Variational Integrators

Book Section VI.6

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Seminar on Geometric Numerical Integration

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Outline

Hamilton's Principle

- Lagrangian $L = T - U$
- Action

$$\mathcal{S}(q) = \int_{t_a}^{t_b} L(q(t), \dot{q}(t), t)dt$$

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The physical motion $q(t)$ extremizes $\mathcal{S}(q)$ under condition $q(t_a) = q_a$ and $q(t_b) = q_b$.

equivalent: Euler-Lagrange equation

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$$\mathcal{S}(q) = \int_{t_a}^{t_b} L(q(t), \dot{q}(t), t)dt = \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} L(q(t), \dot{q}(t), t)dt$$

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The physical motion $\{q_n\}_{n=0}^N$ extremizes, for given q_0 and q_N,

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where q extremizes the integral with $q(t_n) = q_n$, $q(t_n + h) = q_{n+1}$.

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for $n = 1, \ldots, N-1$.

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for $n = 1, \ldots, N-1$.
$\rightsquigarrow$ three-term difference scheme for q_{n+1}.

Construction of Variational Methods

Lemma

$$\frac{\partial}{\partial q_n} \int_{t_n}^{t_n+h} L(q(t), \dot{q}(t), t)dt = -p(t_n) \quad \left(= -\frac{\partial L}{\partial \dot{q}}(q_n, \dot{q}_n, t_n) \right)$$

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if $\partial_1 L_h(q_n, \cdot, t_n)$ is bijective

Variational Method

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Variational Method (simplified)

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Symplecticity of Variational Methods

Theorem

1. *The one-step method* $\Phi_h : (p_n, q_n) \mapsto (q_n, q_{n+1}) \mapsto (p_{n+1}, q_{n+1})$ *given by*

$$p_n = -\partial_1 L_h(q_n, q_{n+1}, t_n) \quad \text{and} \quad p_{n+1} = \partial_2 L_h(q_n, q_{n+1}, t_n)$$

is symplectic.

2. *Every symplectic method is a variational method.*

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Proof.

1. $p_n = -\partial_1 L_h(q_n, q_{n+1}, t_n)$, $p_{n+1} = \partial_2 L_h(q_n, q_{n+1}, t_n)$ imply Φ_h symplectic with generating function L_h.
2. every symplectic map has a generating function L_h.

□

Störmer-Verlet Method

Approximating the discrete Lagrangian

$$L_h(q_n, q_{n+1}, t_n) :\approx \int_{t_n}^{t_n+h} L(q(t), \dot{q}(t), t)dt$$

with the trapezoidal rule,

$$\frac{h}{2}L\left(q_n, \frac{q_{n+1}-q_n}{h}, t_n\right) + \frac{h}{2}L\left(q_{n+1}, \frac{q_{n+1}-q_n}{h}, t_n + h\right)$$

for a mechanical Lagrangian

$$L(q, \dot{q}, t) = \frac{1}{2}\dot{q}^{\mathsf{T}} M \dot{q} - U(q)$$

leads to

Störmer-Verlet Method

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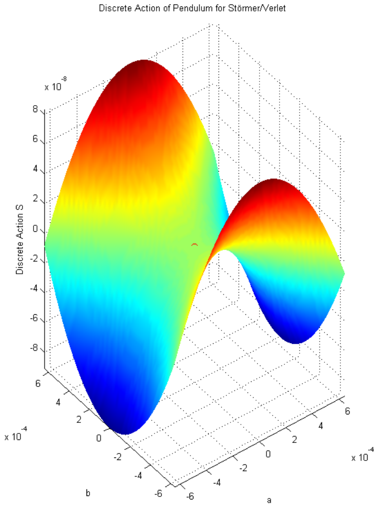
Störmer-Verlet Method

$$\begin{aligned} M v_{n+1/2} &= p_n - \frac{h}{2}\nabla U(q_n) \\ q_{n+1} &= q_n + h v_{n+1/2} \\ p_{n+1} &= M v_{n+1/2} - \frac{h}{2}\nabla U(q_{n+1}) \end{aligned}$$

Demonstration



Mathematical Pendulum with Störmer-Verlet method.

- solve ode
- add small cubic polynomials to solution
- calculate discrete action of all perturbations

The numerical solution should be an extremum.

Partitioned Runge-Kutta Methods for Hamiltonian systems

For partitioned systems such as

$$\dot{q} = \frac{\partial H}{\partial p}(p, q, t) \qquad \dot{p} = -\frac{\partial H}{\partial q}(p, q, t)$$

$$q_1 = q_0 + h\sum_{i=1}^{s} b_i\dot{Q}_i \qquad p_1 = p_0 + h\sum_{i=1}^{s} \hat{b}_i\dot{P}_i$$

$$Q_i = q_0 + h\sum_{j=1}^{s} a_{ij}\dot{Q}_j \qquad P_i = q_0 + h\sum_{j=1}^{s} \hat{a}_{ij}\dot{P}_j$$

$$\dot{Q}_i = \frac{\partial H}{\partial p}(P_i, Q_i, t_i) \qquad \dot{P}_i = -\frac{\partial H}{\partial q}(P_i, Q_i, t_i)$$

Symplecticity conditions:

$$a_{ji}\hat{b}_j + \hat{a}_{ij}b_i = b_i\hat{b}_j \qquad b_i = \hat{b}_i$$

Ansatz for Discrete Lagrangian

- $L_h(q_0, q_1, t_0) = h \sum_{i=1}^{s} b_i L(Q_i, \dot{Q}_i, t_i)$
- $t_i = t_0 + h \sum_{j=1}^{s} a_{ij}$
- $Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} \dot{Q}_j$
- $\dot{Q}_i$ extremize the first sum under condition

  $$q_1 = q_0 + h \sum_{i=1}^{s} b_i \dot{Q}_i$$

Equivalent Formulation as Partitioned RK Method

The following methods are equivalent:

Variational Method

- $L_h = h\sum_i b_i L(Q_i, \dot{Q}_i, t_i)$
- $Q_i = q_0 + h\sum_j a_{ij}\dot{Q}_j$
- $q_1 = q_0 + h\sum_i b_i\dot{Q}_i$
- $\dot{Q}_i$ extremize $\sum_i b_i L(Q_i, \dot{Q}_i, t_i)$

Partitioned RK Method

- $q_1 = q_0 + h\sum_i b_i\dot{Q}_i$
  $p_1 = p_0 + h\sum_i b_i\dot{P}_i$
- $Q_i = q_0 + h\sum_j a_{ij}\dot{Q}_j$
  $P_i = q_0 + h\sum_j \hat{a}_{ij}\dot{P}_j$
- $\dot{Q}_i = \frac{\partial H}{\partial p}(P_i, Q_i, t_i)$
  $\dot{P}_i = -\frac{\partial H}{\partial q}(P_i, Q_i, t_i)$
- $a_{ji}b_j + \hat{a}_{ij}b_i = b_i b_j$

Noether's Theorem

Theorem

Let $\{g_\epsilon; \epsilon \in \mathbb{R}\}$ be a one-parameter group of transformations and

$$I(p,q) := p^\mathsf{T} \frac{d}{d\epsilon}\Big|_{\epsilon=0} g_\epsilon(q) \ .$$

1. *If for all ϵ, q, $\dot{q}$ and t*

$$L(g_\epsilon(q), g'_\epsilon(q)\dot{q}, t) = L(q, \dot{q}, t) \ ,$$

   then $I(p,q)$ is a first integral of the Hamiltonian system.

2. *If for all ϵ, q_0, q_1 and t_0*

$$L_h(g_\epsilon(q_0), g_\epsilon(q_1), t_0) = L_h(q_0, q_1, t_0) \ ,$$

   then $I(p,q)$ is a first integral of the method Φ_h.

Existence of First Integrals

If conditions of the cont. Noether Theorem are satisfied:

Theorem

All symplectic partitioned Runge-Kutta methods conserve integrals of the form

$$I(p,q) = p^{\mathsf{T}}(Aq + w)\ .$$

In particular, linear and angular momenta are conserved.

Theorem

For a mechanical Lagrangian $L = \frac{1}{2}\dot{q}^{\mathsf{T}} M \dot{q} - U(q)$ *, the Störmer-Verlet method conserves all first integrals*

$$I(p,q) = p^{\mathsf{T}} \frac{d}{d\epsilon}\Big|_{\epsilon=0} g_\epsilon(q)\ .$$

Summary

- Discretization of Hamilton's principle leads to the discrete Euler-Lagrange equation and variational methods.
- Variational methods are characterized by their discrete Lagrangians.
- Variational methods are exactly symplectic one-step methods.
- Symplectic partitioned Runge-Kutta methods can be described as variational methods.
- The discrete Noether theorem describes a connection between symmetries of the discrete Lagrangian and first integrals of variational methods.