CS 101

Numerical Geometric Integration

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Today: More Symplecticity

We've seen some examples

- Symplectic Euler, Stormer-Verlet, implicit midpoint

Generating Functions

- Continuous & discrete picture

Variational Integrators

- Another approach to symplecticity

Condition of Symplecticity

$$(p,q) \rightarrow (\hat{P}(p,q), \hat{Q}(p,q))$$

Initial condition — Final state

When is it symplectic?

$$\left(\frac{\partial(\hat{P},\hat{Q})}{\partial(p,q)}\right)^T J \left(\frac{\partial(\hat{P},\hat{Q})}{\partial(p,q)}\right) = J$$

Let's (i.e. you) write it out…

Condition of Symplecticity

$$\hat{P}_p^T \hat{Q}_p = \hat{Q}_p^T \hat{P}_p$$

$$\hat{Q}_q^T \hat{P}_q = \hat{P}_q^T \hat{Q}_q$$

Just says these quantities are symmetric

$$\hat{P}_p^T \hat{Q}_q - I = \hat{Q}_p^T \hat{P}_q$$

$(\hat{P}(p,q), \hat{Q}(p,q))$ is symplectic iff these are true

Condition of Symmetry

Out of the blue:

$$f(p,q) = \hat{P}^T \nabla \hat{Q} - p^T \nabla q$$

If $\nabla f(p,q)$ is symmetric then*

$$f(p,q) = \nabla S(p,q)$$

for some S

- When is this $\nabla f(p,q)$ symmetric?
  - First step: $\nabla \hat{Q} = \hat{Q}_p \nabla p + \hat{Q}_q \nabla q$

Same Conditions

Symmetry of $\nabla f(p,q)$ same as symplecticity of $(\hat{P},\hat{Q})$!

So what?

- $S(p,q)$ exists iff map is symplectic

Change of variable*: $S(q,\hat{Q})$

$$\nabla S(q,\hat{Q}) = \frac{\partial S}{\partial q}\nabla q + \frac{\partial S}{\partial \hat{Q}}\nabla \hat{Q}$$

Generating Function

$$\nabla S(q,\hat{Q}) = \frac{\partial S}{\partial q}\nabla q + \frac{\partial S}{\partial \hat{Q}}\nabla \hat{Q}$$
$$= \hat{P}^T \nabla \hat{Q} - p^T \nabla q = f(p,q)$$
$$\hat{P}^T = \frac{\partial S}{\partial \hat{Q}}(q,\hat{Q}) \qquad p^T = -\frac{\partial S}{\partial q}(q,\hat{Q})$$

- Any [smooth] $S(q,\hat{Q})$ "generates" a symplectic map $(p,q) \to (\hat{P}(p,q),\hat{Q}(p,q))$
- Similar for $S(q,\hat{P})$, $S(p,\hat{Q})$, etc.

How is this useful?

One useful variant: $S(q,\hat{P})$

$$\hat{Q}^T = \frac{\partial S}{\partial \hat{P}}(q,\hat{P}) \qquad p^T = \frac{\partial S}{\partial q}(q,\hat{p})$$

Take: $S = \bar{S} + \hat{P}^T q$

$$\hat{Q}^T = q^T + \frac{\partial \bar{S}}{\partial \hat{P}}(q,\hat{P}) \qquad \hat{P}^T = p^T - \frac{\partial \bar{S}}{\partial q}(q,\hat{P})$$

Try $\bar{S}(q,\hat{P}) = hH(q,\hat{P})$ We get symplectic Euler

Creating More Integrators

Choice of S gives integrator

- Symplectic euler, midpoint, RK
- More clever choices
  - See book
- All symplectic integrators have a generating function.

That Was Not Easy

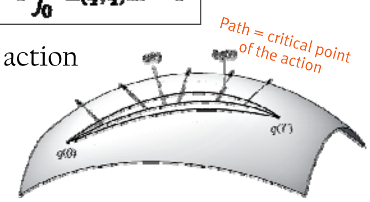
We're going to see this again....

Reminder

Physical path **extremizes** action

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

- stationary action

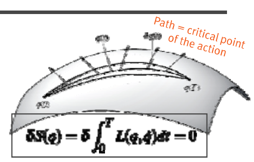


Variational Mechanics

Hamilton's Principle

Lagrangian: $L(q,\dot{q}) = K(\dot{q}) - W(q)$

Action: $S(q) = \int_0^T L(q,\dot{q})dt$



$$\delta S(q) = \delta \int_0^T L(q(t),\dot{q}(t))\,dt = \int_0^T \left[\frac{\partial L}{\partial q}\cdot\delta q + \frac{\partial L}{\partial \dot{q}}\cdot\delta\dot{q}\right] dt$$
$$= \int_0^T \left[\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)\right]\delta q\,dt + \left[\frac{\partial L}{\partial \dot{q}}\delta q\right]_0^T,$$

= 0

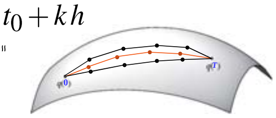
Euler-Lagrange Equation ≈ Newton's Second Law

Discrete Variational Mechanics

Hamilton's Stationary Action Principle:

a *discrete* dynamical system always finds an optimal course from one position to another

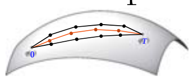
- discrete time $t_k = t_0 + kh$
- so path = "polyline"
- use same recipe!
  - but with variations of states $q_k := q(t_k)$



Discrete Variational Mechanics

Hamilton’s Stationary Action Principle:

- Discrete Lagrangian



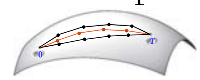
$$\int_{t_k}^{t_{k+1}} L(q,\dot{q})\,dt \approx L_d(q_k, q_{k+1})$$

  - obtained, for instance, through quadrature
    - $L_d(q_k,q_{k+1}) = hL\left(\frac{q_k+q_{k+1}}{2}, \frac{q_{k+1}-q_k}{h}\right)$

Discrete Variational Mechanics

Hamilton’s Stationary Action Principle:

- Discrete Action



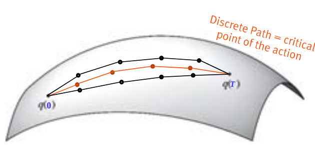
$$S_d(q) = \sum_{k=0}^{N} L_d(q_k, q_{k+1})$$

  - integral of L, like before $S(q) = \int_0^T L(q,\dot{q})\,dt$

Discrete Variational Mechanics

Hamilton’s Stationary Action Principle:

$$\delta S_d(q) = \delta \sum_{k=0}^{N} L_d(q_k, q_{k+1}) = 0$$



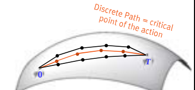
Discrete Variational Mechanics

Turning the crank:

Discrete Euler-Lagrange

$$D_1L_d(q_{k+1}, q_{k+2}) + D_2L_d(q_k, q_{k+1}) = 0$$

derivatives with respect to first or second variable



$$\delta S_d(q) = \delta \sum_{k=0}^{N} L_d(q_k, q_{k+1}) = 0$$

- must be true for each q_{k+1}
- so in particular…

solve DEL for time integration: $(q_k, q_{k+1}) \to q_{k+2}$

Summary

So Time Integration's a Breeze

- start from q_0 and q_1
  - can start with momemtum instead too
- use DEL $(q_k, q_{k+1}) \to q_{k+2}$
- iterate…

Discrete path optimal btw 0 and T

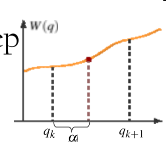
- discrete Hamilton's principle

Discrete Lagrangian: More Details

$$\int_{t_k}^{t_{k+1}} L(q,\dot{q})\,dt = \int_{t_k}^{t_{k+1}} [K(\dot{q}) - W(q)]\,dt$$

$$L_d(q_k,q_{k+1}) = h\left[\tfrac{1}{2}\left(\tfrac{q_{k+1}-q_k}{h}\right)^T M \left(\tfrac{q_{k+1}-q_k}{h}\right) - W((1-\alpha)q_k + \alpha q_{k+1})\right]$$

- integral over one time step
- use any quadrature
  - trapezoidal, midpoint, …
- discretize potential W



Simple Discrete Example

Let's try the free-falling mass again:

$$L_d(q_k, q_{k+1}) = h(\tfrac{1}{2}m(\tfrac{q_{k+1}-q_k}{h})^2 - mg\tfrac{q_k+q_{k+1}}{2})$$

midpoint quadrature

$$D_2 L_d(q_k, q_{k+1}) = m\frac{q_{k+1}-q_k}{h} - \frac{hmg}{2}$$

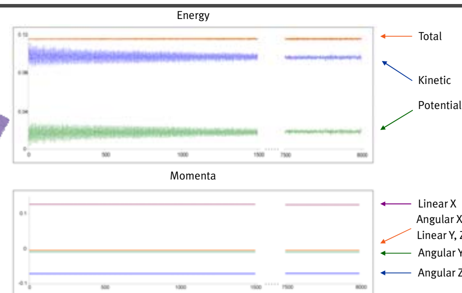
$$D_1 L_d(q_{k+1}, q_{k+2}) = -m\frac{q_{k+2}-q_{k+1}}{h} - \frac{hmg}{2}$$

So, we get:

$$D_1 L_d(q_{k+1}, q_{k+2}) + D_2 L_d(q_k, q_{k+1}) = 0 \Leftrightarrow \frac{q_{k+2}-2q_{k+1}+q_k}{h^2} = g$$

$$\ddot{q} = g$$

Conservation Laws



Where's Waldo?

The momentum p disappeared

- or did it?

Legendre transform to the rescue

- see slide 11 of lecture 3: $p = \frac{\partial L(q,\dot{q})}{\partial \dot{q}}$
- here: $p_n = -D_1 L(q_n, q_{n+1})$
- allows you to switch: $(p_n, q_n) \to (q_n, q_{n+1})$
  - perfect for initial conditions...

DEL in Momentum/Position

We can rewrite the DEL equations as:

$$p_n = -D_1 L(q_n, q_{n+1}) = D_2 L(q_{n-1}, q_n)$$

- rewrite one more time

$$p_{n+1} = \frac{\partial L}{\partial q_{n+1}}(q_n, q_{n+1}) \qquad p_n = -\frac{\partial L}{\partial q_n}(q_n, q_{n+1})$$

$$\hat{p}^T = \frac{\partial S}{\partial \hat{Q}}(q, \hat{Q}) \qquad p^T = -\frac{\partial S}{\partial q}(q, \hat{Q})$$

L is a generating function so these are symplectic!