Adaptive Time-Stepping, Part I

How Control Theory and Digital Filters Enhance IVP Solver Performance

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1. What is the problem?

Time-stepping methods for initial value problem $\dot{y} = f(t, y)$

Given an approximation $y_n \approx y(t_n)$ compute

$$y_n \mapsto y_{n+1}$$

with time step size $h = t_{n+1} - t_n$

Work/accuracy trade-off

Rather than using constant step size, put grid points where they matter to accuracy

Adaptive methods

Given an *error tolerance* TOL, adaptive methods select the *time step* h_n to make the *local error* $r_n = \text{TOL}$

Asymptotic step size – error model (as $h \to 0$)

$$r_n = \varphi_n h_n^k$$

If φ is constant, then $h_{n+1} = (\text{TOL}/r_n)^{1/k} h_n$ makes $r_{n+1} \equiv \text{TOL}$

. . . and scientific computing stopped thinking, right there. . .

2. Control and signal processing

Classical time-step control

$$h_{n+1} = \left(\frac{\mathrm{TOL}}{r_n}\right)^{1/k} h_n$$

In logarithmic form

$$\log h_{n+1} - \log h_n = -\frac{1}{k}\left(\log r_n - \log \mathrm{TOL}\right)$$

Integrating control *Summation of control errors*

Linear difference equation, $\log r \mapsto \log h$, where $\log r = \{\log r_n\}_{n=1}^{\infty}$

Linear control and signal processing

Signal processing How to map observed error sequence $\log r$ to suitable step size sequence $\log h$ while keeping $r \approx \text{TOL}$

General control law (linear difference equations)

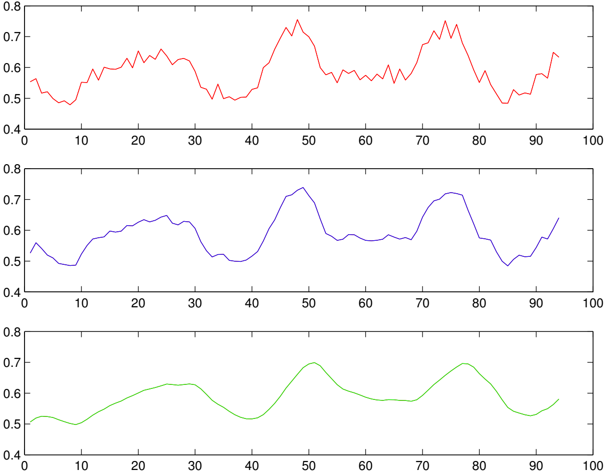
$$(q-1)Q(q) \cdot \log h = P(q) \cdot (\log r - \log \text{TOL})$$

P, Q polynomial operators in forward shift operator q

New possibilities

Q “autoregressive” part; P “moving average” part

What step size properties can be achieved?



Elementary control

FIR filter

Noise shaping filter

Will it have an impact on computations?

Standard, elementary time-step control

$$h_{n+1} = \left(\frac{\mathrm{TOL}}{r_n}\right)^{1/k} h_n$$

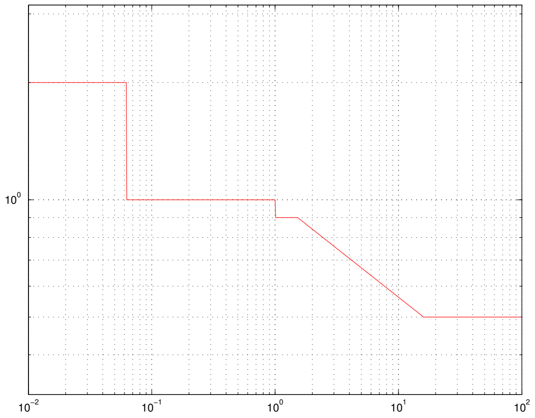
in logarithmic form is a *negative feedback control law*

$$\log \frac{h_{n+1}}{h_n} = -\frac{1}{k} \log \frac{r_n}{\mathrm{TOL}}$$

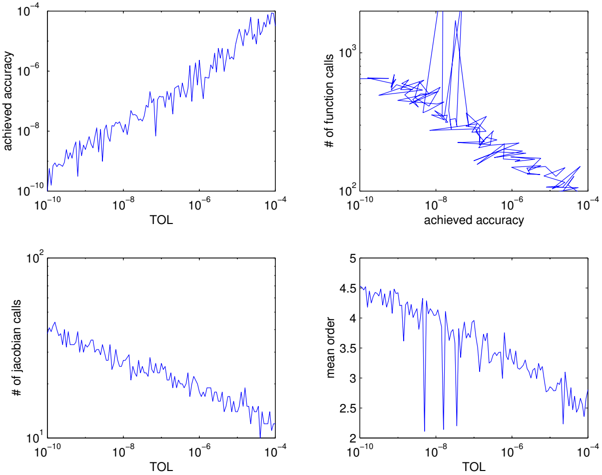
Actual implementations add substantial safety nets and heuristics

. . . so scientific computing didn't quite stop thinking right there

Typical plot of $\log(h_{n+1}/h_n)$ *vs.* $\log(r_n/\mathrm{TOL})$



Nonlinear, discontinuous and nonsymmetric!



Small changes in TOL *have large effects on output*

What is computational stability?

Continuous data dependence

$$c \cdot \mathrm{TOL} \leq \|e\| \leq C \cdot \mathrm{TOL}$$

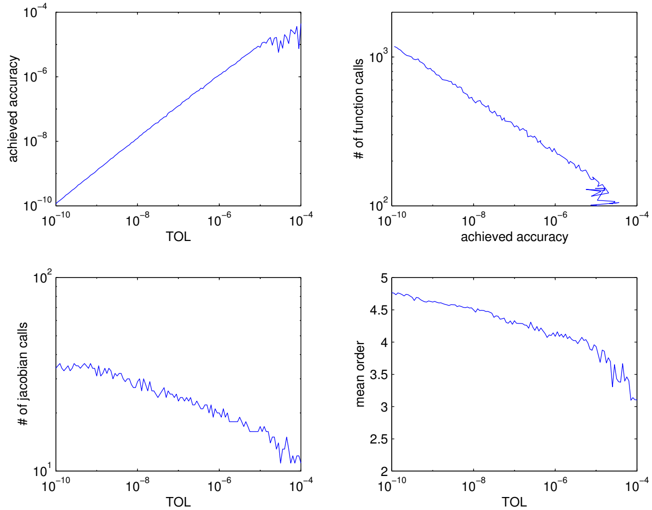
with $\log_{10}(C/c) \ll 1$

How can it be improved?

- *Digital filtering of error estimates*
- *Control theory for time–step selection*
- *Order selection controller*
- *Appropriate Newton iteration termination*

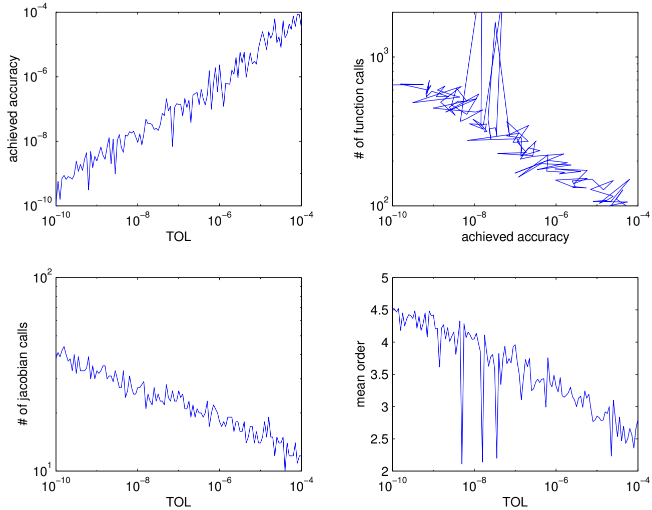
$\Rightarrow \log_{10}(C/c) \approx 0.05$ possible *at no extra cost!*

. . . and it works a lot better!



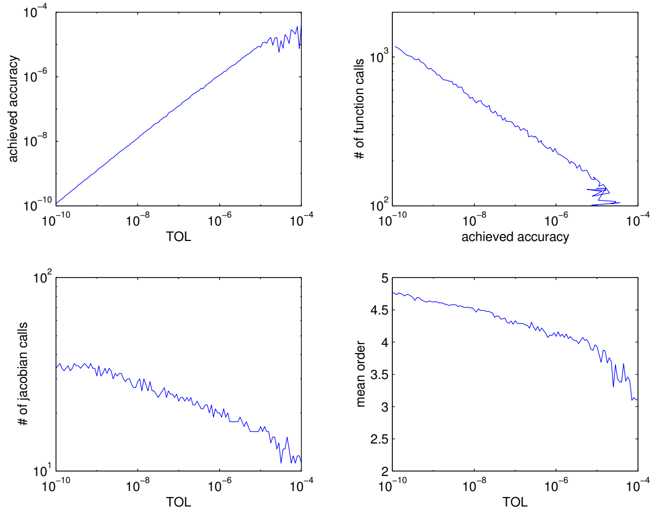
High computational stability

Compare to standard implementation *Chemakzo problem*

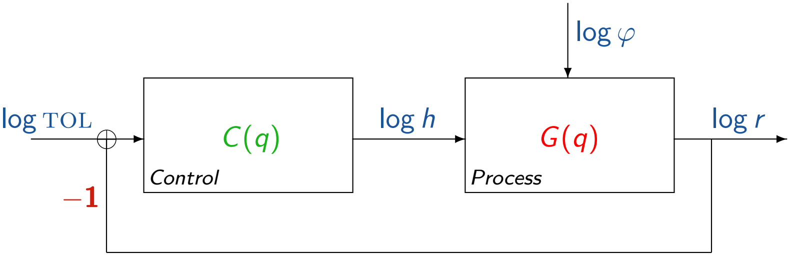


Poor computational stability

Digital filter based controller *Chemakzo problem*



High computational stability



Asymptotic process model

$$r = \varphi h^k \quad \Rightarrow \quad \log r = k \cdot \log h + \log \varphi \qquad (G(q) = k)$$

Control law $\log h = C(q) \cdot (\log \mathrm{TOL} - \log r)$

Closed loop

To find controller–process interaction, solve the linear system

$$\log r = k \cdot \log h + \log \varphi$$
$$\log h = C(q) \cdot (\log \mathrm{TOL} - \log r)$$

for $\log r$ and $\log h$, to find the maps

$$H_\varphi(q): \quad \log \varphi \mapsto \log h$$
$$R_\varphi(q): \quad \log \varphi \mapsto \log r$$

revealing how the differential equation (external disturbance $\log \varphi$) affects the error $\log r$ and step size $\log h$

Closed loop response functions

Step size response $H_\varphi(q) : \log\varphi \mapsto \log h$

$$-kH_\varphi(q) = \frac{k \cdot C(q)}{1 + k \cdot C(q)}$$

Error response $R_\varphi(q) : \log\varphi \mapsto \log r$

$$R_\varphi(q) = \frac{1}{1 + k \cdot C(q)}$$

Control design *Low-pass* filter for h and *high-pass* filter for r

The most general choice of controller is

$$C(q) = \frac{P(q)}{(q-1)Q(q)}$$

with $\deg P = \deg Q$ correponding explicit step size recursion

$$(q-1)Q(q) \cdot \log h = P(q) \cdot (\log r - \log \text{TOL})$$

Consistency Difference operator $q - 1$ is necessary

Stability Interaction between $C(q)$ and the process $G(q) = k$

Convergence to the set point, $r \to \text{TOL}$, then follows

What is a digital filter? $\mathcal{F} : u \mapsto v = \mathcal{F}u$

Let $u = \{u_n\}_0^\infty$ be a given time sequence

A causal linear digital filter is a *difference equation*

$$R(q)v = P(q)u$$

where P and R are polynomials, with $\deg P < \deg R$

Stable filter $R(q) = 0 \Rightarrow |q_\nu| < 1$

If $u_n = \mathrm{e}^{\mathrm{i}\omega n}$ for $\omega \in [0, \pi]$ then the *particular solution* is

$$v_n = A(\omega)\, \mathrm{e}^{\mathrm{i}\omega n}$$

Attenuation $|A(\omega)| = |P(\mathrm{e}^{\mathrm{i}\omega})/R(\mathrm{e}^{\mathrm{i}\omega})|$ affects frequency content

Step size response for $C(q) = P(q)/[(q-1)Q(q)]$

Closed loop recursion $\big((q-1)Q(q) + kP(q)\big)\log h = -P(q)\log\varphi$

Control designs

Elementary control	$Q \equiv 1; \quad P \equiv 1/k$
Convolution filter	$Q \equiv 1; \quad P \equiv \gamma < 1/k$
I control	$Q \equiv 1; \quad \deg P = 0$
PI control	$Q \equiv 1; \quad \deg P = 1$
PID control	$Q \equiv 1; \quad \deg P = 2$
FIR filter	$(q-1)Q(q) + k \cdot P(q) = q^m$
Autoregressive (AR)	Q has zero(s) at $q = 1$
Moving average (MA)	P has zero(s) at $q = -1$

Remove logarithms to get multiplicative recursion

$$h_{n+1} = \left(\frac{\mathrm{TOL}}{r_n}\right)^{1/(bk)} \left(\frac{\mathrm{TOL}}{r_{n-1}}\right)^{1/(bk)} \left(\frac{h_n}{h_{n-1}}\right)^{-1/b} h_n$$

The *filter coefficients* are determined by order conditions

Properties

- Stable for $b \in [1, \infty)$ with poles at $q = 0,\, 1 - 2/b$
- 1st order low-pass FIR filter (deadbeat) at $b = 2$
- Increasing b increases noise suppression

Let the sequence $c = \{\mathrm{TOL}/r_n\}_1^\infty$ denote the *control errors*

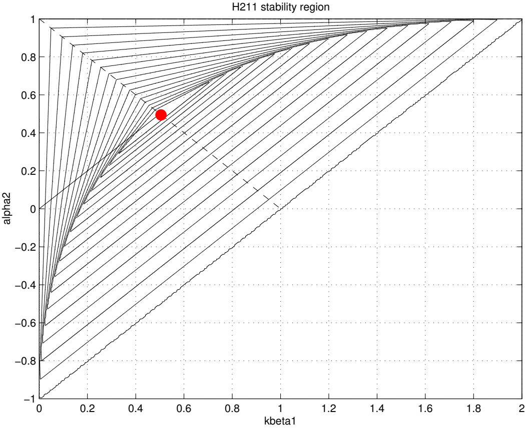
Let the sequence $\rho = \{h_n/h_{n-1}\}_2^\infty$ denote the *step size ratios*

Recursive digital filter *Process errors and step ratios*

$$\rho_{n+1} = c_n^{1/(bk)} \cdot c_{n-1}^{1/(bk)} \cdot \rho_n^{-1/b}$$

Single integrating control *Update step size*

$$h_{n+1} = \rho_{n+1} \cdot h_n$$



FIR filter at ●, other $H211b$ on straight line segment

Filter design in the frequency domain

Quasi periodic input $\log \varphi_n = \mathrm{e}^{\mathrm{i}\omega n}$ for $\omega \in [0, \pi]$

Output $\log h_n = A(\omega)\mathrm{e}^{\mathrm{i}\omega n}$ with amplitude $|A(\omega)| = |H_\varphi(\mathrm{e}^{\mathrm{i}\omega})|$

The *attenuation* of $\mathrm{e}^{\mathrm{i}\omega n}$ is measured by

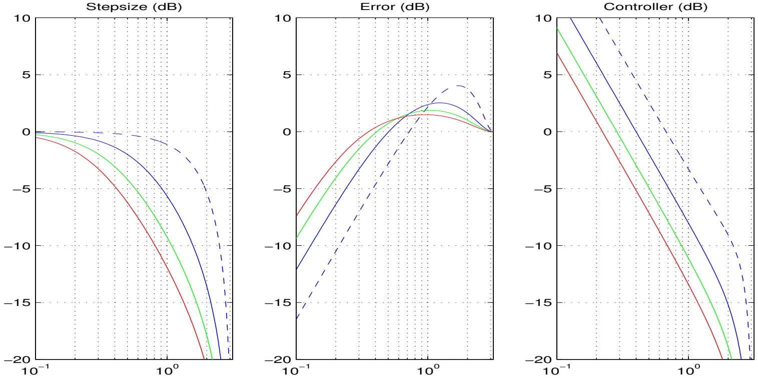
$$|kH_\varphi(\mathrm{e}^{\mathrm{i}\omega})| = \left| \frac{kP(\mathrm{e}^{\mathrm{i}\omega})}{(\mathrm{e}^{\mathrm{i}\omega} - 1)Q(\mathrm{e}^{\mathrm{i}\omega}) + kP(\mathrm{e}^{\mathrm{i}\omega})} \right|$$

Zeros of $H_\varphi(q)$ block signal transmission!

Low-pass filter Make $|H_\varphi(\mathrm{e}^{\mathrm{i}\pi})| = 0$ by taking $P(-1) = 0$

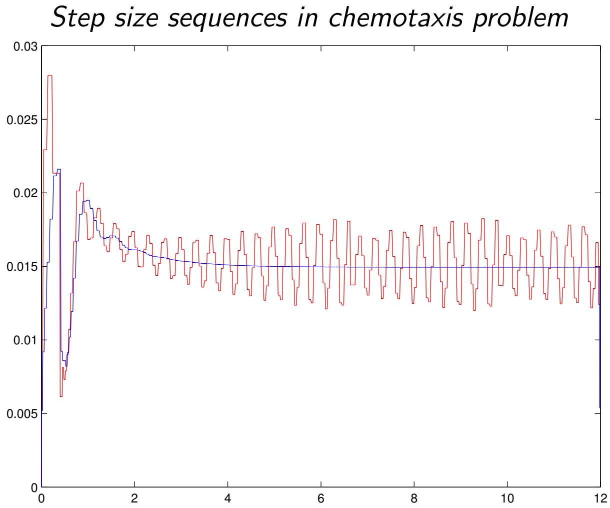
$H211b$ frequency response on $[0.1, \pi]$

$\log \varphi \mapsto k \log h$ $\qquad$ $\log \varphi \mapsto \log r$ $\qquad$ $\log r \mapsto \log h$



FIR filter (dashed, $b = 2$), noise shaping: $b = 4$; $b = 6$; $b = 8$

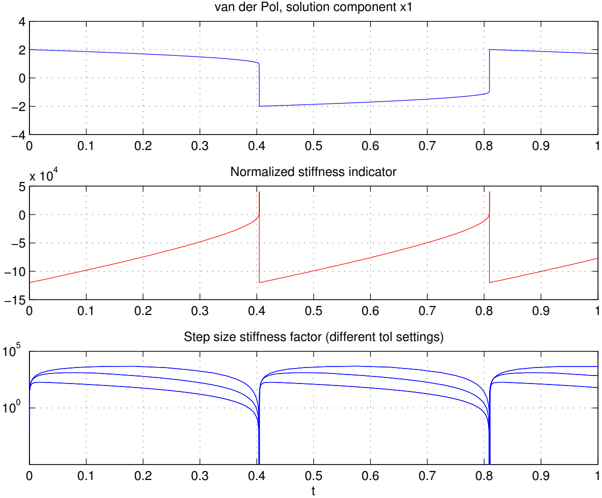
Example. Modifying ode45 in MATLAB to ode45dc



Original vs. modified code (PI controller)

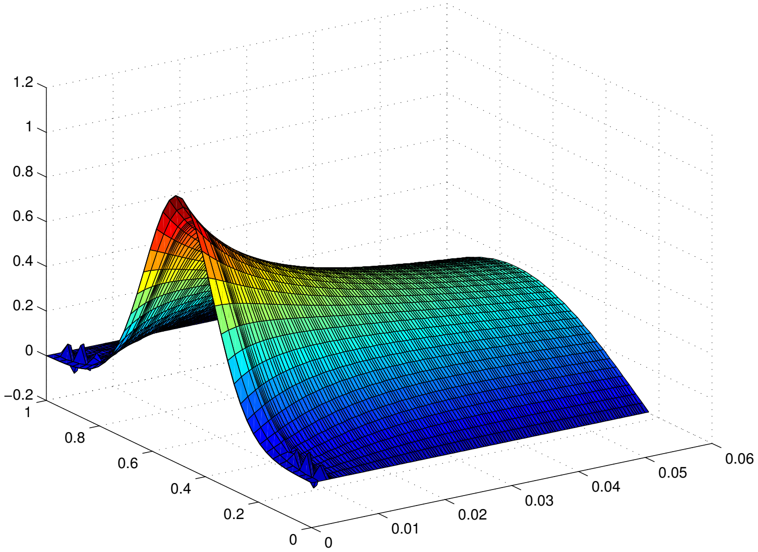
Example. Modifying ode23s in MATLAB to ode23sdc

Step size sequences van der Pol problem, $\mu = 200$

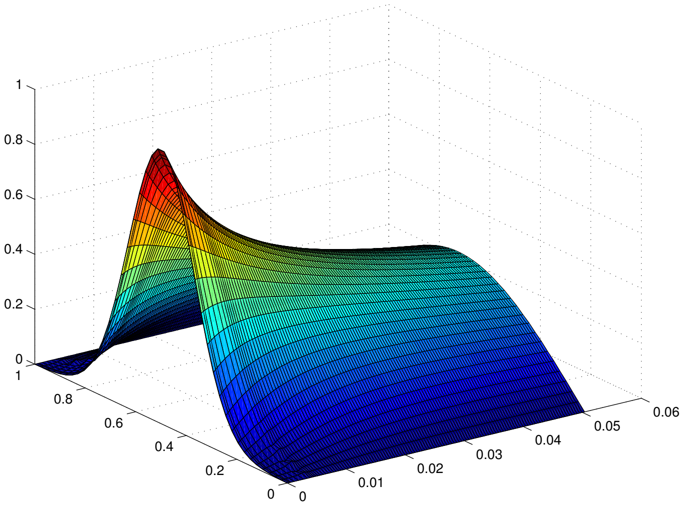


Modified code with *H*211*PI* controller, for various TOL

Elementary deadbeat grid in diffusion problem



PI controlled grid in diffusion problem



A selection of digital filters for step size control

Recursive error filter $\rho_{n+1} = c_n^{\beta_1/k} \cdot c_{n-1}^{\beta_2/k} \cdot {\rho_n}^{-\alpha}$

Controller	Type	β_1	β_2	α
Elementary	I (deadbeat integral control)	1	0	0
PI3040	PI (proportional-integral)	7/10	−4/10	0
PI3333	PI (proportional-integral)	2/3	−1/3	0
PI4020	PI (proportional-integral)	3/5	−1/5	0
H211PI	PI digital filter	1/6	1/6	0
H211b	Noise shaping digital filter	$1/b$	$1/b$	$1/b$

Step size control $h_{n+1} = \rho_{n+1} h_n$

Coming attractions

- **Dedicated controllers for multistep methods**

  The asymptotic model $r \sim \phi h^p$ is questionable

  Develop proper error model based on actual error estimate

  Prove convergence as $\text{TOL} \to 0$ for adaptive scheme

- **Tracking CFL conditions**

  In conservation laws one wants to use the max stable step size

  This is about controlling stability rather than accuracy

- **Automatic detection of stiffness**

- **Automatic detection of oscillatory behavior**

- **Replace heuristics by mathematics in software**

Thank you!