrm{Rg}\,(f, \mathbf{x}) = [-0.337, 0]$

IA vs. TMA: Wrapping

- $$f(x,y) = \begin{pmatrix} x + \sin(\frac{\pi}{2} y) \\ \cos(\frac{\pi}{2} x) - y \end{pmatrix}, \quad A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

  $x,\ y \in [0,1]$: $\quad A\,f,\ A\,(A\,f) = ?$

- IA: $\quad \mathrm{Rg}\,(f) \subseteq \begin{pmatrix} [0,2] \\ [-1,1] \end{pmatrix},$

  $$A\,f \subseteq \frac{1}{\sqrt{2}} \begin{pmatrix} [-1,3] \\ [-1,3] \end{pmatrix}, \quad A\,(A\,f) \subseteq \begin{pmatrix} [-2,2] \\ [-1,3] \end{pmatrix}$$

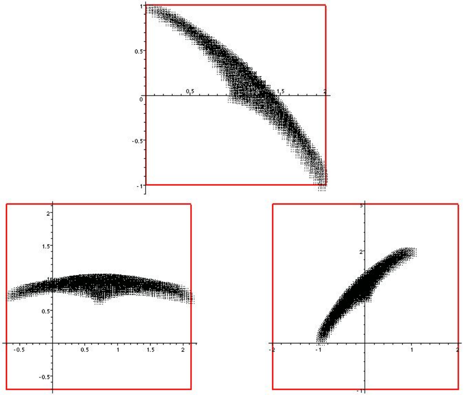
IA vs. TMA: Wrapping

- TMA: $T_{4,f} = \begin{pmatrix} x + \frac{\pi}{2}y - \frac{\pi^3 y^3}{48} + \frac{[0,\pi^5]}{3840} \\ 1 - y - \frac{\pi^2 x^2}{8} + \frac{\pi^4 x^4}{384} - \frac{[0,\pi^5]}{3840} \end{pmatrix}$,

$$A\,T_{4,f} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 + x + (1+\frac{\pi}{2})y + \frac{\pi^2 x^2}{8} - \frac{\pi^3 y^3}{48} - \frac{\pi^4 x^4}{384} + \frac{[0,\pi^5]}{1920} \\ 1 + x + (\frac{\pi}{2}-1)y - \frac{\pi^2 x^2}{8} - \frac{\pi^3 y^3}{48} + \frac{\pi^4 x^4}{384} + \frac{[-\pi^5,\pi^5]}{3840} \end{pmatrix},$$

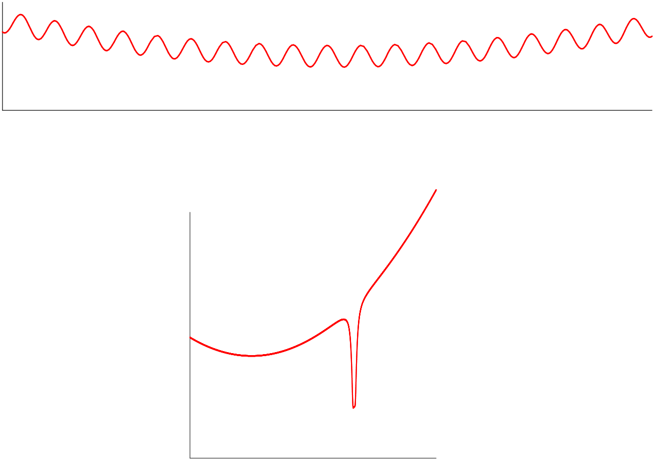
$$A\,(A\,T_{4,f}) = \begin{pmatrix} -1 + y + \frac{\pi^2 x^2}{8} - \frac{\pi^4 x^4}{384} + \frac{[-\pi^5,3\pi^5]}{7680} \\ x + \frac{\pi}{2}y - \frac{\pi^3 y^3}{48} + \frac{[-\pi^5,3\pi^5]}{7680} \end{pmatrix}$$

IA vs. TMA: Wrapping

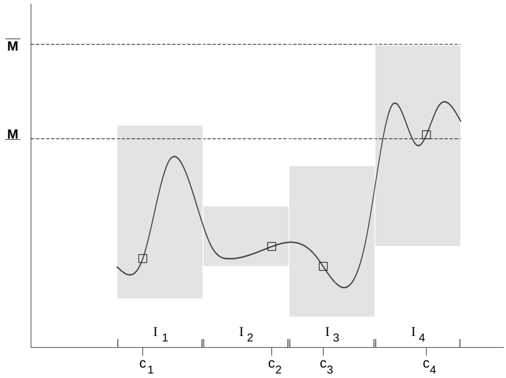


Applications

Global Optimization: Challenges



Global Optimization: Branch-and-Bound Method



Global Optimization: Benefits from Taylor Models

- Reduced dependency
- Range computation with symbolic preconditioning:

  Linear dominated bounder, quadratic fast bounder

  (Berz, Kim, Makino, 2005-)
- QFB: $p_{n,f} + \mathbf{i}_{n,f} = (p_{n,f} - Q) + Q + \mathbf{i}_{n,f}$,

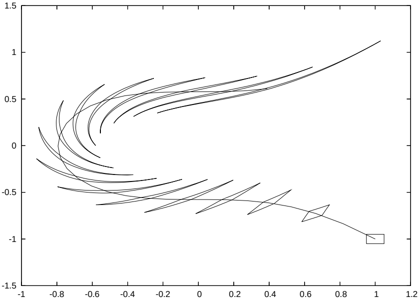
  $\min(p_{n,f} + \mathbf{i}_{n,f}) = \min(p_{n,f} - Q) + \min(Q) + \min \mathbf{i}_{n,f}$

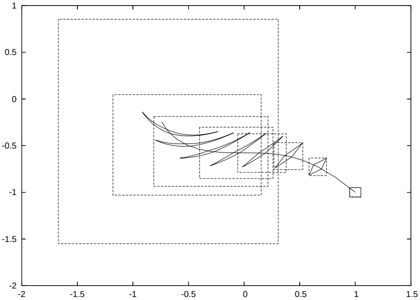
ODEs: Verified Integration of IVPs

- Interval methods for ODEs:
  - Moore (1965), Lohner (1987), Nedialkov & Jackson (1999), and **many** others
  - Inclusion of flow subject to wrapping
  - Available enclosure sets are convex
- Taylor model methods for ODEs:
  - Berz & Makino (1990s – today)
  - Reduced dependency problem
  - Reduced wrapping effect from non-convex enclosure sets

Integration of Model Problem: COSY Infinity vs. AWA

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





Taylor Models of Type II

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

Ex. 1:

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

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

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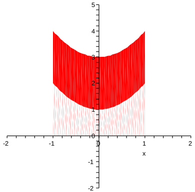
Range of a TM: $\mathrm{Rg}\,(\mathcal{U}) = \{ z = p(x) + \xi \mid x \in \mathbf{x}, \xi \in \mathbf{i} \} \subset \mathbb{R}^m$

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

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



Taylor Models of Type II

Multiplication example: $\mathbf{x} = [-\frac{1}{2}, \frac{1}{2}]$, $x_0 = 0$:

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

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

$$\begin{aligned} \mathcal{U}_1 \cdot \mathcal{U}_2 \;&\subseteq\; (1 + x + \tfrac{1}{2}x^2)(1 - \tfrac{1}{2}x^2) + \mathrm{Rg}\left(1 + x + \tfrac{1}{2}x^2\right)\mathbf{i}_2 \\ &\quad + \mathrm{Rg}\left(1 - \tfrac{1}{2}x^2\right)\mathbf{i}_1 + \mathbf{i}_1 \cdot \mathbf{i}_2 \\ &\subseteq\; 1 + x + [-0.281, 0.281] \end{aligned}$$

Taylor Models of Type II

Composition example: $\mathbf{x} = [-\frac{1}{2}, \frac{1}{2}]$, $x_0 = 0$:

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

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

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

Taylor Model Arithmetic: Composition

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

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

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

but

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

For example,

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

Taylor Model Arithmetic: Composition

Cause of failure: The interval term of $\mathcal{U}_1$ does not fit the range of $\mathcal{U}_2$ (which is not contained in $\mathbf{x}$).

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Compositions of Taylor models may be computed as above, but
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Valid $\mathbf{i}_1$ for e^x, $x \in \square\big(\mathrm{Rg}\,(\mathcal{U}_2) \cup \{0\}\big)$: $[0.106, 0.472]$

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

Conclusion

- Interval methods are useful for:
  - Modelling of uncertain data
  - Enclosing discretization or truncation errors
  - Bounding of roundoff errors
- Drawbacks of IA:
  - Dependency problem
  - Wrapping effect
- Taylor models:
  - Interval arithmetic enhanced with symbolic computations
  - Reduced dependency problem
  - Reduced wrapping effect

Challenges

- Multivariate Taylor models of order n in m dimensions

  No. of Taylor coefficients: $N(m,n) = \binom{m+n}{m}$

N(4,10)	N(4,20)	N(6,10)	N(6,20)	N(20,10)
1,001	10,626	8,008	230,230	30,045,015

- Memory management for sparse Taylor models
- Software

Thank you.

Questions or Remarks?