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Variational Integrator for Hamiltonian Neural Networks

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Abstract—Hamiltonian neural networks are a type of neural networks for learning equations of motion that describe physical phenomena from given observed data. Such models should be used in physical simulations; however, it is known that when general-purpose numerical integrators are used for discretization, the energy conservation law and other laws of physics are destroyed. Structure-preserving numerical methods such as the variational integrator are effective to address this problem. We propose a variational integrator for Hamiltonian neural networks in this paper.

1. Introduction

In recent years, neural network models that learn equations of motion that explain observed data of physical phenomena have been attracting much attention. The Hamiltonian neural network proposed by Greydanus et al. in 2019 is an example of such a study [1]. In Hamiltonian neural networks, given data is assumed to satisfy the Hamiltonian equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} O & I \\ -I & O \end{pmatrix} \nabla H \tag{1}$$

In this equation, q and p represent generalized coordinates and generalized momenta, respectively. H is a function that depends on q and p and represents the total energy of the system. This function H is also called the Hamiltonian of the system. By learning the Hamiltonian H in this equation using a neural network, Hamiltonian neural networks learn the equations of motion that the data obey. In this paper, we refer to neural network models that learn equations of motion as deep physical models.

In the last three years, research on deep physical models has intensively performed, and numerous extensions have been proposed, including the neural symplectic form [7], Lagrangian neural networks[2] based on Lagrangian dynamics, DGNet[3] and VIN[4], as well as other models discretized in the time direction.

Additionally, [5] also includes theoretical analyses such as proofs of universal approximation properties and generalization error analysis. A primal application of these models is physical simulations. Therefore, models discretized in the time direction are particularly useful, as such models do not require a further discretization for simulations. On the other hand, discrete-time models have a disadvantage of being unable to be simulated with time steps other than that used in the training process. As a result, developing a way to discretize continuous-time deep physical models for simulation is important. In addition, discretization methods of deep physical models are also useful for designing discrete-time models.

We propose a variational integrator for Hamiltonian neural networks as such a method. The variational integrator is a numerical method of the Euler–Lagrange equation, which is the fundamental equations of Lagrangian mechanics [6]. By discretizing the variational principle, which is a fundamental principle of analytical mechanics, the variational integrator discretizes the equations without breaking various conservation laws. The variational integrator network, one of the discrete-time deep physics models, is based on this approach. On the other hand, for Hamiltonian neural networks, however, such a discretization method has not been established. In this paper, we propose a variational integrator for Hamiltonian neural networks, and to this end, we need to solve the following two questions.

- Is it possible to formulate a discrete variational problem similar to the variational problem for the Hamilton equation using the energy function given by a neural network?

- Can the discrete Hamilton equation be derived from the formulated discrete variational problem?

In particular, regarding the second question, because the Hamiltonian is provided by a neural network, it is not possible to execute variational calculus manually. Therefore, it is necessary to successfully apply automatic differentiation to perform the discrete variational calculus.

The following is the outline of this paper. First, in Section 2, the variational integrator for Lagrangian mechanics is explained. Next, in Section 3, we explain the Hamiltonian equation and the variational principle that derives it. Finally, in Section 4, we propose a variational integrator for Hamiltonian neural networks.

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2. Outline of the varitaional integrator

The variational integrator was proposed as a method to discretize the Euler–Lagrange equation, which is the fundamental equation of Lagrangian mechanics, by using the variational principle. First, the variational principle and the Euler–Lagrange equation are explained briefly. Let $q(t) : t \in \mathbb{R} \mapsto q(t) \in \mathbb{R}^n$ denote a variable that represents the state. Consider the case of a mass point in motion under a force derived by a potential energy $V(q)$. The Lagrangian $\mathcal{L}(q, \dot{q})$, which depends on q and its time derivative $\dot{q}$, is defined as the difference between the kinetic and the potential energy:

$$\mathcal{L}(q, \dot{q}) := \frac{m}{2}\dot{q} \cdot \dot{q} - V(q), \tag{2}$$

where the mass is denoted by m. The Euler–Lagrange equation, which is the equation of motion in Lagrangian mechanics, is defined as follows:

$$\frac{\partial \mathcal{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q}} = 0. \tag{3}$$

This equation is known to be equivalent to Newton's equation of motion. The variational principle states that the Euler–Lagrange equation is obtained by computing the stationary points of the action integral S, which is defined as

$$S := \int_0^T \mathcal{L}(q, \dot{q})\mathrm{d}t.$$

The variational integrator uses this principle for discretization. More precisely, in general, numerical integrators of differential equations are derived by discretizing a given differential equation; however, to obtain the variational integrator, the variational principle is discretized, that is, the action integral is discretized and stationary points of the discretized action integral are computed. In the following, the approximate value of $q(n\Delta t)$ is denoted by $q^{(n)}$, where Δt is the time step size. Then, $\dot{q}$ can be approximated, for example, as follows:

$$\dot{q} \simeq \frac{q^{(n+1)} - q^{(n)}}{\Delta t}.$$

Suppose that the Lagrangian is given as (2). Then the Lagrangian can be approximated by

$$\mathcal{L}_\mathrm{d}(q^{(n)}, q^{(n+1)}) := \frac{m}{2}\frac{q^{(n+1)} - q^{(n)}}{\Delta t} \cdot \frac{q^{(n+1)} - q^{(n)}}{\Delta t} - V(q^{(n)}).$$

Using this discretized Lagrangian, the action sum S_d is defined as follows:

$$S_\mathrm{d} = \sum_{n=0}^{N-1} \mathcal{L}_\mathrm{d}(q^{(n)}, q^{(n+1)})\Delta t.$$

It is easy to confirm that this is an approximation of the action integral S. In the variational integrator, as in ordinary Lagrangian mechanics, the discrete equations of motion are derived by computing the variation of the action sum. Let $\delta q^{(n)}$ be a variation with $q^{(n)}$ with both ends fixed

$$\delta q^{(0)} = \delta q^{(N)} = 0$$

as is common in the original variational principle. Ignoring higher-order terms, the computation of difference of S_d leads to

$$\begin{aligned}
&\sum_{n=0}^{N-1} \mathcal{L}_\mathrm{d}(q^{(n)}+\delta q^{(n)}, q^{(n+1)}+\delta q^{(n+1)})\Delta t - \sum_{n=1}^{N} \mathcal{L}_\mathrm{d}(q^{(n)}, q^{(n+1)})\Delta t \\
&= \sum_{n=0}^{N-1} \left(D_1\mathcal{L}_\mathrm{d}(q^{(n)}, q^{(n+1)})\delta q^{(n)} + D_2\mathcal{L}_\mathrm{d}(q^{(n)}, q^{(n+1)})\delta q^{(n+1)}\right)\Delta t \\
&= \sum_{n=0}^{N-1} \left(D_1\mathcal{L}_\mathrm{d}(q^{(n)}, q^{(n+1)}) + D_2\mathcal{L}_\mathrm{d}(q^{(n-1)}, q^{(n)})\right)\delta q^{(n)}\Delta t,
\end{aligned}$$

where D_1 and D_2 are derivatives with respect to the first and second variables, respectively. Note that the final equality uses $\delta q^{(0)} = \delta q^{(N)} = 0$. To be zero for any variation $\delta q^{(n)}$, the following conditions must be satisfied

$$D_1\mathcal{L}_\mathrm{d}(q^{(n)}, q^{(n+1)}) + D_2\mathcal{L}_\mathrm{d}(q^{(n-1)}, q^{(n)}) = 0.$$

This is an approximation to the Euler–Lagrange equation and is known as the discrete Euler–Lagrange equation.

3. Variational principle behind the Hamilton equation

Similar to the Euler–Lagrange equation, the Hamilton equation is known to be derived by the variational principle. Instead of S, consider the following integral:

$$\int_0^T (p \cdot \dot{q} - H(q, p))\,\mathrm{d}t \tag{4}$$

By ignoring the higher-order terms and fixing both ends, the variation of this integral becomes

$$\begin{aligned}
&\int_0^T ((p + \delta p) \cdot (\dot{q} + \delta\dot{q}) - H(q + \delta q, p + \delta p))\,\mathrm{d}t \\
&- \int_0^T (p \cdot \dot{q} - H(q, p))\,\mathrm{d}t \\
&= \int_0^T (p \cdot \delta\dot{q} + \delta p \cdot \dot{q} - D_1 H \delta q - D_2 H \delta p)\,\mathrm{d}t \\
&= \int_0^T \left(-\dot{p} \cdot \delta q + \delta p \cdot \dot{q} - \frac{\partial H}{\partial q} \cdot \delta q - \frac{\partial H}{\partial p} \cdot \delta p\right)\mathrm{d}t + [p \cdot \delta q]_0^T \\
&= \int_0^T \left((-\dot{p} - \frac{\partial H}{\partial q}) \cdot \delta q + (\dot{q} - \frac{\partial H}{\partial p}) \cdot \delta p\right)\mathrm{d}t
\end{aligned}$$

For this variation to be zero for any δq and δp, the following conditions must be hold:

$$-\dot{p} - \frac{\partial H}{\partial q} = 0, \quad \dot{q} - \frac{\partial H}{\partial p} = 0.$$

This corresponds to the Hamilton equation (1).

4. Proposed variational integrator for Hamiltonian neural networks

In this section, we propose a variational integrator for Hamiltonian neural networks. Suppose that a trained Hamiltonian neural network is given, of which Hamiltonian is given by a neural network H_{NN}. First, as in the Lagrangian formalism, consider the following sum that approximates the integral (4)

$$\sum_{n=0}^{N-1}\left(p^{(n)}\cdot\frac{q^{(n+1)}-q^{(n)}}{\Delta t}-H_{\mathrm{NN}}(q^{(n)},p^{(n)})\right)\Delta t$$

where $q^{(n)}$ and $p^{(n)}$ are approximations of $q(n\Delta t)$ and $p(n\Delta t)$, respectively. Computing the variation of the above sum with respect to the infinitesimal perturbations $\delta q^{(n)}$ and $\delta p^{(n)}$ of $q^{(n)}$ and $p^{(n)}$ under the assumption that $\delta q^{(0)}=\delta q^{(N)}=0$, we obtain

$$\begin{aligned}
&\sum_{n=0}^{N-1}\Big((p^{(n)}+\delta p^{(n)})\cdot(\frac{q^{(n+1)}-q^{(n)}}{\Delta t}+\frac{\delta q^{(n+1)}-\delta q^{(n)}}{\Delta t})\\
&-H_{\mathrm{NN}}(q^{(n)}+\delta q^{(n)},p^{(n)}+\delta p^{(n)})\Big)\Delta t\\
&-\sum_{n=0}^{N-1}\left(p^{(n)}\cdot\frac{q^{(n+1)}-q^{(n)}}{\Delta t}-H_{\mathrm{NN}}(q^{(n)},p^{(n)})\right)\Delta t\\
&=\sum_{n=0}^{N-1}\Big(p^{(n)}\cdot\frac{\delta q^{(n+1)}-\delta q^{(n)}}{\Delta t}+\delta p^{(n)}\cdot\frac{q^{(n+1)}-q^{(n)}}{\Delta t}\\
&-D_1H_{\mathrm{NN}}(q^{(n)},p^{(n)})\cdot\delta q^{(n)}-D_2H_{\mathrm{NN}}(q^{(n)},p^{(n)})\cdot\delta p^{(n)}\Big)\Delta t.
\end{aligned}$$

For the first term, the following equality holds:

$$\begin{aligned}
&\sum_{n=0}^{N-1}p^{(n)}\cdot\frac{\delta q^{(n+1)}-\delta q^{(n)}}{\Delta t}\Delta t\\
&=\sum_{n=0}^{N-1}p^{(n)}\cdot\delta q^{(n+1)}-\sum_{n=0}^{N-1}p^{(n)}\cdot\delta q^{(n)}\\
&=\sum_{n=1}^{N}p^{(n-1)}\cdot\delta q^{(n)}-\sum_{n=0}^{N-1}p^{(n)}\cdot\delta q^{(n)}\\
&=\sum_{n=0}^{N-1}p^{(n-1)}\cdot\delta q^{(n)}-\sum_{n=0}^{N-1}p^{(n)}\cdot\delta q^{(n)}\\
&=\sum_{n=0}^{N-1}\left(-\frac{p^{(n)}-p^{(n-1)}}{\Delta t}\cdot\delta q^{(n)}\right)\Delta t
\end{aligned}$$

where $\delta q^{(0)}=\delta q^{(N)}=0$ is used. This is often referred to as "summation by parts." Using this, the above variation can be rewritten as follows:

$$\begin{aligned}
&\sum_{n=0}^{N-1}\Big(-\frac{p^{(n)}-p^{(n-1)}}{\Delta t}\cdot\delta q^{(n)}+\delta p^{(n)}\cdot\frac{q^{(n+1)}-q^{(n)}}{\Delta t}\\
&-D_1H_{\mathrm{NN}}(q^{(n)},p^{(n)})\delta q^{(n)}-D_2H_{\mathrm{NN}}(q^{(n)},p^{(n)})\delta p^{(n)}\Big)\Delta t\\
&=\sum_{n=0}^{N-1}\Big(\Big(-\frac{p^{(n)}-p^{(n-1)}}{\Delta t}-D_1H_{\mathrm{NN}}(q^{(n)},p^{(n)})\Big)\cdot\delta q^{(n)}\\
&+\Big(\frac{q^{(n+1)}-q^{(n)}}{\Delta t}-D_2H_{\mathrm{NN}}(q^{(n)},p^{(n)})\Big)\cdot\delta p^{(n)}\Big)\Delta t.
\end{aligned}$$

Hence for the vatiation to be zero the following equation must hold:

$$\begin{aligned}
&-\frac{p^{(n)}-p^{(n-1)}}{\Delta t}-D_1H_{\mathrm{NN}}(q^{(n)},p^{(n)})=0,\\
&\frac{q^{(n+1)}-q^{(n)}}{\Delta t}-D_2H_{\mathrm{NN}}(q^{(n)},p^{(n)})=0.
\end{aligned}$$

These equations can be rearranged to

$$\begin{pmatrix}\dfrac{q^{(n+1)}-q^{(n)}}{\Delta t}\\ \dfrac{p^{(n)}-p^{(n-1)}}{\Delta t}\end{pmatrix}=\begin{pmatrix}O & I\\ -I & O\end{pmatrix}\begin{pmatrix}D_1H_{\mathrm{NN}}(q^{(n)},p^{(n)})\\ D_2H_{\mathrm{NN}}(q^{(n)},p^{(n)})\end{pmatrix}. \quad (5)$$

It turns out that this is certainly an approximation of the Hamilton equation (1).

We now consider whether $q^{(n+1)}$ and $p^{(n+1)}$ can be computed using this equation for a Hamiltonian H_{NN} given by a neural network. First, because each expression of (5) is valid for any n, so (5) can be rewritten as

$$\begin{pmatrix}\dfrac{q^{(n+1)}-q^{(n)}}{\Delta t}\\ \dfrac{p^{(n+1)}-p^{(n)}}{\Delta t}\end{pmatrix}=\begin{pmatrix}O & I\\ -I & O\end{pmatrix}\begin{pmatrix}D_1H_{\mathrm{NN}}(q^{(n+1)},p^{(n+1)})\\ D_2H_{\mathrm{NN}}(q^{(n)},p^{(n)})\end{pmatrix}. \quad (6)$$

This defines the simultaneous equations for $q^{(n+1)},p^{(n+1)}$, when $q^{(n)},p^{(n)}$ are given. This system of equations can be solved numerically as explained below. The D_1 and D_2 are the derivatives of the neural network from the first and second variables, respectively. Therefore, if the values of $H_{\mathrm{NN}}(q^{(n)},p^{(n)})$ and $H_{\mathrm{NN}}(q^{(n+1)},p^{(n+1)})$ can be calculated, D_1H_{NN} and D_2H_{NN} can be obtained by using automatic differentiation.

For simplicity, let us solve the above system of equations by using a simple fixed-point iteration method. Let $q^{(n+1)}_{(k)},p^{(n+1)}_{(k)}$ be the approximations of $q^{(n+1)},p^{(n+1)}$ at the kth iteration. The algorithm of the fixed-point iteration method is as follows:

$$\begin{aligned}
&q^{(n+1)}_{(0)}=q^{(n)},p^{(n+1)}_{(0)}=p^{(n)},\\
&\begin{pmatrix}q^{(n+1)}_{(k+1)}\\ p^{(n+1)}_{(k+1)}\end{pmatrix}=\begin{pmatrix}q^{(n)}\\ p^{(n)}\end{pmatrix}+\Delta t\begin{pmatrix}O & I\\ -I & O\end{pmatrix}\begin{pmatrix}D_1H_{\mathrm{NN}}(q^{(n+1)}_{(k)},p^{(n+1)}_{(k)})\\ D_2H_{\mathrm{NN}}(q^{(n)},p^{(n)})\end{pmatrix}.
\end{aligned}$$

The right-hand side can be computed using automatic differentiation. Thus, when the algorithm converges, the numerical method (6) certainly determines $q^{(n+1)},p^{(n+1)}$.

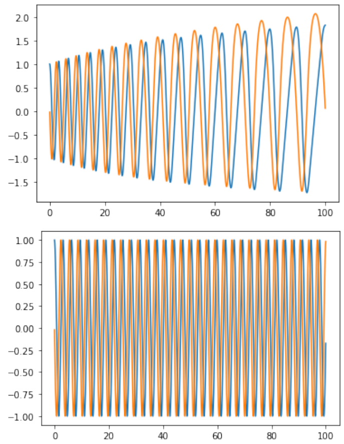

Figure 1: Predicted solutions (q: blue, p: orange) by the Euler method (top) and those by the variational integrator (bottom).

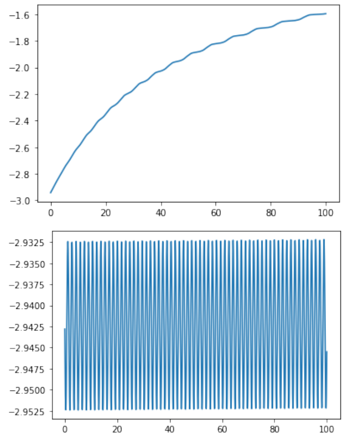

Figure 2: Predicted energies by the Euler method (top) and by the variational integrator (bottom).

5. Numerical Example

We trained Hamiltonian neural networks using a data set of a simple harmonic oscillator:

$$\dot{q} = p, \quad \dot{p} = -q.$$

We performed physical simulations by using the trained model discretized by the explicit Euler method and the proposed variational integrator. The time step size was set to $\Delta t = 0.01$. The numerical solutions are computed from $t = 0$ to $t = 100$. When the neural network was trained, it was confirmed that the loss function was certainly small enough. Fig. 1 shows the simulation results by the two methods, while Fig. 2 shows the energy behaviors. When the explicit Euler method was employed, the energy increased and the numerical solution diverged. When the proposed method was used, however, the energy was very well conserved and the solution continued to oscillate within a certain range.

6. Concluding Remarks

In this paper, we have proposed a variational integrator for Hamiltonian neural networks. In Hamiltonian neural networks, the variational calculus cannot be performed by hand because the energy function is given by a neural network. Therefore, it was necessary to confirm that this principle can be certainly applied and the solutions of the derived numerical method can be computed by using automatic differentiation. In addition, the energy conservation property of the proposed method was confirmed by the numerical experiment.

Acknowledgments

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