

# Variational integrators

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**Discretizing Hamilton's principle.** The idea behind variational integrators is to discretize directly the action integral

$$S(q) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t)) dt$$

This means that we split the time interval into subintervals, and on each of these we replace the Lagrangian with some discrete approximation, the resulting discrete action sum is

$$S_h(\{q_j\}_{j=0}^N) = \sum_{j=0}^{N-1} L_h(q_j, q_{j+1}) \quad (1)$$

where we have defined the function  $L_h(x, y)$ ,  $L_h : Q \times Q \rightarrow \mathbb{R}$  called the discrete Lagrangian. One has

$$L_h(q_j, q_{j+1}) \approx \int_{t_j}^{t_{j+1}} L(q(t), \dot{q}(t)) dt$$

where  $q(t)$  is the solution to the Euler-Lagrange equations with boundary conditions  $q(t_j) = q_j$ ,  $q(t_{j+1}) = q_{j+1}$ . We extremize (1) by requiring

$$\frac{\partial S_h}{\partial q_n} = 0, \quad n = 1, \dots, N-1$$

This leads to

$$\frac{\partial L_h}{\partial y}(q_{n-1}, q_n) + \frac{\partial L_h}{\partial x}(q_n, q_{n+1}) = 0 \quad (\text{DEL})$$

These are the *discrete Euler-Lagrange equations*.

For given  $q_0, q_N$  we can solve (DEL) for  $q_1, \dots, q_{N-1}$ .

We now introduce the *discrete momenta* and the *discrete Legendre transformation*

$$p_n = -\frac{\partial L_h}{\partial x}(q_n, q_{n+1}) \quad (\text{DLT})$$

If (DLT) can be solved for  $q_{n+1}$ , then we have an invertible transformation

$$FL_h : Q \times Q \rightarrow T^*Q, \quad (q_n, q_{n+1}) \mapsto (q_n, p_n)$$

We can present an integrator  $\Phi_h$  that takes a step on  $T^*Q$  by mapping  $(q_n, p_n)$  to  $(q_{n+1}, p_{n+1})$ .

$$\begin{array}{ccc}
(q_n, q_{n+1}) & \xrightarrow{\text{DEL}} & (q_{n+1}, q_{n+2}) \\
\uparrow FL_h^{-1} & & \downarrow FL_h \\
(q_n, p_n) & \xrightarrow{\Phi_h} & (q_{n+1}, p_{n+1})
\end{array}$$

In practice, we can make a short cut since (DLT) with  $n$  replaced by  $n+1$  yields

$$p_{n+1} = -\frac{\partial L_h}{\partial x}(q_{n+1}, q_{n+2}) \stackrel{\text{DEL}}{=} \frac{\partial L_h}{\partial y}(q_n, q_{n+1}) \quad (2)$$

Then the integrator can be understood as follows

$$(q_n, p_n) \xrightarrow{FL_h^{-1}} (q_n, q_{n+1}) \xrightarrow{(2)} (q_{n+1}, p_{n+1})$$

**Symplecticity of the variational integrator** We discuss the symplecticity of the form in terms of local coordinates  $q_1, \dots, q_d, p_1, \dots, p_d$ . First consider the following lemma

**Lemma 1.** *A map  $\Psi : (q, p) \mapsto (Q, P)$  preserves the symplectic form*

$$\omega = dp_1 \wedge dq_1 + \dots + dp_d \wedge dq_d$$

*if and only if there exists locally a function  $S(q, p)$  such that*

$$dS = PdQ - pdq = \sum_{i=1}^d P_i dQ_i - \sum_{i=1}^d p_i dq_i$$

*Proof.* This follows from the fact that the symplectic two-form is closed, and closed forms are locally exact, meaning that there in this case exists locally a one-form  $\theta_0$  such that  $\Psi^*\omega - \omega = d\theta_0$  (note that  $d$  commutes with pull-back). To this one-form, one can add any element in the kernel of  $d$ , the kernel consists precisely of exact one-forms. This means that any one-form  $\theta$  such that  $d\theta = \omega$  is of the form  $\theta = \theta_0 + dS$  where  $S$  is a 0-form (function). So

$$\begin{aligned}
dS &= PdQ - pdq \\
&\Downarrow \text{apply } d \\
0 &= dP \wedge dQ - dp \wedge dq = \Psi^*\omega - \omega
\end{aligned}$$

□

Then we have

**Theorem 1.** *The variational integrator derived here preserves the symplectic form*

$$\omega = dp_1 \wedge dq_1 + \dots + dp_d \wedge dq_d$$

*Proof.* We now consider the action sum to be just a function of  $q_0$  and  $q_N$ , assuming that we solve for all the other  $q_n$  by using the equations (DEL), this means that we have  $q_n = q_n(q_0, q_N)$  for  $n = 1, \dots, N-1$ .

$$S_h(q_0, q_N) = \sum_{n=0}^{N-1} L_h(q_n, q_{n+1})$$

So differentiating with respect to  $q_0$  we get

$$\frac{\partial S_h}{\partial q_0}(q_0, q_N) = \frac{\partial L_h}{\partial x}(q_0, q_1) + \sum_{n=1}^{N-1} \left( \frac{\partial L_h}{\partial x}(q_n, q_{n+1}) + \frac{\partial L_h}{\partial y}(q_{n-1}, q_n) \right) \frac{\partial q_n}{\partial q_0}$$

So using (DEL) we simply obtain

$$\frac{\partial S_h}{\partial q_0}(q_0, q_N) = \frac{\partial L_h}{\partial x}(q_0, q_1)$$

In a similar way, we differentiate with respect to  $q_N$  and get

$$\frac{\partial S_h}{\partial q_N}(q_0, q_N) = \frac{\partial L_h}{\partial y}(q_{N-1}, q_N)$$

So we can write down  $dS$  in terms of  $dq_0$  and  $dq_N$  and we make use of the discrete Legendre transformation (DLT)

$$dS = \frac{\partial S_h}{\partial q_0} dq_0 + \frac{\partial S_h}{\partial q_N} dq_N = \frac{\partial L_h}{\partial x}(q_0, q_1) dq_0 + \frac{\partial L_h}{\partial y}(q_{N-1}, q_N) dq_N = -p_0 dq_0 + p_N dq_N$$

and we can use Lemma 1 to conclude that the numerical method that maps  $(q_0, p_0)$  to  $(q_N, p_N)$  is a symplectic map.  $\square$

**Example 1** We consider the “mechanical Lagrangian”

$$L(q, \dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q} - V(q), \quad q \in \mathbb{R}^d.$$

where  $M$  is a diagonal matrix with positive diagonal elements. The exact Euler-Lagrange equations are obtained from the formula

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

giving the second order differential equations

$$M \ddot{q} = -\frac{\partial V}{\partial q}$$

To transform the problem to  $T^*Q$ , we introduce the Legendre transformation  $p = \frac{\partial L}{\partial \dot{q}}$  and the Hamiltonian  $H(q, p) = p^T \dot{q} - L(q, \dot{q})$ . We get  $\dot{q} = M^{-1}p$  such that

$$H(q, p) = p^T M^{-1}p - L(q, M^{-1}p) = \frac{1}{2} p^T M^{-1}p + V(q)$$

Then the Hamiltonian equations read

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} = M^{-1}p \\ \dot{p} &= -\frac{\partial H}{\partial q} = -\frac{\partial V}{\partial q} \end{aligned}$$

So now let us consider the discrete case. We first need to define  $L_h(q_n, q_{n+1})$ . A plausible way to do this is to set

$$L_h(q_n, q_{n+1}) = hL \left( \frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h} \right)$$

In our case with the mechanical Lagrangian, this leads to

$$L_h(x, y) = h \left[ \frac{1}{2} \left( \frac{y-x}{h} \right)^T M \left( \frac{y-x}{h} \right) - V \left( \frac{x+y}{2} \right) \right]$$

We invoke (DEL) to obtain

$$M \frac{q_{n+1} - 2q_n + q_{n-1}}{h^2} = -\frac{1}{2} \left( \frac{\partial V}{\partial q} \left( \frac{q_n + q_{n+1}}{2} \right) + \frac{\partial V}{\partial q} \left( \frac{q_{n-1} + q_n}{2} \right) \right)$$

The next thing to do is to compute the discrete Legendre transformation. Using (DLT) we get

$$p_n = M \frac{q_{n+1} - q_n}{h} + \frac{h}{2} \frac{\partial V}{\partial q} \left( \frac{q_n + q_{n+1}}{2} \right) \quad (3)$$

so contrary to the continuous Legendre transformation, there is no way we can solve explicitly for  $q_{n+1}$ . We can however find an explicit expression of  $p_{n+1}$  by using (2).

$$p_{n+1} = M \frac{q_{n+1} - q_n}{h} - \frac{h}{2} \frac{\partial V}{\partial q} \left( \frac{q_n + q_{n+1}}{2} \right) \quad (4)$$

We add (3) and (4), and then solve for  $q_{n+1}$

$$q_{n+1} = q_n + h \frac{p_n + p_{n+1}}{2} = q_n + h \frac{\partial H}{\partial p} \left( \frac{p_n + p_{n+1}}{2} \right)$$

Similarly, subtracting (3) from (4) and solving for  $p_{n+1}$ , we get

$$p_{n+1} = p_n - h \frac{\partial V}{\partial q} \left( \frac{q_n + q_{n+1}}{2} \right) = p_n - h \frac{\partial H}{\partial q} \left( \frac{q_n + q_{n+1}}{2} \right)$$

so we conclude that the variational integrator derived here is nothing else than the implicit midpoint rule. □