Rigorous Defect Control and the Numerical Solution of ODEs

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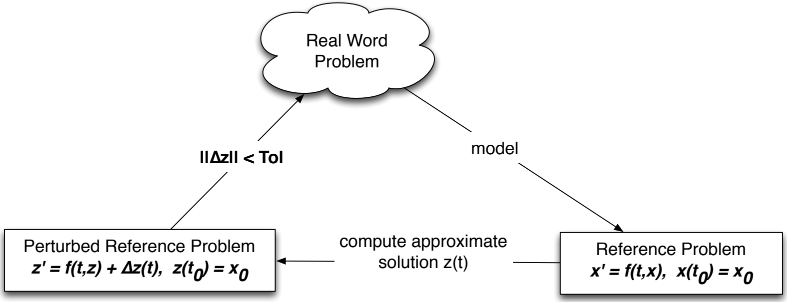
Problem statement



Defect control literature

- Enright advocates asymptotic defect control
  Enright and Coworkers and Students (1989-2012)
- Defect control and ODE boundary value problem
  Enright and Muir, Shampine and Muir (1993-2004)
- Corless and Corliss proposed rigorous defect control
  Corless and Corliss (1991)

Numerical problem

Given TOL, approximate z on $[t_i, t_{i+1}]$ near x_i get defect

$$\Delta z(t) \stackrel{\text{def}}{=} z'(t) - f(t, z(t))$$

Find stepsize so that z satisfies on $[t_i, t_{i+1}]$

$$z'(t) = f(t, z(t)) + \Delta z(t) \quad z(t_i) = x_i \quad \|\Delta z\|_\infty \leq TOL$$

Then z exactly solves on $[t_0, t_f]$

$$z'(t) = f(t, z(t)) + \Delta z(t) \quad z(t_0) = x_0 \quad \|\Delta z\|_\infty \leq TOL$$

How to do it?

- Construct approximate solution z
- Rigorously bound Δz on $[t_0, t_f]$
- Find good stepsize

Approximate solution

Numerical ODE solvers for the initial value problem

$$x'(t) = f(t, x(t)) \quad x(t_0) = x_0 \quad t \in [t_0, t_f]$$

- control local error on each step
- return skeletal solution (t_i, x_i)
- return a continuously differentiable approximation z to x

Taylor series method

Computation often regarded as expensive

This is not the case

Computing defect inexpensive

Compared to cost of Taylor series method itself

$$z(t) = \sum_{k=0}^{n} (z)_k (t - t_i)^k \quad \text{where} \quad (z)_k = \frac{1}{k} (f)_{k-1}$$

Data management: ApproximateSolution class

Automatic differentiation via operator overloading

From f to its Computational Graph, a DAG

Bendtsen and Stauning [FADBAD++, TADIFF] (1997)

Idea: Taylor arithmetic

- Assume user equations are elementary functions
- Construct an efficient computational graph
- Nodes (basic functions): sin, asin, sqrt, pow, log, exp
- Edges (basic operators): add, sub, mul, div, composition

High precision machine representation format

Zheng Gu (M Eng)

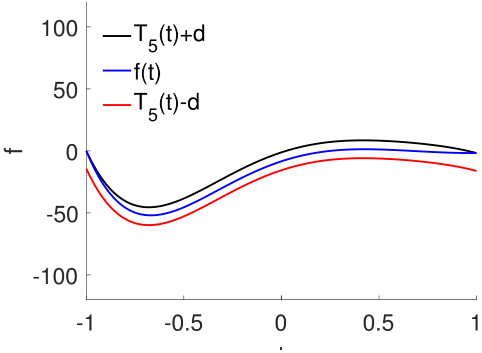
Interface to TADIFF: TaylorExpansion class

Rigorous Polynomial Approximations (RPA)

$$f(t) = -8.4 + t\,(51.7 + t\,(-74.05 + t\,(-9.4 + t\,(74.35 + t\,(-43.2 + t\,7.2)))))$$

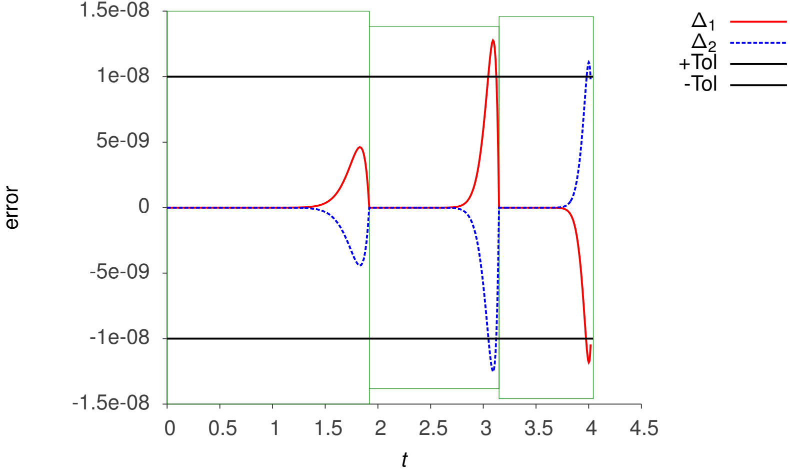
on $[-1, 1]$ has RPA $\left(T_5, [-7.2, 7.2]\right)$ then

$$7.2\ t^6 = f(t) - T_5(t) \in [-7.2, 7.2] \ \ \forall t \in [-1, 1]$$



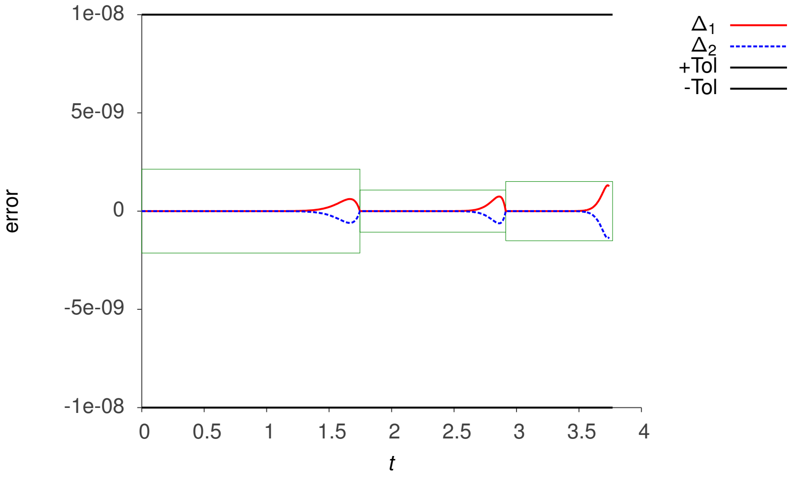
Rigorous bounds

Observed rigorous defect



Rigorous bounds

Controlled rigorous defect



Rigorous bounds

Natural interval extension rigorous (overestimation) sup-norm

Interval arithmetic

Rigorous polynomial approximation and sup-norm in 1D

Joldes (2011)

SOLLYA

Chevillard, Lauter, Joldes [SOLLYA] (2006-2016)

SOLLYA interface: Tmodel class

Controller

Traditional error model

$$\text{err} = Ch^{p+1}$$

Elementary controller

$$\frac{h_{\text{new}}}{h_{\text{trial}}} = 0.9 \left(\frac{\text{Tol}}{\text{err}}\right)^{1/(p+1)}$$

Rigorous error model

$$\Delta z = d_0 + d_1 h + \ldots + d_p h^p + d_{p+1} h^{p+1} \quad d_k \neq 0$$

Roots controller

$$\Delta z - TOL = 0 \quad \Delta z + TOL = 0$$

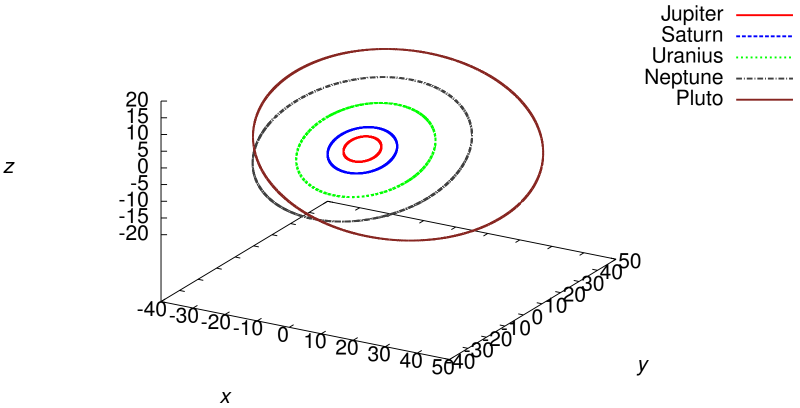
ODETS: Putting it all together

Guaranteed ODE defect control

Corless and Corliss (1991), Nedialkov (1999)

- Evaluate computational graph
  TaylorExpansion class
- Compute approximate solution using taylor arithemetic
  ApproximateSolution class
- Compute rigorous polynomial and bound it
  Tmodel class
- Apply stepsize control to rigorously control error
  ODETS class

Planets


Jupiter
Saturn
Uranius
Neptune
Pluto
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x
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