CS 101

Numerical Geometric Integration

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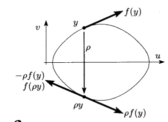
ρ-Reversible Systems

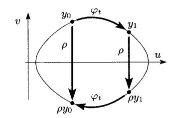
$\dot{y} = f(y)$ is *ρ-reversible* if:

$$\rho \circ f(y) = -f(\rho \circ y) \;\; \forall y$$



A map Φ(y) is *ρ-reversible* if:

$$\rho \circ \Phi = \Phi^{-1} \circ \rho$$



(continuous)

Time-Reversible Systems

$$\rho(u, v) = (u, -v)$$

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

Example: $$\begin{aligned} f(u,-v) &= -f(u,v) \\ g(u,-v) &= g(u,v) \end{aligned}$$

Special Cases:

$$\dot{u} = v, \dot{v} = g(u)$$

$$H(p,q) = H(-p,q)$$

The Discrete Picture

What can we conserve?
- Can't always get everything.

What should we conserve?
- What's the proper discrete definition.

How do we do it?
- Often more than one approach.

Symmetric Integrators

$$y_{k+1} = \Phi_h(y_k)$$

Symmetric (time-reversible) if

$$\Phi_h \circ \Phi_{-h} = id \;\Leftrightarrow\; \Phi_h = \Phi_{-h}^{-1}$$ Adjoint Φ^*

Practically: $y_k \leftrightarrow y_{k+1}$ and $h \leftrightarrow -h$

Examples
- Midpoint, Trapezoidal
- Symmetric Euler (composition)

The Least We Can Ask

Linear Invariants (First Integrals)

$$I'(y)f(y) = 0 \;\; \forall y$$

$$I(y) = d^T y$$

Examples
- Linear Momentum, Mass

Which methods conserve this?
- all explicit and implicit RK methods.
  - Simple proof
  - Clearly not always enough

Quadratics

Quadratic Invariants

$$I(y) = y^T C y$$

$$y^T C f(y) = 0 \quad \forall y$$

Examples

- Angular Momentum, Some Energies

Which methods conserve this?

- Implicit Midpoint (Proof!)
- Gauss methods
  - Specific conditions for RK methods

Higher Order Polynomials

$n \geq 3$?

Examples

- Volume Preservation (determinant)

Any RK methods?

- Nope, at least not all of a given order
- RK isn't always the answer

Hamiltonian Systems

Energy Preservation

- Midpoint gets quadratic energies
  - Also gets angular momentum
- Modify it to get energy preservation?

$$\dot{q} = \frac{1}{m}p \quad \dot{p} = -\nabla U(q)$$

$$q_{k+1} = q_k + \frac{h}{m}p_{k+\frac{1}{2}} \quad p_{k+1} = p_k - \alpha h \nabla U(q_{k+1})$$

$$p_{k+1} = p_k - h\frac{U(q_{k+1}) - U(q_k)}{||q_{k+1}|| - ||q_k||}\frac{q_{k+\frac{1}{2}}}{\frac{1}{2}(||q_{k+1}|| + ||q_k||)}$$

More General: Discrete Gradients

Discrete-Gradient Methods

$$y_{k+1} = y_k + h\bar{B}(y_{k+1}, y_k)\bar{\nabla}H(y_{k+1}, y_k)$$

skew-symmetric "discrete gradient"

Discrete Gradient:

$$\bar{\nabla}H(y,y) = \nabla H(y,y)$$ "pointwise"

$$\bar{\nabla}H(\hat{y},y)^T(\hat{y}-y) = H(\hat{y}) - H(y)$$ "integrated" (linear)

These Preserve Energy (Proof!)

Some Discrete Gradients

Modified Midpoint

$$\bar{B}(\hat{y},y) = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \quad \bar{\nabla}H(\hat{y},y) = \begin{pmatrix} \frac{1}{2}(\hat{p}+p) \\ \sigma(\hat{q},q)\frac{1}{2}(\hat{q}+q) \end{pmatrix}$$

Midpoint Discrete Gradient

$$\bar{\nabla}H(\hat{y},y) = \nabla H(\frac{1}{2}(\hat{y}+y)) + \frac{H(\hat{y}) - H(y) - \nabla H(\frac{1}{2}(\hat{y}+y))^T(\hat{y}-y)}{||\hat{y}-y||^2}(\hat{y}-y)$$

Bonus: Symmetric

Symplectic Integrators

Remember Sympectic Map:

$$\left(\frac{\partial\phi_t}{\partial z_0}\right)^t J \left(\frac{\partial\phi_t}{\partial z_0}\right) = J \text{ for all time, for all } z_0$$

One-step map

$$y_{k+1} = \Phi_h(y_k)$$

Method is symplectic if $\Phi_h(y_k)$ is a symplectic map

First Symplectic Integrator

Symplectic Euler Methods

$$p_{k+1} = p_k - hH_q(p_{k+1}, q_k)$$
$$q_{k+1} = q_k + hH_p(p_{k+1}, q_k)$$

or

$$p_{k+1} = p_k - hH_q(p_k, q_{k+1})$$
$$q_{k+1} = q_k + hH_p(p_k, q_{k+1})$$

(first order)

Why is it symplectic?

$$p_{k+1} = p_k - hH_q(p_{k+1}, q_k)$$
$$q_{k+1} = q_k + hH_p(p_{k+1}, q_k)$$

Differentiate wrt (p_k, q_k):

$$\begin{pmatrix} I + hH_{qp}^T & 0 \\ -hH_{pp} & I \end{pmatrix} \left(\frac{\partial(p_{k+1}, q_{k+1})}{\partial(p_k, q_k)} \right) = \begin{pmatrix} I & -hH_{qq} \\ 0 & I + hH_{qp} \end{pmatrix}$$

Verify:

$$\left(\frac{\partial(p_{k+1}, q_{k+1})}{\partial(p_k, q_k)} \right)^T J \left(\frac{\partial(p_{k+1}, q_{k+1})}{\partial(p_k, q_k)} \right) = J$$

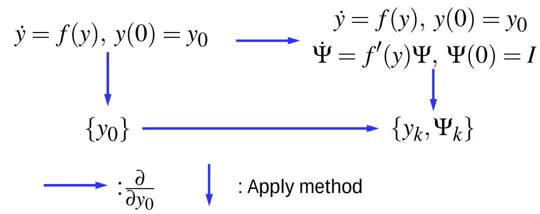
Another Famous One

Störmer-Verlet (2nd order)

$$p_{k+\frac{1}{2}} = p_k - \frac{h}{2} H_q(p_{k+\frac{1}{2}}, q_k)$$
$$q_{k+1} = q_k + \frac{h}{2}(H_p(p_{k+\frac{1}{2}}, q_k) + H_p(p_{k+\frac{1}{2}}, q_{k+1}))$$
$$p_{k+1} = p_{k+\frac{1}{2}} - \frac{h}{2} H_q(p_{k+\frac{1}{2}}, q_{k+1})$$

- Why?
- Bonus: symmetric

RK Methods (Lemma)



This diagram commutes (Proof: Explicit Euler)

Symplectic RK Methods

$$\dot{y} = J^{-1}\nabla H(y), \quad \dot{\Psi} = J^{-1}\nabla^2 H(y)\Psi$$

So $\Psi^T J \Psi$ is a quadratic 1st integral

- Proof!

RK methods that preserve quadratic first integrals are symplectic

- Implicit Midpoint included