CS 101

Numerical Geometric Integration

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Today

Multistep Methods

- Classical & Structure Preserving
- Only the big picture
  - Many statements, few proofs (in books)
  - Tried to hit "interesting" parts

High-order Variational Integrators

- Different interpretations

Multistep Methods

Idea: Use several previous values

- As opposed to "one-step" methods

Simplest: Linear Multistep Methods

$$\dot{y} = f(y)$$

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f(y_{n+j})$$

Explicit When?

$$\alpha_k \neq 0 \qquad |\alpha_0| + |\beta_0| > 0$$

We've seen these before

Adams Methods

- Explicit: Adams-Bashforth
  - $\alpha_{k-1} = -1$, others 0
  - Solve for β's using degree s-1 polynomial
    - Polynomial matches derivatives, then integrate
- Implicit: Adams-Moulton
  - β_k not 0, so use degree s polynomial

Backward Differentiation

"BDF" – good for stiff systems

- Implicit
- Interpolate y(t) using backward differences $\nabla y_n = \frac{1}{h}(y_n - y_{n-1})$
  - Differentiate and evaluate at t_{n+k}
  - Set this equal to $f(y_{n+k})$
- Ex: $\frac{3}{2} y_{n+2} - 2 y_{n+1} + \frac{1}{2} y_n = h f(y_{n+2})$

Handwave Analysis

Generating/Characteristic Polynomials

$$\rho(z) = \sum_{j=0}^{k} \alpha_j z^j \qquad \sigma(z) = \sum_{j=0}^{k} \beta_j z^j$$

Stable if ρ(z) has roots $|z_i| \leq 1$

- And all roots on unit circle are simple
- Strictly stable if 1 only for $z_i = 1$

Symmetric Multistep Methods

No Surprise:

- $\alpha_{k-j} = -\alpha_j$ and $\beta_{k-j} = \beta_j$
- Implies

  $$\rho(z_i) = 0 \Rightarrow \rho(z_i^{-1}) = 0$$

- Stable+Symmetric:
  - All zeros simple and on unit circle
- These can behave nicely (not always)

2nd Order Differential Equation

Same idea $\ddot{y} = f(y)$

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f(y_{n+j})$$

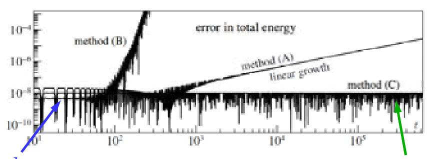
Stable - similar

- Can have double zeros on unit circle

Symmetry: same story

How well do they work?

3 different 4th-order methods



All good at start

A: Strictly Stable

B&C: Symmetric!

Lambert & Watson 1976

C: No Double Zeros (except z=1)

B: Exponential Error Growth (Dahlquist 1956)

"Stabilized" Version

Split ρ to remove double zeros

$$\rho(z) = \rho_A(z)\rho_B(z)$$

Define $hv_n = \sum_{j=0}^{k_A} \alpha_j^A y_{n+j}$

So we get $\sum_{j=0}^{k_B} \alpha_j^B v_{n+j} = h \sum_{j=0}^{k} \beta_j f(y_{n+j})$

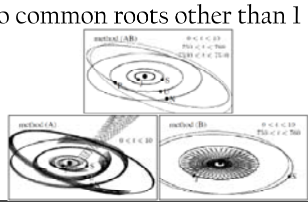
Use this idea for partitioned methods…

Partitioned Multistep Methods

$$\dot{y} = f(y, v) \qquad \dot{v} = g(y, v)$$

Same idea: ρ_A for y, ρ_B for v

- No common roots other than 1



Symplecticity?

Nope* (at least for linear ones)

- Based on "underlying one-step method"
- At least not in the standard sense
  - "G-symplecticity" (see book)
    - Doesn't guarantee anything (by itself)
- Still possible to get good behavior
  - Analysis gets deeper (Chapter XV)
  - Battle between structure and sensitivity

Higher-Order Var. Integrators

See thesis by Matt West for more

Discrete Lagrangian of order r

- Approximates action integral

$$L_d(q_0, q_1) = \int_0^h L(q(t), \dot{q}(t))\, dt + O(h^{r+1})$$

- Can show this gives order r integrator

$$q_k = q(kh) + O(h^{r+1})$$

  - Just need a way to build Lagrangians…

Composition Approach

We've seen composition before

- Can use it to increase order of schemes
  - Works for discrete Lagrangians too
- Break a step into multiple steps:

$$(q_k, q_{k+1}) \to (q_k = q_k^0, q_k^1, q_k^2, \ldots, q_k^s = q_{k+1})$$

- Different discrete Lagrangian for each

$$A = \sum_{k=0}^{N} \sum_{i=1}^{s} L_d^i(q_k^{i-1}, q_k^i, \gamma^i h) \qquad \sum_{i=1}^{s} \gamma^i = 1$$

Composition Approach

Do variations wrt all points

$$D_2 L_d^i(q_k^{i-1}, q_k^i, \gamma^i h) + D_1 L_d^{i+1}(q_k^i, q_k^{i+1}, \gamma^{i+1} h) = 0$$

for $i = 1, \ldots, s-1$ and

$$D_2 L_d^s(q_k^{s-1}, q_k^s, \gamma^s h) + D_1 L_d^1(q_{k+1}^0, q_{k+1}^1, \gamma^1 h) = 0$$

since $q_k^s = q_{k+1}^0$

- Symplectic since it's a composition of symplectic substeps

Equivalent Interpretations

Substeps: $L_d(q_k^0, q_k^1, \ldots, q_k^s, h) = \sum_{i=1}^{s} L_d^i(q_k^{i-1}, q_k^i, \gamma^i h)$

$$A = \sum_{k=0}^{N} L_d(q_k^0, q_k^1, \ldots, q_k^s, h)$$

Single Step:

$$L_d(q_k, q_{k+1}, h) = \underset{(q_k^1, \ldots, q_k^{s-1})}{\text{ext}} L_d(q_k = q_k^0, q_k^1, \ldots, q_k^s = q_{k+1}, h)$$

$$A = \sum_{k=0}^{N} L_d(q_k, q_{k+1}, h)$$

What if this wasn't from composition?

Galerkin Approach

Choose a space for the sub-interval

- Locally extremize action in that space
- E.g. polynomial interpolation

$$L_d(q_k, q_{k+1}) = \underset{q \in P^s}{\text{ext}}\ A(q)$$

- Parameterize $P^s = \sum_{i=0}^{s} q^i \phi^i$ ← Lagrange polynomial basis functions

$$L_d(q_k, q_{k+1}) = \underset{(q_k^1, \ldots, q_k^{s-1})}{\text{ext}} A\left(\sum_{i=0}^{s} q_k^i \phi^i\right)$$

Solved for simultaneously → $(q_k^1, \ldots, q_k^{s-1})$