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Hamiltonian Neural Network Exploration for Electron Particle Tracking

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Motivation

A Hamiltonian Neural Network (HNN) utilizes Hamiltonian mechanics so that the NN can learn conservation laws from data. This research explores electron particle tracking through machine learning using HNN, Dissipative Neural Networks (D-HNNs), and a multilayer perceptron (MLP). Electron particle tracking in 6D phase space can be computationally expensive (for this research 2D will be used as proof of principle). Particle tracking is an important step in designing particle accelerators. Can we utilize a HNN to train on limited data and track electron particles to advance the design of particle accelerators?

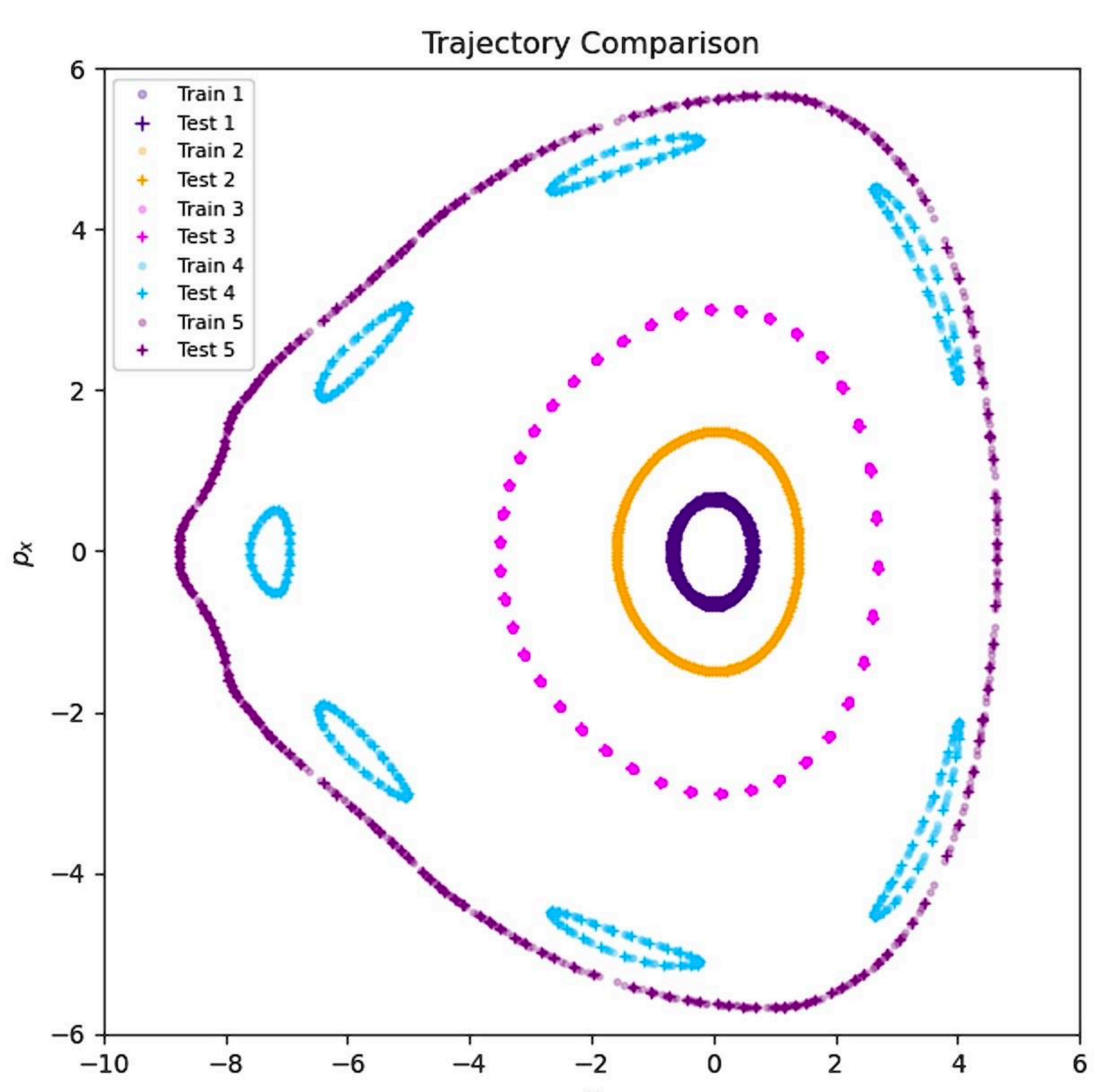


Figure 1. We choose 5 electron particle trajectory data sets with 1000 points each and split the coordinates into an 80/20 train-to-test ratio.

Theory

A HNN uses the Hamiltonian equations as an inductive bias within a neural network to map phase space coordinates to their approximate time derivative. The Hamiltonian, $H(x, p_x)$, is a scalar function such that

$$\frac{\partial H}{\partial p_x} = \frac{\partial x}{\partial t}, \; -\frac{\partial H}{\partial x} = \frac{\partial p_x}{\partial t}$$

Our Hamiltonian function is given by

$$H(x, p_x) = \frac{x^2}{2} + \frac{{p_x}^2}{2} + V(x)$$

with the sextupole potential

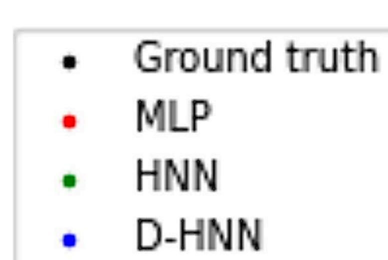
$$V(x) = \frac{\alpha x^3}{3}$$

where $\alpha = 0.113$ is the estimated strength for the sextupole potential. A D-HNN combines Hamiltonian mechanics and Helmholtz decomposition that can separate dissipative effects such as friction. See [2] for more information about D-HNNs.

Method

The 5 trajectory data sets from Figure 1 were made by applying the action of each element on a particle iteratively. The HNN, D-HNN, and MLP are trained on this data to learn particle behavior, then tested, and their losses are recorded in Table 1. To understand the models' performance, we reserve the testing data to serve as the ground truth and compare it with the predictions. The Hamiltonian function, $H(x, p_x)$, is used to compare the total energies of the system to each time step.

Legend on the right for figures 2-6. For readability, only HNN was shown for the total energy.



Results

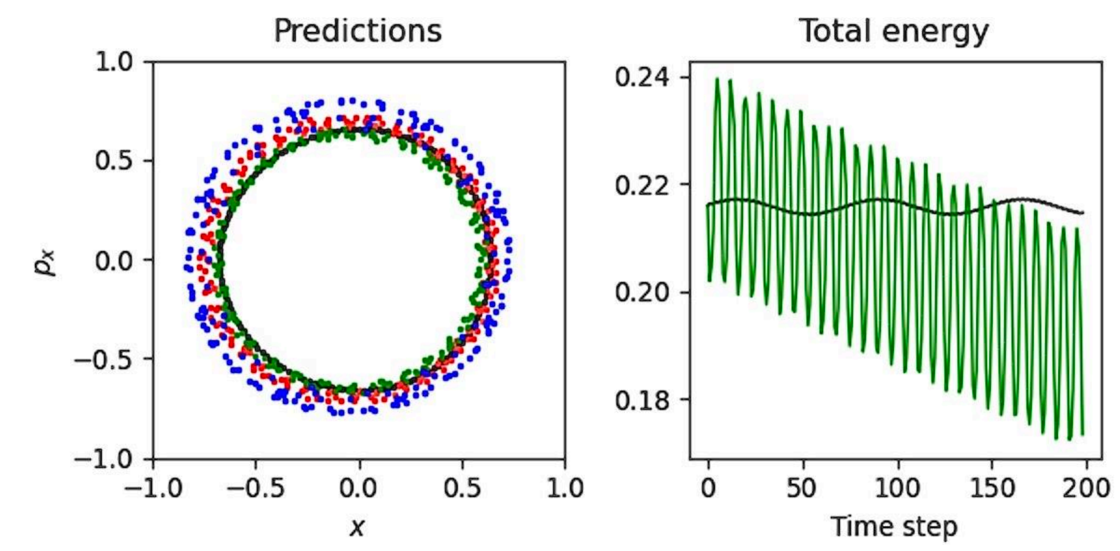


Figure 2. Left: The predicted dynamics for all the models on trajectory 1. The HNN clearly performs better when predicting coordinates. **Right:** Modeling the system of the dissipation rate over time for trajectory 1.

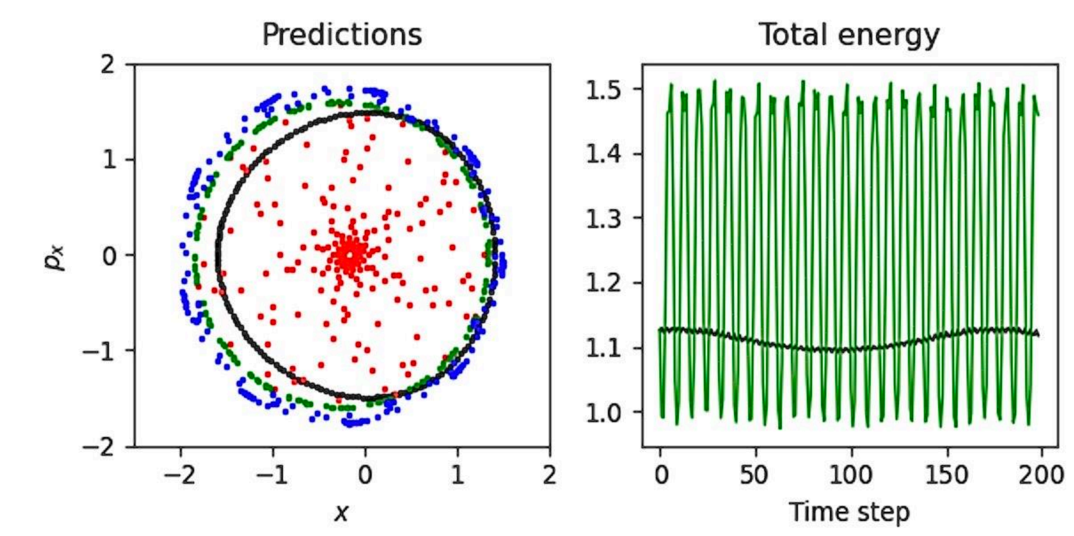


Figure 3. Left: The predicted dynamics for all the models on trajectory 2. The HNN losses accuracy for points to the left of $x = 0$. **Right:** Modeling the system of the dissipation rate over time for trajectory 2.

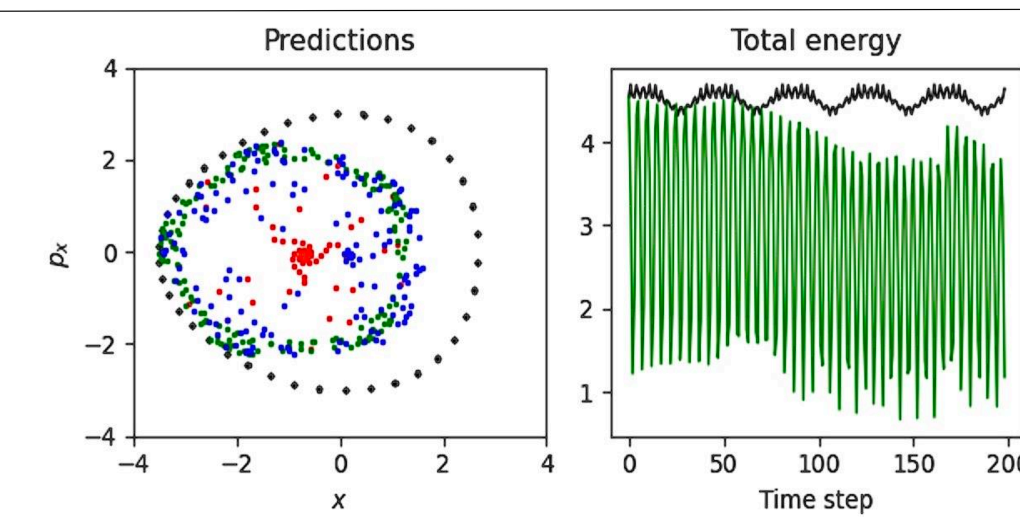


Figure 4. Left: The predicted dynamics for all the models on trajectory 3. The HNN loses accuracy for most points, underestimating the position. **Right:** Modeling the system of the dissipation rate over time for trajectory 3.

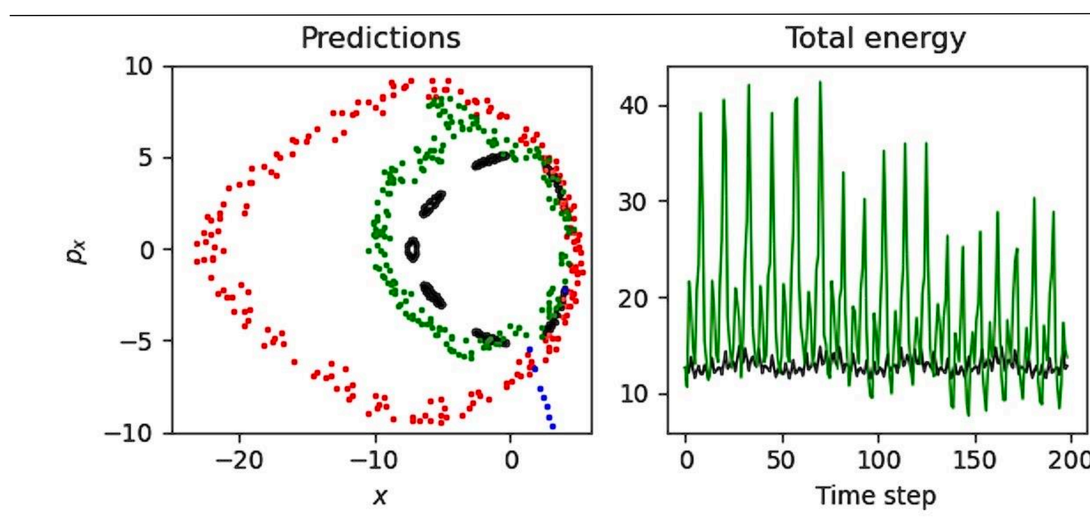


Figure 5. Left: The predicted dynamics for all the models on trajectory 4. The D-HNN fails to get a moderate prediction. **Right:** Modeling the system of the dissipation rate over time for trajectory 4.

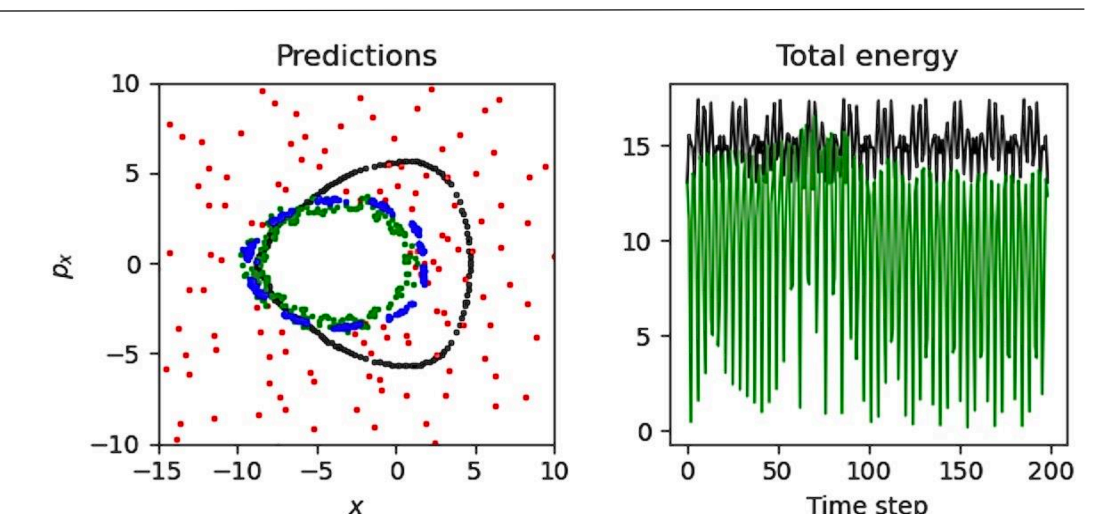


Figure 6. Left: The predicted dynamics for all the models on trajectory 5. The MLP fails to predict most points. **Right:** Modeling the system of the dissipation rate over time for trajectory 5.

Trajectory	HNN	D-HNN	MLP
1	1.12e-05	3.48e-06	7.83e-06
2	2.15e-05	2.25e-04	1.95e-05
3	4.28e-05	8.78e-05	3.18e-04
4	1.50e-02	8.04e-04	1.88e-04
5	1.61e-03	6.59e-03	7.71e-04

Table 1: Test loss from training for each of the three models on each trajectory. The average test losses were as follows: HNN = 3.34E-03, D-HNN = 1.54E-03, and MLP = 2.61E-04

Conclusion

The above results do not show sufficient evidence that HNNs can predict particle trajectories. Possible new ML algorithms, or a combination of them, can be created to capture a system's dynamics.

[1] L. Gupta, Analytic and Machine Learning Methods for Controlling Nonlinearities in Particle Accelerators. 2021

[2] S. Greydanus, A. Sosanya. Dissipative Hamiltonian Neural Networks: Learning Dissipative and Conservative Dynamics Separately. *arXiv preprint arXiv:2201.10085*, 2022.

This study was based on data from [1] with adapted python code from [2]