Hamiltonian formalism for discrete equations. Symmetries and first integrals.

Roman Kozlov

Norwegian School of Economics and Business Administration
Bergen, Norway

joint work with **Vladimir Dorodnitsyn**
Keldysh Institute of Applied Mathematics, Moscow, Russia

Content

1. Symmetries of differential equations

We consider canonical Hamiltonian equations

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

and their Lie group transformation

$$\bar{t} = \bar{t}(t,q,p,a) \approx t + \xi(t,q,p)a$$

$$\bar{q} = \bar{q}(t,q,p,a) \approx q + \eta(t,q,p)a$$

$$\bar{p} = \bar{p}(t,q,p,a) \approx p + \zeta(t,q,p)a$$

Lie group transformations in the space (t,q,p) are generated by operators of the form

$$X = \xi(t,q,p)\frac{\partial}{\partial t} + \eta(t,q,p)\frac{\partial}{\partial q} + \zeta(t,q,p)\frac{\partial}{\partial p}$$

Symmetries $\longleftrightarrow$ transformed equations have the same form

Example: Harmonic oscillator $H = \frac{1}{2}(p^2 + q^2)$.

The canonical Hamiltonian equations

$$\dot{q} = p, \qquad \dot{p} = -q$$

are invariant, for example, for

1. Translation in time

$$\bar{t} = t + a, \qquad \bar{q} = q, \qquad \bar{p} = p,$$

   generated by the operator

$$X_1 = \frac{\partial}{\partial t}$$

2. Scaling

$$\bar{t} = t, \qquad \bar{q} = e^a q \approx q + qa, \qquad \bar{p} = e^a p \approx p + pa,$$

   generated by the operator

$$X_2 = q\frac{\partial}{\partial q} + p\frac{\partial}{\partial p}$$

Infinitesimal criterion of invariance

We prolong the operator on $\dot{q}$ and $\dot{p}$:

$$X = \xi\frac{\partial}{\partial t} + \eta\frac{\partial}{\partial q} + \zeta\frac{\partial}{\partial p} + (D(\eta) - \dot{q}D(\xi))\frac{\partial}{\partial \dot{q}} + (D(\zeta) - \dot{p}D(\xi))\frac{\partial}{\partial \dot{p}}$$

The equations are invariant with respect to operator X if

$$X\left(\dot{q} - \frac{\partial H}{\partial p}\right)\bigg|_{\dot{q}=\frac{\partial H}{\partial p},\ \dot{p}=-\frac{\partial H}{\partial q}} = 0, \qquad X\left(\dot{p} + \frac{\partial H}{\partial q}\right)\bigg|_{\dot{q}=\frac{\partial H}{\partial p},\ \dot{p}=-\frac{\partial H}{\partial q}} = 0$$

Example: Harmonic oscillator.

1. Translation in time

$$X_1 = \frac{\partial}{\partial t}, \qquad X_1(\dot{q} - p) \equiv 0, \qquad X_1(\dot{p} + q) \equiv 0.$$

2. Scaling

$$X_2 = q\frac{\partial}{\partial q} + p\frac{\partial}{\partial p} + \dot{q}\frac{\partial}{\partial \dot{q}} + \dot{p}\frac{\partial}{\partial \dot{p}}$$

$$X_2(\dot{q} - p) = \dot{q} - p, \qquad X_2(\dot{p} + q) = \dot{p} + q.$$

2. Canonical Hamiltonian equations

2.a. Hamiltonian symmetries and first integrals

Hamiltonian symmetries have the form

$$X = 0\frac{\partial}{\partial t} + \eta(t,q,p)\frac{\partial}{\partial q} + \zeta(t,q,p)\frac{\partial}{\partial p},$$

where

$$\eta = \frac{\partial I}{\partial p}, \qquad \zeta = -\frac{\partial I}{\partial q}, \qquad I = I(t,q,p).$$

They generate transformations which preserve the canonical Hamiltonian form of the equations, i.e. generate **canonical transformations**, which are usually known as provided by generating functions $S_1(q,\bar{q})$, $S_2(\bar{p},q)$, $S_3(p,\bar{q})$ and $S_4(p,\bar{p})$. For example,

$$S_1(q,\bar{q}): \qquad p = \frac{\partial S_1}{\partial q}(q,\bar{q}), \qquad \bar{p} = -\frac{\partial S_1}{\partial \bar{q}}(q,\bar{q}).$$

Invariance of the equation $\dot{q} = \frac{\partial H}{\partial p}$ with respect to a Hamiltonian symmetry

$$\eta_t + \eta_q \dot{q} + \eta_p \dot{p} = \eta \frac{\partial}{\partial q}\left(\frac{\partial H}{\partial p}\right) + \zeta \frac{\partial}{\partial p}\left(\frac{\partial H}{\partial p}\right), \quad \text{where} \quad \eta = \frac{\partial I}{\partial p}, \quad \zeta = -\frac{\partial I}{\partial q}$$

on the solutions $\dot{q} = \frac{\partial H}{\partial p}$, $\dot{p} = -\frac{\partial H}{\partial q}$ yields

$$\frac{\partial^2 I}{\partial t \partial p} + \frac{\partial H}{\partial p}\frac{\partial^2 I}{\partial q \partial p} - \frac{\partial H}{\partial q}\frac{\partial^2 I}{\partial p \partial p} = \frac{\partial I}{\partial p}\frac{\partial^2 H}{\partial q \partial p} - \frac{\partial I}{\partial q}\frac{\partial^2 H}{\partial p \partial p}.$$

This can be rewritten as

$$\frac{\partial}{\partial p}\left(\frac{\partial I}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial I}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial I}{\partial p}\right) = 0.$$

Similarly, invariance of $\dot{p} = -\frac{\partial H}{\partial q}$ leads to

$$\frac{\partial}{\partial q}\left(\frac{\partial I}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial I}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial I}{\partial p}\right) = 0.$$

Therefore,

$$\frac{\partial I}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial I}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial I}{\partial p} = f(t).$$

Since

$$\frac{\partial I}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial I}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial I}{\partial p} = \left.\frac{\partial I}{\partial t} + \frac{\partial I}{\partial q}\dot{q} + \frac{\partial I}{\partial p}\dot{p}\right|_{\dot{q}=\frac{\partial H}{\partial p},\ \dot{p}=-\frac{\partial H}{\partial q}} = D(I)|_{\dot{q}=\frac{\partial H}{\partial p},\ \dot{p}=-\frac{\partial H}{\partial q}}$$

we get a first integral $I(t) - F(t)$. Function $F(t)$ is to be found from the Hamiltonian equations.

- PROBLEM: How to consider discrete case?

2.b. Variational formulation

Canonical Hamiltonian equations

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

can be obtained by the variational principle from the action functional

$$\int_{t_1}^{t_2} (p\dot{q} - H(t, q, p))\, dt, \qquad \delta q(t_1) = \delta q(t_2) = 0$$

Indeed,

$$\delta \int_{t_1}^{t_2} (p\dot{q} - H(t, q, p))\, dt = \int_{t_1}^{t_2} \left(\delta p \dot{q} + p \delta \dot{q} - \frac{\partial H}{\partial q} \delta q - \frac{\partial H}{\partial p} \delta p \right) dt$$

$$= \int_{t_1}^{t_2} \left[\left(\dot{q} - \frac{\partial H}{\partial p} \right) \delta p - \left(\dot{p} + \frac{\partial H}{\partial q} \right) \delta q \right] dt + [p \delta q]_{t_1}^{t_2}.$$

2.c. Variational symmetries and first integrals

Invariance of **elementary action**

$$(p\dot{q} - H)dt = pdq - Hdt$$

Theorem. The elementary Hamiltonian action (we say a Hamiltonian) is invariant with respect to a symmetry operator if and only if

$$\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi) = 0.$$

Proof. Application of prolonged X yields:

$$X\,(pdq - Hdt) = (\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi))\,dt = 0.$$

□

Lemma. (The Hamiltonian identity) The identity

$$\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi) \equiv \xi\left(D(H) - \frac{\partial H}{\partial t}\right)$$

$$-\eta\left(\dot{p} + \frac{\partial H}{\partial q}\right) + \zeta\left(\dot{q} - \frac{\partial H}{\partial p}\right) + D\left[p\eta - \xi H\right]$$

is true for any smooth function $H = H(t, q, p)$.

Theorem. (Noether theorem) The canonical Hamiltonian equations possess a first integral

$$I = p\eta - \xi H$$

if and only if the Hamiltonian function is invariant with respect to the corresponding symmetry operator on the solutions of Hamiltonian equations.

Remark. If the Hamiltonian is divergence invariant, i.e.

$$\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi) = D(V), \qquad V = V(t, q, p),$$

then there is a first integral

$$I = p\eta - \xi H - V.$$

Invariance of canonical Hamiltonian equations

Let us consider variation operators

$$\frac{\delta}{\delta p} = \frac{\partial}{\partial p} - D\frac{\partial}{\partial \dot{p}}, \qquad \frac{\delta}{\delta q} = \frac{\partial}{\partial q} - D\frac{\partial}{\partial \dot{q}}, \qquad D = \frac{\partial}{\partial t} + \dot{q}\frac{\partial}{\partial q} + \dot{p}\frac{\partial}{\partial p} + ...$$

Lemma. Application of variational operators to invariance condition yields

$$\frac{\delta}{\delta p}\left(\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi)\right) = \left[D(\eta) - \dot{q}D(\xi) - X\left(\frac{\partial H}{\partial p}\right)\right]$$

$$+\xi_p\left(D(H) - \frac{\partial H}{\partial t}\right) - \eta_p\left(\dot{p} + \frac{\partial H}{\partial q}\right) + (\zeta_p + D(\xi))\left(\dot{q} - \frac{\partial H}{\partial p}\right).$$

and

$$\frac{\delta}{\delta q}\left(\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi)\right) = -\left[D(\zeta) - \dot{p}D(\xi) + X\left(\frac{\partial H}{\partial q}\right)\right]$$

$$+\xi_q\left(D(H) - \frac{\partial H}{\partial t}\right) - (\eta_q + D(\xi))\left(\dot{p} + \frac{\partial H}{\partial q}\right) + \zeta_q\left(\dot{q} - \frac{\partial H}{\partial p}\right).$$

Theorem. If a Hamiltonian is invariant with respect to a symmetry operator, then the canonical Hamiltonian equations are also invariant.

Remark. The same is true for divergence symmetries of the Hamiltonian, because the term $D(V)$ belongs to the kernel of the variational operators.

Theorem. Canonical Hamiltonian equations are invariant with respect to an operator X if and only if the following conditions are true (on the solutions of the canonical Hamiltonian equations):

$$\frac{\delta}{\delta p}\left(\zeta \dot{q} + pD(\eta) - X(H) - HD(\xi)\right)\Big|_{\dot{q}=\frac{\partial H}{\partial p},\ \dot{p}=-\frac{\partial H}{\partial q}} = 0,$$

$$\frac{\delta}{\delta q}\left(\zeta \dot{q} + pD(\eta) - X(H) - HD(\xi)\right)\Big|_{\dot{q}=\frac{\partial H}{\partial p},\ \dot{p}=-\frac{\partial H}{\partial q}} = 0.$$

Example

The Hamiltonian equations

$$\dot{q} = p, \qquad \dot{p} = \frac{1}{q^3},$$

provided by the Hamiltonian function

$$H(t, q, p) = \frac{1}{2}\left(p^2 + \frac{1}{q^2}\right),$$

admit symmetries

$$X_1 = \frac{\partial}{\partial t}, \qquad X_2 = 2t\frac{\partial}{\partial t} + q\frac{\partial}{\partial q} - p\frac{\partial}{\partial p}, \qquad X_3 = t^2\frac{\partial}{\partial t} + tq\frac{\partial}{\partial q} + (q - tp)\frac{\partial}{\partial p}.$$

1. Variational symmetries

Variational symmetry operators X_1 and X_2 provide first integrals

$$I_1 = -H = -\frac{1}{2}\left(p^2 + \frac{1}{q^2}\right), \qquad I_2 = pq - t\left(p^2 + \frac{1}{q^2}\right).$$

Operator X_3 is a divergence symmetry with $V_3 = q^2/2$. It yields the following conserved quantity

$$I_3 = -\frac{1}{2}\left(\frac{t^2}{q^2} + (q - tp)^2\right).$$

Putting $I_1 = A/2$ and $I_2 = B$, we find the solution as

$$Aq^2 + (At - B)^2 + 1 = 0, \qquad p = \frac{B - At}{q}.$$

2. Hamiltonian symmetries

We rewrite symmetry operators in the evolutionary form

$$\bar{X}_1 = -\dot{q}\frac{\partial}{\partial q} - \dot{p}\frac{\partial}{\partial p}, \quad \bar{X}_2 = (q - 2t\dot{q})\frac{\partial}{\partial q} - (p + 2t\dot{p})\frac{\partial}{\partial p},$$

$$\bar{X}_3 = (tq - t^2\dot{q})\frac{\partial}{\partial q} + (q - tp - t^2\dot{p})\frac{\partial}{\partial p}.$$

On the solutions of the canonical Hamiltonian equations $\dot{q} = p$, $\dot{p} = \frac{1}{q^3}$ these operators are equivalent to the set

$$\tilde{X}_1 = -p\frac{\partial}{\partial q} - \frac{1}{q^3}\frac{\partial}{\partial p}, \quad \tilde{X}_2 = (q - 2tp)\frac{\partial}{\partial q} - \left(p + \frac{2t}{q^3}\right)\frac{\partial}{\partial p},$$

$$\tilde{X}_3 = \left(tq - t^2 p\right)\frac{\partial}{\partial q} + \left(q - tp - \frac{t^2}{q^3}\right)\frac{\partial}{\partial p}.$$

To find first integrals one should integrate the equations

$$\eta = \frac{\partial I}{\partial p}, \qquad \zeta = -\frac{\partial I}{\partial q}, \qquad \tilde{X} = \eta\frac{\partial}{\partial q} + \zeta\frac{\partial}{\partial p}$$

for each symmetry. Integration provides us with the same first integrals.

3. Discrete Hamiltonian equations

3.a. Discrete variational equations in Lagrangian framework

We consider a finite–difference functional

$$\mathbb{L}_h = \sum_{\Omega} \mathcal{L}(t, t_+, q, q_+) h_+,$$

defined on some one-dimensional lattice Ω with step $h_+ = t_+ - t$.

Let us take a variation of the functional along some curve $q = \phi(t)$ at some point (t, q). The variation will effect only two terms in the sum:

$$\mathbb{L}_h = ... + \mathcal{L}(t_-, t, q_-, q) h_- + \mathcal{L}(t, t_+, q, q_+) h_+ + ...,$$

so we get the following expression for the variation of the difference functional

$$\delta \mathbb{L}_h = \frac{\delta \mathcal{L}}{\delta q} \delta q + \frac{\delta \mathcal{L}}{\delta t} \delta t,$$

where $\delta q = \phi' \delta t$ and

$$\frac{\delta\mathcal{L}}{\delta q} = h_+\frac{\partial\mathcal{L}}{\partial q} + h_-\frac{\partial\mathcal{L}^-}{\partial q}, \qquad \frac{\delta\mathcal{L}}{\delta t} = h_+\frac{\partial\mathcal{L}}{\partial t} + h_-\frac{\partial\mathcal{L}^-}{\partial t} + \mathcal{L}^- - \mathcal{L},$$

where $\mathcal{L} = \mathcal{L}(t, t_+, q, q_+)$ and $\mathcal{L}^- = \underset{-h}{S}(\mathcal{L}) = \mathcal{L}(t_-, t, q_-, q)$.

Thus, for an arbitrary curve the stationary value of difference functional is given by any solution of the 2 equations, called **quasiextremal equations**,

$$\frac{\delta\mathcal{L}}{\delta q} = 0, \qquad \frac{\delta\mathcal{L}}{\delta t} = 0.$$

These equations represent the entire difference scheme (approximation of ODE and mesh) and could be called "the discrete Euler–Lagrange system".

- Noether theorem links variational symmetries and first integrals.

3.b. Discrete Legendre transform and discrete Hamiltonian equations

We consider discrete Legendre transform $(t, t_+, q, q_+) \to (t, t_+, q, p_+)$:

$$p_+ = h_+ \frac{\partial \mathcal{L}}{\partial q_+}(t, t_+, q, q_+),$$

$$\mathcal{H}(t, t_+, q, p_+) = p_+ \underset{+h}{D}(q) - \mathcal{L}(t, t_+, q, q_+), \qquad \underset{+h}{D}(q) = \frac{q_+ - q}{t_+ - t},$$

which is a slightly modified version of the transform proposed in

Lall S, West M, Discrete variational Hamiltonian mechanics,
J. Phys. A **39**, 19 (2006) 5509-5519,

where the discrete Hamiltonian equations were developed as the dual, in the sense of optimization, to discrete Euler–Lagrange equations.

Alternatively, on can use discrete Legendre transform $(t, t_+, q, q_+) \to (t, t_+, p, q_+)$:

$$p = -h_+ \frac{\partial \mathcal{L}}{\partial q}(t, t_+, q, q_+),$$

$$\mathcal{H}(t, t_+, q_+, p) = p \underset{+h}{D}(q) - \mathcal{L}(t, t_+, q, q_+).$$

Relations for derivatives of the Lagrangian and Hamiltonian:

$$h_+ \frac{\partial \mathcal{H}}{\partial t} - \mathcal{H} = -h_+ \frac{\partial \mathcal{L}}{\partial t} + \mathcal{L}, \qquad h_+ \frac{\partial \mathcal{H}}{\partial t_+} + \mathcal{H} = -h_+ \frac{\partial \mathcal{L}}{\partial t_+} - \mathcal{L},$$

$$h_+ \frac{\partial \mathcal{H}}{\partial q} = -p_+ - h_+ \frac{\partial \mathcal{L}}{\partial q}, \qquad h_+ \frac{\partial \mathcal{H}}{\partial p_+} = q_+ - q.$$

Transforming 2 quasiextremal equations (discrete Euler–Lagrange equations) into Hamiltonian framework, we obtain **discrete Hamiltonian equations**.

$$\begin{cases} \underset{+h}{D}(q) = \dfrac{\partial \mathcal{H}}{\partial p_+}, \qquad \underset{+h}{D}(p) = -\dfrac{\partial \mathcal{H}}{\partial q}, \\ \\ h_+ \dfrac{\partial \mathcal{H}}{\partial t} - \mathcal{H} + h_- \dfrac{\partial \mathcal{H}^-}{\partial t} + \mathcal{H}^- = 0, \end{cases}$$

where $\mathcal{H} = \mathcal{H}(t, t_+, q, p_+)$ and $\mathcal{H}^- = \mathcal{H}(t_-, t, q_-, p)$.

3.c. Variational formulation

We consider the finite–difference functional

$$\mathbb{H}_h = \sum_{\Omega} (p_+(q_+ - q) - \mathcal{H}(t, t_+, q, p_+)h_+).$$

A variation of this functional along a curve $q = \phi(t)$, $p = \psi(t)$ at some point (t, q, p) will effect only two term of the sum:

$$\mathbb{H}_h = ... + p(q - q_-) - \mathcal{H}(t_-, t, q_-, p)h_- + p_+(q_+ - q) - \mathcal{H}(t, t_+, q, p_+)h_+ + ...$$

Therefore, we get the following expression for the variation

$$\delta\mathbb{H}_h = \frac{\delta\mathcal{H}}{\delta p}\delta p + \frac{\delta\mathcal{H}}{\delta q}\delta q + \frac{\delta\mathcal{H}}{\delta t}\delta t,$$

where $\delta q = \phi'\delta t$, $\delta p = \psi'\delta t$ and

$$\frac{\delta \mathcal{H}}{\delta p} = q - q_- - h_- \frac{\partial \mathcal{H}^-}{\partial p}, \qquad \frac{\delta \mathcal{H}}{\delta q} = -\left(p_+ - p + h_+ \frac{\partial \mathcal{H}}{\partial q} \right),$$

$$\frac{\delta \mathcal{H}}{\delta t} = -\left(h_+ \frac{\partial \mathcal{H}}{\partial t} - \mathcal{H} + h_- \frac{\partial \mathcal{H}^-}{\partial t} + \mathcal{H}^- \right),$$

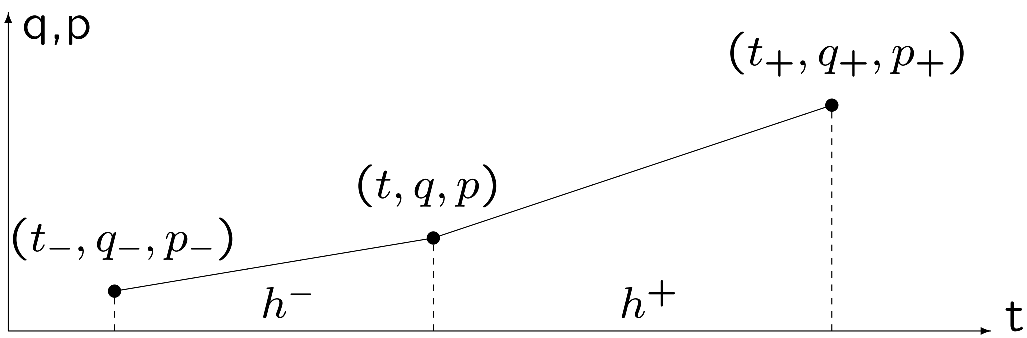
where $\mathcal{H} = \mathcal{H}(t, t_+, q, p_+)$ and $\mathcal{H}^- = \mathcal{H}(t_-, t, q_-, p)$.

For the stationary value of the finite–difference functional we obtain the system of 3 equations

$$\frac{\delta \mathcal{H}}{\delta p} = 0, \qquad \frac{\delta \mathcal{H}}{\delta q} = 0, \qquad \frac{\delta \mathcal{H}}{\delta t} = 0,$$

which are equivalent to the discrete Hamiltonian equations.

3.d. Variational symmetries and first integrals



Discrete prolongation of the operator X:

$$X = \xi\frac{\partial}{\partial t} + \eta\frac{\partial}{\partial q} + \zeta\frac{\partial}{\partial p} + \xi_-\frac{\partial}{\partial t_-} + \eta_-\frac{\partial}{\partial q_-} + \zeta_-\frac{\partial}{\partial p_-} + \xi_+\frac{\partial}{\partial t_+} + \eta_+\frac{\partial}{\partial q_+} + \zeta_+\frac{\partial}{\partial p_+}$$

where

$$\xi_- = \xi(t_-, q_-, p_-), \qquad \eta_- = \eta(t_-, q_-, p_-), \qquad \zeta_- = \zeta(t_-, q_-, p_-),$$

$$\xi_+ = \xi(t_+, q_+, p_+), \qquad \eta_+ = \eta(t_+, q_+, p_+), \qquad \zeta_+ = \zeta(t_+, q_+, p_+).$$

Let us consider the finite–difference functional

$$\mathbb{H}_h = \sum_{\Omega} (p_+(q_+ - q) - \mathcal{H}(t, t_+, q, p_+)h_+).$$

on some lattice given by equation

$$\Omega(t, h_+, h_-, q, p) = 0.$$

The lattice is provided by the discrete Hamiltonian equations.

Theorem. The discrete action functional (we say a Hamiltonian function) considered together with the mesh is invariant with respect to a group generated by operator X if and only if the conditions

$$\zeta_+ \underset{+h}{D}(q) + p_+ \underset{+h}{D}(\eta) - X(\mathcal{H}) - \mathcal{H} \underset{+h}{D}(\xi)\bigg|_{\Omega=0} = 0,$$

$$X\Omega(t, h_+, h_-, q, p)|_{\Omega=0} = 0$$

hold on the solutions of the discrete Hamiltonian equations.

- Since the mesh is provided by discrete Hamiltonian equations we need their invariance

Lemma. (Discrete Hamiltonian identity) The following identity is true for any smooth function $\mathcal{H} = \mathcal{H}(t, t_+, q, p_+)$:

$$\zeta_+ \underset{+h}{D}(q) + p_+ \underset{+h}{D}(\eta) - X(\mathcal{H}) - \mathcal{H} \underset{+h}{D}(\xi) \equiv \xi \left(\frac{h_-}{h_+} \underset{-h}{D}(\mathcal{H}) - \frac{\partial \mathcal{H}}{\partial t} - \frac{h_-}{h_+} \frac{\partial \mathcal{H}^-}{\partial t} \right)$$

$$-\eta \left(\underset{+h}{D}(p) + \frac{\partial \mathcal{H}}{\partial q} \right) + \zeta_+ \left(\underset{+h}{D}(q) - \frac{\partial \mathcal{H}}{\partial p_+} \right) + \underset{+h}{D} \left[\eta p - \xi \left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \right) \right]$$

Theorem. (Noether theorem) The invariant with respect to symmetry operator X discrete Hamiltonian equations possess a first integral

$$\mathcal{I} = \eta p - \xi \left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \right)$$

if and only if the Hamiltonian function is invariant with respect to the same symmetry on the solutions of the equations.

Remark 1. If the operator X is a divergence symmetry of the Hamiltonian action, i.e.

$$\zeta_+ \underset{+h}{D}(q) + p_+ \underset{+h}{D}(\eta) - X(\mathcal{H}) - \mathcal{H} \underset{+h}{D}(\xi) = \underset{+h}{D}(V), \qquad V = V(t, q, p),$$

then there is a first integral

$$\mathcal{I} = \eta p - \xi \left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \right) - V.$$

Remark 2. If Hamiltonian is invariant with respect to time translations, i.e. $\mathcal{H} = \mathcal{H}(h_+, \mathbf{q}, \mathbf{p}^+)$, where $h_+ = t_+ - t$, then there is a conservation of energy

$$\mathcal{E} = \mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial h_-} = \mathcal{H} + h_+ \frac{\partial \mathcal{H}}{\partial h_+}.$$

Example: Discrete harmonic oscillator.

Let us consider the one-dimensional harmonic oscillator

$$\dot{q} = p, \qquad \dot{p} = -q,$$

which is generated by the Hamiltonian function

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

As a discretization we consider the application of the midpoint rule

$$\frac{q_+ - q}{h_+} = \frac{p + p_+}{2}, \qquad \frac{p_+ - p}{h_+} = -\frac{q + q_+}{2}$$

on a uniform mesh $h_+ = h_- = h$.

- The midpoint rule conserves quadratic first integral. Therefore, H is conserved.

This discretization can be rewritten as the system

$$\underset{+h}{D}(q) = \frac{4}{4 - h_+^2}\left(p_+ + \frac{h_+}{2}q\right), \qquad \underset{+h}{D}(p) = -\frac{4}{4 - h_+^2}\left(q + \frac{h_+}{2}p_+\right), \qquad h_+ = h_- = h.$$

It can be shown that this system provides discrete Hamiltonian equations

$$\begin{cases} \underset{+h}{D}(q) = \dfrac{\partial \mathcal{H}}{\partial p_+}, \qquad \underset{+h}{D}(p) = -\dfrac{\partial \mathcal{H}}{\partial q}, \\ h_+ \dfrac{\partial \mathcal{H}}{\partial t} - \mathcal{H} + h_- \dfrac{\partial \mathcal{H}^-}{\partial t} + \mathcal{H}^- = 0, \end{cases}$$

generated by the discrete Hamiltonian

$$\mathcal{H}(t, t_+, q, p_+) = \frac{2}{4 - h_+^2}(q^2 + p_+^2 + h_+ q p_+).$$

The system admits, in particular, symmetries

$$X_1 = \sin(\omega t)\frac{\partial}{\partial q} + \cos(\omega t)\frac{\partial}{\partial p}, \qquad X_2 = \cos(\omega t)\frac{\partial}{\partial q} - \sin(\omega t)\frac{\partial}{\partial p},$$

$$X_3 = \frac{\partial}{\partial t}, \qquad X_4 = q\frac{\partial}{\partial q} + p\frac{\partial}{\partial p}, \qquad X_5 = p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p},$$

where

$$\omega = \frac{\arctan(h/2)}{h/2}.$$

Operators X_1 and X_2 are divergence symmetries with functions $V_1 = q\cos(\omega t)$ and $V_2 = -q\sin(\omega t)$ respectively. Therefore, we obtain two first integrals

$$\mathcal{I}_1 = p\sin(\omega t) - q\cos(\omega t), \qquad \mathcal{I}_2 = p\cos(\omega t) + q\sin(\omega t).$$

From the first integrals $\mathcal{I}_1$ and $\mathcal{I}_2$ we have conservation

$$\mathcal{I}_1^2 + \mathcal{I}_2^2 = q^2 + p^2 = \text{const}.$$

Operator X_3 is a variational symmetry. It provides the first integral

$$\mathcal{I}_3 = -\frac{4}{4-h_-^2}\left(\frac{4+h_-^2}{4-h_-^2}\frac{q_-^2+p^2}{2} + \frac{4h_-}{4-h_-^2}q_-p\right).$$

Using the equations, we can simplify it as

$$\mathcal{I}_3 = -\frac{4}{4+h_-^2}\frac{q^2+p^2}{2}$$

Using $q^2+p^2 = \text{const}$, we can take the third first integrals equivalently as

$$\tilde{\mathcal{I}}_3 = h_-.$$

Finally, we have three first integrals $\mathcal{I}_1$, $\mathcal{I}_2$, $\tilde{\mathcal{I}}_3$, which are sufficient for integration of the discrete system. We obtain the solution

$$q = \mathcal{I}_2 \sin(\omega t) - \mathcal{I}_1 \cos(\omega t), \qquad p = \mathcal{I}_1 \sin(\omega t) + \mathcal{I}_2 \cos(\omega t)$$

on the lattice

$$t_i = t_0 + ih, \qquad i = 0, \pm 1, \pm 2, ..., \qquad h = \tilde{\mathcal{I}}_3.$$

Example.

The discrete Hamiltonian

$$\mathcal{H}(t, t_+, q, p_+) = \frac{1}{2}\left(p_+^2 + \frac{1}{q^2}\right)$$

yields the discrete Hamiltonian equations:

$$\underset{+h}{D}(q) = p_+, \qquad \underset{+h}{D}(p) = \frac{1}{q^3}, \qquad p_+^2 + \frac{1}{q^2} = p^2 + \frac{1}{q_-^2}.$$

Operators

$$X_1 = \frac{\partial}{\partial t}, \qquad X_2 = 2t\frac{\partial}{\partial t} + q\frac{\partial}{\partial q} - p\frac{\partial}{\partial p}$$

are variational symmetries. They provide first integrals

$$\mathcal{I}_1 = -\frac{1}{2}\left(p^2 + \frac{1}{q_-^2}\right), \qquad \mathcal{I}_2 = qp - t\left(p^2 + \frac{1}{q_-^2}\right).$$

Therefore, the solution satisfies the relation

$$\mathcal{I}_2 = qp + 2t\mathcal{I}_1$$

in all points of the lattice.

4. Concluding remarks

1. For canonical Hamiltonian equations and discrete Hamiltonian equations there is a relation:

$$\text{Variational (divergence) symmetries} \quad \longleftrightarrow \quad \text{first integrals}$$

2. The same holds for n degrees of freedom

$$\mathbf{q} = (q_1, ..., q_n), \qquad \mathbf{p} = (p_1, ..., p_n).$$

3. Two discrete versions of discrete Legendre transform

$$(t, t_+, \mathbf{q}, \mathbf{q}_+) \rightarrow (t, t_+, \mathbf{q}, \mathbf{p}_+), \quad \text{and} \quad (t, t_+, \mathbf{q}, \mathbf{q}_+) \rightarrow (t, t_+, \mathbf{p}, \mathbf{q}_+)$$

let us obtain $2n+1$ discrete Hamiltonian equations from $n+1$ discrete Euler–Lagrangian equations.

4. For discrete Hamiltonian equations with Hamiltonian functions invariant with respect to time translations, i.e. $\mathcal{H} = \mathcal{H}(h_+, \mathbf{q}, \mathbf{p}_+)$, where $h_+ = t_+ - t$, there is a conservation of energy

$$\mathcal{E} = \mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} .$$

Note that $\mathcal{H}$ is not the discrete energy, it has a meaning of a generating function for discrete Hamiltonian flow.

This is related to

Kane C., Marsden J.E., Ortiz M.,
Symplectic–energy–momentum preserving variational integrators,
J. Math. Phys. **40** (1999) no. 7, 3353-3371.

5. It is possible to consider complete discrete Legendre transform.

Given a discrete Lagrangian $\mathcal{L}(t, t_+, \mathbf{q}, \mathbf{q}_+)$, we can consider, for example, a discrete Legendre transform $(t, t_+, \mathbf{q}, \mathbf{q}_+) \to (t, E_+, \mathbf{q}, \mathbf{p}_+)$:

$$\mathbf{p}_+ = \frac{\partial \mathcal{L}}{\partial \mathbf{q}_+}, \qquad E_+ = -\frac{\partial \mathcal{L}}{\partial t_+},$$

$$\mathcal{S}(t, E_+, \mathbf{q}, \mathbf{p}_+) = \mathbf{p}_+(\mathbf{q}_+ - \mathbf{q}) - E_+(t_+ - t) - \mathcal{L}(t, t_+, \mathbf{q}, \mathbf{q}_+).$$

In this case $n+1$ discrete Euler–Lagrange equations are transformed into the system of $2n+2$ equations

$$\mathbf{q}_+ - \mathbf{q} = \frac{\partial \mathcal{S}}{\partial \mathbf{p}_+}, \qquad \mathbf{p}_+ - \mathbf{p} = -\frac{\partial \mathcal{S}}{\partial \mathbf{q}}, \qquad E_+ - E = \frac{\partial \mathcal{S}}{\partial t}, \qquad t_+ - t = -\frac{\partial \mathcal{S}}{\partial E_+}.$$

- Stepsize $h_+ = t_+ - t$ becomes a complicated expression.