Phase Space Visualization and Neural Networks: Learning Hamiltonian Dynamics in the Duffing System

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1. Introduction

The intersection of artificial intelligence (AI) and natural sciences has seen significant advances in recent years, particularly in modeling physical dynamics. Among these developments, Hamiltonian Neural Networks (HNNs) [1] have emerged as a novel framework for learning and preserving Hamiltonian dynamics. HNNs are designed to directly learn the Hamiltonian of a system. This makes HNNs especially suitable for modeling systems governed by conservation laws.

Building on this foundation, several extensions have been proposed. For instance, Symplectic Recurrent Neural Networks [2], SympNets [3] and HenonNets [4], which explore intrinsic symplectic structures. A recent study [5] introduced Generalized Hamiltonian Neural Networks (GHNNs), offering a unified framework that connects these various approaches.

Despite these advancements, the global visualization and analysis of phase-space structures, particularly invariant manifolds, remains unexplored in visualizing the neural network modeling of Hamiltonian systems. Invariant manifolds, such as stable and unstable manifolds, define boundaries between regions of behavior and are essential for predicting long-term system evolution. To address this, we propose the use of Lagrangian Descriptors [6, 7] to visualize the phase space of learned dynamics, enabling a deeper understanding of global features.

This paper has two primary objectives: (1) to evaluate the ability of neural network models to learn Hamiltonian systems and (2) to employ LDs for phase-space visualization, assessing how well these models reconstruct critical structures such as invariant manifolds.

As a test case, we use the Duffing equation, a nonlinear oscillator with rich Hamiltonian dynamics. A key feature of the Duffing system is the homoclinic orbit, which separates the basins of attraction. By applying GHNNs and leveraging LDs, we aim to demonstrate the effectiveness of our method in uncovering the intricate structures of phase space learned by neural networks.

2. Methods

2.1 The Datasets

The Duffing equation's Hamiltonian, derived through an appropriate transformation, takes the form:

$$H = \frac{1}{2}\dot{x}^2 - \frac{1}{2}x^2 - \frac{\alpha}{4}x^4 \tag{1}$$

This system becomes particularly interesting when $\alpha < 0$, corresponding to a softening spring in the context of spring dynamics. This condition results in a double-well potential, introducing bistable behavior. Specifically, the system exhibits three fixed points: two center points at $(x, \cdot x) = (0, \pm\alpha)$ and a saddle point at $(x, \cdot x) = (0, 0)$. The homoclinic orbit, connecting the saddle point to itself, serves as a boundary between the basins of attraction of the two stable equilibria, playing a critical role in the system's dynamics.

Here we used $\alpha = -1$. The training datasets are generated by numerically solving the Duffing equation with the initial conditions $\cdot x(0) = 0$ while $x(0)$ randomly chosen from the interval $(-3, 3)$. Each trajectory simulates 100 time units of dynamics. The datasets vary in the number of trajectories, with totals of 10, 20, 50, 100, and 200 trajectories. For each dataset, the trajectories are divided into 80% for training, 10% for validation, and 10% for testing.

2.2 Neural Network Models

In this article, we compare the performance of SympNet, HenonNet, and GHNN models. We refer to [5] for details of the architectures of the models. The model parameters are chosen to align with those described in [5] and summarized in Table 1

NN type	Learned Hamiltonians	Neurons per Layer	Trainable parameters
SympNet	10	50	3000
HénonNet	10	50	755
GHNN	5	25	7250

Table 1: Hyperparameters of the Neural Network

An advantageous property of the neural network (NN) models considered in this study is their inherent invertibility, which significantly simplifies LD computation. Specifically, the invertibility allows for efficient computation of the backward-time portion of the trajectory without resorting to solving nonlinear equations at each step. For general NN models lacking this property, computing the backward trajectory would require iterative solutions, leading to prohibitively high computational costs. Due to this reason, we are not considering comparing our result with the baseline MLP.

2.3 *Lagrangian Descriptors*

Lagrangian Descriptors (LDs) are a powerful tool for uncovering phase-space structures in dynamical systems due to their simplicity and straightforward implementation. In this study, the LDs are computed by evaluating the finite-time arc length of trajectories in the phase space for each model. Specifically, for a given initial state, the LD is defined as:

$$M(x_0, \dot{x}_0) = \int_{-\tau}^{\tau} \sqrt{|\dot{x}|^2 + |\ddot{x}|^2} dt \tag{2}$$

where we use $\tau = 5$ is the integration time. Through experimentation, we determined that this integration time is sufficient to reveal the homoclinic structure in the phase space. Remark that, in general, for LD other positive scalar valued functions might be used rather than the arc length of the trajectory[7].

The LD computation is performed on a phase-space grid defined by $x_0 \in [-1.5, 1.5]$ and $\dot{x}_0 \in [-0.8, 0.8]$, using a resolution of 400 grid points in each direction. This fine grid ensures a detailed visualization of the phase space structure.

3. Result

For datasets containing 200 trajectories, all the evaluated methods - SympNet, HenonNet, and GHNN - successfully captured the presence of a homoclinic orbit in phase space, as shown in the first three plots of Fig. 1. However, subtle differences in the location of the homoclinic orbit are evident, particularly in the bottom panel of Fig. 1, where we plot the exact homoclinic orbit for comparison. Among the methods, the HenonNet model exhibits the most noticeable deviation from the exact orbit.

Reducing the number of training datasets enables the capture of the homoclinic orbit, albeit with greater deviations. In extreme cases, the neural network models to capture the homoclinic orbit entirely, as indicated by the Lagrangian Descriptors, which identified that the learned phase space structure consists only of a central fixed point. Among the datasets used, GHNN requires a minimum of 20 datasets to capture the homoclinic orbit, while HenonNet needs at least 50 datasets, and SympNet requires 200 datasets. Due to space constraints, detailed visualizations of these cases are not included here..

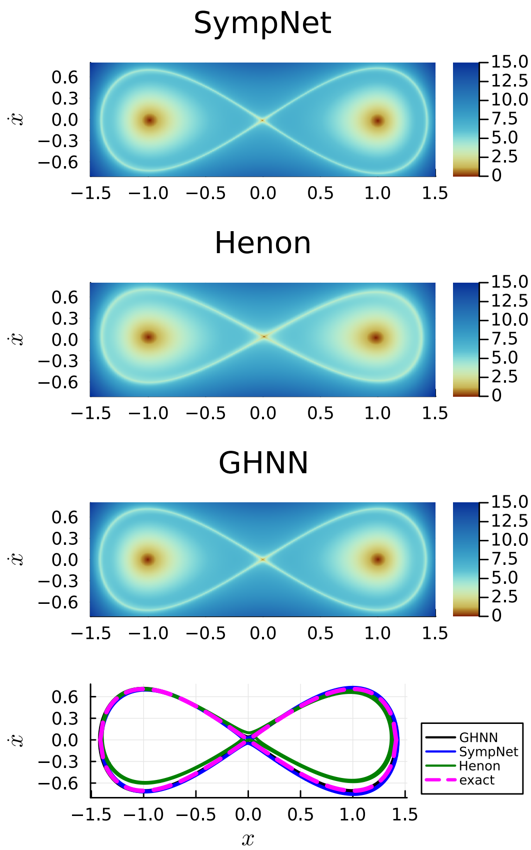

Fig. 1: Lagrangian Descriptors for SympNet, HenonNet, and GHNN across 200 datasets (top three plots). The bottom panel shows the homoclinic structure extracted from the Lagrangian Descriptors. The dashed line represents the exact homoclinic orbit of the Duffing Equation.

4. DISCUSSION AND CONCLUSION

This study demonstrates that some class Hamiltonian Neural Networks (HNNs), namely SympNet, HenonNet, and GHNN, , can effectively learn the dynamics of Hamiltonian systems, as evaluated through their ability to reconstruct the homoclinic orbit of the Duffing equation. By employing Lagrangian Descriptors (LDs) for phase-space analysis, we verified that all models successfully capture the homoclinic orbit, a key structure in the Duffing system. However, subtle discrepancies in the learned orbits were observed, with HenonNet exhibiting the most significant deviation from the exact trajectory. Moreover, we found that the number of training datasets plays a critical role in the accuracy of learned dynamics.

A key contribution of this work is the application of Lagrangian Descriptors as a diagnostic tool for assessing phase-space structures in learned dynamics. LDs provided a detailed and intuitive visualization of the reconstructed manifolds, highlighting both the strengths and limitations of each model. This demonstrates the potential of LDs for evaluating the accuracy and reliability of data-driven models in capturing essential dynamical features.

Future work will extend this analysis to chaotic regimes of the Duffing equation, where intricate manifold structures and sensitivity to initial conditions pose significant challenges. Additionally, we aim to investigate the use of LDs in analyzing the phase space dynamics of neural networks trained on the nonlinear Schrödinger equation, a system with rich and diverse behavior, including solitons and modulational instability. These extensions will further explore the capabilities of HNNs in learning complex dynamical systems and reinforce the role of LDs as a valuable tool for phase-space analysis.

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