CS 101

Numerical Geometric Integration

Patrick Mullen
Mathieu Desbrun

Today's Show

Three main points:

Pontryagin added to the mix

- mixing Lagrangian, Hamiltonian, and Legendre into a unifying approach

Non-conservative forces

Noether & Legendre in discrete world

Hamilton-Pontryagin

Continuous Hamilton-Pontryagin

$$\delta \int_0^T \big(p(\dot q - v) + L(q,v)\big)\, dt = 0$$

- equivalent to Hamilton's principle
- decouples velocity and position

Hamilton-Pontryagin

$$\delta \int_0^T \big(p(\dot q - v) + L(q,v)\big)\, dt = 0$$

Lagrange multiplier = momentum

- builds in the Legendre transformation, both Hamilton's configuration space and phase space principles
- synthesizes Lagrangian and Hamiltonian viewpoints
- closely related to Pontryagin's principle in optimal control

Hamilton-Pontryagin

Continuous Hamilton-Pontryagin

$$\delta \int_0^T \big(p(\dot q - v) + L(q,v)\big)\, dt = 0$$

Discrete version:

$$\delta \sum_{k=0}^{N} \left(h p_{k+1} \left(\frac{q_{k+1} - q_k}{h} - v_{k+1} \right) + L^d(q_k, v_{k+1}) \right) = 0$$

taking variations with respect to all discrete variables gives the algorithm for update

Derivations

Take variations w.r.t. all variables

$$\delta \sum_{k=0}^{N} \left(h p_{k+1} \left(\frac{q_{k+1} - q_k}{h} - v_{k+1} \right) + L^d(q_k, v_{k+1}) \right) = 0$$

$$\begin{aligned} \delta p: &\quad q_{k+1} - q_k = h v_{k+1} \\ \delta q: &\quad p_{k+1} - p_k = D_1 L^d(q_k, v_{k+1}) \\ \delta v: &\quad h\, p_{k+1} = D_2 L^d(q_k, v_{k+1}) \end{aligned}$$

Discrete Integration

Algorithm

- set initial q_0 and p_0
- solve for v_{k+1} (non-linear root finding)

$$D_2L^d(q_k,v_{k+1}) - h\,D_1L^d(q_k,v_{k+1}) - h\,p_k = 0$$

- explicit update

$$q_{k+1} = q_k + hv_{k+1}$$
$$p_{k+1} = D_2L^d(q_k,v_{k+1})/h$$

Fully Variational Update

Algorithm when $\exists P / D_2P(q_k,v_{k+1}) = D_1L^d(q_k,v_{k+1})$

- set initial q_0 and p_0
- solve for v_{k+1} (non-linear function minimization)

$$L^d(q_k,v_{k+1}) - hP(q_k,v_{k+1}) - hp_kv_{k+1}$$

- explicit update

$$q_{k+1} = q_k + hv_{k+1}$$
$$p_{k+1} = D_2L^d(q_k,v_{k+1})/h$$

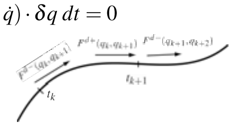
Back to Regular Hamilton's

Treatment of non-conservative forces

- remember Lagrange-d'Alembert?

$$\delta \int_0^T L(q,\dot{q})dt + \int_0^T F(q,\dot{q}) \cdot \delta q\, dt = 0$$

- discrete version

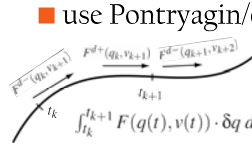


$$D_2L(q_{k-1},q_k) + D_1L(q_k,q_{k+1}) + F^{d-}(q_{k-1},q_k) + F^{d+}(q_k,q_{k+1}) = 0$$

Non-Conservative Systems w/ HP

Full control over dissipation forces too

- use Pontryagin/d'Alembert principle

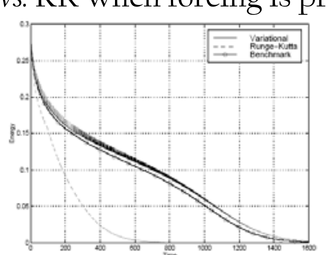


$$\int_{t_k}^{t_{k+1}} F(q(t),v(t)) \cdot \delta q\, dt \approx F^{d-}(q_k,v_{k+1}) + F^{d+}(q_k,v_{k+1})$$

- can be used to add a damping model
  - damping not a side effect of bad numerics
  - captures energy decay correctly

Benefit on Numerics

VarInt *vs.* RK when forcing is present



Discrete Noether Theorem

Discrete Invariance to translation?

$$L(q_k + \varepsilon T, v_{k+1}) = L(q_k, v_{k+1}) \qquad T = (\mathbf{t}\ldots\mathbf{t})^t$$

- variation w.r.t ε

$$D_1L(q_k,v_{k+1}) \cdot T = 0$$

- Therefore:

$$D_2L(q_k,v_{k+1}) \cdot T = D_2L(q_{k-1},v_k) \cdot T$$

  - proof?

Discrete Noether Theorem

Discrete Invariance to Rotations?

$$L(R_\omega(\varepsilon)q_k, R_\omega(\varepsilon)v_{k+1}) = L(q_k, v_{k+1})$$

- same deal

$$D_1L(q_k, v_{k+1}) \cdot (\omega \times q_k) + D_2L(q_k, v_{k+1}) \cdot (\omega \times v_{k+1}) = 0$$

- thus:

$$(D_2L(q_k, v_{k+1}) \times q_{k+1}) \cdot \begin{pmatrix} \omega \\ \vdots \\ \omega \end{pmatrix} = (D_2L(q_{k-1}, v_k) \times q_k) \cdot \begin{pmatrix} \omega \\ \vdots \\ \omega \end{pmatrix}$$

  - remember: triple product rule!

Discrete Noether Theorem

More generally

- if the discrete Lagrangian $L : Q \times Q \to \mathbb{R}$ is (infinitesimally) invariant under a (left or right) action, there's an associated discrete momentum exactly preserved

More Properties [Marsden & West '01]

Discrete Legendre Transforms

$$\mathbb{F}^+ L_d : (q_0, q_1) \mapsto (q_1, p_1) = (q_1, D_2L_d(q_0, q_1))$$
$$\mathbb{F}^- L_d : (q_0, q_1) \mapsto (q_0, p_0) = (q_0, -D_1L_d(q_0, q_1))$$

- equivalent in the limit

Symmetry of discrete Lagrangian?

- $L(q_k, q_{k+1}, h) = -L(q_{k+1}, q_k, -h)$
  - then DEL is symmetric
    - thus time reversible, and even order