CS 101

Numerical Geometric Integration

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Today

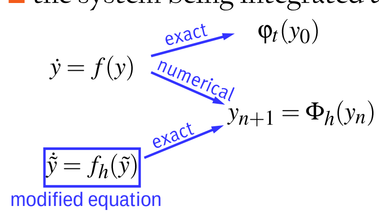
Analysis of long-time behavior

- Hopefully fulfill my promises ☺
- Backward Error Analysis (BEA)
  - Symmetric Integrators (more later)
  - Symplectic Integrators
- High-level
  - Many theorem details omitted for brevity – see book for formal statements

Backward Error Analysis (BEA)

Find the modified Diff. Eq.

- the system being integrated *exactly*



Finding the Modified Equation

Look for the form

Won't always converge (will truncate)

$$\dot{\tilde{y}}(t) = f(\tilde{y}(t)) + hf_2(\tilde{y}(t)) + h^2 f_3(\tilde{y}(t)) + \cdots$$

Define $y = \tilde{y}(t)$ for t fixed and expand

$$\tilde{y}(t+h) = \tilde{y}(t) + h\dot{\tilde{y}}(t) + \frac{h^2}{2}\ddot{\tilde{y}}(t) + \cdots$$

$$= y + h(f(y) + hf_2(y) + h^2 f_3(y) + \cdots)$$

$$+ \frac{h^2}{2}(f'(y) + hf_2'(y) + \cdots)(f(y) + hf_2(y) + \cdots) + \cdots$$

Finding the Modified Equation

Expand the numerical method*

$$\Phi_h(y) = y + hf(y) + h^2 d_2(y) + h^3 d_3(y) + \cdots$$

Set $\tilde{y}(t+h) = \Phi_h(y)$ and group h^i terms

$$f_2(y) = d_2(y) - \frac{1}{2}f'f(y)$$

$$f_3(y) = d_3(y) - \frac{1}{2}(f'f_2(y) + f_2'f(y))$$

Computer can help ☺

$$-\frac{1}{3!}(f''(f,f)(y) + f'f'f(y))$$

Simple Example

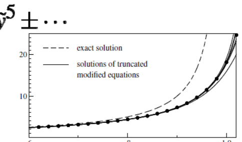
Explicit Euler

$$\Phi_h(y) = y + hf(y)$$

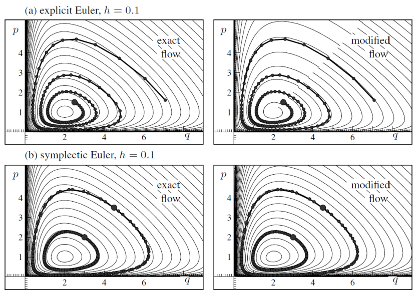
$$\dot{y} = y^2$$

- Use Mathematica (HW!)...

$$\dot{\tilde{y}} = \tilde{y}^2 - h\tilde{y}^3 + h^2\frac{3}{2}\tilde{y}^4 - h^3\frac{8}{3}\tilde{y}^5 \pm \cdots$$



Lotka-Volterra Example



Examples & Observations

$$\dot{y} = y^2$$

Midpoint

$$\dot{\tilde{y}} = \tilde{y}^2 + h^2 \frac{1}{4}\tilde{y}^4 + h^4 \frac{1}{8}\tilde{y}^6 + h^6 \frac{11}{192}\tilde{y}^8 \pm \cdots$$

Order of method

Even (due to symmetry)

RK4

$$\dot{\tilde{y}} = \tilde{y}^2 - h^4 \frac{1}{24}\tilde{y}^6 + h^6 \frac{65}{576}\tilde{y}^8 - h^7 \frac{17}{96}\tilde{y}^9 \pm \cdots$$

Symmetric Methods

Adjoint Method:

$$\Phi_h^* = \Phi_{-h}^{-1}$$

$$f_j^*(y) = (-1)^{j+1} f_j(y)$$

- Proof: start with $\tilde{y}(t) = \Phi_{-h}(\tilde{y}(t+h))$

Symmetric Method

$$f_j(y) = 0 \quad \forall j \text{ even}$$

$$\dot{\tilde{y}}(t) = f(\tilde{y}(t)) + h f_2(\tilde{y}(t)) + h^2 f_3(\tilde{y}(t)) + \cdots$$

ρ-Reversible Systems

Sidenote: ρ-compatibility

- If $\rho \circ \Phi_h = \Phi_{-h} \circ \rho$ then Φ_h is ρ-reversible iff Φ_h is symmetric
  - Typically true

BEA for ρ-reversible system

- If Φ_h is ρ-reversible then each f_i is ρ-reversible
- Proof by induction on f_i

Every truncation of modified system is ρ-reversible

Symplectic Methods

Applied to Hamiltonian system

- Modified system is Hamiltonian
- In particular, H_j exists s.t.

$$f_j(y) = J^{-1} \nabla H_j(y)$$

- 2 Proofs
  - Induction on f_i (like symmetric)
  - Expand generating function

Example: Symplectic Euler

$$S(P,q,h) = hH(P,q)$$

$$\tilde{H} = H - \frac{h}{2} H_p H_q + \frac{h^2}{12}\left(H_{pp} H_q^2 + H_{qq} H_p^2 + 4 H_{pq} H_q H_p\right) + \cdots$$

Applied to pendulum: $H(p,q) = \frac{p^2}{2} - \cos q$

$$\tilde{H}(p,q) = H(p,q) - \frac{h}{2} p \sin q + \frac{h^2}{12}\left(\sin^2 q + p^2 \cos q\right) + \cdots$$

- Not separable
- Not second order ($\ddot{q} = -\nabla U(q)$)

Extensions

BEA for most things we've covered

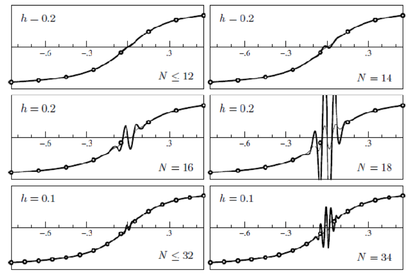
- Constrained Systems
- Adaptive step sizes
- Splitting methods

Similar results for other properties

- Preservation of first integrals

Truncation

$$f(t) = \frac{1}{1+25t^2}$$



What Can We Really Say?

Goal

- Explain long-time energy behavior of symplectic methods
- Fairly pessimistic

Assume:

- f(y) complex analytic around y_0
- $||f(y)|| \leq M$ for $||y - y_0|| \leq 2R$

What Can We Really Say?

Then:

- Can bound $d_j(y)$ for most methods
  - Cauchy's estimate – bound is uniform
- Estimate and bound $f_j(y)$
- Find optimal truncation N
- Bound $||\Phi_h(y_0) - \tilde{\varphi}_{N,h}(y_0)||$ ← Skipping to here
- Bound change in $\tilde{H}$ and H

$\dot{\tilde{y}}(t) = f(\tilde{y}(t)) + hf_2(\tilde{y}(t)) + h^2 f_3(\tilde{y}(t)) + \cdots$ $\Phi_h(y) = y + hf(y) + h^2 d_2(y) + h^3 d_3(y) + \cdots$

Error of modified equation

Theorem 7.6. *Let $f(y)$ be analytic in $B_{2R}(y_0)$, let the coefficients $d_j(y)$ of the method (7.3) be analytic in $B_R(y_0)$, and assume that (7.2) and (7.5) hold. If $h \leq h_0/4$ with $h_0 = R/(e\eta M)$, then there exists $N = N(h)$ (namely N equal to the largest integer satisfying $hN \leq h_0$) such that the difference between the numerical solution $y_1 = \Phi_h(y_0)$ and the exact solution $\widetilde{\varphi}_{N,t}(y_0)$ of the truncated modified equation (7.11) satisfies*

$$\|\Phi_h(y_0) - \widetilde{\varphi}_{N,h}(y_0)\| \leq h\gamma M e^{-h_0/h},$$

where $\gamma = e(2 + 1.65\eta + \mu)$ depends only on the method (we have $5 \leq \eta \leq 5.18$ and $\gamma \leq 31.4$ for the methods of Table 7.1).

Long-Time Energy Conservation

Φ_h symplectic method

- Then* there exists h_0 and N s.t

truncated after N terms → $\tilde{H}(y_n) = \tilde{H}(y_0) + O(e^{h_0/2h})$

$H(y_n) = H(y_0) + O(h^p)$ ← doesn't depend on n

for $nh \leq e^{h_0/2h}$ ← "exponentially long" time interval

- Good: rigor Bad: very conservative