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VARIATIONAL INTEGRATORS FOR HIGHER ORDER DIFFERENTIAL EQUATIONS[*1)]

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Abstract

We analyze three one parameter families of approximations and show that they are symplectic in Lagrangian sence and can be related to symplectic schemes in Hamiltonian sense by different symplectic mappings. We also give a direct generalization of Veselov variational principle for construction of scheme of higher order differential equations. At last, we present numerical experiments.

Key words: Variational integrator, Symplectic mapping

1. Introduction

The two main formalisms of mechanics are Lagrangian mechanics based on variational principle and Hamiltonian mechanics based on symplectic structure of cotangent bundle. In many cases two formalisms are equivalent. For a mechanical system once a n-dimensional configuration space Q is chosen, then its Lagrangian flow F_t is defined on the tangent bundle TQ with its coordinates $(q_i, \dot{q}_i)$ and its Hamiltonian flow G_t is defined on cotangent bundle T^*Q with its coordinates (p_i, q_i). The equivalence between these two flows is realized by the well known Legendre transformation $FL : TQ \longrightarrow T^*Q$, which depends on the Lagrangian function $L : TQ \longrightarrow R$ and is a local diffeomorphism in general. Consequently, we have the following commutative diagram

$$\begin{tikzcd} TQ \arrow[r, "F_t"] \arrow[d, "FL"'] & TQ \arrow[d, "FL"] \\ T^*Q \arrow[r, "G_t"'] & T^*Q \end{tikzcd}$$

$FL^{-1} \circ G_t \circ FL = F_t$, F_t preserves the symplectic form $\omega_L = FL^*\omega$, i.e., $F_t^*\omega_L = \omega_L$, in canonical coordinates,

$$\omega_L = \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j} dq_i \wedge dq_j + \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} dq_i \wedge d\dot{q}_j.$$

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Note that $G_t^*\omega = \omega$, in canonical coordinates,

$$\omega = dq_i \wedge dp_i.$$

Taking $Q \times Q$ as the discrete version of TQ, we can define the specific discrete Legendre transformations $\mathbf{FL} : Q \times Q \longrightarrow T^*Q, \quad \mathbf{FL}(q^{n+1}, q^n) = (p^n, q^n)$ which are symplectic mappings between $Q \times Q$ and T^*Q, and have the following commutative diagram

$$\begin{tikzcd} Q \times Q \arrow[r, "\mathbf{F}"] \arrow[d, "\mathbf{FL}"'] & Q \times Q \arrow[d, "\mathbf{FL}"] \\ T^*Q \arrow[r, "\mathbf{G}"'] & T^*Q \end{tikzcd}$$

therefore, the discrete Lagrangian flow $\mathbf{F}$ preserves the symplectic form $\omega_{\mathbf{L}} = \mathbf{FL}^*\omega$, i.e., $\mathbf{F}^*\omega_{\mathbf{L}} = \omega_{\mathbf{L}}$, in canonical coordinates,

$$\omega_{\mathbf{L}} = \frac{\partial^2 \mathbf{L}(q^{n+1}, q^n)}{\partial q_i^{n+1} \partial q_j^n} dq_i^n \wedge dq_j^{n+1}.$$

Note that the discrete Hamiltonian flow $\mathbf{G}$ preserves the canonical symplectic form, i.e., $\mathbf{G}^*\omega = \omega$, in canonical coordinates,

$$\omega = dq_i^n \wedge dp_i^n.$$

In [1] Veselov developed a variational way to construct numerical integrators for Lagrangian mechanical systems based on a discretization of Hamilton's principle. Such an integrator is derived from the corresponding discrete Euler-Lagrange equations and preserves some symplectic forms on the discrete tangent space. The idea was highlighted by Marsden et al in [2] where the "variational integrators" of Veselov type were generalized to PDEs for field theory in the framework of multisymplectic geometry. Variational integrators often enjoy some amazing properties such as the preservation of the integrability of mechanical systems. In the case of Hamiltonian mechanics, however, symplectic integrators have been extensively studied and some nice results in both quantitative and qualitative aspects of numerical analysis are obtained. Therefore, it is interesting to bridge the gap between the variational integrators and symplectic ones, which should be an analogue to the continuous case as described above.

An outline of the paper is as follows. The variational descriptions of one parameter families of approximations studied in [3] for mechanical systems are presented in section 2. A direct generalization to higher order differential equations of Euler-Lagrange type is given in section 3. In section 4, we give some numerical results.

2. Variational descriptions of symplectic integrators

Consider the following system of ODEs

$$M\frac{\partial^2 q}{\partial t^2} = -\frac{\partial V(q)}{\partial q} = F(q), \tag{1}$$

where q is the collective position vector, M is a positive symmetric matrix and F is the collective force vector. (1) can be rewritten as following two equivalent forms

$$\dot{q} = M^{-1}p, \qquad \dot{p} = -\frac{\partial V(q)}{\partial q} \tag{2}$$

and

$$\frac{\partial L}{\partial q} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}, \tag{3}$$

where $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$.