Stepsize Selection in the Rigorous Defect Control of Taylor Series Methods

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The initial-value problem (IVP)

Consider

$$x'(t) = f(t, x(t)) \quad x(t_0) = x_0 \quad x \in \mathbb{R}^d \quad t \in [t_0, t_{\text{end}}]$$

Given any $u \in C^1([t_0, t_{\text{end}}], \mathbb{R}^d)$, $u(t) = (u_1(t), \ldots, u_d(t))$

you have space, increase line spacing

- the residual or defect at u is

  $$\Delta u(t) \stackrel{\text{def}}{=} u'(t) - f(t, u(t)) \quad \Delta u(t_0) \stackrel{\text{def}}{=} u(t_0) - x_0$$

- $u(t)$ solves exactly

  $$u'(t) = f(t, u(t)) + \Delta u(t) \quad u(t_0) = x_0 + \Delta u(t_0)$$

Approximate solution and defect control

Approximate solution (AS)

consistency with caps smalls

- Piecewise differentiable function
- defined in a neighborhood of start time
- nearly satisfies the initial condition

Given tolerance TOL

- modern numerical IVP solvers provide polynomial AS
- a defect control method tries to achieve (Enright 1989)
  $\|\Delta u\|_{[t_0,\, t_{\mathrm{end}}],\infty} \leq \mathrm{TOL}$

Is this definition needed for 10 min?
Talk is more informal

$\|w\|_{\mathcal{J},\infty} \stackrel{\mathrm{def}}{=} \sup\{\|w(t)\|_\infty \mid t \in \mathcal{J}\}$ for $w \in C^0(\mathcal{J}, \mathbb{R}^d)$

Residual-based backward-error and analysis

Suppose $\Delta u(t)$ is smaller than the perturbations inherent in the modelling context of the IVP

Don't see what the colors emphasize

Suppose Δu satisfies $\|\Delta u\|_{[t_0,\, t_{\text{end}}],\infty} \leq \text{TOL}$

Then u can be considered a satisfactory solution to

$$x'(t) = f\left(t, x(t)\right) \quad x(t_0) = x_0$$

Forward vs. backward error

Forward error

- Standard IVP ODE solvers control local error on each step
  Local error control can be deceived
  No guaranteed bounds for the global error
- Interval methods compute such bounds
  Hard to keep them tight

Backward error

- Defect control methods estimate $\|\Delta u\|_{[t_0,\, t_{\mathrm{end}}],\infty}$
- We bound rigorously $\|\Delta u\|_{[t_0,\, t_{\mathrm{end}}],\infty}$

Previous work

- Enright advocates asymptotic defect control for Runge-Kutta (RK) methods
  Enright with coworkers and students (1989–2012)
- Defect control and ODE boundary value problem
  Enright and Muir, Shampine and Muir (1993–2004)
- Corless and Corliss (1991) "Rationale for Guaranteed ODE Defect Control" outlined an algorithm, no implementation details

Outline

Scheme to integrate ODE by time stepping

Given initial condition y_n at t_n and tolerance TOL, solve sequence of local problems

$$y'(t) = f(t, y(t)) \quad y(t_n) = y_n \quad y_0 = x_0$$

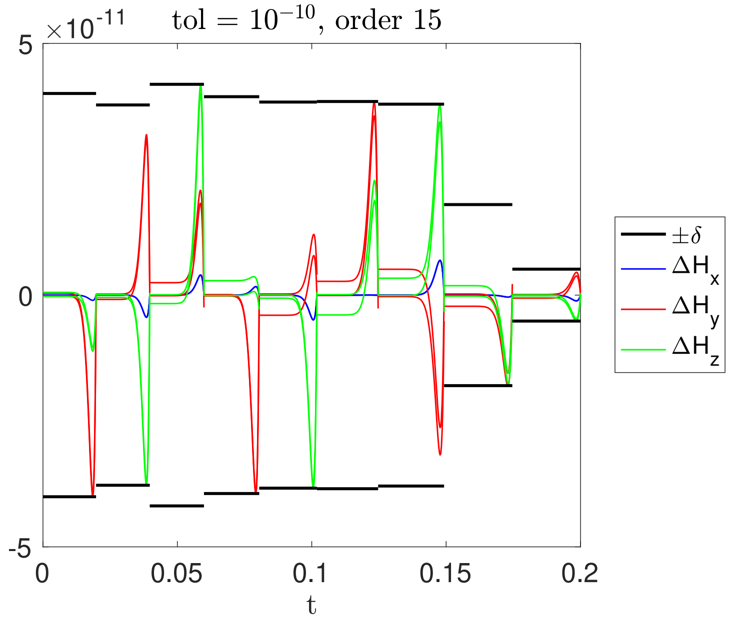
Misleading: AD is for TCs, from which H is formed after

- Compute Hermite polynomial approximate solution H
  automatic differentiation in floating-point arithmetic
  FADBAD++ (Bendtsen and Stauning)
- if validated, Bound the defect $\|\Delta H\|_{[t_n,\, t_{n+1}],\infty} \leq \text{TOL}$
  rigorous Taylor model arithmetic and rigorous sup-norm
  SOLLYA (Joldes et. al.)
- Stepsize controller provides h_n, take step $t_{n+1} = t_n + h_n$
  floating-point arithmetic, very challenging to get right

Example: Lorenz system

$$x' = 10(y - x)$$
$$y' = x(28 - z) - y$$
$$z' = xy - 8/3z$$
$$x(0) = (15, 15, 36)^T$$

Enclosures of $\Delta H(t)$ and computed bounds



Rigorous numerical results: Lorenz system

Integrated for $t \in [0, 20]$
An entry under *defect* is the largest defect bound over all the steps
Under *error* is the largest global error over $[0, 20]$

		max		num. steps	
k	TOL	defect	error	accept	reject
15	1.0e-06	6.7e-07	3.1e-01	358	0
	1.0e-08	5.2e-09	3.3e-03	487	0
	1.0e-10	4.9e-11	7.0e-05	662	0
	1.0e-12	4.9e-13	1.6e-04	900	0
20	1.0e-06	9.1e-07	1.9e+00	251	0
	1.0e-08	6.9e-09	6.2e-03	317	0
	1.0e-10	5.6e-11	1.2e-04	399	0
	1.0e-12	5.0e-13	1.8e-04	503	0

Rigorous numerical results: van der Pol

$$x_1' = x_2 \qquad x(0) = (2,0)^T, \quad t \in [0,20]$$
$$x_2' = 2(1 - x_1^2)x_2 - x_1$$

New table more informative, but this one still OK

		max		num. steps	
k	TOL	defect	error	accept	reject
15	1.0e-06	8.3e-07	2.8e-07	79	0
	1.0e-08	9.4e-09	3.7e-09	105	5
	1.0e-10	7.7e-11	1.5e-10	142	4
	1.0e-12	8.9e-13	3.3e-12	194	5
20	1.0e-06	9.2e-07	5.8e-07	58	3
	1.0e-08	9.6e-09	1.3e-08	74	6
	1.0e-10	7.3e-11	8.6e-11	93	4
	1.0e-12	9.0e-13	8.2e-13	116	3

Stepsize control appears very effective!

Non-rigorous results for 25 DETEST problems at $p = 8$

TOL	NSTP	DMAX	Frac-D	RMAX	Frac-G
10^{-2}	571	2.04	0.02	2.82	1.0
10^{-4}	919	3.82	0.02	1.66	1.0
10^{-6}	1549	3.13	0.01	0.63	1.0
10^{-8}	2675	4.73	0.0	1.85	1.0

- Defect at H by 100 equidistant point evaluation over $[t_n, t_{n+1}]$
- NSTP total number of steps
- DMAX max defect/tol over all steps
- Frac-D fraction of steps where $\texttt{DMAX} > 1$
- RMAX max defect$/\|(f)_p h^p\|_\infty$ over all steps
- Frac-G fraction of steps where $\texttt{RMAX} \leq 1.01$

(Enright and Yan, 2010)

Consider color
(f)_ph^p out of the blue
max defect/error estimate

The last two columns
don't seem compatible
Look carefully at the numbers

Non-rigorous results for 25 DETEST problems at $p = 20$

TOL	NSTP	DMAX	Frac-D	RMAX	Frac-G
10^{-2}	345	2.71	0.06	2.0	0.99
10^{-4}	413	5.83	0.04	2.0	0.99
10^{-6}	502	3.22	0.03	2.0	1.0
10^{-8}	616	4.62	0.02	2.0	1.0

- Add 10^{-10}, can't do 10^{-12} surely you can do -12
- How Enright and Yan paper relates, why order 8
- What we are trying to show
- What we have shown
- Conclusions

Conclusion

- We have a simple defect control method for Taylor series solutions with an effective stepsize control
- Method can be applied with or without the validation phase
- With validation, we have achieved rigorous defect control, an open problem for over 25 years
- Without validation, the stepsize controller computes stepsizes that satisfy $\|\Delta u\|_{[t_n,\, t_{n+1}],\infty} \leq \mathrm{TOL}$ for 25 DETEST problems
- Validation phase can be applied to any ODE polynomial approximate solution

Open problem is
NP != P
This is hardly an
open problem.
Remove