Neural ODE for Hamiltonian Systems with Irregular and Noisy Data

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Abstract: Learning generalizing models from measurements is a challenging task, especially when the data is noisy or irregular. Real data is almost never noise-free and often irregular. Therefore noise removal is necessary if we want to learn good models. In this work we will focus on Hamiltonian systems, which can fully be described by the associated Hamiltonian. We discuss a methodology for learning the Hamiltonian from noisy measurements. To do this, we train a neural network to implicitly represent the data. We simultaneously use a Hamiltonian-Neural-Network (HNN) to learn the Hamiltonian and combine both networks by the neural ODE approach. Another important property of Hamiltonian systems is their symplectic phase flow. If we want to predict future states of the system, we can learn an explicit symplectic integrator by using intrinsic structure-preserving symplectic networks (SympNets). We also combine the SympNets with the implicit representation of the data via the neural ODE approach to deal with noise or irregular measurements. The proposed method can handle data where dependent variables are not available on the same time grid. This is particularly remarkable since standard SympNets only work on equidistant full state variables. We show the effectiveness of the proposed method by comparing it against standard HNNs and SympNets, which do not consider noisy or irregular data.

Keywords: Hamiltonian Systems, Machine Learning, Neural ODE, Noisy Data, Structure-Preserving Methods

Novelty statement:

- We combine machine learning methods for Hamiltonian systems like HNNs and SympNets with a neural network, which works as an implicit representation of the data, by using the integral formulation of the Hamiltonian equations of motion.
- Derivative Information is not required to train HNNs in this framework, as it can be recovered from the implicit representation of the data.
- The proposed methodology is capable of a situation when the dependent variables are sampled irregularly. Moreover, they need not be measured on the same irregular time grid.
- This creates the possibility to use SympNets outside of data sampled on equidistant time grids.