Rigorous Computation with Function Enclosures in Chebyshev Basis

Tomáš Dzetkulič

Institute of Computer Science Academy of Sciences of the Czech Republic

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Rigorous Computation and Initial Value Problem in ODE

Lorentz system:

$$\dot{x} = 10(y - x)$$

 $\dot{y} = x(28 - z) - y$
 $\dot{z} = xy - 8z/3$

x(0) = 15; y(0) = 15; z(0) = 36

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Using Matlab ode45, we get numerical solution:

 $\begin{array}{rrrr} & \text{ATol} = \text{RTol} = 10^{-10} & \text{ATol} = \text{RTol} = 10^{-16} \\ \text{x(50)} & 6.85806551 & 4.89309707 \\ \text{y(50)} & -1.82131145 & 7.51188676 \\ \text{z(50)} & 34.13364729 & 16.64840204 \end{array}$

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Rigorous solution:

 $egin{aligned} x(50) \in [-0.4737, -0.4738] \ y(50) \in [-5.13, -5.14] \ z(50) \in [26.93, 26.94] \end{aligned}$

The Overview of the Contribution

We extend the work of Makino and Berz on Taylor Models

We replace the Taylor polynomial approximation in the Taylor Model with the Chebyshev polynomial approximation

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Method is applied to the initial value problem of ordinary differential equations

Chebyshev Polynomials

Chebyshev polynomials of the first kind:

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_i(x) = 2x \ T_{i-1}(x) - T_{i-2}(x) \text{ for } i \in \{2..\infty\}$$

$$T_2(x) = 2x^2 - 1; \ T_3(x) = 4x^3 - 3x; \ T_4(x) = 8x^4 - 8x^2 + 1$$

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Alternative form: $T_i(x) = \cos(i \arccos(x))$



Polynomial Function Enclosure

Taylor Model by Makino and Berz [1]:

For the function $f(x_1, \ldots, x_n)$ on the domain $[-1, 1]^n$: $f(x_1, \ldots, x_n) \in (\sum_{(i_1, \ldots, i_n)} a_{(i_1, \ldots, i_n)} \prod_j x_j^{i_j}) + [-e_{lo}, e_{hi}]$

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Example: $f(x, y) = y \sin(x)$ on $[-1, 1]^2$:

$$xy + 0.1666x^3y + [-0.01, 0.01]$$

Makino and Berz in [1] claim, that:

- Magnitude of the Chebyshev series coefficients is higher compared to the Taylor series
- Chebyshev polynomial multiplication sub-optimal
- \rightarrow Chebyshev polynomials not suitable for rigorous computation

Chebyshev Function Enclosure

We show that:

- The Chebyshev series never lead to an increase in the magnitude of the coefficients
- Although sub-optimal, the Chebyshev polynomial multiplication gives better approximation compared to the Taylor multiplication

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We introduce the Chebyshev function enclosure of the form:

For the function $f(x_1, ..., x_n)$ on the domain $[-1, 1]^n$: $f(x_1, ..., x_n) \in (\sum_{(i_1, ..., i_n)} a_{(i_1, ..., i_n)} \prod_j T_{i_j}(x_j)) + [-e, e]$

Function Enclosure Operations

The operations with function enclosures:

- Addition and substraction simple term based algorithm
- Multiplication new recursive algorithm

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- Multiplication new recursive algorithm
- Composition Clenshaw algorithm
- Division, square root, exp application of composition
- Integration and derivative reordering of coefficients

Problems with Chebyshev Polynomials Multiplication

$$T_i(x) \times T_j(x) = (T_{i+j}(x) + T_{|i-j|}(x))/2$$

Low order terms of the result depend on high order terms

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Given the truncated Chebyshev series of $f_1(x)$ and $f_2(x)$: - impossible to compute the truncated series for $f_1(x) \times f_2(x)$

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Multiplication of two *n*-variate terms gives 2^n term result:

 $(T_1(x)T_1(y)) \times (T_2(x)T_3(y)) =$ $(T_1(x)T_2(y) + T_1(x)T_4(y) + T_3(x)T_2(y) + T_3(x)T_4(y))/4$

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- 4. Add $P_{(i,j)}/2$ to R_{i+j} and $R_{|i-j|}$

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- 5. Construct the result: $\sum_{i=0}^{2 \text{ deg}} R_i(x_2, \ldots, x_n) T_i(x_1)$
- 2 deg^2 function enclosures $P_{(i,j)}/2$, but only $2 \text{ deg } R_i$ \rightarrow huge cancellation in step 4 of the algorithm

Initial Value Problem

Given the input:

• system of *n* differential equations $\dot{\mathbf{x}} = f(\mathbf{x})$

▶ initial values over *m* free variables $\{\mathbf{x} \mid \exists \mathbf{a} \in [-1, 1]^m : g(\mathbf{a}) = \mathbf{x}\}$

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Compute the function $h(t, \mathbf{a})$:

▶ it is the solution to the ODE: $dh(t, \mathbf{a})/dt = f(h(t, \mathbf{a}))$

$$\blacktriangleright h(0,\mathbf{a}) = g(\mathbf{a})$$

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 $f(\mathbf{x})$ and $g(\mathbf{a})$ given as Chebyshev function enclosures

Picard Iteration

We set $h_0(t, \mathbf{a}) := 0$

Application of **Picard operator**:

Compute a sequence of enclosures for the recurrence $h_{i+1}(t, \mathbf{a}) := g(\mathbf{a}) + t_{max} \int_0^t f(h_i(t, \mathbf{a})) dt$

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In case of convergence, the sequence of h_i converges to $h(t, \mathbf{a})$

In case of non-convergent sequence: t_{max} can be reduced and muli-step method can be applied

Wrapping Effect

The exponential growth of the error due to re-packaging of the solution in each step



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The wrapped object may be of complex non-convex shape

New Method for Wrapping Effect Suppression

In rigorous Picard operator: $H_{i+1}(t, \mathbf{a}) := G(\mathbf{a}) + t_{max} \int_0^t F(H_i(t, \mathbf{a})) dt$

if $G(\mathbf{a})$ contains non-empty error interval:

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Additional variables **p** are used to parametrize the error interval

We construct error-free $G'(\mathbf{a}, \mathbf{p})$ that describes the same initial set

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Similar idea used for multi-step wrapping effect suppression

Implementation and Extensions

Rigorous IVP solver implemented in C++ with both Taylor and Chebyshev function enclosures

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- High precision results can be used to verify numerical results and low-precision results

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Multi-processor support:

- ► All data structures can be used in parallel execution
- Solving high dimension problems is executed in parallel

Computational Experiments

Comparison of Taylor and Chebyshev polynomial enclosures:

Problem (degree)	Taylor	Chebyshev
Volterra (10)	1.1E-6	5.7E-9
Volterra (12)	3.4E-8	5.2E-11
Volterra (14)	1.1E-9	9.8E-13
Roessler (12)	1.8E-6	1.4E-8
Roessler (14)	1.2E-7	2.7E-10
Roessler (16)	9E-9	5.7E-12
Roessler (18)	6.6E-10	5.3E-13

VERICOMP Computation Experiments

VERICOMP - A System for Comparing Verified IVP Solvers
http://vericomp.inf.uni-due.de/

		Best result in VERICOMP				Our tool	
#	Ν	VNODE_LP		RIOT		Width	Time
1	2	4.67079	0.01s	10.1	2s	4.6707 <mark>8</mark>	0.08s
2	3	0.232544	0.01s	0.235	0.7s	0.232544	0.03s
3	1	0.89	0.01s	0.44	40s	0. <mark>38</mark>	0.12s
4	2	0.073	0.02s	0.067569	38s	0.06756 <mark>1</mark>	0.4s
5	51	0.21527	2s	N/A		0.21527	18s
6	30	2.95E-5	3s	N/A		2. <mark>54</mark> E-5	160s
28	2	N/A		N/A		1.018	6s

In benchmarks 1 to 5, the results from our tool match optimal interval width in all displayed digits.

Method for rigorous computation with multivariate function enclosures in Chebyshev basis

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Provides verified enclosure for various polynomial operations

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Implementation available (open source) from: http://odeintegrator.souceforge.net

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- Allow trigonometric functions on input
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Thank you for you attention.

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 K. Makino and M. Berz. Taylor models and other validated functional inclusion methods. *International Journal of Pure and Applied Mathematics*, 4(4):379–456, 2003.