Local error estimation and step size control in adaptive linear multistep methods

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Outline

Adaptive linear multistep methods

We are interested in the numerical solution of IVPs

$$\dot{y} = f(t, y),$$
$$y(0) = y_0,$$

by using adaptive linear multistep methods (LMMs)

$$y_{n+1} + \sum_{j=1}^{k} a_{k-j,n}\, y_{n-j+1} = h_n \sum_{j=0}^{k} b_{k-j,n}\, f(t_{n-j+1}, y_{n-j+1}).$$

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- approximation $y_{n+1} \approx y(t_{n+1})$ depends on previously accepted states $y_{n-j+1} \approx y(t_{n-j+1})$, $j = 1, \ldots, k$;
- coefficients $a_{k-j,n}$ and $b_{k-j,n}$ depend on previous step ratios $\rho_{n-j} = h_{n-j+1}/h_{n-j}$;
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How to estimate the local asymptotic error?
How to control the step size?

Elementary control error model

Classical asymptotic error model:

$$r_n = \varphi_n h_n^q,$$

r_n: norm of the error estimate;
φ_n: norm of the principal error function, i.e., $||c\, y^{(p+1)}(t)||$;

$$q : \begin{cases} p, & \text{if EPUS (non-stiff computation)} \\ p+1, & \text{if EPS (stiff computation).} \end{cases}$$

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Assume $\varphi_n = \varphi_{n+1}$, then for a given tolerance TOL we want $r_{n+1} = \mathrm{TOL}$:

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- works well for one-step methods;
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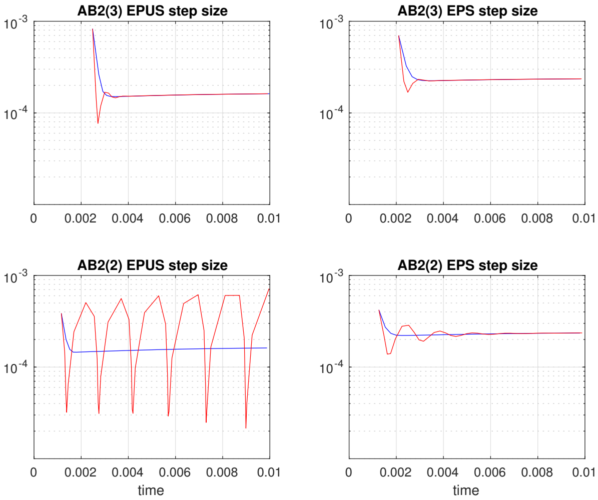
We want a model that dynamically describes the interaction between method, controller and error estimator.

An example



The 2-step Adams–Bashforth (AB2) method combined with two different error estimators and two different controllers, running in EPUS and EPS modes.

Objectives

Our goal:

- Construct dynamic error models of multiplicative form
$$r_n = \varphi_n h_n^q \cdot \prod_{j=1}^{s} \rho_{n-j}^{\delta_j};$$
- Apply discrete control theory by coupling error estimators with suitable controllers;
- Manage local error and the interaction between method and controller.

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How this can be achieved?

- Separate the static and dynamic part of asymptotic error model;
- Update step size by applying digital filters from linear control theory.

As a result, local errors are controlled resulting in smooth and reliable step size sequences.

Outline

Error analysis

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Then the global error satisfies the variational equation $\dot{u} = \dfrac{\partial f(t, y)}{\partial y(t)} u + w$.

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The function w is the scaled local truncation error (l_n), given by

$$w = \frac{l_n}{b(\bar{\rho}_n) h_n} = y^{(p+1)}(t_n)\, h_n^p \cdot \pi(\bar{\rho}_n),$$

where $\bar{\rho}_n = (\rho_{n-1}, \ldots, \rho_{n-k+1})$ and $b(\bar{\rho}_n) = \sum_0^k b_{k-j,n}$.

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Keeping the magnitude of w bounded by a given TOL, controls the global error and enables tolerance proportionality.

Why considering multiplicative error models?

Compansating for the LMM normalization we extract the error constant $\pi(\mathbf{1})$, arriving at

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Then, linearization gives $\hat{\pi}(\bar{\rho}_n) \approx \prod_1^s \rho_{n-j}^{\delta j}$ and the error model can be written as

$$r_n = \varphi_n\, h_n^q \cdot \prod_{j=1}^{s} \rho_{n-j}^{\delta_j}.$$

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Linear control theory

Error model in multiplicative form:

$$r_n = \varphi_n \, h_n^q \cdot \prod_{j=1}^{s} \rho_{n-j}^{\delta_j}.$$

Taking logarithms we derive linear differential equations.

Then, we can obtain the process and control models that determine the stability and frequency response.

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Process model:
Employing the ***z transform***, the linear difference equation becomes

$$\log r = G(z) \log h + \log \varphi,$$

$G(z)$: z transform of the linear difference operator related to the ***process***.
$\log h$: z transform of the sequence $\{\log h_j\}_0^\infty$;
$\log \varphi$: ***external disturbance***.

Process and control models

Control model:

To minimize the ***control error***

$$\left\{ \log \frac{\mathrm{TOL}}{r_j} \right\}_0^\infty = \log \mathrm{TOL} - \log \mathbf{r}$$

we use a ***control law***

$$\log h = C(z) \cdot (\log \mathrm{TOL} - \log r),$$

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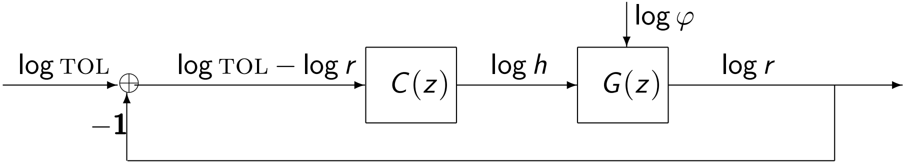

Time step adaptivity viewed as a feedback control system.

Outline

Control analysis for LMMs

Given a LMM, the process model is determined by an asymptotic error estimate

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Combined with a step-size control law

$$h_{n+1} = \left(\frac{\mathrm{TOL}}{r_n}\right)^{\beta/q} h_n \cdot \prod_{j=1}^{s} \rho_{n-j}^{\alpha_j},$$

where $\alpha_j = \delta_j \cdot \beta/q$ for all j, ***then the closed loop has a single nontrivial pole at $z = 1 - \beta$, with all other poles at $z = 0$.***

If in addition $\beta = 1$, the controller is deadbeat (i.e., has a finite impulse response).

Control analysis for LMMs (cont.)

Therefore, any LMM characterized by its asymptotic error parameters $\{\delta_j\}_1^s$ and q can be coupled with a single-parameter controller

$$h_{n+1} = \left(\frac{\mathrm{TOL}}{r_n} \cdot \prod_{j=1}^{s} \rho_{n-j}^{\delta_j} \right)^{\beta / q} h_n.$$

Closed loop is stable whenever $\beta \in (0, 2)$.

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Considering a ***dynamically compensated error***

$$\tilde{r}_n = r_n \cdot \prod_{j=1}^{s} \rho_{n-j}^{-\delta_j},$$

we can recover the *static model* since $\tilde{r}_n \approx \varphi_n h_n^q$ and also achieve deadbeat control.

Thus, the controller can be written as $h_{n+1} = \left(\frac{\mathrm{TOL}}{\tilde{r}_n} \right)^{\beta/q} h_n$.

Outline

1. Motivation
2. Error analysis
3. Linear control theory
4. Dynamic error models for LMMs
   - Asymptotic error estimators
5. Numerical results
6. Conclusion and future work

How to calculate the error estimates?

Case 1: Comparison LMM of higher order

If the comparison LMM is one order higher ($p_z = p_y + 1$), then the error estimate is the one of the lower order LMM:

$$l_n = \|y_{n+1} - z_{n+1}\| \approx |c_y(\mathbf{1})| \cdot \|y^{(p_y+1)}(t_n)\| \cdot h_n^{p_y+1} \cdot \hat{\pi}_l(\bar{\rho}).$$

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Case 2: Comparison LMM of same order

If the comparison LMM has the same order ($p_z = p_y$) or polynomial extrapolation is used for z_{n+1}, then the error estimate is

$$e_n = \|y_{n+1} - z_{n+1}\| \approx |c_y(\mathbf{1}) - c_z(\mathbf{1})| \cdot \|y^{(p_y+1)}(t_n)\| \cdot h_n^{p_y+1} \cdot \hat{\pi}_e(\bar{\rho}_n).$$

Error control process

1. Given (t_n, y_n), compute $y_{n+1} = P_{n+1}(t_{n+1})$ at $t_{n+1} = t_n + h_n$.
2. Compute the ***dynamically compensated error estimate***

$$\tilde{r}_n = \tilde{K} \cdot \frac{\|y_{n+1} - z_{n+1}\|}{h_n} \cdot \prod_{j=1}^{s} \rho_{n-j}^{-\delta_j}, \qquad \tilde{K}: \text{ depends on error estimator}$$

3. Compute the ***scaled control errors*** $c_n = \left(\mathrm{TOL}/\tilde{r}_n\right)^{1/p_y}$.
4. Apply recursive digital filter with coefficients $(\beta_1, \beta_2, \gamma)$:

$$\rho_n = c_n^{\beta_1} c_{n-1}^{\beta_2} \rho_{n-1}^{-\gamma}.$$

and update the step size according to $h_{n+1} = \rho_n h_n$.

Error parameters for selected LMMs

Method	C_l	C_e	Parameters $\{\delta_j\}_1^s$			k	p_y	p_z	$b_y(\mathbf{1})$	$c_y(\mathbf{1})$
AB2(2)		$\frac{5}{23}$	$-\frac{45}{23}$	$-\frac{12}{23}$		2	2	2		
AB2(3)	1		$-\frac{3}{5}$			2	2	3	1	$-\frac{5}{12}$
AB3(3)		$\frac{9}{55}$	$-\frac{148}{55}$	$-\frac{182}{165}$	$-\frac{56}{165}$	3	3	3		
AB3(4)	1		$-\frac{4}{3}$	$-\frac{10}{27}$		3	3	4	1	$-\frac{3}{8}$
EDF2(2)		$\frac{1}{3}$	$-\frac{71}{36}$	$-\frac{5}{9}$		2	2	2		
EDF2(3)	$\frac{3}{2}$		$-\frac{5}{8}$			2	2	3	$\frac{2}{3}$	$-\frac{4}{9}$
EDF3(3)		$\frac{99}{320}$	$-\frac{217}{80}$	$-\frac{183}{160}$	$-\frac{121}{320}$	3	3	3		
EDF3(4)	$\frac{11}{6}$		$-\frac{37}{27}$	$-\frac{11}{27}$		3	3	4	$\frac{6}{11}$	$-\frac{9}{22}$
Nyström3(3)		$\frac{4}{51}$	$-\frac{181}{68}$	$-\frac{317}{306}$	$-\frac{437}{1224}$	3	3	3		
Nyström3(4)	$\frac{1}{2}$		$-\frac{41}{32}$	$-\frac{19}{48}$		3	3	4	2	$-\frac{1}{3}$

Error coefficients and $\{\delta_j\}_1^s$ of dynamically compensated error for explicit LMMs.

Examples of filter coefficients

Filter type	β_1	β_2	γ	Property
Elementary	1	0	0	Deadbeat with compensator
Exponential forgetting	2/3	0	0	Medium gain I controller
PI3333	2/3	$-1/3$	0	Low gain PI controller
$H211$PI	1/6	1/6	0	Low-pass filter of PI type
$H211b$	1/4	1/4	1/4	Noise-shaping low-pass filter

Filter coefficients for various controllers.

Outline

ODE problems

Problem 1: *two-compartment dilution process*

$$\begin{aligned} y_1' &= -\frac{1}{5}y_1, \\ y_2' &= -\frac{2}{5}(y_2 - y_1). \end{aligned}$$

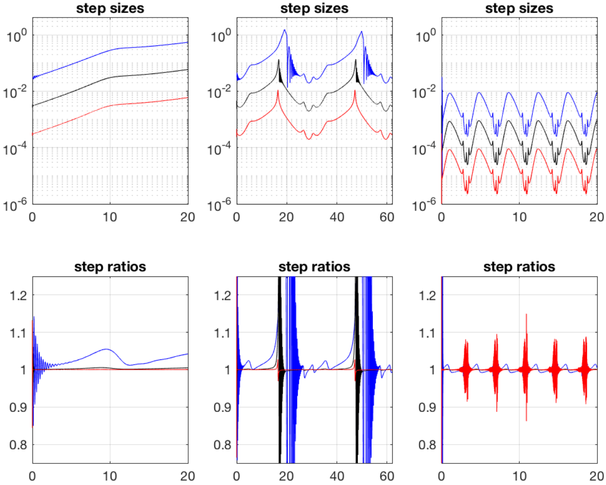
Problem 2: *Lotka–Volterra* equation

$$\begin{aligned} y_1' &= 0.1y_1 - 0.3y_1y_2, \\ y_2' &= 0.5(y_1 - 1)y_2. \end{aligned}$$

Problem 3: *van der Pol* equation

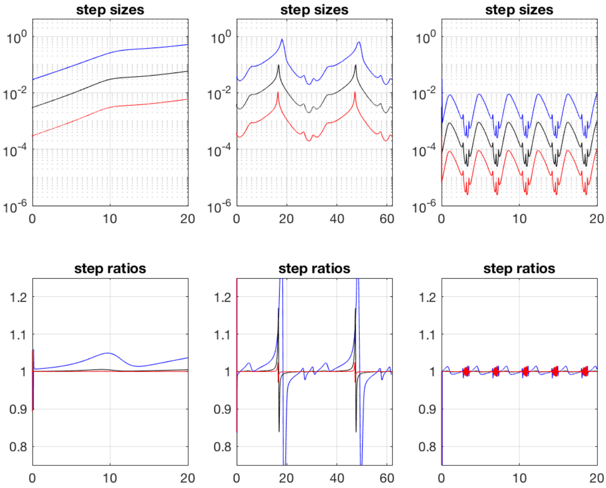
$$\begin{aligned} y_1' &= y_2, \\ y_2' &= \mu(1 - y_1^2)y_2 - y_1. \end{aligned}$$

Numerical test 1



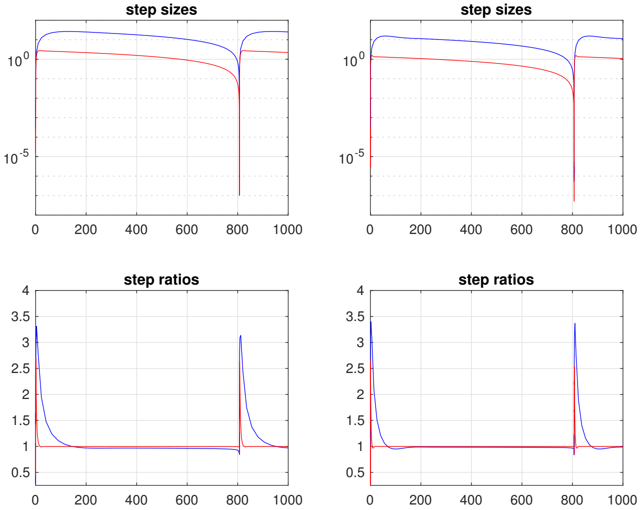
The AB2(2) method, using polynomial extrapolation as error estimation, is combined with the elementary controller, running in EPUS mode with $\text{TOL} = 10^{-5}, 10^{-7}, 10^{-9}$.

Numerical test 1 (cont.)



The AB2(2) method, using polynomial extrapolation as error estimation, is combined with the compensated exponential forgetting controller with gain 2/3, running in EPUS mode with TOL $= 10^{-5}, 10^{-7}, 10^{-9}$.

Numerical test 2



Stiff van der Pol equation is solved using the BDF2 method in EPS mode and $H211$PI control with $\text{TOL} = 10^{-6}, 10^{-9}$. AM2 error estimation (left) is compared to polynomial extrapolation (right).

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Conclusion and future work

- Obtained a dynamic asymptotic error model in multiplicative form for variable step size LMMs.
- The structure of the error model and compensator allows the application of linear control theory and easy implementation.
- Different filters and controllers were tested, showing that elementary controller may suffer in certain cases.
- Parameters for error estimates for various LMMs have been calculated; these error estimates coupled with appropriate controllers are essential for smooth step size sequences and tolerance proportionality.

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Thanks for your attention!