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Exterior difference systems and invariance properties of discrete mechanics

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Abstract
Invariance properties describe the fundamental physical laws in discrete mechanics. Can those properties be described in a geometric way? We investigate an exterior difference system called the discrete Euler–Lagrange system, whose solution has one-to-one correspondence with solutions of discrete Euler–Lagrange equations, and use it to define the first integrals. The preservation of the discrete symplectic form along the discrete Hamilton phase flows and the discrete Noether's theorem is also described in the language of difference forms.

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1. Introduction

In recent years, there has been a substantial growth of interest in discrete mechanics [2–13, 19]. In this renascent field, invariance properties such as desirable symmetry also describe the fundamental physical laws and exhibit many geometric properties such as the conservation laws as the continuous mechanics. It should be an interesting problem to describe those properties in a geometric way. In continuous mechanics, it is well known that utilizing techniques from exterior differential systems such as the derived flag and prolongation allows a systematic treatment of the variational principles in greater generality than customary and sheds new light on even the classical Noether's theorem [1]. Naturally, we consider how to apply the techniques in discrete differential geometry and exterior difference systems [13–18] to the discrete variations in discrete mechanics:

- A difference 1-form called discrete Poincáre–Cartan integral invariant is investigated, which preserves the discrete Hamilton phase flows. This form can derive the discrete symplectic form, which is equivalent to the form given by Wendlandt and Marsden [11], if the space variables are continuous (section 3).
- The discrete Euler–Lagrange system is investigated here, whose solution has one-to-one correspondence with solutions of discrete Euler–Lagrange equations. A remarkable application of this system is deriving the discrete Hamilton equations (section 4).
- The discrete Euler–Lagrange system can define the first integrals of discrete Euler–Lagrange equations. We described the discrete Noether's theorem in the language of difference forms and show that this theorem can derive Marsden and West's results [10] (section 5).

The first author wishes to thank professors Wu and Guo for many valuable suggestions concerning the various contents of this paper. The readers can also find some motivation in their theory [13] about discrete exterior calculus. There are two approaches to discrete exterior calculus. One approach to consider the discrete mesh as the only given thing and developing an entire calculus using only discrete combinatorial and geometric operations [17]. Another approach is to approximate a smooth exterior calculus and to consider the given mesh as approximating some smooth manifold at least locally, and then defining the discrete operators by truncating the smooth ones. The derivations may require that the objects on the discrete mesh, but not the mesh itself, are interpolated. It is this latter route that Wu *et al* have taken and this leads to a discrete exterior calculus.

2. Preliminaries

In this section, we recall some concepts in exterior difference systems and discrete variational problems [10, 13–19], which are used in this paper.

2.1. Exterior difference operator

We denote $Z^m = \{(x^i)\}$ by a regular lattice $Z^m = \underbrace{Z \times Z \times \cdots \times Z}_{m}$ with coordinates $\{(x^1, \ldots, x^m)\}$, where Z is a ring of integers.

Let Δ_i be a difference operator in the direction of x^i such that

$$\Delta_i g(x^1, \ldots, x^m) = E_i g(x^1, \ldots, x^m) - g(x^1, \ldots, x^m),$$

where

$$E_i g(x^1, \ldots, x^m) = g(x^1, \ldots, x^i + 1, \ldots, x^m),$$

and g is an R-valued function on Z^m, R is the field of real numbers.

The discrete tangent space at the node $p \in Z^m$ is

$$T_p Z^m := R \otimes \{\Delta_i|_p, i = 1, \ldots, m\},$$

The discrete tangent bundle is

$$TZ^m := \bigcup_{p\in Z^m} T_p Z^m$$

The dual spaces of them are called discrete tangent and cotangent bundles, denoted by

$$T_p^* Z^m := R \otimes \{d_D x^i|_p, i = 1, \ldots, m\}, \qquad T^* Z^m := \bigcup_{p\in Z^m} T_p^* Z^m,$$

where $d_D x^i$ satisfies

$$\langle d_D x^i, \Delta_j \rangle_D := \Delta_j(x^i) = \delta^i_j.$$

Sections on TZ^m and T^*Z^m are called discrete tangent vector fields and difference 1-forms, respectively. In this paper, we denote the set of sections of any discrete bundle $*$ by $\Gamma *$. As in the differential case, we can construct the exterior difference forms algebra [13]

$$\Omega^* = \oplus_{n\in Z} \Omega^n,$$

where Ω^n is a set of difference n-forms

$$K \otimes \{d_D x^{j_1} \wedge \cdots \wedge d_D x^{j_n} | j_1, \ldots, j_n \in 1, \ldots, m\},$$

where K is a ring of R-valued functions on Z^m and $\wedge$ is the anticommutative product.

The exterior difference operator $d_D : \Omega^k \to \Omega^{k+1}$ is defined as

$$d_D w = \sum_{i=1}^{m} \Delta_i h d_D x^i \wedge d_D x^{j_1} \wedge \cdots \wedge d_D x^{j_k},$$

where $w = h d_D x^{j_1} \wedge \cdots \wedge d_D x^{j_k}$. The d_D should satisfy the Leibnitz law and $d_D^2 = 0$ [13]. So we have

$$d_D x^i h = E_i h d_D x^i, \qquad d_D x^i \wedge d_D x^j = -d_D x^j \wedge d_D x^i.$$

2.2. *Exterior difference systems*

Let $Z^m \times R^n = \{(x^i, u^i)\}$ be a discrete vector bundle on Z^m, where x^i and u^i are coordinates of Z^m and R^n, respectively. Consider a section f,

$$u^i = f^i(x^1, \ldots, x^m), \qquad 1 \leqslant i \leqslant n.$$

Define the map $f^* : \wedge T^* f(Z^m) \to \wedge T^* Z^m$ as follows:

$$f^* d_D u^{i_1} := d_D(u^{i_1} \circ f)$$
$$f^*(h d_D u^{i_1} \wedge \cdots \wedge d_D u^{i_r}) := (h \circ f) f^* d_D u^{i_1} \wedge \cdots \wedge f^* d_D u^{i_r}.$$

The f^* is a linear map and commutes with $\wedge$ and d_D, called the discrete cotangent map of f [18].

The dual map of f^* is called discrete tangent map, denoted by f_*. So we can define

$$\begin{pmatrix} \Delta_{u^1} \\ \cdots \\ \Delta_{u^n} \end{pmatrix} := \begin{pmatrix} \Delta_1 u^1 & \cdots & \Delta_1 u^n \\ \cdots & \cdots & \cdots \\ \Delta_m u^1 & \cdots & \Delta_m u^n \end{pmatrix}^{-1} \begin{pmatrix} \Delta_1 \\ \cdots \\ \Delta_m \end{pmatrix}.$$

For any $a \in Z^m \times R^n$, we define

$$T(Z^m \times R^n)_a := R \otimes \{\Delta_i|_a, \Delta_{u^j}|_a | i = 1, \ldots, m, j = 1, \ldots, n\}$$
$$T(Z^m \times R^n) := \bigcup_{a \in Z^m \times R^n} T(Z^m \times R^n)_a$$
$$T^*(Z^m \times R^n)_a := R \otimes \{d_D x^i|_a, d_D u^j|_a | i = 1, \ldots, m, j = 1, \ldots, n\}$$
$$\widetilde{\Omega}^k|_a := \underbrace{T^*(Z^m \times R^n)_a \wedge \cdots \wedge T^*(Z^m \times R^n)_a}_{k}$$
$$\widetilde{\Omega}^* := \bigoplus_{k \in Z} \Big(\bigcup_{a \in Z^m \times R^n} \widetilde{\Omega}^k|_p \Big).$$

Now we can give the exterior difference system as a local approximation of exterior differential system.

Definition 2.1.

(1) A subring of $I \subset \Gamma\widetilde{\Omega}^*$ *is called a right ideal, if:*

(a) $\alpha \in I$ *implies* $\alpha \wedge \beta \in I$ *for all* $\beta \in \Gamma\widetilde{\Omega}^*$.

(b) $\alpha \in I$ *implies that all its components in* $\Gamma\widetilde{\Omega}^*$ *are contained in I.*

(2) An exterior difference system is given by a right ideal $I \subset \Gamma\widetilde{\Omega}^*$ *that is closed under* d_D.

(3) An integral lattice of the system is given by a section $f : Z^m \to Z^m \times R^n$ *such that* $f^*\theta = 0$ *for all* $\theta \in I$.

This system can include all the local ordinary and partial difference equations on a regular lattice, if introducing the discrete jet bundle on a regular lattice.

Definition 2.2. *Let* $Z^m \times R^n = \{(x^i, u^i)\}$ *be a discrete vector bundle on* Z^m *and* $\Delta^k_{i_1\cdots i_k} = \Delta_{i_1}\cdots\Delta_{i_k}$. *The discrete k-jet bundle of this bundle is a discrete vector bundle with coordinates*

$$\left\{\left(x^i, u^j, \Delta_i u^j, \ldots, \Delta^k_{i_1\cdots i_k}u^j\right)\right\}, \qquad 1 \leqslant i, i_1, \ldots, i_k \leqslant m, \qquad 1 \leqslant j \leqslant n,$$

denoted by $J^k_D\alpha$.

In the similar way as Beauce *et al* did [14], we can define the *discrete contract operator* i_Y,

$$i_Y w := \sum_{j=1}^{m} f \sum_{j=i_s} (-1)^s d_D x^{i_1} \wedge \cdots \wedge d_D \check{x}^{i_s} \wedge \cdots \wedge d_D x^{i_k} Y^j,$$

where $Y = Y^i\Delta_i \in TZ^m$, $w = f d_D x^{i_1} \wedge \cdots \wedge d_D x^{i_k} \in \Omega^k$. If w is a difference 1-form, then we denote $i_Y w$ by $\langle w, Y\rangle_D$.

Using the Cartan formula, we define the *discrete Lie derivative operator*

$$L_X\omega := i_X d_D\omega + d_D i_X\omega.$$

More information about those or the similar operators can be found in [10, 13–18].

2.3. Discrete variational problem

Let

$$I = \{\theta^1, \ldots, \theta^k | \theta^i \in \Gamma T^*(Z \times R^{2n})\}$$

be an exterior difference system and $V(I)$ be the set of integral lattice of *I*. For each $\varphi \in \Gamma T^*(Z \times R^{2n})$ and $f \in V(I)$, we set

$$\Phi(Z, f) = \sum_{t\in Z} \langle f^*\varphi, \Delta_t\rangle_D$$

be an *R*-valued function on lattice *Z*.

Consider a subset of discrete vector bundle

$$Z^{2n+1} \times R^{2n} = \{(t, s^i, x^i, q^i, \dot{q}^i)\}$$

such that

$$q^i(s^i, t) = s^i + q^i(t)|_{t\neq\pm\infty}, \qquad q^i(s^i, \pm\infty) = q^i(\pm\infty), \qquad q^i(x^i, t) = q^i(t)$$
$$\dot{q}^i(x^i, t) = x^i + \dot{q}^i(t)|_{t\neq\pm\infty}, \qquad \dot{q}^i(x^i, \pm\infty) = \dot{q}^i(\pm\infty), \qquad \dot{q}^i(s^i, t) = \dot{q}^i(t).$$

So we can extend *I* and φ to this subset, still denote by *I* and φ. In this paper, we omit some pull back and extended maps for simple. We always extend the forms to the extended bundle and pull back them after calculating.

We denote by (I, φ) the discrete variational problem associated with the function $\Phi(Z, f)$, $f \in V(I)$. The associated discrete Euler–Lagrange equations are

$$f^*(i_v d_D(\varphi + \theta^\alpha \lambda_\alpha)|_{Z\times R^{2n}}) = 0, \tag{1}$$

for any $v \in \Gamma(TZ^{2n+1})$ such that $\Delta_v(q^i \circ f)|_{\pm\infty} = 0$.

3. Discrete symplectic structure

Let $Z^{2n+1} \times R^{2n} = \{(s^i, w^i, t, q^i, p^i)\}$ be a discrete vector bundle and

$$\omega^1 = d_D q^i p^i - H(t, E_t p^i, q^i) d_D t, \qquad \text{summation},$$

where $q^i(s^i, t) = s^i + q^i(t)$, $p^i(w^i, t) = w^i + p^i(t)$.

The discrete curve f on $Z \times R^{2n} = \{t, q^i, p^i\}$ such that

$$i_{\Delta_t} f^* d_D \omega^1|_{Z\times R^{2n}} = 0$$

is called the *vortex line* of the form ω^1.

Theorem 3.1. *The vortex line of the form ω^1 on the $Z^{2n+1} \times R^{2n}$ satisfies the discrete Hamilton equations [19]*

$$\dot{p}^i = -H_{q^i}(t, E_t p^i, q^i), \qquad \dot{q}^i = H_{E_t p^i}(t, E_t p^i, q^i), \tag{2}$$

where

$$H_{E_t p^i}(t, E_t p^i, q^i) := \Delta_{w^i} H(t, E_t p^i(t, x^i), q^i(t))|_{w^i=0}$$
$$H_{q^i}(t, E_t p^i, q^i) := \Delta_{s^i} H(t, E_t p^i(t), q^i(t, s^i))|_{s^i=0},$$

$\dot{p}^i = \Delta_t p^i$ *and* $\dot{q}^i = \Delta_t q^i$.

Proof. The exterior difference of the form ω^1 is

$$\begin{aligned} d_D\omega^1 &= d_D q^i \wedge d_D p^i - d_D H(t, E_t p^i, q^i) \wedge d_D t \\ &= d_D s^i \wedge d_D w^i + (\dot{p}^i + H_{q^i}) d_D t \wedge d_D s^i + (\dot{q}^i - H_{E_t p^i}) d_D w^i \wedge d_D t. \end{aligned}$$

Thus the integral lattice of (2) is the vortex line of the form ω^1. □

The vortex line of ω^1 is also called *discrete Hamiltonian phase flows*. Let γ be a discrete curve on $Z^{2n} \times R^{2n} \times t_0 = \{(s^i, x^i, q^i, p^i, t_0)\}$. Since

$$\begin{aligned} \sum_\gamma i_{\Delta_{s^i}} E_t \omega^1|_{t=t_0} - \sum_\gamma i_{\Delta_{s^i}} \omega^1|_{t=t_0} &= \sum_\gamma -i_{\Delta_{s^i}} i_{\Delta_t}(\Delta_t \omega^1 \wedge d_D t)|_{t=t_0} \\ &= \sum_\gamma i_{\Delta_{s^i}} i_{\Delta_t}(d_D\omega^1)|_{t=t_0} \\ \sum_\gamma i_{\Delta_{w^i}} E_t \omega^1|_{t=t_0} - \sum_\gamma i_{\Delta_{w^i}} \omega^1|_{t=t_0} &= \sum_\gamma -i_{\Delta_{w^i}} i_{\Delta_t}(\Delta_t \omega^1 \wedge d_D t)|_{t=t_0} \\ &= \sum_\gamma i_{\Delta_{w^i}} i_{\Delta_t}(d_D\omega^1)|_{t=t_0}, \end{aligned}$$

so the discrete Hamiltonian phase flows preserve the integral of $d_D q^i p^i$ over the discrete curves on $Z^{2n} \times R^{2n} = \{(s^i, w^i, q^i, p^i)\}$. So we call the difference 1-form ω^1 the *discrete Poincáre–Cartan integral invariant*.

If γ is closed discrete curve (connected by links), then there is a two-dimensional oriented chain σ such that $\gamma = \partial\sigma$ (use the notation in general case). As in the differential case, we call difference 2-form

$$\omega^2 = d_D q^i \wedge d_D p^i$$

the *discrete symplectic structure*.

From the discrete Stokes formula, we have

$$\sum_{\sigma} i_{\Delta_{w^i}} i_{\Delta_{s^i}} (d_D q^i \wedge d_D p^i) = \sum_{\gamma} i_{\Delta_{s^i}} \omega^1 - \sum_{\gamma} i_{\Delta_{w^i}} \omega^1.$$

Hence the discrete Hamiltonian phase flows preserve the integral of the oriented sublattice in $Z^{2n} \times R^{2n}$. In other words, ω^2 is an absolute integral invariant of the discrete Hamiltonian phase flows.

Further, the interested reader would probably benefit from a detailed description of the relationship of ω^2 and discrete symplectic structure given by Marsden and Wendlandt [11].

Let $Z^{n+1} \times R^{2n} = \{(s^i, t, q^i, \dot{q}^i)\}$ be a discrete vector bundle on Z^{n+1} and $\dot{q}^i(s^i, t) = s^i + \dot{q}^i(t)$. If s^i, x^i are continuous variables then

$$L_{\dot{q}^i(\varepsilon s^i, t)}|_{w^i=0} := \frac{L(t, q^i(t), \dot{q}^i(\varepsilon, t)) - L(t, q^i(t), \dot{q}^i(t))}{\varepsilon}$$

$$L_{q^i(\varepsilon s^i, t)}|_{s^i=0} := \frac{L(t, q^i(\varepsilon, t), \dot{q}^i(t)) - L(t, q^i(t), \dot{q}^i(t))}{\varepsilon}.$$

Since

$$\begin{aligned}
\dot{q}^i(\varepsilon s^i, t) &= \dot{q}^i(t) + \varepsilon s^i \\
&= (q^i(t+1) + \varepsilon s^i) - q^i(t) \\
&= q^i(\varepsilon s^i, t+1) - q^i(t)
\end{aligned}$$

and $\Delta_{s^i} \dot{q}^i(\varepsilon s^i, t) = \Delta_{s^i} q^i(\varepsilon s^i, t+1) = \varepsilon$, so

$$\begin{aligned}
D_2 L(q^i(t), q^i(t+1)) &= \lim_{\varepsilon \to 0} \frac{\Delta_{s^i} L(q^i(t), q^i(\varepsilon s^i, t+1))}{\varepsilon}\bigg|_{s^i=0} \\
&= \lim_{\varepsilon \to 0} \frac{\Delta_{s^i} L(q^i(t), \dot{q}^i(\varepsilon s^i, t))}{\varepsilon}\bigg|_{s^i=0} \\
&= \lim_{\varepsilon \to 0} L_{\dot{q}^i(\varepsilon s^i, t)}\bigg|_{s^i=0}
\end{aligned}$$

$$\begin{aligned}
\lim_{\varepsilon \to 0} L_{q^i(\varepsilon s^i, t)}|_{s^i=0} &= \lim_{\varepsilon \to 0} \frac{\Delta_{s^i} L(q^i(\varepsilon s^i, t), q^i(\varepsilon s^i, t+1))}{\varepsilon}\bigg|_{s^i=0} \\
&= \lim_{\varepsilon \to 0} \frac{\Delta_{s^i} L(q^i(\varepsilon s^i, t), q^i(\varepsilon, t+1))}{\varepsilon}\bigg|_{s^i=0} \\
&\quad + \lim_{\varepsilon \to 0} \frac{\Delta_{s^i} L(q^\alpha(t), q^\alpha(\varepsilon s^i, t+1))}{\varepsilon}\bigg|_{s^i=0} \\
&= D_1 L(q^i(t), q^i(t+1)) + \lim_{\varepsilon \to 0} L_{\dot{q}^i(\varepsilon s^i, t)}|_{s^i=0}
\end{aligned}$$

$$\begin{aligned}
D_{12} L dq^i(t) \wedge dq^j(t+1)|_{t=t_0} &= \frac{\partial^2 L(q^i(t), q^j(t+1))}{\partial q^i(t) \partial q^j(t+1)} dq^i(t) \wedge dq^j(t+1)|_{t=t_0} \\
&= \frac{\partial^2 L(q^i, q^j)}{\partial(q^i - \dot{q}^i) \partial \dot{q}^j} d_D q^i \wedge d_D(\dot{q}^j + q^j)|_{t=t_0} \\
&= \frac{\partial^2 L(q^i, q^j)}{\partial q^i \partial \dot{q}^j} d_D q^i \wedge d_D \dot{q}^j|_{t=t_0} \\
&\quad + \frac{\partial^2 L(q^i, q^j)}{\partial q^i \partial \dot{q}^j} d_D q^i \wedge d_D q^j|_{t=t_0} \\
&\quad - \frac{\partial^2 L(q^i, q^j)}{\partial \dot{q}^i \partial \dot{q}^j} d_D q^i \wedge d_D \dot{q}^j|_{t=t_0}.
\end{aligned}$$

Recall the discrete Euler–Lagrange equations [19]

$$\Delta_t E_{-t} L_{\dot{q}^i} = L_{q^i}, \tag{3}$$

where

$$L_{\dot{q}^i} := \Delta_{s^i} L(t, q^i(t), \dot{q}^i(s^i, t))|_{s^i=0}$$
$$L_{q^i} := \Delta_{s^i} L(t, q^i(s^i, t), \dot{q}^i(t))|_{s^i=0}$$

and the equations derived from discrete Legendre transformation

$$H_{q^i} = -L_{q^i}, \qquad \dot{q}^i = H_{E_t p^i}, \qquad E_t p^i = L_{\dot{q}^i}, \tag{4}$$

we have

$$\begin{aligned}
d_D q^i \wedge d_D p^i|_{t=t_0} &= d_D q^i \wedge d_D E_{-t} L_{\dot{q}^i}|_{t=t_0} \\
&= d_D q^i \wedge d_D \left(\frac{\partial L(q^i, q^j)}{\partial q^i} - \frac{\partial L(q^i, q^j)}{\partial \dot{q}^i} \right) \bigg|_{t=t_0} \\
&= d_D q^i \wedge \left(\frac{\partial^2 L(q^i, q^j)}{\partial q^i \partial q^j} d_D q^j + \frac{\partial^2 L(q^i, q^j)}{\partial q^i \partial \dot{q}^j} d_D \dot{q}^j \right) \bigg|_{t=t_0} \\
&\quad - d_D q^i \wedge \left(\frac{\partial^2 L(q^i, q^j)}{\partial \dot{q}^i \partial q^j} L_{\dot{q}^i q^j} d_D q^j + \frac{\partial^2 L(q^i, q^j)}{\partial \dot{q}^i \partial \dot{q}^j} d_D \dot{q}^j \right) \bigg|_{t=t_0} \\
&= \frac{\partial^2 L(q^i, q^j)}{\partial q^i \partial \dot{q}^j} d_D q^i \wedge d_D \dot{q}^j \bigg|_{t=t_0} + \frac{\partial^2 L(q^i, q^j)}{\partial q^i \partial \dot{q}^j} d_D q^i \wedge d_D q^j \bigg|_{t=t_0} \\
&\quad - \frac{\partial^2 L(q^i, q^j)}{\partial \dot{q}^i \partial \dot{q}^j} d_D q^i \wedge d_D \dot{q}^j \bigg|_{t=t_0}.
\end{aligned}$$

So ω^2 is equivalent to $D_{12} L dq^i(t) \wedge dq^j(t+1)$.

From a simple example, we show the discrete Euler–Lagrange equations' relationship with the symplectic Euler schemes.

Example 3.2. For the system of harmonic oscillator we have

$$\begin{aligned}
L &= \sum_0^{\dot{q}^i} m_i \dot{q}^i h_{\dot{q}^i} - \sum_0^{q^i} k q^i h_{q^i} \\
&= \frac{1}{2} m_i \dot{q}^i (\dot{q}^i - h_{\dot{q}^i}) - \frac{1}{2} k q^i (q^i - h_{q^i}) \\
H &= L - \dot{q}^i L_{\dot{q}^i} \\
&= -\frac{1}{2} m_i \dot{q}^i (\dot{q}^i + h_{\dot{q}^i}) - \frac{1}{2} k q^i (q^i - h_{q^i}) \\
&= -\frac{1}{2} E_t p^i \left(\frac{E_t p^i}{m^i} + h_{\dot{q}^i}\right) - \frac{1}{2} k q^i (q^i - h_{q^i}) \\
&\cong -\frac{1}{2} \frac{E_t p^i}{m^i} (E_t p^i - h_{p^i}) - \frac{1}{2} k q^i (q^i - h_{q^i}),
\end{aligned}$$

where h_* is the equal footing of $*$.

The corresponding Euler–Lagrange and Hamilton equations are

$$m_i \ddot{q}^i = k E_t q^i \begin{cases} \dot{p}^i = -k q^i \\ \dot{q}^i = \dfrac{E_t p^i}{m^i}. \end{cases}$$

Both of them are equivalent to

$$\begin{cases} E_t p^i = -kq^i + p^i \\ E_t q^i = -\left(\dfrac{k}{m_i} + 1\right) q^i + \dfrac{p^i}{m_i}, \end{cases}$$

whose coefficient matrix is symplectic.

4. Discrete Euler–Lagrange system

As in the differential case, we want to write the discrete Euler–Lagrange equations (1) as an exterior difference system on a proper discrete bundle. This construction will hopefully help to clarify the role of the functions λ_i to be determined. Now we follow the Griffiths' method in differential case [1] to do that job.

On a subset of $Z^{3n+1} \times R^{3n} = \{(s^i, x^i, w^i, t, q^i, \dot{q}^i, \lambda_i)\}$ such that

$$\begin{array}{lll} q^i(s^i, t) = s^i + q^i(t)|_{t \neq \pm\infty}, & q^i(s^i, \pm\infty) = q^i(\pm\infty), & q^i(x^i, t) = q^i(w^i, t) = q^i(t) \\ \dot{q}^i(x^i, t) = x^i + \dot{q}^i(t)|_{t \neq \pm\infty}, & \dot{q}^i(x^i, \pm\infty) = \dot{q}^i(\pm\infty), & \dot{q}^i(s^i, t) = \dot{q}^i(w^i, t) = \dot{q}^i(t) \\ \lambda^i(w^i, t) = w^i + \lambda^i(t)|_{t \neq \pm\infty}, & \lambda^i(w^i, \pm\infty) = \lambda^i(\pm\infty), & \lambda^i(s^i, t) = \lambda^i(x^i, t) = \lambda^i(t), \end{array}$$

suppose we are given a closed 2-form $\psi = d_D(\varphi + \theta^i \lambda_i)$ with the associated exterior difference system generated by the set of 1-forms

$$i_v \psi, \qquad \forall v \in \Gamma(TZ^{3n+1}).$$

Denote by $C(\psi)$ the exterior difference system generated by the collection of 1-forms $i_v \psi$ restricting on $Z \times R^{3n} = \{(t, q^i, \dot{q}^i, \lambda_i)\}$.

Theorem 4.1. *The solutions to the discrete Euler–Lagrange equations (1) are in a natural one-to-one correspondence with the integral lattice of $C(\psi)$, which is called the discrete Euler–Lagrange system of ψ.*

Proof. Let f be an integral lattice of I. Then we may determine functions $\lambda_i(t)$ in (1). Associated with f and the functions $\lambda_i(t)$ is a discrete curve $\widetilde{f} \in Z \times R^{3n}$ such that $\pi \widetilde{f} = f$, where $\pi : Z \times R^{3n} = \{(t, q^i, \dot{q}^i, \lambda_i)\} \to Z \times R^{2n} = \{(t, q^i, \dot{q}^i)\}$. We claim that $\widetilde{f}$ is an integral lattice of $C(\psi)$. In fact

$$d_D(\varphi + \theta^i \lambda_i) = d_D\varphi + d_D\theta^i \lambda_i + \theta^i \wedge d_D\lambda_i.$$

It will suffice to show that

$$i_{\Delta_{w^i}}(d_D\varphi + d_D\theta^i \lambda_i + \theta^i \wedge d_D\lambda_i)|_{\widetilde{f}} = 0. \tag{5}$$

But clearly

$$i_{\Delta_{w^i}}(d_D\varphi + d_D\theta^i \lambda_i + \theta^i \wedge d_D\lambda_i) = -\theta^i, \tag{6}$$

so that (5) follows form $\theta^i|_f = 0$.

Conversely, let $\widetilde{f}$ be an integral lattice of $C(\psi)$ with the projection $\pi(\widetilde{f}) = f \in Z^{2n+1} \times R^{2n}$. Then from (6) it follows that f is an integral lattice of I. Moreover, the conditions

$$i_v d_D(\varphi + \theta^i \lambda_i)|_{\widetilde{f}} = 0 \qquad \text{for} \qquad v \in \Gamma(TZ^{2n+1}) = \Gamma(TZ^{3n+1})$$

are just the (1) for f. $\square$

Example 4.2. Consider discrete 1-jet bundle of $Z \times R^n = \{t, q^1, \ldots, q^n\}$ and let L be a function on $J^1_D(Z \times R^n)$.

We set $\varphi = L(t, q^i, \dot{q}^i)d_D t$ and take $I = \{d_D q^i - \dot{q}^i d_D t\}$. Using

$$\begin{cases} \varphi = L(t, q^i, \dot{q}^i)d_D t \\ \theta^i = d_D q^i - \dot{q}^i d_D t. \end{cases}$$

From

$$\begin{aligned} i_v\psi &= i_v(L_{q^i} d_D s^i \wedge d_D t + L_{\dot{q}^i} d_D x^i \wedge d_D t + d_D\theta^i \lambda_i + \theta^i d_D \lambda_i) \\ &= i_v(L_{q^i} d_D s^i \wedge d_D t + L_{\dot{q}^i} d_D x^i \wedge d_D t + d_D x^i \wedge d_D t \lambda_i + \theta^i d_D \lambda_i) \end{aligned}$$

and $v = \Delta_{s^i}, \Delta_{w^i}, \Delta_{x^i}$, we obtain the discrete Euler–Lagrange system

$$\begin{cases} (L_{\dot{q}^i} - E_t\lambda_i)d_D t = 0 \\ (L_{q^i} - \Delta_t\lambda_i)d_D t = 0 \\ d_D q^i - \dot{q}^i d_D t = 0. \end{cases}$$

A remarkable application of the discrete Euler–Lagrange system is deriving the discrete Hamilton equations.

We have

$$\psi = (L - \dot{q}^i E_t\lambda_i)d_D t + d_D q^i \lambda_i.$$

Letting $H(q^i, \dot{q}^i, E_t\lambda_i, t) = L - \dot{q}^i E_t\lambda_i$ be a function on $Z \times R^{3n}$, we consider the discrete Euler–Lagrange system for the 2-form $d_D\psi$,

$$i_v(H_{s^i} d_D s^i \wedge d_D t + H_{w^i} d_D w^i \wedge d_D t + H_{x^i} d_D x^i \wedge d_D t - d_D q^i \wedge d_D \lambda^i),$$

where $v \in \Gamma(TZ^{3n+1}) = \Gamma(\{\Delta_{s^i}, \Delta_{w^i}, \Delta_{x^i}, \Delta_t\})$. By contraction with the generated elements of $\Gamma(TZ^{3n+1})$, we find that $C(\psi)$ is generated by

$$\begin{cases} H_{x^i} d_D t = 0 \\ H_{w^i} d_D t - d_D q^i = 0 \\ d_D \lambda^i + H_{s^i} d_D t = 0. \end{cases}$$

From the first equation, we can see that H is independent of x^i. It is also possible to write $\lambda_i = p^i$, which we may recognize as discrete Legendre transform and H the discrete Hamilton function. Letting $H_{q^i} := H_{s^i}$, $H_{E_t\lambda_i} := H_{w^i}$ and $H_{\dot{q}^i} := H_{x^i}$, we see that the solutions of $C(\psi)$ satisfy the discrete Hamilton's equations [19]

$$\begin{cases} \dot{p}^i = -H_{q^i}(t, E_t p^i, q^i) \\ \dot{q}^i = H_{E_t p^i}(t, E_t p^i, q^i). \end{cases}$$

5. Discrete Noether's theorem

We consider a discrete variational problem (I, φ) given by the functional

$$\Phi(Z, f) = \sum_{t\in Z} \langle f^*\varphi, \Delta_t\rangle_D,$$

where $f \in V(I)$ is an integral lattice of the difference system I on discrete jet bundle of $Z \times R^{2n}$.

Definition 5.1. *A first integral of the discrete variational problem (I, φ) is given by a function V defined on $Z \times R^{2n} = \{(t, q^i, \dot{q}^i)\}$ such that V is constant on the integral lattice of $C(\psi)$.*

The condition that V be constant on integral lattice of $C(\psi)$ is equivalent to

$$d_D V = 0 \bmod C(\psi).$$

Continuous first integrals arose as conserved quantities for mechanical systems. In the discrete case, there are some new features. The energy of the system cannot be kept conserved discretely if the time step length is fixed [9]. We will discuss this and several examples later. For the moment we pause to give a further

Definition 5.2. *Let* (I, φ) *be a variational problem on* $Z \times R^{2n}$. *Given functions* U, V *defined on* $Z \times R^{2n}$ *their discrete Poisson bracket* $[U, V]_D$ *is the function on* $Z \times R^{2n}$ *defined by*

$$[U, V]_D \psi \wedge (d_D\psi)^n = d_D U \wedge d_D V \wedge \psi \wedge (d_D\psi)^{n-1}$$

on $Z^{2n+1} \times R^{2n}$.

By direct computation, we can show that the discrete Poisson bracket is like in the differential case

$$[U, V]_D = U_{q^i} V_{\dot{q}^i} - V_{q^i} U_{\dot{q}^i},$$

where

$$U_{q^i} := E_{s^i} U(q^i, \dot{q}^i, t) - U(q^i, \dot{q}^i, t), \qquad V_{q^i} := E_{s^i} V(q^i, \dot{q}^i, t) - V(q^i, \dot{q}^i, t),$$
$$U_{\dot{q}^i} := E_{x^i} U(\dot{q}^i, \dot{q}^i, t) - U(q^i, \dot{q}^i, t), \qquad V_{\dot{q}^i} := E_{x^i} V(q^i, \dot{q}^i, t) - V(q^i, \dot{q}^i, t).$$

The importance of the discrete modified Poisson brackets lies in the following observation:

Theorem 5.3. *If* U, V *are each first integrals of* (I, φ) *and* $\Delta_t\varphi = 0$, *then so is their discrete Poisson bracket* $[U, V]_D$.

Proof. Let f be the discrete integral lattice of $C(\psi)$ on $Z \times R^{2n}$. Saying that U is a first integral is equivalent to

$$L_{\Delta t} U = \Delta_t U = 0.$$

Since $L_{\Delta_t} d_D U = d_D L_{\Delta_t} U$, if U and V are each first integrals it follows that

$$\begin{aligned} L_{\Delta_t} d_D U \wedge d_D V \wedge \psi \wedge (d_D\psi)^{n-1} &= (i_{\Delta_t} d_D + d_D i_{\Delta_t}) d_D U \wedge d_D V \wedge \psi \wedge (d_D\psi)^{n-1} \\ &= d_D(d_D U \wedge d_D V \wedge i_{\Delta_t}\psi \wedge (d_D\psi)^{n-1}) \\ &= d_D U \wedge d_D V \wedge \Delta_t\psi \wedge (d_D\psi)^{n-1} \\ &= 0. \end{aligned}$$

So

$$\begin{aligned} \Delta_t[U, V]_D \psi \wedge (d_D\psi)^n &= L_{\Delta_t}[U, V]_D \psi \wedge (d_D\psi)^n \\ &= L_{\Delta_t} d_D U \wedge d_D V \wedge \psi \wedge (d_D\psi)^{n-1} \\ &= 0., \end{aligned}$$

which implies that $\Delta_t[U, V] = 0$. □

A major source of first integrals is provided by invariant movement of variational problems. To explain this we need the following:

Definition 5.4. *An invariant movement of discrete variational problem* (I, φ) *is given by a discrete vector field* v *on* $Z^{2n+1} = \{(t, s^i, x^i)\}$ *that satisfies*

$$L_v I = 0 \quad L_v(\varphi) = 0 \bmod I. \tag{7}$$

If $v = A^i \Delta_{s^i} + B^i \Delta_{x^i} + C\Delta_t$, these conditions are equivalent to

$$E_{A^i s^i + B^i x^i + Ct} I = I \qquad E_{A^i s^i + B^i x^i + Ct}\varphi = \varphi \bmod I.$$

Example 5.5. If the invariant movement induces by $v = \Delta_{s^i}$, then condition (7) is equivalent to

$$L(t, q^i(t, s^i), \dot{q}^i(t)) = L(t, q^i(t), \dot{q}^i(t)),$$

which is also called L admit the discrete variation [19].

In fact $L_{\Delta_{s^i}}(d_D q^i - \dot{q}^i d_D t) = 0$ and $L_{\Delta_{s^i}} L d_D t = 0$. More directly,

$$d_D(q^i + s^i) - \dot{q}^i d_D t = d_D q^i - \dot{q}^i d_D t$$
$$L(t, q^i(t, s^i), \dot{q}^i(t)) d_D t = L(t, q^i(t), \dot{q}^i(t)) d_D t.$$

The v can induce a discrete vector field $\widetilde{v}$ on $Z^{3n+1} = \{(t, s^i, x^i, w^i)\}$ by the product structure. Now we give the main result of this paper

Theorem 5.6. *Discrete Noether's theorem. If v induces an invariant movement of (I, φ), then the function $V = i_{\widetilde{v}}\psi$ is a first integral of the discrete variational problem.*

Proof. By discrete Cartan's formula

$$d_D V = d_D(i_{\widetilde{v}}\psi) = L_{\widetilde{v}}\psi - i_{\widetilde{v}} d_D \psi.$$

By the very definition of $C(\psi)$

$$i_{\widetilde{v}} d_D \psi \in C(\psi),$$

while on the other hand since

$$i_{\Delta_{w^i}} d_D \psi = \theta^\alpha$$

we have $I \subset C(\psi)$. Combining these gives $d_D V \in C(\psi)$. Here we omit some pull back and extended maps. □

We note that discrete Noether's theorem used here is a local form. But we will see that the theorem in this form has it own merit from the following examples.

Example 5.7. If

$$\psi = L(q^i(t), \dot{q}^i(t), t) d_D t + (d_D q^i - \dot{q}^i d_D t) L_{\dot{q}^i}$$

and

$$\widetilde{v} = A^i \Delta_{s^i} + B^i \Delta_{x^i} + C \Delta_t,$$

then

$$i_{\widetilde{v}}\psi = CL + A^i L_{\dot{q}^i}.$$

We have discussed that $i_{\Delta_{s^i}}\psi = L_{\dot{q}^i}$, which is equivalent to the discrete Noether's theorem given by Marsden and West [10, 19]. More precisely, we want to point out one further easy source of first integrals.

Definition 5.8. *If the variable q^i does not appear in the discrete Lagrangian of (I, φ), then q^i is called a cyclic coordinate.*

In this case, the discrete vector field Δ_{s^i} gives an invariant movement of the corresponding variational problem with first integral $L_{\dot{q}^i}$. Actually, for this we do not need discrete Noether's theorem, it is clear from the discrete Euler–Lagrange equations.

In continuous case, we know that if the Lagrangian L is independent of time t, then the Hamiltonian H is a first integral. But this is not always true in discrete case, unless

$\widetilde{v} = q^i \Delta_{s^i} - \Delta_t$ induces an invariant movement of the variational problem (I, φ). In fact, the discrete Noether's theorem gives the first integral

$$\begin{aligned} V &= i_{\dot{q}^i \Delta_{s^i} - \Delta_t}(L d_D t + (d_D q^i - \dot{q}^i d_D t) L_{\dot{q}^i}) \\ &= -L + E_t L_{\dot{q}^i} \dot{q}^i \\ &= H. \end{aligned}$$

Now we consider a detail problem by above methods.

Example 5.9. In R^3 with cylindrical coordinates (r, ω, z) the numerical approximation of a particle's movement on a surface of revolution given by $z = f(r)$ with little discrete time Δt is

$$\begin{aligned} \Delta s^2 &= (1 + \Delta f(r)^2)\Delta r^2 + r^2 \Delta\omega^2 \\ &= F(r)\Delta r^2 + r^2 \Delta\omega^2 \end{aligned}$$

where the second equation defines $F(r)$.

Let h_* be the footing of $*$, $\dot{r} = \frac{\Delta r}{\Delta t}$ and $\dot{\omega} = \frac{\Delta\omega}{\Delta t}$. The discrete Lagrangian has the form

$$\begin{aligned} L &= m \frac{\sqrt{F(r)\dot{r}^2 + r^2\dot{\omega}^2}\left(\sqrt{F(r)\dot{r}^2 + r^2\dot{\omega}^2} - h_v\right)}{2} + U(r) \\ &\cong m \frac{F(r)\dot{r}^2 + r^2\dot{\omega}^2}{2} - h_v \frac{\sqrt{F(r)}\dot{r} + r\dot{\omega}}{2} + U(r) \\ &\cong m \frac{F(r)\dot{r}(\dot{r} - h_{\dot{r}}) + r(r - h_r)\dot{\omega}(\dot{\omega} - h_{\dot{\omega}})}{2} + U(r), \end{aligned}$$

where $U(r)$ is the potential energy and m is the mass of the particle.

If L is independent of t, then L is a first integral. Since ω is a cyclic coordinate, $L_{\dot{\omega}} = r(r - h_r)\dot{\omega}$ is the first integral that corresponds to conservation of angular momentum about the vertical axis.

From the discrete Legendre transform (4)

$$\begin{aligned} E_t p^r &= L_{\dot{r}} = F(r)\dot{r} \\ E_t p^\omega &= L_{\dot{\omega}} = r(r - h_r)\dot{\omega}, \end{aligned}$$

the discrete symplectic form is

$$\omega^2 = d_D r \wedge d_D E_{-t}(F(r)\dot{r}) + d_D \omega \wedge d_D E_{-t}(r(r - h_r)\dot{\omega}).$$

Now, we use the discrete Euler–Lagrange equation to simulate the movement of a particle on the surface of revolution $y = \cos(\sqrt{x^2 + z^2})$ with horizontal linear velocity v_h, mass $m = 1$ and gravitational acceleration $g = 1$. The continuous Euler–Lagrange equation is

$$(1 + \sin^2(r(t)))r\ddot{(t)} = \sin(r(t)) - \sin(r(t))\cos(r(t))\dot{r}^2(t).$$

The corresponding discrete equations are

$$\begin{aligned} &r(t + h_t) = r(t) + h_t v(t) \\ &v(t + h_t) \\ &= \frac{h_t \sin(r(t + h_t)) - {h_t}^2((\sin(r(t + h_t)))^2 - (\sin(r(t)))^2)v(t) + (1 + (\sin(r(t + h_t)))^2)v(t)}{1 + (\sin(r(t + h_t)))^2 - {h_t}^2((\sin(r(t + h_t) + h_t))^2 - (\sin(r(t + h_t)))^2)v(t)}. \end{aligned}$$

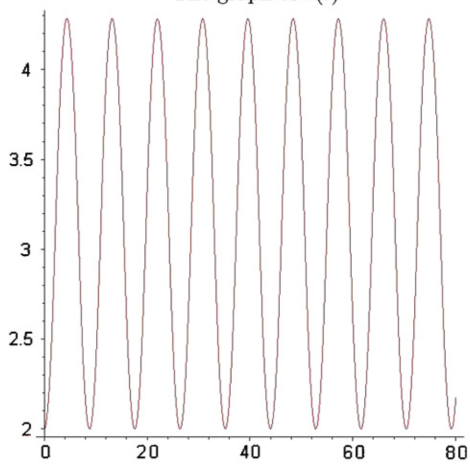
Here we let $h_t = h_r = h_v$ for convenience.

So the numerical simulation of the particle's movement is described by following equations:

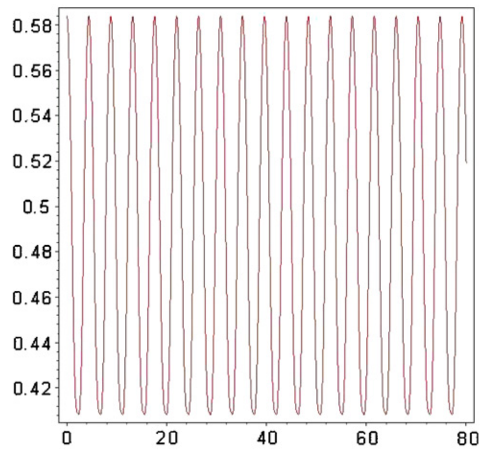
$$x(t) = r(t)\cos\frac{v_h t}{r(t)}, \qquad z(t) = r(t)\sin\frac{v_h t}{r(t)}, \qquad y(t) = \cos r(t) + 1. \quad (8)$$

Choosing $r(0) = 2$, $v(0) = 0$, $v_h = 1$ and $h_t = h_r = h_v = 0.01$, we have the following graphs:

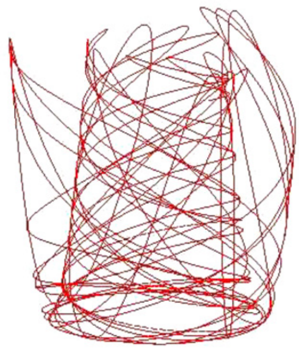
The graph of $r(t)$



The graph of total energy



The graph of (8)



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