Hamiltonian Neural Network

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Introduction

Hamiltonian Neural Networks (HNN) are a class of models that leverage the Hamiltonian Mechanic framework to learn the dynamics of physical systems. Hamiltonian Mechanics is a reformulation of classical mechanics that describes a system's evolution using Hamilton's Equations, which are second order Ordinary Differential Equations (ODEs). We define the

Mathematical Formulation:

- In Hamiltonian mechanics, the state of a system is described by its position q and momentum p.
- The Hamiltonian H(q,p)H(q, p)H(q,p) represents the total energy of the system (kinetic + potential energy).
- The evolution of the system is governed by Hamilton's equations:

Hamilton's equations

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

#Weeqly @TamasGorbe

- In Hamiltonian Neural Networks, a neural network is used to approximate the Hamiltonian function H(q,p;θ) with parameters θ.
- The learned Hamiltonian is then used to predict the time evolution of the system's state.

Predicting The Motion Of A Double Pendulum Using HNNs

Problem Description:

The double pendulum is a classic problem in physics known for its chaotic behavior. It consists of two pendulums attached end to end. Predicting its motion accurately is challenging due to its sensitive dependence on initial conditions.

Objective:

To use a Hamiltonian Neural Network (HNN) to learn the dynamics of the double pendulum and predict its motion over time.

Solution And Implementation

Data Generation:

- Simulate the double pendulum system using known physics-based models to generate training data.
- The state of the double pendulum is described by the angles θ1 and θ2, and their corresponding angular momenta p1and p2.
- Generate a dataset of state transitions (θ1,θ2,p1,p2) over time.

Hamiltonian Function:

- Define the Hamiltonian H(θ1,θ2,p1,p2)which represents the total energy of the double pendulum system (kinetic + potential energy).
- Use a neural network to approximate the Hamiltonian: HNN(θ1,θ2,p1,p2;θ) where θ are the parameters of the neural network.

Training the HNN:

- Use the training data to learn the parameters of the neural network such that it approximates the true Hamiltonian of the system.
- Define the loss function based on Hamilton's equations:

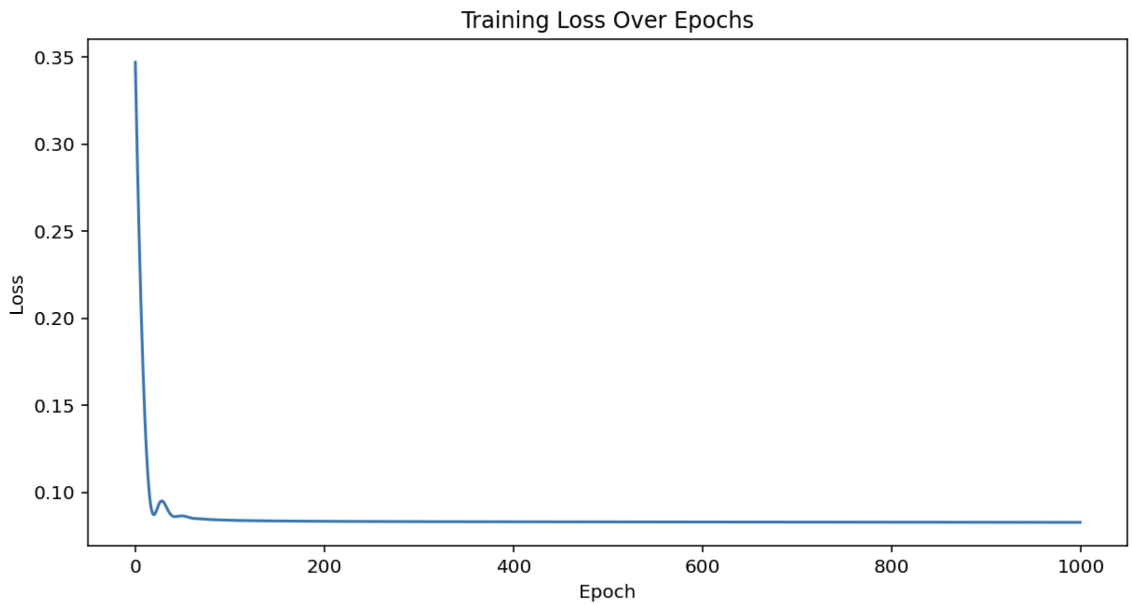
$$\mathcal{L} = \left\| \frac{d\theta_1}{dt} - \frac{\partial H_{\mathrm{NN}}}{\partial p_1} \right\|^2 + \left\| \frac{dp_1}{dt} + \frac{\partial H_{\mathrm{NN}}}{\partial \theta_1} \right\|^2 + \left\| \frac{d\theta_2}{dt} - \frac{\partial H_{\mathrm{NN}}}{\partial p_2} \right\|^2 + \left\| \frac{dp_2}{dt} + \frac{\partial H_{\mathrm{NN}}}{\partial \theta_2} \right\|^2$$

- Minimize the loss function using gradient-based optimization techniques.

Prediction and Evaluation:

- Use the trained HNN to predict the state of the double pendulum over time given initial conditions.
- Compare the predicted motion with ground truth data from the physics-based simulation to evaluate the performance of the HNN.

Results



We observed that the Training Loss drops significantly over epochs indicating the correctness of the model.

Conclusion:

1. **Effectiveness of HNNs:**
   - **Physical Consistency:** By using Hamiltonian mechanics, HNNs ensure that the learned dynamics respect the conservation of energy, which is crucial for accurate modeling of physical systems.
   - **Generalization:** HNNs can generalize well to unseen states and longer time horizons due to their grounding in physical principles, making them suitable for complex dynamical systems like the double pendulum.
2. **Training Progress:**
   - The plot of training loss over epochs showed a decreasing trend, indicating that the model was effectively learning the system's dynamics.
   - Periodic monitoring of the loss (e.g., every 100 epochs) provided insights into the training progress and model performance.

Hamiltonian Neural Networks offer a robust framework for modeling complex dynamical systems by leveraging the principles of Hamiltonian mechanics. The approach's success in predicting the motion of a double pendulum demonstrates its potential in various applications, from physics-based modeling to robotics and beyond. Continued research and development in this area can lead to more sophisticated models capable of handling increasingly complex systems.

Key References

- Greydanus, S., Dzamba, M., & Yosinski, J. (2019). Hamiltonian Neural Networks. In *Advances in Neural Information Processing Systems* (*NeurIPS* 2019).