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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 $\varphi$ is constant, then

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

makes $r_{n+1} \equiv \text{TOL}$

...and scientific computing stopped thinking, right there...
2. Control and signal processing

Classical time-step control

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

In logarithmic form

\[ \log h_{n+1} - \log h_n = -\frac{1}{k} (\log r_n - \log TOL) \]

**Integrating control**  *Summation of control errors*

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

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

in logarithmic form is a *negative feedback control law*

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

Actual implementations add substantial safety nets and heuristics

...so scientific computing didn’t quite stop thinking right there
Example of actual heuristic implementation

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

Nonlinear, discontinuous and nonsymmetric!
How well does it work?

Chemakzo problem

Small changes in TOL have large effects on output
What is computational stability?

Continuous data dependence

\[ c \cdot \text{TOL} \leq \|e\| \leq C \cdot \text{TOL} \]

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

\[ \Rightarrow \log_{10}(C/c) \approx 0.05 \text{ possible at no extra cost!} \]
... and it works a lot better!

Chemakzo problem

High computational stability
Compare to standard implementation

Chemakzo problem

Poor computational stability
Digital filter based controller

Chemakzo problem

High computational stability
Control theoretic approach

Feedback loop

Asymptotic process model

\[ r = \varphi h^k \quad \Rightarrow \quad \log r = k \cdot \log h + \log \varphi \quad \text{ (} G(q) = k \text{)} \]

Control law

\[ \log h = C(q) \cdot (\log \text{TOL} - \log r) \]
Closed loop

To find controller–process interaction, solve the linear system

\[ \log r = k \cdot \log h + \log \varphi \]
\[ \log h = C(q) \cdot (\log TOL - \log r) \]

for \( \log r \) and \( \log h \), to find the maps

\[ H_{\varphi}(q) : \log \varphi \mapsto \log h \]
\[ R_{\varphi}(q) : \log \varphi \mapsto \log r \]

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 $\text{deg } P = \text{deg } Q$ corresponding 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 \textit{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 \( u_n = e^{i\omega n} \) for \( \omega \in [0, \pi] \) then the \textit{particular solution} is

\[ v_n = A(\omega)e^{i\omega n} \]

**Attenuation** \( |A(\omega)| = |P(e^{i\omega})/R(e^{i\omega})| \) affects frequency content.
Step size response for \( C(q) = P(q)/[(q - 1)Q(q)] \)

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

**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 \( q = -1 \)
A digital filter for step size control

LP filter $H_{211b}$

Remove logarithms to get multiplicative recursion

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

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 \( c = \{\text{TOL}/r_n\}_{1}^{\infty} \) 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

\[
h_{n+1} = \rho_{n+1} \cdot h_n
\]
Pole placement

The effect of choosing $b$

FIR filter at $\bullet$, other $H211b$ on straight line segment
Filter design in the frequency domain

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

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

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

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

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

**Low-pass filter** Make $|H_\varphi(e^{i\pi})| = 0$ by taking $P(-1) = 0$
$H_{211b}$ frequency response on $[0.1, \pi]$

\[ \log \varphi \mapsto k \log h \quad \log \varphi \mapsto \log r \quad \log r \mapsto \log h \]

FIR filter (dashed, $b = 2$), noise shaping: $b = 4; \ b = 6; \ b = 8$
Example. Modifying ode45 in MATLAB to ode45dc

Step size sequences in chemotaxis problem

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 $H_{211PI}$ 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** \( \rho_{n+1} = c_n^{\beta_1/k} \cdot c_{n-1}^{\beta_2/k} \cdot \rho_n^{-\alpha} \)

<table>
<thead>
<tr>
<th>Controller</th>
<th>Type</th>
<th>( \beta_1 )</th>
<th>( \beta_2 )</th>
<th>( \alpha )</th>
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<td>I (deadbeat integral control)</td>
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<td>PI (proportional-integral)</td>
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<td>PI digital filter</td>
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<tr>
<td>H211b</td>
<td>Noise shaping digital filter</td>
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<td>1/b</td>
<td>1/b</td>
</tr>
</tbody>
</table>

**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!