CS 101

Numerical Geometric Integration

Patrick Mullen
Mathieu Desbrun

Today's Show

Lagrangian/Hamiltonian mechanics
- just an intro
  - pointing to geometric characteristics
  - presenting some crucial notions for later
  - but all in the continuous world for now
- not intended to be complete
  - restricted to conservative systems
  - we will extend it later when we need it!

Second Order Systems

Fundamental differential equation

$$\mathbf{F} = m\,\mathbf{a}$$

- Newtonian point of view
- second order in time

Introducing Lagrange and Hamilton…
- physical path has geometric properties
- rewrite foundations accordingly

Setup

Consider a dynamical system
- call its configuration q
  - generalized coordinates of the components of the system
    - positions, angles, …
- we need to describe $q(t)$
- "path" of the system in space-time

How to define the path given $q(0)$?

Core of Lagrangian Mechanics

Lagrangian function

$$L(q,\dot q) = K(\dot q) - W(q)$$

- K: kinetic energy $K(\dot q) = \frac{1}{2}\dot q^t M \dot q$
- W: potential energy
  - expression based on model
    - gravity, elasticity, …
- careful: integral over volume of system

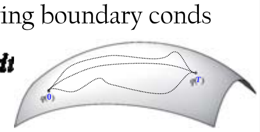
Variational Mechanics

Hamilton's Stationary Action Principle

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

Notion of Action
- scores paths satisfying boundary conds

$$S(q) = \int_0^T L(q,\dot q)\,dt$$

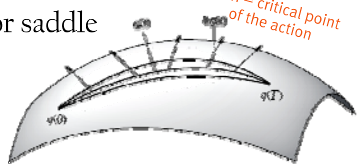


Path Property

Physical path **extremizes** action

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

- min, max, or saddle



Reminder

Calculus of Variations

- To derive this critical point condition...
- Assume a small variation (fixed ends)

$$q \rightsquigarrow q + \varepsilon \delta q$$

- Do Taylor expansion
- identify the linear terms in δq

$$\delta F = \lim_{\varepsilon \to 0} \frac{F(q+\varepsilon\delta q) - F(q)}{\varepsilon}$$

Euler-Lagrange Eqns

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

Consequence on physical path

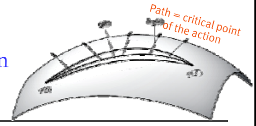
$$\delta S(q) = \delta \int_0^T L(q(t),\dot{q}(t))\,dt = \int_0^T \left[\frac{\partial L}{\partial q}\cdot \delta q + \frac{\partial L}{\partial \dot{q}}\cdot \delta \dot{q}\right] dt$$

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

$= 0$

Euler-Lagrange Equation

≈ Newton's Second Law!



Example of Euler-Lagrange

Falling mass (1D, with gravity):

- q: altitude
- Kinetic energy: $K(\dot{q}) = \frac{1}{2} m \dot{q}^2$
- Potential energy: $W(q) = m g q$
- Lagrangian: $L(q,\dot{q}) = K(\dot{q}) - W(q)$

Therefore, the equation of motion is:

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}}\right] = -mg - \frac{d}{dt}(m\dot{q}) = 0$$

$$-mg = m\ddot{q}$$

Hamiltonian Systems

Hamiltonian function $H(p,q)$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}$$

can (often) be deduced from Lagrangian through Legendre transformation

$$H(p,q) = p\dot{q} - \mathcal{L}(q,\dot{q})$$

with $p = \frac{\partial \mathcal{L}(q,\dot{q})}{\partial \dot{q}}$

- q = position
- p = momentum ("mass" times "velocity)
- H = total energy (kinetic + potential)

Phase space

p: generalized momentum

- for Cartesian coordinates: $p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$
  - usual linear momenta

Phase space simple

$$q = (q_1, q_2, \ldots, q_n)$$
$$p = (p_1, p_2, \ldots, p_n)$$
$$z := (p_1, p_2, \ldots, p_n, q_1, q_2, \ldots, q_n)^T$$

Notice then that:

$$\dot{z} = J^{-1}\nabla H(z) \text{ with } J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$$

Conservation

Take time derivative of Hamiltonian

$$\frac{dH}{dt} = \frac{\partial H}{\partial p}\frac{dp}{dt} + \frac{\partial H}{\partial q}\frac{dq}{dt}$$

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$$= \frac{\partial H}{\partial p}\frac{\partial H}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial H}{\partial p} = 0$$

- the Hamiltonian is constant of motion
- value implied by initial conditions

Simple Example

Spring of mass m and stiffness k

$$H(p,q) = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

Equations of motion:

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \qquad \dot{p} = -\frac{\partial H}{\partial x} = -kx$$

First Integrals

Advection in Hamiltonian flow

Poisson bracket

$$\{H,L\} = \sum_i \left(\frac{\partial H}{\partial p_i}\frac{\partial L}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial L}{\partial p_i}\right)$$

L is "**First Integral**" of Ham. system if

$$\{H,L\} = 0$$

- generally, physical quantities
  - angular momentum for 2-body problems
- if n integrals, system called integrable

HamiltonianFlow

For any initial condition (p_0, q_0),
call the *map*

$$\phi_t(p_0,q_0) = (p(t),q(t))$$

the "flow" of the system

Hamiltonian dynamics implies flows with special properties....

Symplecticity

In particular, the map is symplectic

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

First off, why?

- we know: $\left(\frac{\partial \phi_t}{\partial t}\right) = \frac{dz(t)}{dt} = J^{-1}\nabla H(z)$
- then: $\left(\frac{\partial \dot{\phi}_t}{\partial z_0}\right) = J^{-1}\nabla^2 H(\phi_t(z_0)) \left(\frac{\partial \phi_t}{\partial z_0}\right)$
- we thus derive: $\frac{d}{dt}\left[\left(\frac{\partial \phi_t}{\partial z_0}\right)^t J \left(\frac{\partial \phi_t}{\partial z_0}\right)\right] = 0$
  - just expand
  - use symmetry of Hessian, antisymmetry of J

Now, What Does It Mean?

Notion of area

$$\text{area}(u,v) = u \times v = u_1 v_2 - u_2 v_1 = u^t J v$$

- area-preserving 2D linear map A iff

$$A^t J A = J$$

Simplecticity=extension to higher dims!

- area-preserv. over 2D cross-sections
- preservation of summed projected area
  - i.e., $\omega = \sum_i dq_i \wedge dp_i$

Consequences

For a pendulum (1 variable)

- if you start off a set of trajectories occupying some region in phase space, that region may get distorted but it will maintain its area

More complex for more variables

- volume in phase space preserved too!

A Look Back

Why Is Euler's Bad?

$$\begin{aligned} H(x_{k+1}, p_{k+1}) &= \frac{p_{k+1}^2}{2m} + \frac{1}{2} k x_{k+1}^2 \\ &= \frac{1}{2m}(p_k - h k x_k)^2 + \frac{1}{2} k (x_k + h \frac{p_k}{m})^2 \\ &= H(x_k, p_k) + \frac{kh^2}{m}(\frac{p_k^2}{2m} + \frac{1}{2} k x_k^2) \\ &= H(x_k, p_k)[1 + \frac{kh^2}{m}] \end{aligned}$$

Look at What's Coming Up

General ODE methods not symplectic

- numerics don't mimic continuous world.

Guess what

- we'll develop methods that fix this
- ... and it will make a huge difference