Symmetries and variational calculation of discrete Hamiltonian systems*

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We present a numerical simulation method of Noether and Lie symmetries for discrete Hamiltonian systems. The Noether and Lie symmetries for the systems are proposed by investigating the invariance properties of discrete Lagrangian in phase space. The numerical calculations of a two-degree-of-freedom nonlinear harmonic oscillator show that the difference discrete variational method preserves the exactness and the invariant quantity.

Keywords: discrete Hamiltonian systems, discrete variational integrators, symmetry, conserved quantity

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1. Introduction

Noether theorem reveals that the conserved quantities can be obtained by the corresponding Noether symmetries.[1] The Noether symmetry has gained considerable attention from many researchers, such as Djukic and Vujanovic,[2] and Sarlet and Cantrijn.[3] Lutzky[4,5] proposed the definition of Lie symmetry on the basis of extended Lie groups which leave the differential equation invariant. Mei[6] derived a new type of symmetry (called the form invariance or Mei symmetry) which is different from the Noether symmetry and Lie symmetry. Symmetries are the intrinsic and fundamental features of the differential equations of mathematical physics.[7,8]

Discrete systems defined by difference equations provide us with a potentially powerful way to deal with model dynamics in real-world problems.[9] Due to the theoretical significance of the symmetries and the first integrals, there have been many attempts to develop discrete symmetries and conserved quantities. Logan[10] and Dorodnitsyn[11] constructed the discrete Noether theorem by studying the difference Lagrangian systems. Dorodnitsyn and Kozlov[12] also gave the Noether theorem of difference Hamiltonian systems. Fu[13] devised a discrete variational principle and a method to build first integrals for finite-dimensional Lagrange–Maxwell mechanico-electrical systems and extended discrete Noether symmetries to mechanico-electrical dynamical systems. Levi *et al.*[14] proposed a method to find the Lie point symmetry transformations, acting simultaneously on difference equations and lattices. Xia and Chen[15] studied the Mei symmetries and constructed the discrete versions of Noether conserved quantities for non-conservative Hamiltonian systems.

Variational integrators often perform better than their non-variational counterparts. Simulations and animations using these integrators usually have great physical and visual fidelity with low computing cost.[16] Cadzow[17] presented a discrete variational principle and obtained the discrete Euler–Lagrange equation. Wendlandt and Marsden[18] developed the numerical implementation of discrete mechanics on the basis of discrete variational principle. Extensive research has been extended to study the discrete variational principle, which has been reviewed by Marsden *et al.*,[19] Kane *et al.*,[20] and Cortés and Martínez.[21] Guo and his cooperators[22] obtained the difference discrete variational principle, which both keeps the advantages of Lie's and Veselov's methods. This method can be applied to the Lagrangian mechanical systems,[23] the Hamiltonian mechanical systems,[24] the nonholonomic systems,[25] and the field theory.[26] However, there has been no sufficient investigation of the symmetries and discrete variational calculation based on the difference discrete variational principle. Liu[27] studied the discrete variational calculation of Birkhoffian systems and reached the conclusion that the discrete method is as effective as a symplectic scheme. Zhang *et al.*[28] investigated the invariance properties of the discrete Lagrangian in phase space by discretizing the phase $(\boldsymbol{p}, \boldsymbol{q})$ and showed the discrete version of Noether's theorem for Hamiltonian systems. However, the numerical simulation method of solving symmetric problems is lacking. In the present work,

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we study the difference discrete variational principle and the Lie point symmetry on the base of the Lie group transformation on the discretization of the phase space $(t, \boldsymbol{p}, \boldsymbol{q})$ and apply it to a harmonic oscillator system. This paper also demonstrates that the Lie symmetry of the Hamiltonian systems can lead to discrete Noether conserved quantities indirectly. Finally, the numerical curves of these symmetries of discrete Hamilton systems can be obtained.

This paper is organized as follows In Section 2, the Hamilton's equations and the variational integrators are recalled on the discretization of both time and space. In Section 3, the Lie group transformations acting both on the difference equations and the lattice are considered. The determining equations of Lie symmetry are derived for the systems by using the Lie point symmetries. In Section 4, the discrete version of gauge functions and the Noether conserved quantities are constructed via the Logan's method. In Section 5, the numerical calculation of a two-degree-of-freedom nonlinear harmonic oscillator shows that the difference discrete variational method preserves a symplectic form and invariant quantity. Section 6 draws the conclusion of the present paper.

2. Discrete variational integrators in Hamiltonian formalism

Let Q denote the configuration space with coordinates q_i, and T^*Q the phase space with coordinate (p_i, q_i), where $i = 1, 2, \ldots, n$. Consider the extended phase space $R \times T^*Q$ with coordinates (t, q_i, p_i). We use $P \times P$ for discrete version of $R \times T(T^*Q)$. Here P is the discrete version of $R \times T^*Q$. A discrete L is defined as $L_{\rm d}$: $P \times P \to R$. According to the discrete variational principle in total variation of the correspond action, the discrete Hamiltonian canonical equations and the discrete energy conservation law are[24]

$$\begin{aligned}
&(t_{k+1}-t_k)D_2L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+(t_k-t_{k-1})D_5L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (1)\\
&(t_{k+1}-t_k)D_3L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+(t_k-t_{k-1})D_6L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (2)\\
&(t_{k+1}-t_k)D_1L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+(t_k-t_{k-1})D_4L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\\
&-L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (3)
\end{aligned}$$

where D_i denotes the partial derivative of $L_{\rm d}$ with respect to the i-th argument. The $2n$ equations (Eqs. (1) and (2)) are first-order difference equations, which are the discrete Hamilton canonical equations, also called variational integrators. In the continuous limit, that is, the time $t \in T \simeq R$, the generalized coordinates q_s $(s = 1, 2, \ldots, n)$ and p_s vary continuously with time, both equations (1) and (2) become the differential Euler equation. Equation (3) is the discrete energy conservation law associated to Eqs. (1) and (2). It defines the lattice on which the canonical Hamiltonian equations are discretized. In the continuous limit, the lattice equation disappears. The discrete flow determined by Eqs. (1)–(3) preserves a discrete version of extended canonical two-form ω. Chen *et al.*[24] have proved that the integrator determined by Eqs. (1) and (2) is a symplectic energy integrator. One proof can be achieved by a straightforward calculation. We can also draw the conclusion via an example of numerical calculations in Section 5.

There are different types of equations according to different Lagrangian schemes for Eqs. (1)–(3). Suppose that $L_{\rm d}$ is obtained by approximating the action function associated with a given Lagrangian[29]

$$\begin{aligned}
&L_{\rm d}^{\alpha}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&=((1-\alpha)p_k+\alpha p_{k+1})\frac{q_{k+1}-q_k}{t_{k+1}-t_k}\\
&\quad -H((1-\alpha)q_k+\alpha q_{k+1},(1-\alpha)p_k+\alpha p_{k+1}), \quad (4)
\end{aligned}$$

where $h \in R^+$ is the time step and $\alpha \in [0, 1]$ is a real parameter. Equations (1) and (2) can be written as

$$\begin{aligned}
&(1-\alpha)(p_{k-1}-p_k)+\alpha(p_k-p_{k+1})\\
&-(t_{k+1}-t_k)D_2H(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&-(t_k-t_{k-1})D_5H(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (5)\\
&(1-\alpha)(q_{k+1}-q_k)+\alpha(q_k-q_{k-1})\\
&-(t_{k+1}-t_k)D_3H(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&-(t_k-t_{k-1})D_6H(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0. \quad (6)
\end{aligned}$$

Equation (3) can be expressed as

$$\begin{aligned}
&((1-\alpha)p_k+\alpha p_{k+1})\frac{q_{k+1}-q_k}{t_{k+1}-t_k}\\
&-L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&-((1-\alpha)p_{k-1}+\alpha p_k)\frac{q_k-q_{k-1}}{t_k-t_{k-1}}\\
&+L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (7)
\end{aligned}$$

which is the energy-conserved quantity

$$\begin{aligned}
&H(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&-H(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0. \quad (8)
\end{aligned}$$

Different discrete schemes can be obtained by choosing α correctly. Dorodnitsyn and Kozlov[12] obtained the difference Hamiltonian equations in the case of $\alpha = 1/2$ in Eqs. (5)–(7).

3. Lie symmetry of discrete Lagrangian in phase space

The first steps in the construction of Lie symmetries for difference equations were taken by Maeda in 1980,[30] and later extended by Levi and Winternitz,[31] and Dorodnitsyn and Winternitz.[32] Based on these, the Lie point symmetry of the discrete Hamiltonian systems is proposed.

In what follows, the case of one independent variable t_k and depended variable $q_{i,k}$ and $p_{i,k}$ will be considered

$$t_k^* = t + \varepsilon\tau_k, \quad q_{i,k}^* = q_{i,k} + \varepsilon\xi_{i,k}, \quad p_{i,k}^* = p_{i,k} + \varepsilon\eta_{i,k}, \tag{9}$$

where ε is a small parameter, the infinitesimal generators $\tau_k = \tau(t_k, q_{i,k}, p_{i,k})$, $\xi_{i,k} = \xi_i(t_k, q_{i,k}, p_{i,k})$, and $\eta_{i,k} = \eta_i(t_k, q_{i,k}, p_{i,k})$ are the sequences depending on t_k, $q_{i,k}$, and $p_{i,k}$. The prolongation of the Lie group operator (5) is expressed as follows:[32]

$$\begin{aligned}\mathrm{Pr}X \;=\; & \tau_k\frac{\partial}{\partial t_k} + \xi_{i,k}\frac{\partial}{\partial q_{i,k}} + \eta_{i,k}\frac{\partial}{\partial p_{i,k}} + \tau_{k-1}\frac{\partial}{\partial t_{k-1}} \\ & + \xi_{i,k-1}\frac{\partial}{\partial q_{i,k-1}} + \eta_{i,k-1}\frac{\partial}{\partial p_{i,k-1}} + \tau_{k+1}\frac{\partial}{\partial t_{k+1}} \\ & + \xi_{i,k+1}\frac{\partial}{\partial q_{i,k+1}} + \eta_{i,k+1}\frac{\partial}{\partial p_{i,k+1}},\end{aligned} \tag{10}$$

where $\tau_{k+1} = \tau(t_{k+1}, q_{k+1}, p_{k+1})$, $\xi_{i,k+1} = \xi_i(t_{k+1}, q_{k+1}, p_{k+1})$, $\eta_{i,k+1} = \eta_i(t_{k+1}, q_{k+1}, p_{k+1})$, $\tau_{k-1} = \tau(t_{k-1}, q_{k-1}, p_{k-1})$, $\xi_{i,k-1} = \xi_i(t_{k-1}, q_{k-1}, p_{k-1})$, and $\eta_{i,k-1} = \eta_i(t_{k-1}, q_{k-1}, p_{k-1})$. For simplification, we obtain

$$\begin{aligned}\Pi_1 \;=\; & (t_{k+1} - t_k)D_2L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + (t_k - t_{k-1})D_5L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}),\end{aligned} \tag{11}$$

$$\begin{aligned}\Pi_2 \;=\; & (t_{k+1} - t_k)D_3L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + (t_k - t_{k-1})D_6L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}),\end{aligned} \tag{12}$$

$$\begin{aligned}\Pi_3 \;=\; & (t_{k+1} - t_k)D_1L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + (t_k - t_{k-1})D_4L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}) \\ & - L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}).\end{aligned} \tag{13}$$

The requirement is that equations (11)–(13), which are invariant under the considered group, are translated into

$$\mathrm{Pr}X\prod_\rho|_{\Pi_1=0,\Pi_2=0,\Pi_3=0} = 0, \quad \rho = 1,2,3. \tag{14}$$

Equation (14) is the discrete determining equations of Lie symmetry for Hamiltonian systems.

Definition 1 If the infinitesimal generators τ_k, $\xi_{i,k}$, and $\eta_{i,k}$ satisfy the determining equation (14), then the symmetry is the Lie symmetry of discrete Hamiltonian systems (1)–(3).

4. Noether symmetry and conserved quantities

Conservation laws of the dynamical mechanical systems can always be obtained by certain symmetries. Lie symmetries can have the Noether conserved quantities under certain conditions.[7] Using the analogy with the continuous case, many results[12,28,33] based on symmetries of discrete functions provide a simple and clear way to construct first integrals of difference Hamiltonian equations. In this section, we propose the discrete Noether theorem in Hamiltonian formalism $L_\mathrm{d} = L(t_k, t_{k+1}, q_k, q_{k+1}, p_k, p_{k+1})$. A systematic procedure for the establishment of the first integrals of the discrete Hamiltonian canonical equation can be developed from a direct study of the invariance properties of the discrete Lagrangian $L_\mathrm{d} = L(t_k, t_{k+1}, q_k, q_{k+1}, p_k, p_{k+1})$ in phase space.

Definition 2 If there exists a sequence $g(t_k, t_{k+1}, q_k, q_{k+1}, p_k, p_{k+1})$ such that

$$\delta L_\mathrm{d}(\varepsilon\tau, \varepsilon\xi, \varepsilon\eta) = \varepsilon\Delta g(t_k, t_{k+1}, q_k, q_{k+1}, p_k, p_{k+1}), \tag{15}$$

where

$$\begin{aligned}\delta L_\mathrm{d} \;=\; & (h_{k+1}D_2L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + h_kD_5L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}))\delta q_{i,k} \\ & + \Delta\left(-\delta q_{i,k-1}D_2L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k})\right) \\ & + (h_{k+1}D_3L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + h_kD_6L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}))\delta p_{i,k} \\ & + \Delta\left(-\delta p_{i,k-1}D_3L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k})\right) \\ & + (h_{k+1}D_1L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + h_kD_4L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}) \\ & - L_\mathrm{d}(t_k, q_{i,k}, p_{i,k}, t_{k+1}, q_{i,k+1}, p_{i,k+1}) \\ & + L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}))\delta t_{i,k} \\ & + \Delta\left(-\delta t_{i,k-1}D_1L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k})\right),\end{aligned} \tag{16}$$

where $h_{k+1} = t_{k+1} - t_k$ and $h_k = t_k - t_{k-1}$ for each k, then the discrete Lagrangian in phase space is difference invariance with respect to the infinitesimal transformation (9).

Conservation laws have a deep relevance because they express the conservation of physical quantities, such as mass, momentum, angular momentum, energy, and electrical charge. They are also important due to their use in investigating integrability, stability of solutions, or in implementing efficient numerical methods of integration. The point of the Noether theorem is that every symmetry (transformation) corresponds to a conserved quantity. The discrete analogues of Noether theorem for difference equations were reported in Refs. [9]–[12], [28], and [33].

Theorem 1 If the discrete Lagrangian L_d in phase space is difference invariance with respect to the infinitesimal transformations and equations (1)–(3) hold, then one has

$$\begin{aligned}I_{N,k} \;=\; & \xi_{i,k-1}D_2L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}) \\ & + \eta_{i,k-1}D_3L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}) \\ & + \tau D_1L_\mathrm{d}(t_{k-1}, q_{i,k-1}, p_{i,k-1}, t_k, q_{i,k}, p_{i,k}) + g.\end{aligned} \tag{17}$$

The difference equations (17) are called the discrete counterparts of Noether conservation laws for the discrete Hamiltonian systems. If a discrete regular function $g_{i,k} = g(t_k, t_{k+1}, q_{i,k}, q_{i,k+1}, p_{i,k}, p_{i,k+1})$ exists such that the infinitesimal transformation generators τ_k, $\xi_{i,k}$, and $\eta_{i,k}$ satisfy the discrete Noether identity (15), then the systems possess the discrete conserved quantities (17).

Proof The variation of $L_{\rm d}$ is the linear part of the increments of ε

$$L_{\rm d}(t_k^*,t_{k+1}^*,q_k^*,q_{k+1}^*,p_k^*,p_{k+1}^*)-L_{\rm d}(t_k,t_{k+1},q_k,q_{k+1},p_k,p_{k+1}). \tag{18}$$

Denote this variation by $\delta L_{\rm d}(\delta t_k,\delta q_{i,k},\delta p_{i,k})$, then

$$\begin{aligned}
&\delta L_{\rm d}(\delta t_k,\delta q_{i,k},\delta p_{i,k})\\
&=\left.\frac{\partial L_{\rm d}(t_k,t_{k+1},q_{i,k},q_{i,k+1},p_{i,k},p_{i,k+1})}{\partial\varepsilon}\right|_{\varepsilon=0}\\
&\quad+D_3L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\delta q_{i,k}\\
&\quad+D_4L_{\rm d}(t_{k+1},q_{i,k+1},p_{i,k+1},t_{k+2},q_{i,k+2},p_{i,k+2})\delta q_{i,k+1}\\
&\quad+D_5L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\delta p_{i,k}\\
&\quad+D_6L_{\rm d}(t_{k+1},q_{i,k+1},p_{i,k+1},t_{k+2},q_{i,k+2},p_{i,k+2})\delta p_{i,k+1}\\
&\quad+D_1L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\delta t_k\\
&\quad+D_2L_{\rm d}(t_{k+1},q_{i,k+1},p_{i,k+1},t_{k+2},q_{i,k+2},p_{i,k+2})\delta t_{k+1}.
\end{aligned} \tag{19}$$

A procedure analogous to the integration by parts in classical calculus of variations can be performed on Eq. (19) using the method of the monograph.[34] For $L_{\rm d}=L(t_k,t_{k+1},q_k,q_{k+1},p_k,p_{k+1})$, $\delta L_{\rm d}(\delta t_k,\delta q_{i,k},\delta p_{i,k})$ can be expressed as

$$\begin{aligned}
\delta L_{\rm d}\ =\ &(h_{k+1}D_2L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+h_kD_5L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}))\delta q_{i,k}\\
&+\Delta\left(-\delta q_{i,k-1}D_2L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)\\
&+(h_{k+1}D_3L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+h_kD_6L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}))\delta p_{i,k}\\
&+\Delta\left(-\delta p_{i,k-1}D_3L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)\\
&+(h_+D_1L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+h_-D_4L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\\
&-L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}))\delta t_{i,k}\\
&+\Delta\left(-\delta t_{i,k-1}D_1L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right).
\end{aligned} \tag{20}$$

Considering Eqs. (15) and (20), we have

$$\begin{aligned}
&(h_{k+1}D_2L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+h_kD_5L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}))\delta q_{i,k}\\
&+\Delta\left(-\delta q_{i,k-1}D_2L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)\\
&+(h_{k+1}D_3L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+h_kD_6L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}))\delta p_{i,k}\\
&+\Delta\left(-\delta p_{i,k-1}D_3L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)\\
&+(h_{k+1}D_1L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+h_kD_4L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\\
&-L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})\\
&+L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}))\delta t_{i,k}\\
&+\Delta\left(-\delta t_{i,k-1}D_1L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)=\varepsilon\Delta g.
\end{aligned} \tag{21}$$

Utilizing Eqs. (1)–(3) yields

$$\begin{aligned}
&\Delta\left(\delta q_{i,k-1}D_2L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)\\
&+\Delta\left(\delta p_{i,k-1}D_3L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)\\
&+\Delta\left(\delta t_{i,k-1}D_1L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\right)+\Delta g=0.
\end{aligned} \tag{22}$$

That is,

$$\begin{aligned}
&\Delta(\delta q_{i,k-1}D_2L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\\
&+\delta p_{i,k-1}D_3L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})\\
&+\delta t_{i,k-1}D_1L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})+g)=0.
\end{aligned} \tag{23}$$

Equation (17) can be obtained.

In the Hamiltonian formulation, the Lie point symmetry can have Noether conserved quantity under certain conditions. The discrete Noether theorem of the Hamiltonian systems are proposed.

Theorem 2 If the infinitesimal transformation generators τ_k, $\xi_{i,k}$, and $\eta_{i,k}$ satisfy the determining equation (14), the discrete regular function $g_{i,k}=g_i(t_k,t_{k+1},q_{i,k},q_{i,k+1},p_{i,k},p_{i,k+1})$ exists and the discrete Noether identity (15) is satisfied, then the Lie point symmetry of the Hamiltonian systems possess the discrete conserved quantities (17).

5. Example

The harmonic oscillator is an extremely important physical problem. Many potentials look like a harmonic oscillator near their minimum. Many more physical systems can, at least approximately, be described in terms of harmonic oscillator models. In this paper, a coupled nonlinear two-degree-of-freedom harmonic oscillator will be studied to illustrate the theory. The Lagrangian function of the coupled nonlinear harmonic oscillator is

$$L=\frac{1}{2}m\dot{q}_i^2+\gamma\cos q_i+\frac{1}{2}K(q_1-q_2)^2,\ \ i=1,2, \tag{24}$$

where m is a particle of mass, and γ and K are constants. This system's configuration is determined by generalized coordinates q_i. Consider the discretization of the uniform mesh. According to the Verlet scheme,[35,36] the difference Lagrangian function of a two-degree-of-freedom nonlinear harmonic oscillator can be constructed

$$L_{\rm d}=\frac{h}{2}\left((p_{i,k+1}+p_{i,k})\frac{q_{i,k+1}-q_{i,k}}{h_{k+1}}-H_{\rm d}\right),\ \ i=1,2, \tag{25}$$

where

$$H_{\rm d} = \frac{1}{2}\left((p_{i,k+1})^2+(p_{i,k})^2\right)-\cos q_{i,k}-\cos q_{i,k+1} + \frac{1}{2}(q_{1,k}-q_{2,k})^2+\frac{1}{2}(q_{1,k+1}-q_{2,k+1})^2. \quad (26)$$

The time step $h_{k+1}\in R^+$, $m=1$, $K=-1$, and $\gamma=1$. The difference equations (1) and (2) for the discrete nonlinear harmonic oscillator have the difference discrete variational algorithm. On the discretization of the uniform mesh, they can be rewritten as

$$-\frac{p_{1,k+1}+p_{1,k}}{2} - \frac{h}{2}D_2H_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})+\frac{p_{1,k}+p_{1,k-1}}{2} + \frac{h}{2}D_5H_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (27)$$

$$\frac{q_{1,k+1}-q_{1,k}}{2} - \frac{h}{2}D_3H_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})+\frac{q_{1,k+1}-q_{1,k}}{2} - \frac{h}{2}D_6H_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (28)$$

$$-\frac{p_{2,k+1}+p_{2,k}}{2} - \frac{h}{2}D_2H_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})+\frac{p_{2,k}+p_{2,k-1}}{2} - \frac{h}{2}D_5H_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0, \quad (29)$$

$$\frac{q_{2,k+1}-q_{2,k}}{2} - \frac{h}{2}D_3H_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1})+\frac{q_{2,k+1}-q_{2,k}}{2} - \frac{h}{2}D_6H_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})=0. \quad (30)$$

Under the infinitesimal transformation,

$$t_k^*=t+\varepsilon,\quad q_{i,k}^*=q_{i,k},\quad p_{i,k}^*=p_{i,k}. \quad (31)$$

The corresponding operator is

$$X=\frac{\partial}{\partial t}. \quad (32)$$

The determining equations of Lie symmetry are

$$\mathrm{Pr}X\left(p_{1,k-1}-p_{1,k+1}-2h\sin q_{1,k}-2\left(q_{1,k}-q_{2,k}\right)\right)=0, \quad (33)$$

$$\mathrm{Pr}X\left(q_{1,k+1}-q_{1,k}-2hp_{1,k}\right)=0, \quad (34)$$

$$\mathrm{Pr}X\left(p_{2,k-1}-p_{2,k+1}-2h\sin q_{2,k}+2(q_{1,k}-q_{2,k})\right)=0, \quad (35)$$

$$\mathrm{Pr}X(q_{2,k+1}-q_{2,k}-2hp_{2,k})=0. \quad (36)$$

The operator (31) or (32) satisfies the discrete determining equations (33)–(36). It is the Lie symmetry. Direct verification shows that equation (25) is difference invariant with

$$g=\frac{h}{2}\left(\frac{1}{2}(p_{i,k-1}^2+p_{i,k}^2)-\cos q_{i,k}-\cos q_{i,k-1} + \frac{1}{2}(q_{1,k}-q_{2,k})^2+\frac{1}{2}(q_{1,k+1}-q_{2,k+1})^2\right). \quad (37)$$

It is the Noether symmetry. The operator (31) is of both the Lie and Noether symmetries. From Theorem 1, the Noether symmetry of the discrete Hamiltonian systems can possess the discrete conserved quantities directly. From Theorem 2, the Lie symmetry can possess the discrete Noether conserved quantities indirectly. The discrete nonlinear harmonic oscillator possess the discrete conserved quantities

$$I_{N,k} = \xi_{i,k-1}D_2L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}) + \eta_{i,k-1}D_3L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}) + \tau D_1L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})+g, \quad (38)$$

or

$$I=\frac{h}{2}\left(\frac{1}{2}(p_{i,k-1}^2+p_{i,k}^2)-\cos q_{i,k}-\cos q_{i,k-1} + \frac{1}{2}(q_{1,k}-q_{2,k})^2+\frac{1}{2}(q_{1,k+1}-q_{2,k+1})^2\right). \quad (39)$$

Equation (3) has

$$H_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1}) = H_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})$$

under the transformation operators. The difference conserved quantity (39) is consistent with the energy equation (3) of the system.

Equations (1) and (2) are the result of the difference discrete variational principle for difference equations. It is the key point for the following numerical algorithm. In order to implement the variational integrators of the harmonic oscillator, the difference equations can be written as

$$D_5L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}) = -D_2L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1}), \quad (40)$$

$$D_6L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k}) = -D_3L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1}). \quad (41)$$

Taking $b_{i,k}=D_5L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})$ and $c_{i,k}=D_6L_{\rm d}(t_{k-1},q_{i,k-1},p_{i,k-1},t_k,q_{i,k},p_{i,k})$ for each k, this equation is simply written as

$$b_{i,k+1}=-D_2L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1}),\quad c_{i,k+1}=-D_3L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1}), \quad (42)$$

together with the next update

$$b_{i,k+1}=D_5L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1}),\quad c_{i,k+1}=D_6L_{\rm d}(t_k,q_{i,k},p_{i,k},t_{k+1},q_{i,k+1},p_{i,k+1}). \quad (43)$$

By solving the implicit equation (42) for $q_{i,k+1}$ and $p_{i,k+1}$ and then evaluating the explicit equation (43) to

give $b_{i,k+1}$ and $c_{i,k+1}$, so we update $(q_{i,k}, p_{i,k}, b_{i,k}, c_{i,k})$ to $(q_{i,k+1}, p_{i,k+1}, b_{i,k+1}, c_{i,k+1})$.

According to the difference discrete variational integrators (27)–(30), the discrete results of the nonlinear harmonic oscillator are derived when we give the same initial conditions $p_1 = 0.01$, $q_1 = 0.01$, $p_2 = 0.011$, $q_2 = 0.01$, and $h = 0.01$. A numerical result of the preservation of energy is shown for a short time in Fig. 1 for the constant time step case $t^+ - t = t - t^- =$ const between the calculation implementations of variational Verlet and the four-step Runge–Kutta methods. The same pattern is observed if the simulation is carried out for essentially arbitrarily long times. The energy of the nonlinear harmonic oscillator is constant in the variational Verlet scheme. It is consistent with the conclusion that the energy of nonlinear harmonic oscillator system is conservative. It is immediately apparent from this figure that the variational Verlet is typical of symplectic methods compared with the Runge–Kutta scheme. Thus, the difference discrete variational algorithm is more accurate than the four-step Runge–Kutta method in Fig. 2 which shows that the computational result of the trajectories of phase space. The variational Verlet scheme is still periodically orbital, but is unstable from Runge–Kutta.

Figure 3 shows the discrete Noether conserved quantity (39) of the nonlinear harmonic oscillator. From the computational result shown in Fig. 3, equation (39) is stable and conservative. The discrete Noether theorem proposes the conserved quantity (39) from the Noether symmetry. The numerical integration result is consistent with that obtained by the Noether theorem. It can follow that the discrete variational method is effective and reasonable for the system. The discrete variational method has theoretical significance for the numerical simulations.

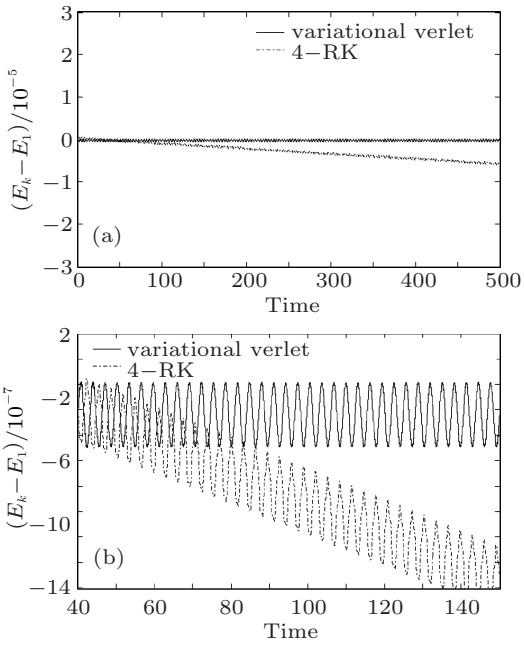


Fig. 1. (a) Comparison of error of energies of coupled nonlinear harmonic oscillators. (b) The partial enlarged view.

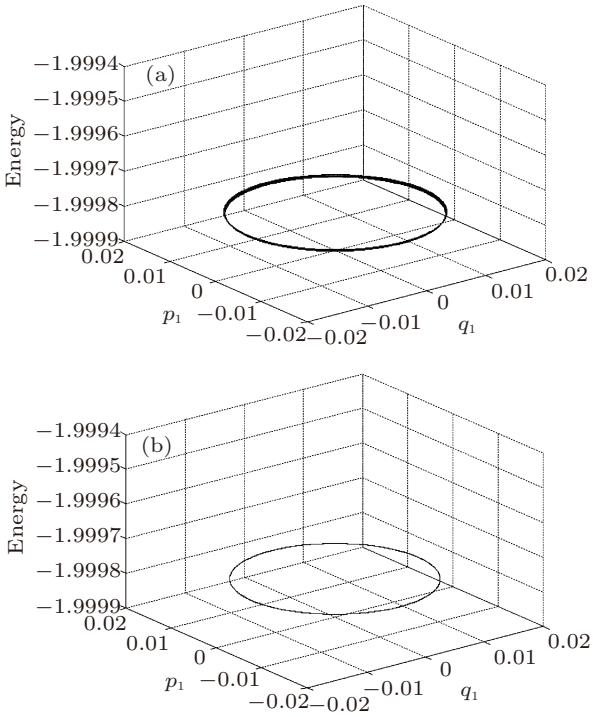


Fig. 2. Trajectories of the phase space computed with variational Verlet (a) and the Runge–Kutta methods (b).

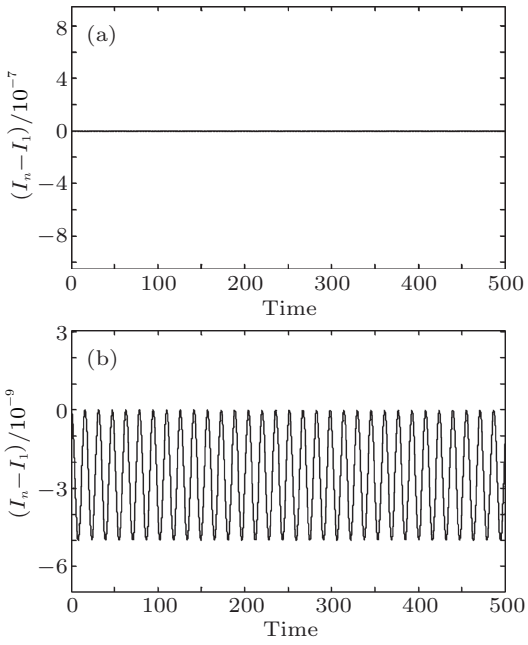


Fig. 3. (a) Error of the Noether conserved quantity (38). (b) The partial enlarged view.

6. Conclusion

We investigate the discretization of Lagrangian in phase space via the difference discrete variational principle. The Lie and Noether symmetries are constructed for discrete Hamiltonian systems based on the discrete variational integrators. Both the Lie and Noether symmetries can lead to discrete Noether conserved quantity. The numerical calculations of the two-degree-of-freedom nonlinear harmonic oscillator demon-

strate that the difference discrete variational method preserves the invariant quantity.

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