Deep Discrete-Time Lagrangian Mechanics

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Introduction

Goal: a deep neural network that
• learns the physical dynamics only from the position.
• ensures the energy conservation laws strictly in discrete time.

Background
• Recent studies demonstrated that neural networks learn the physical dynamics associated with the conservation law of energy in continuous time [1].
• The method is no longer conserved after numerical integrators discretize the time for computer simulations.
• Symplectic integrators conserve a modified energy and a discrete gradient method conserves energy strictly in discrete time [2, 3].
• They need velocity or momentum but measuring an accurate velocity is troublesome.
• Without an accurate velocity, a learned dynamics may be greatly different from the teacher system.
• The Verlet method is a symplectic integrator and depends only on the position.
• No method that conserves energy strictly in discrete time is available when only the position is available.

Proposed approach
• models discrete-time Lagrangian mechanics, which is expressed only with the position.
• ensures the energy conservation laws strictly in discrete time by the automatic discrete differential (AAD) algorithm [3].

Method: Theory

Target system
• The potential energy $V$ is expressed as a function of the position $q$.
• The kinetic energy $T$ is expressed as a function of the velocity $q$ or momentum $p$.

Hamiltonian mechanics
A system
- has a state $u = (q, p)$.
- has a Hamiltonian $H = T + V$.

Hamilton’s equation

\[
\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}\]

Lagrangian mechanics
A system
- has a state $u = (q, q')$.
- has a Lagrangian $L = T - V$.

Euler-Lagrangian equation

\[
\frac{dq}{dt} = \frac{\partial L}{\partial q'}, \quad \frac{dq'}{dt} = \frac{\partial L}{\partial q}\]

The conservation law of energy.
For conserving energy strictly in discrete time, a discrete gradient has been devised [4].

Method: Proposed Approach

Method
- Eliminating the momentum from Hamiltonian mechanics in discrete time.

\[
\frac{q^{(n+1)} - q^{(n)}}{\Delta t} = \frac{\partial}{\partial p} T(p^{(n+1)}, p^{(n)}) - \frac{\partial}{\partial q'} V(q^{(n+1)}, q^{(n)})
\]

Proposed: discrete-time Lagrangian mechanics

\[
M \frac{q^{(n+1)} - q^{(n)}}{(\Delta t)^2} = \frac{1}{2} \left[ \frac{\partial}{\partial q'} V(q^{(n+1)}, q^{(n)}) + \frac{\partial}{\partial q'} V(q^{(n)}, q^{(n-1)}) \right]
\]

- The potential energy $V$ is modeled by a neural network.
- A discrete gradient $\nabla q'$ is obtained by the AAD algorithm [3].
- $M$ is a mass matrix.

Since the proposed equation (1) converges to the Euler-Lagrangian equation, it is considered as a discrete-time Lagrangian mechanics.

Proposed approach
- learns the physical dynamics only from the position by modeling a discrete-time Lagrangian mechanics.
- ensures the conservation law of energy strictly in discrete time using a discrete gradient.

Training
- Minimizing mean squared error between left- and right-hand sides of Eq. (1).

Experiments and Results

Datasets
- mass-spring system, pendulum system, and 2-body system

Comparative methods
- Euler method, symplectic Euler method, and leapfrog integrator
- “leapfrog + proposed” use leapfrog integrator for training and the proposed approach for prediction.

Results
- The proposed approach and the leapfrog integrator predict the state at a similar level.
- For the mass-spring and pendulum systems, the proposed approach conserves energy accurately, symplectic Euler method and leapfrog integrator conserve a modified energy only from the position but they do not conserve energy strictly.
- For the 2-body system, “leapfrog + proposed” conserves energy accurately.
- The proposed approach conserves modeled energy.

Table 1: Mean squared errors averaged over 15 trials across all three tasks.

<table>
<thead>
<tr>
<th>Model</th>
<th>Position $q$</th>
<th>Energy</th>
<th>Position $q$</th>
<th>Energy</th>
<th>Position $q$</th>
<th>Energy</th>
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<tbody>
<tr>
<td>Euler</td>
<td>4.46 $\times$ 10^{-2}</td>
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<tr>
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<td>1.03 $\times$ 10^{-1}</td>
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Table 2: The variance of modeled energy.

<table>
<thead>
<tr>
<th>Model</th>
<th>Mass-Spring</th>
<th>Pendulum</th>
<th>2-Body</th>
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References