# STIFFNESS-AWARE NEURAL NETWORK FOR LEARNING HAMILTONIAN SYSTEMS

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## ABSTRACT

We propose stiffness-aware neural network (SANN), a new method for learning Hamiltonian dynamical systems from data. SANN identifies and splits the training data into stiff and nonstiff portions based on a stiffness-aware index, a simple, yet effective metric we introduce to quantify the stiffness of the dynamical system. This classification along with a resampling technique allows us to apply different time integration strategies such as step size adaptation to better capture the dynamical characteristics of the Hamiltonian vector fields. We evaluate SANN on complex physical systems including a three-body problem and billiard model. We show that SANN is more stable and can better preserve energy when compared with the state-of-the-art methods, leading to significant improvement in accuracy.

## 1 INTRODUCTION

Data-driven modeling of dynamical systems provides a computationally inexpensive approach for exploiting the scientific law of the physical processes and predicting future phenomena (Giannakis & Majda, 2014; Harlim et al., 2021; Gu et al., 2021). With the superior approximation and generalization capacity (Lu et al., 2020; Shen et al., 2021) of neural networks (NNs), important advances have been made in learning Hamiltonian systems (Greydanus et al., 2019; Finzi et al., 2020; Tong et al., 2021). Based on the physical property that the total energy of the system (also called Hamiltonian) must be conserved, many studies model the Hamiltonian system by learning this conserved quantity from data (Greydanus et al., 2019; Chen et al., 2019; DiPietro et al., 2020). Even though some successes have been achieved, it remains challenging to learn the estimated system to capture the exact physical law, because of the elusive and chaotic characteristics of the systems (Choudhary et al., 2020; Marchal, 1990), especially for complex systems that are intrinsically stiff. When learning stiff dynamics, the NN optimization easily leads to an unstable solution or biased estimation due to the lack of constraint on parameters (Kim et al., 2021; Wang et al., 2020).

To illustrate the difficulty in learning stiff Hamiltonian dynamics, let us consider a three-body problem that describes the interactions of three particles under gravitational force. According to physical law, the repulsive force of two particles increases dramatically when they get close to each other. Hence, the close three-body interaction intensifies stiffness phenomena (Huang & Leimkuhler, 1997). Figure 1 shows the reference orbits of three particles and the orbits learned by the Hamiltonian neural network (HNN) (Greydanus et al., 2019), a famous approach that directly approximates the Hamiltonian with a neural network. In Fig. 1(a, e), the HNN orbits coincide with the reference when the three particles are far from each other, which is consistent with the results in (Greydanus et al., 2019). However, the particles deviate from the reference orbits rapidly after collision, and the energy becomes nonconserved (Fig. 1(c, f)). This reveals that although the NN is trained with the data containing collision, the NN does not fully capture the dynamics and easily diverges when stiffness grows. Two primary factors may affect the accuracy of the learned Hamiltonian.

**Implicit bias.** NN-based optimization has an implicit bias toward fitting a smooth function with the fast decay in the frequency domain (Xu et al., 2020; Cao et al., 2019). This implicit bias impedes the NN from capturing high-frequency components, such as singularities in an N-body problem.

**Imbalanced stiffness proportion.** The stiffness of the dynamical system changes with time and varies across different trajectories (e.g., the same system with different initial conditions). It is not uncommon that only a small proportion of trajectories corresponds to stiff dynamics. As a statistical

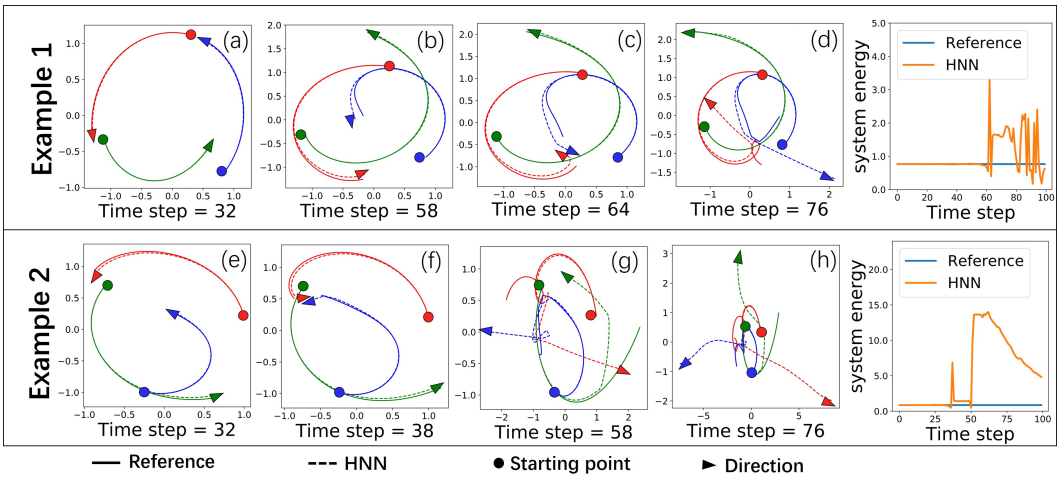


Figure 1: First four columns show a comparison of the reference orbits and the Hamiltonian neural network (HNN) orbits of three particles. The orbits of the different particles are displayed with different colors. The rightmost figures show the energy comparison. The reference orbits are simulated by the RKF45 solver with the ground truth Hamiltonian, and the energy is conserved. The energy of the HNN changes dramatically at the close interaction of two particles (see c, f), and eventually the HNN orbits diverge from the reference.

example, in the $1,000$ independent simulations of three-body trajectories following (Chen et al., 2019), 91.4% of the trajectories contain collision, but on average only $4.2\%$ of the time intervals within the trajectories contain collision or close interaction.

To mitigate the implicit bias caused by NN-based optimization and the imbalanced stiffness proportion problem, we propose a new method called the stiffness-aware neural network (SANN) based on the stiffness classification of the training data. In our approach, we introduce a stiffness-aware index (SAI) as a simple, yet effective metric to classify the time intervals into stiff and nonstiff portions. For training efficiency, we integrate the Hamiltonian dynamics over different intervals with different step sizes based on their classification. To balance the ratio between the stiff group and the nonstiff group and avoid biased training, we resample the stiff intervals. Our contributions are as follows.

1. We identify the importance of the stiffness concept in learning Hamiltonian systems from the time series data. We show that SAI is easy to calculate and can be used to effectively determine stiffness intervals of the data.
2. We validate the SANN method with complex Hamiltonian dynamics including a three-body problem and billiard model. Extensive numerical results show that SANN can accurately predict the the stiff dynamics and significantly outperform the existing methods.

## 2 PRELIMINARIES

### 2.1 HAMILTONIAN SYSTEM

The Hamiltonian system describes the continuous-time evolution of states in the phase space $(\mathbf{p}, \mathbf{q})$, where $\mathbf{p} \in \mathbb{R}^n$ represents the generalized momentum and $\mathbf{q} \in \mathbb{R}^n$ denotes position coordinates. The Hamiltonian $\mathcal{H}(\mathbf{p}, \mathbf{q}) : \mathbb{R}^{2n} \to \mathbb{R}^1$ is denoted as the total energy of the system at $(\mathbf{p}, \mathbf{q})$. The dynamics can be described with $\mathcal{H}(\mathbf{p}, \mathbf{q})$ by

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}}, \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}}. \tag{1}$$

With Eqn. (1), $\mathcal{H}(\mathbf{p}, \mathbf{q})$ is conservative during the evolution as $\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} \cdot \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} + \frac{\partial \mathcal{H}}{\partial \mathbf{q}} \cdot \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = 0$. In classical mechanics, the Hamiltonian is usually expressed as the sum of the kinetic and potential energies. We are interested in learning the separable Hamiltonian, namely, $\mathcal{H}(\mathbf{p}, \mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q})$,

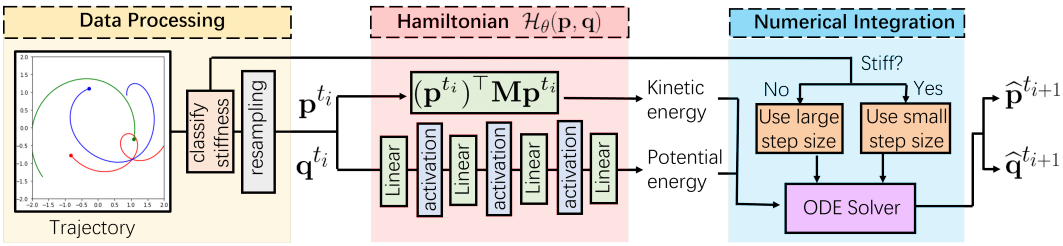


Figure 2: Workflow of SANN.

where $T(\mathbf{p})$ is kinetic energy while $V(\mathbf{q})$ is potential energy. The kinetic energy is proportional to the square of the momentum of the object. In particular, $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^\top \boldsymbol{M}\mathbf{p}$ with mass matrix $\boldsymbol{M} = \text{diag}\{m_1^{-1}, ..., m_n^{-1}\}$, where $m_i > 0$ is the mass associated with the $i$th component of $\mathbf{p}$. In this paper our goal is to learn the Hamiltonian of a dynamical system. What is available is the time series of observations $\{(\mathbf{p}^{t_i}, \mathbf{q}^{t_i})\}_{i=1}^N$. The Hamiltonian is parameterized by a neural network as follows,

$$\mathcal{H}(\mathbf{p},\mathbf{q}) \approx \mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p},\mathbf{q}) \triangleq \mathbf{p}^\top \boldsymbol{M}\mathbf{p} + \phi(\mathbf{q}; \boldsymbol{W}), \tag{2}$$

where $\phi : \mathbb{R}^n \to \mathbb{R}^1$ is a fully connected NN, $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ is a trainable matrix, and $\boldsymbol{\theta} \triangleq \{\boldsymbol{M}, \boldsymbol{W}\}$ is a set of all trainable parameters. Once we obtain $\mathcal{H}_{\boldsymbol{\theta}}$, the trajectories of the learned Hamiltonian system can be simulated by Eqn. (1) with an ordinary differential equation (ODE) solver.

### 2.2 ODE Solver for the Hamiltonian System

We use $\text{Forward}((\mathbf{p}^0, \mathbf{q}^0), \mathcal{H}, \Delta t)$ to denote a one-step integration of Eqn. (1) from $(\mathbf{p}^0, \mathbf{q}^0)$ over the step size $\Delta t$. The Euler method is a first-order Runge–Kutta method adopted in (Greydanus et al., 2019). When the Euler method is used, the integration becomes

$$(\mathbf{p}^{t_{i+1}}, \mathbf{q}^{t_{i+1}}) = \text{Forward}((\mathbf{p}^{t_i}, \mathbf{q}^{t_i}), \mathcal{H}, t_{i+1} - t_i) \triangleq (\mathbf{p}^{t_i}, \mathbf{q}^{t_i}) + (-\frac{\partial \mathcal{H}}{\partial \mathbf{q}^{t_i}}, \frac{\partial \mathcal{H}}{\partial \mathbf{p}^{t_i}})(t_{i+1} - t_i). \tag{3}$$

The Euler method is usually not suitable for stiff dynamics because of its poor stability property. Another popular numerical method (Fehlberg, 1969) for the Hamiltonian system is Runge—Kutta–Fehlberg (RKF45). RKF45 allows the step size to be changed adaptively based on an estimate of the local truncation error. This error-based step size control has great potential for improving computational efficiency. However, its effectiveness may be hampered by the use of minibatches, which are crucial for training. Minibatching adds an additional dimension to Eqn. (1). Controlling the step size requires considering a combined ODE system and estimating the error on all batch elements, as noted in Chen et al. (2018). Moreover, the step size is limited by the stiffest element in a batch, making it difficult to use a large step size especially when the batch size is large.

A symplectic integrator, a numerical method that conserves the energy quantity, is widely used in learning Hamiltonian system (Chen et al., 2019; Zhong et al., 2020). Leapfrog is a second-order symplectic integrator designed for a separable Hamiltonian. The forward scheme of Leapfrog is given in Appendix A.

## 3 Stiffness-Aware Neural Network

In this section we introduce our method, called SANN (stiffness-aware neural network), with its workflow shown in Fig. 2. First, we propose SAI (stiffness-aware index) to classify the time interval as either stiff or nonstiff. During training, we integrate the NN-parameterized Hamiltonian dynamics over the interval with different step sizes based on their classification. Next, we resample the stiff intervals to balance their ratio and avoid biased training.

### 3.1 Identifying the Stiff Interval

In this part we first discuss the stiffness index (SI) that is used to characterize stiffness for an ODE and propose the stiffness-aware index (SAI) to characterize the stiffness for the time series data.

**SI reveals the fastest rate of change of state.** We consider the dynamics of the state $\boldsymbol{u}$,

$$\frac{\mathrm{d}\boldsymbol{u}}{dt} = f(\boldsymbol{u}). \tag{4}$$

SI at the state $\boldsymbol{u}(t)$ is defined by $\max\{|Re(\lambda_i)|\}$, where $\lambda_i$ is the eigenvalue of the Jacobian matrix of Eqn. (4) (Aiken, 1985). To illustrate that SI reveals the fastest rate of change of state, we consider that Eqn. (4) is a linear system with constant coefficients, namely, $\frac{\mathrm{d}\boldsymbol{u}}{dt} = \boldsymbol{A}\boldsymbol{u}$, and $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ is a diagonalizable matrix with eigenvalues $\{\lambda_i\}_{i=1}^n$ and corresponding eigenvectors $\{\boldsymbol{v}_i\}_{i=1}^n$. Then the solution of the linear system is $\boldsymbol{u}(t) = \sum_{i=1}^n c_i \boldsymbol{v}_i e^{\lambda_i t}$. Let us suppose that $Re(\lambda_i) < 0, i = 1, ..., n$. We have $e^{\lambda_i t} \to \mathbf{0}$ as $t \to \infty$. Hence, $\max\{|Re(\lambda_i)|\}$ reveals the fastest speed of decaying to $\mathbf{0}$. If $\max\{|Re(\lambda_i)|\}$ is large, the integrator needs a small step size to reduce the local truncation error.

**Definition of SAI.** Given the observations $\{\boldsymbol{u}^{t_i}\}_{t=1}^N$ from the system (4), we define SAI at $\boldsymbol{u}^{t_i}$ by

$$\frac{1}{\|\boldsymbol{u}^{t_i}\|_2}\Big\|\frac{\boldsymbol{u}^{t_{i+1}} - \boldsymbol{u}^{t_i}}{t_{i+1} - t_i}\Big\|_2. \tag{5}$$

Intuitively, SAI characterizes the relative changing speed of the state $\boldsymbol{u}$ from time $t_i$ to $t_{i+1}$. The norm of finite difference $\big\|\frac{\boldsymbol{u}^{t_{i+1}} - \boldsymbol{u}^{t_i}}{t_{i+1} - t_i}\big\|_2$ approximates $\big\|f(\boldsymbol{u}^{t_i})\big\|_2$, which is used in time parameterization of the adaptive time step method (Huang & Leimkuhler, 1997). In our data-driven setting, we can not compute SI as the analytic expression of $f$ is unavailable. SAI can serve as a proxy of SI in time series data, which will be demonstrated in Section 5.

Next, we split the training data into stiff and nonstiff portions by classifying the time interval as either stiff or nonstiff based on SAI. For a time series observation $\{\boldsymbol{u}^{t_i}\}_{i=1}^N$, we first compute SAI for each time interval. Let $\mathrm{SAI}_i = \frac{1}{\|\boldsymbol{u}^{t_i}\|_2}\big\|\frac{\boldsymbol{u}^{t_{i+1}} - \boldsymbol{u}^{t_i}}{t_{i+1} - t_i}\big\|_2$. We then rank $\{\mathrm{SAI}_i\}_{i=1}^{N-1}$. The interval $(t_i, t_{i+1})$ with the larger $\mathrm{SAI}_i$ is supposed to be the stiffer part. We use $\gamma \in (0, 1)$ to denote the stiff ratio, a hyperparameter to determine the ratio of the stiff portion. The interval belonging to the top-$\gamma$ of $\{\mathrm{SAI}_i\}_{i=1}^{N-1}$ is identified as a stiff interval, and the other is classified as nonstiff.

### 3.2 Training the estimated Hamiltonian

**Loss function.** Let $\{(\mathbf{p}^{t_i}, \mathbf{q}^{t_i})\}_{i=1}^N$ be the given trajectory from Hamiltonian system. Given a pair of consecutive states, $(\mathbf{p}^{t_i}, \mathbf{q}^{t_i})$ and $(\mathbf{p}^{t_{i+1}}, \mathbf{q}^{t_{i+1}})$, we integrate Eqn. (1) from $t_i$ to obtain the estimated solution $(\hat{\mathbf{p}}^{t_{i+1}}, \hat{\mathbf{q}}^{t_{i+1}})$ at $t_{i+1}$. To achieve a more accurate solution, we conduct the integration over $[t_i, t_{i+1}]$ with a small time step $\frac{t_{i+1} - t_i}{S}$, where $S$ is an integer hyperparameter called partition. Specifically, we proceed as follows:

$$(\hat{\mathbf{p}}^{t_{i+s/S}}, \hat{\mathbf{q}}^{t_{i+s/S}}) = \mathrm{Forward}((\hat{\mathbf{p}}^{t_{i+(s-1)/S}}, \hat{\mathbf{q}}^{t_{i+(s-1)/S}}), \mathcal{H}_{\boldsymbol{\theta}}, \frac{t_{i+1} - t_i}{S}), s = 1, \cdots, S, \tag{6}$$

where $(\hat{\mathbf{p}}^{t_i}, \hat{\mathbf{q}}^{t_i}) \triangleq (\mathbf{p}^{t_i}, \mathbf{q}^{t_i})$. For the stiff equation, the step size of the numerical integration must be small enough for the stable solution. Therefore, the large partition $S$ should be chosen for the stiff portion while the small partition $S$ is used for the nonstiff portion. The parameter $\boldsymbol{\theta}$ in $\mathcal{H}_{\boldsymbol{\theta}}$ can be optimized by minimizing the mean squared error between the prediction and the ground truth:

$$\frac{1}{N-1}\sum_{i=1}^{N-1} \|\mathbf{p}^{t_{i+1}} - \hat{\mathbf{p}}^{t_{i+1}}\|_2^2 + \|\mathbf{q}^{t_{i+1}} - \hat{\mathbf{q}}^{t_{i+1}}\|_2^2, \tag{7}$$

with stochastic optimization algorithms such as Adam (Kingma & Ba, 2014).

**Resampling.** As demonstrated in Section 1, the stiff phenomena may comprise only a small proportion in the trajectory of the Hamiltonian system. We usually pick the stiff ratio $\gamma$ with a value less than 0.5. To avoid biased regression and unstable training caused by imbalanced categories of intervals, we adopt a random resampling technique that balances the data by replicating the stiff intervals $K$ times. A typical choice for replication $K$ is $\frac{1-\gamma}{\gamma}$ such that the number of the stiff intervals is comparable to that of the nonstiff intervals.

## 4 Experiments

To evaluate the performance of SANN, we use two complex Hamiltonian systems: the billiard model and the three-body problem. We compare SANN with two famous approaches, including

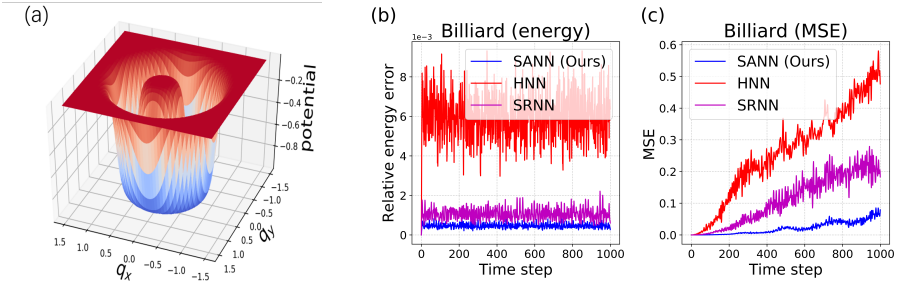


Figure 3: (a) Profile of the potential function for the billiard model; $\mathbf{q} = (q_x, q_y) \in \mathbb{R}^2$ denotes the position. Comparison of (b) relative energy error and (c) MSE for billiard model.

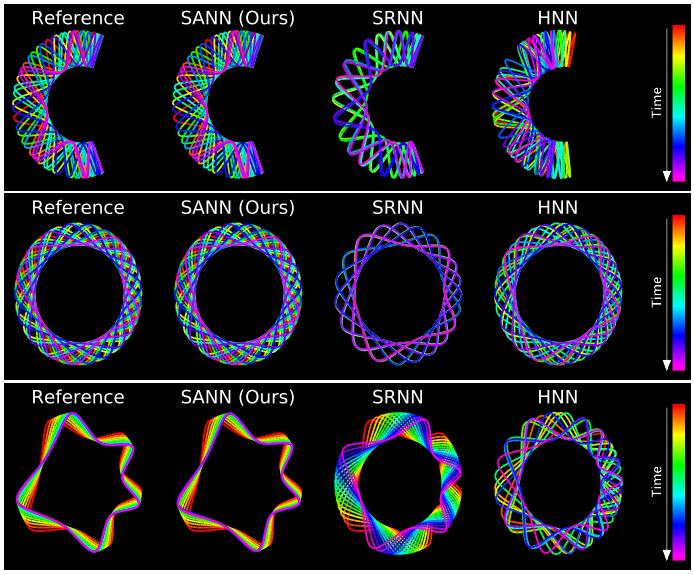


Figure 4: Comparison of billiard orbits simulated using the Hamiltonian learned by different methods. We can see that SANN produces orbits that are almost identical to those of the reference. We provide more results in Appendix C and dynamic graphs on anonymous website.

HNN (Greydanus et al., 2019) and SRNN (Chen et al., 2019). All approaches aim to learn $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ in Eqn. (1) as a representation of the dynamics. HNN trains $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ by minimizing the error between the partial derivatives of $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ and time derivatives approximated by data. SRNN utilizes symplectic solvers to conduct multistep integration and trains $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ by minimizing the error between the prediction and the data. SANN uses a similar loss function but with stiffness awareness as shown in Section 3.2. For a fair comparison, we use the Leapfrog solver for both SRNN and SANN. To evaluate the accuracy of the learned $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ for different methods, we simulate the dynamics using the Leapfrog solver with the same settings during testing.

### 4.1 Billiard Model

The billiard model has wide application in real-world physical systems, spanning quantum-classical correspondence (Stöckmann & Stein, 1990), lasers (Stone, 2010), quantum dots (Ponomarenko et al., 2008), and nanodevices (Chen et al., 2016). The billiard model that we consider describes a billiard bouncing between a ring with soft boundaries (Choudhary et al., 2020). The Hamiltonian is defined as

$$\mathcal{H}(\mathbf{p}, \mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|_2^2 + \Big(1 + \exp\big(\frac{r_\alpha - \|\mathbf{q}\|_2}{s}\big)\Big)^{-1} - \Big(1 + \exp\big(\frac{r_\beta - \|\mathbf{q} - (q_0, 0)\|_2}{s}\big)\Big)^{-1}, \quad (8)$$

where $\mathbf{p} \in \mathbb{R}^2$ and $\mathbf{q} \in \mathbb{R}^2$ are the momentum and the position of a billiard on a 2D plane, respectively; $r_\alpha, r_\beta$ are the radius of the outer circle and the inner circle, respectively; $s$ is the softness of the boundary; and $(q_0, 0)$ is a shift of the inner circle from the center. As shown in Fig. 3(a), the potential function becomes sharp near the boundaries of the ring, causing a rapid change of the momenta of the billiard ball when it gets close to the boundaries.

**Experimental setup.** The parameters $r_\alpha, r_\beta, s$, and $q_0$ are set to be $1.0, 0.5, 0.05$, and $0.1$, respectively. We use the physics-informed model $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ defined in Eqn. (2); $\phi$ is a 3-hidden-layer fully connected NN with width 256 per layer and a rational activation function (Boullé et al., 2020). We simulate the training set with 100 trajectories and the testing set with 30 trajectories by RKF45. Each trajectory contains 1,000 time steps with step size of 0.1. We set the stiff ratio $\gamma$ to be 10% and the partition $S$ to be 10 for the stiff interval and 2 for the nonstiff interval. The loss function (7) is optimized by Adam with a batch size of 1,024, and we use an initial learning rate of 0.001 for 500 epochs. The learning rate follows cosine decay with the increasing training epoch. During testing, we integrate ODE (1) using the Leapfrog integrator with a fixed step size of 0.005.

**Results.** SANN can predict the dynamics more accurately than HNN and SRNN can. Figure 3(b, c) shows the mean square error (MSE) with time and relative energy error, which is defined as the ratio of difference between the current energy and the initial energy to the initial energy. We can see that SANN maintains a much smaller energy error compared with HNN or SRNN. On average, SANN reduces the relative energy error by 56.07% compared with SRNN and 92.13% compared with HNN. The gap in terms of MSE enlarges as the number of time steps increases. At the last time step, the MSE of SANN is 56.91% lower than that of SRNN and 83.44% lower than that of HNN. Figure 4 gives a comparison of the predicted trajectories. SANN recovers visually the same trajectories as the reference, while the trajectories obtained with SRNN and HNN clearly diverge from the reference. Additional results for noisy data are given in Appendix D.

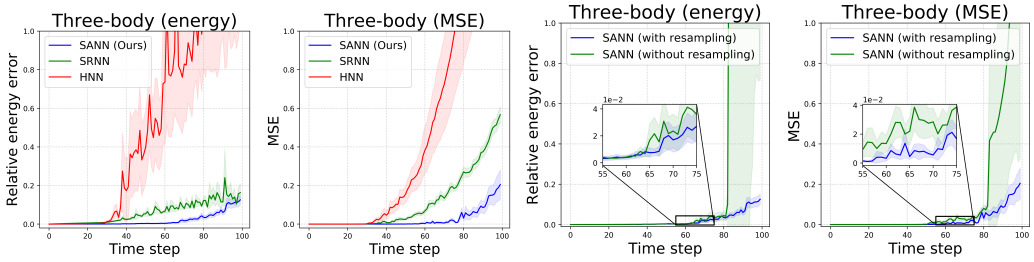


Figure 5: The first two figures show the comparison of relative energy error and MSE with varied time for the three-body problem. The last two figures show the comparison of performance with and without resampling.

### 4.2 Three-body problem

We consider a three-body problem that describes the motion of three particles under Newtonian gravitational force. The Hamiltonian of the three-body system is given by

$$\mathcal{H}(\mathbf{p}, \mathbf{q}) = \frac{1}{2} \sum_{i=1}^{3} \frac{\|\mathbf{p}_i\|_2^2}{m_i} + \sum_{1 \le i < j \le 3} -\frac{G m_i m_j}{\|\mathbf{q}_i - \mathbf{q}_j\|_2}, \tag{9}$$

where $\mathbf{p}_i \in \mathbb{R}^2$, $\mathbf{q}_i \in \mathbb{R}^2$ and $m_i$ are the momentum, position, and mass of the $i$th particle, $i = 1, 2, 3$, $\mathbf{p} \triangleq (\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$ and $\mathbf{q} \triangleq (\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)$, and $G$ is the gravitational constant. From Eqn. (9), we see that the potential function incurs singularities when the distance between any two particles is small.

**Experiment setup.** We set $m_1 = m_2 = m_3 = 1$ and $G = 1$ in our experiments. To approximate the Hamiltonian of three-body dynamics, we use a physics-informed $\mathcal{H}_{\boldsymbol{\theta}}$ as follows,

$$\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q}) \triangleq \mathbf{p}^\top \boldsymbol{M} \mathbf{p} + \phi(\|\mathbf{q}_1 - \mathbf{q}_2\|_2, \|\mathbf{q}_1 - \mathbf{q}_3\|_2, \|\mathbf{q}_2 - \mathbf{q}_3\|_2; \boldsymbol{W}), \tag{10}$$

where $\phi$ is defined as in Section 4.1, and we incorporate the physics information where the potential is a function of pairwise distances. The training data comprises 1,000 trajectories, and the length

of each trajectory $N$ is 60 with the step size $0.1$. The random initialization of initial states follows (Chen et al., 2019). The testing data set consists of 300 trajectories with length $N$ of 100 and step size of $0.1$. We set the stiff ratio $\gamma$ to be 10% and the partition $S$ to be 50 for the stiff interval and 10 for the nonstiff interval. When training, we minimize the loss function (7) by Adam with the batch size of 1,024. $\mathcal{H}_{\boldsymbol{\theta}}$ is trained with an initial learning rate of 0.001; the learning rate decays for 3,000 epochs. During evaluation, the Leapfrog integrator with fixed step size of 0.01 is used.

**Results.** SANN learns a more accurate Hamiltonian than HNN and SRNN do on the three-body problem. Figure 6 shows the orbits of three particles simulated by different methods and a system energy comparison. The relative energy error and MSE of orbits simulated by different methods are presented in Fig. 5. In Fig. 6, in the beginning the orbits of all methods coincide with the reference. However, we see that the orbits of HNN and SRNN rapidly drift away from the reference, and the energy changes dramatically whenever two orbits meet. On the contrary, SANN produces orbits that are nearly identical to the orbits of the reference, and the energy remains roughly constant. From Fig. 5, we see that SANN achieves lower energy error and MSE compared with HNN and SRNN. On average, SANN reduces the relative energy error by 67.80% compared with SRNN and 96.30% compared with HNN. Also, at the last time step SANN's MSE is 63.84% lower than SRNN's and 92.65% lower than HNN's.

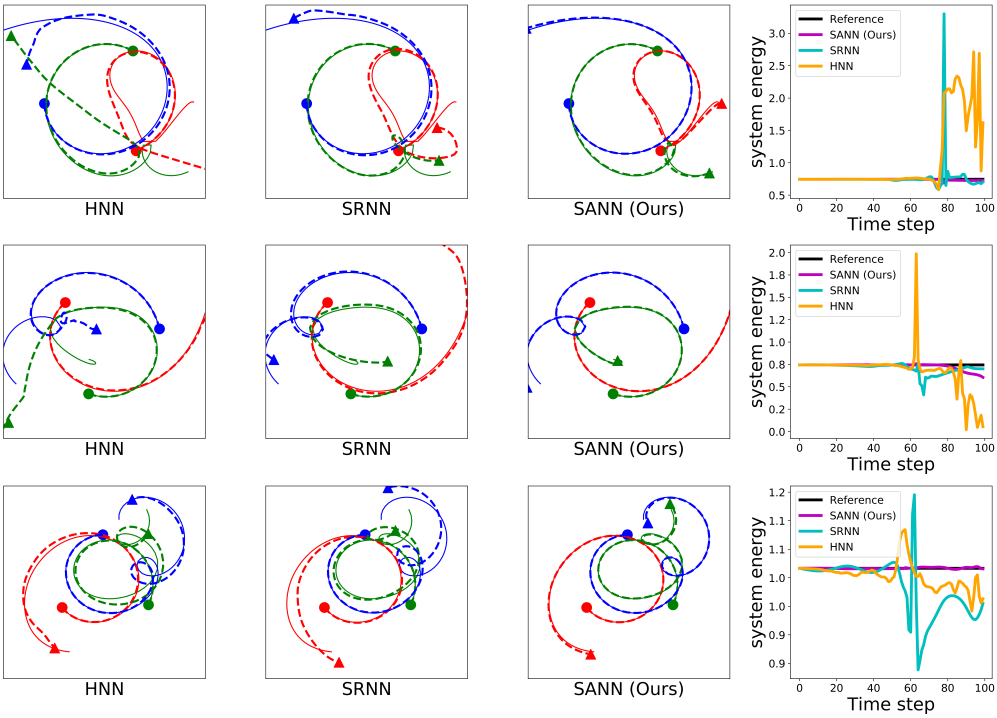


Figure 6: The first three columns show the comparison of the reference orbits (solid curves) and the orbits learned by different method (dotted curves). • is the initial position, and ▶ is the direction. The orbit of the different particles is presented by different colors. The rightmost figures show the energy comparison. We provide more results on Appendix C and dynamic graphs in website.

## 5 Stiffness Metric

In Section 3.1 SAI was introduced in order to characterize the stiffness of a trajectory. In this section we show theoretically and numerically that SAI can serve as a proxy of SI in a data-driven scenario.

**SAI keeps the same trend as SI.** With the analytic expression of dynamics in three-body problem and a given trajectory, we compute the SI and SAI for each time step of the trajectory, respectively. As a representative example, Fig. 7 shows the orbits of three particles and the corresponding curves

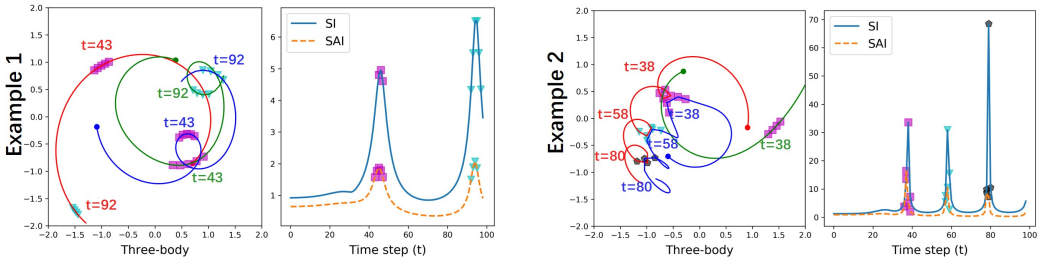


Figure 7: Comparison of SAI and SI with time. The color markers refer to the occurrence of the stiffness phenomena; the same color corresponds to the same time period. The trends of SAI and SI are consistent. We provide more results on Appendix C and dynamic graphs in website.

of SAI and SI with time. We can see that SI remains roughly a small constant when three particles are far away from each other but rises sharply when two particles get close. In three-body dynamics, the stiff phenomena are known to occur at the close interaction of particles, which is in good correspondence to large SI values. More important, SAI keeps the same trend with SI as time goes by, and SAI reaches the peak at the same time interval as SI does. Through extensive numerical validation like this, we find that SAI is capable of characterizing the stiffness of a trajectory very well.

**SAI is a generalized SI.** For a theoretical analysis, we follow the standard technique that linearizes the ODE locally (Arrowsmith & Place, 1992). In our method, SAI is computed by adjacent states with small step size, and the adjacent states satisfy the linearized ODE. By definition, SI depends on the eigenvalue $\lambda_m$ of the linear ODE with the maximum absolute real part. We show in Theorem 1 (with proof in Appendix B) that SAI depends on all the eigenvalues. In an ideal setting where $\ell_m = 1, \ell_i = 0, \forall i \neq m$, SAI is roughly equivalent to SI.

**Theorem 1.** *Let $\boldsymbol{A}$ be a $n \times n$ symmetric real matrix and $\{\lambda_i\}_{i=1}^n$ be its $n$ distinct eigenvalues. Then for the linear system $\frac{\mathrm{d}\boldsymbol{x}}{dt} = \boldsymbol{A}\boldsymbol{x}$ with nonzero initial condition $\boldsymbol{x}(0) = \boldsymbol{u}^0$, we have*

$$\frac{1}{\|\boldsymbol{u}^0\|_2} \Big\| \frac{\boldsymbol{u}^1 - \boldsymbol{u}^0}{\Delta t} \Big\|_2 = \Big( \sum_{i=1}^{n} \ell_i \lambda_i^2 \Big)^{1/2} + \mathcal{O}(\Delta t) \tag{11}$$

*where $\boldsymbol{u}^1 = \boldsymbol{x}(\Delta t)$ and $\ell_i \geq 0, i = 1, ..., n$ with $\sum_{i=1}^n \ell_i = 1$.*

## 6 Ablation Study

In this section we explore the effect of varied resampling replication $K$ introduced in Section 3.2 and activation functions used in $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$. The experiments are conducted on the three-body problem. Table 1 shows the training MSE, testing MSE, relative energy error, and training time (in seconds) for each epoch. Figure 5 shows the performance with and without resampling. Figure 8 displays the performance of different activation functions used in the NN.

**Resampling.** From Exp. 2–Exp. 6, we see that with the increasing resampling replication for stiff portion, the learned Hamiltonian dynamics can achieve smaller errors, but the training time grows accordingly. For example, when the replication $K$ changes from 6 to 8, the testing MSE decreases by 47.61% but the training time increases by 22.72%.

**Efficiency.** In Exp. 7 where all training intervals are integrated with partition 50, we achieve a more accurate solution compared with Exp. 2 where some portions of intervals are integrated with partition 10. However, the training time increases significantly. On the other hand, despite the time increment caused by resampling, Exp. 4 achieves comparable performance to Exp. 7 but reduces over 40% of training time. To trade off between the accuracy and time cost, we can choose an appropriate resampling replication.

**Activation functions.** We compare the performance of ReLU, Tanh, and Rational (Boullé et al., 2020) used in the NN to approximate the Hamiltonian. Even though theoretically ReLU NN has a good approximation property, it has worse performance in our problem where the dynamics involve

a first-order derivative. Rational NN is slightly better than Tanh NN. According to Occam's Razor (Lattimore & Hutter, 2011), we intuitively prefer to formulate the physical system with a simple expression and avoid a complicated one such as Tanh NN, a highly nonlinear function. Rational NN, which has the form of a rational fraction, is more suitable for modeling the Hamiltonian.

| Exp. ID | Stiff Ratio $\gamma$ | Partition (nonstiff) | Partition (stiff) | Replication | Train MSE | Test MSE | Energy Error | Training Time |
|---|---|---|---|---|---|---|---|---|
| Exp. 1 | 0.1 | 10 | 10 | 9 | 2.0e-6 | 0.0513 | 0.0611 | 13.52 |
| Exp. 2 | 0.1 | 10 | 50 | 1 | 2.0e-7 | 0.2173 | 0.7884 | 10.08 |
| Exp. 3 | 0.1 | 10 | 50 | 4 | 1.5e-7 | 0.0460 | 0.1026 | 19.82 |
| Exp. 4 | 0.1 | 10 | 50 | 6 | 7.4e-8 | 0.0294 | 0.0581 | 26.36 |
| Exp. 5 | 0.1 | 10 | 50 | 8 | 5.5e-8 | 0.0154 | 0.0228 | 32.35 |
| Exp. 6 | 0.1 | 10 | 50 | 9 | 4.3e-8 | 0.0234 | 0.0457 | 35.35 |
| Exp. 7 | 0.5 | 50 | 50 | 1 | 6.2e-7 | 0.0554 | 0.0900 | 34.75 |

Table 1: Performance comparison under different parameter settings. "Exp." is short for experiment.

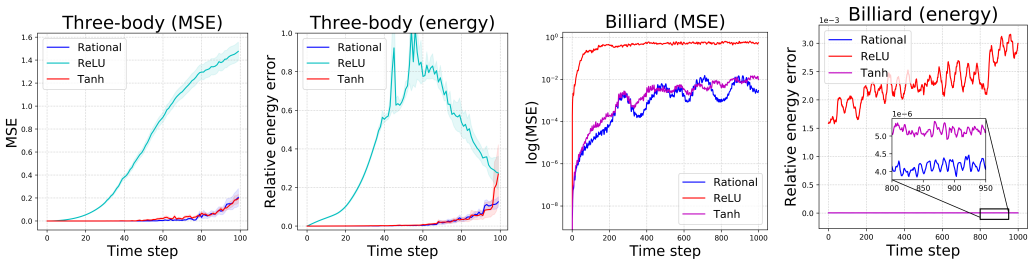


Figure 8: Performance comparison of different activation function on the three-body problem and billiard model.

## 7 Related Work

**Learning Hamiltonian system with neural networks.** There are two main directions to learn the Hamiltonian systems: parameterizing the Hamiltonian with NNs and modeling the dynamics directly. HNN trains $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ by minimizing the error between the partial derivatives of $\mathcal{H}_{\boldsymbol{\theta}}(\mathbf{p}, \mathbf{q})$ and time derivatives approximated by data (Greydanus et al., 2019). SRNN conducts multi-step integration with symplectic solver to enforce the solution close to the given data (Chen et al., 2019). In (Tong et al., 2021; Jin et al., 2020), a neural network with special structure is used to learn the dynamics directly. Furthermore, some methods proposed to improve the accuracy of modeling Hamiltonian system from different perspectives, such as coordinate transformation (Finzi et al., 2020) and physical prior (Zhong et al., 2020).

**The applications of resampling methods.** The resampling technique is an indispensable tool in machine learning. This technique repeatedly samples data from the training set and enforces the model to learn some data with specific purpose. Resampling has been applied in many areas, such as software defect prediction (Hilding, 2020), functional magnetic resonance imaging (Davenport, 2021), remote sensing classification (Lyons et al., 2018), and investment (Borges & Neves, 2020).

## 8 Conclusion

We propose SANN (stiffness-aware neural network) to learn the stiff Hamiltonian system. We also propose a new metric SAI (stiffness-aware index) to classify the training data into stiff and nonstiff portions. This classification along with a resampling technique allows us to apply step size adaptation strategies to better capture the dynamical characteristics of the Hamiltonian vector fields. On complex physical systems including the three-body problem and the billiard model, our method outperforms the state-of-art approaches with a significant margin. Our method has potential to extend to other types of stiff dynamical systems, not limited to learning the Hamiltonian; such an extension is left as future work.

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## A LEAPFROG INTEGRATION METHOD

The forward step of Leapfrog on separable Hamiltonian $\mathcal{H}(\mathbf{p}, \mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q})$ is given as follows (Chen et al., 2019),

$$\begin{aligned}
\mathbf{p}^{t_{i+\frac{1}{2}}} &= \mathbf{p}^{t_i} - \frac{1}{2}(t_{i+1} - t_i)\nabla_{\mathbf{q}} V(\mathbf{q}^{t_i}), \\
\mathbf{q}^{t_{i+1}} &= \mathbf{q}^{t_i} + (t_{i+1} - t_i)\nabla_{\mathbf{p}} T(\mathbf{p}^{t_{i+\frac{1}{2}}}), \\
\mathbf{p}^{t_{i+1}} &= \mathbf{p}^{t_{i+\frac{1}{2}}} - \frac{1}{2}(t_{i+1} - t_i)\nabla_{\mathbf{p}} V(\mathbf{q}^{t_{i+1}}).
\end{aligned}$$

## B PROOF OF THEOREM 1

**Theorem 1**. Let $\boldsymbol{A}$ be an $n \times n$ symmetric real matrix and $\{\lambda_i\}_{i=1}^n$ be its $n$ distinct eigenvalues. Then for the linear system $\frac{\mathrm{d}\boldsymbol{x}}{dt} = \boldsymbol{A}\boldsymbol{x}$ with nonzero initial condition $\boldsymbol{x}(0) = \boldsymbol{u}^0$, we have

$$\frac{1}{\|\boldsymbol{u}^0\|_2}\Big\|\frac{\boldsymbol{u}^1 - \boldsymbol{u}^0}{\Delta t}\Big\|_2 = \big(\sum_{i=1}^n \ell_i \lambda_i^2\big)^{1/2} + \mathcal{O}(\Delta t), \tag{12}$$

where $\boldsymbol{u}^1 = \boldsymbol{x}(\Delta t)$ and $\ell_i \geq 0, i = 1, ..., n$ with $\sum_{i=1}^n \ell_i = 1$.

*Proof.* Let $\{\boldsymbol{v}_i\}_{i=1}^n$ be the eigenvectors corresponding to the eigenvalues $\{\lambda_i\}_{i=1}^n$. Since $\boldsymbol{A}$ is a symmetric real matrix, $\{\boldsymbol{v}_i\}_{i=1}^n$ form a set of orthogonal vectors. Without loss of generalization, we assume $\{\boldsymbol{v}_i\}_{i=1}^n$ is standard orthogonal basis. Let $\boldsymbol{x}(0) = \boldsymbol{u}^0 = \sum_{i=1}^n c_i \boldsymbol{v}_i$; then $\|(c_1, ..., c_n)\|_2 = \|\boldsymbol{u}^0\|_2$. The solution of the linear system is $\boldsymbol{x}(t) = \sum_{i=1}^n c_i \boldsymbol{v}_i e^{\lambda_i t}$. Therefore,

$$\begin{aligned}
\lim_{\Delta t \to 0} \frac{1}{\|\boldsymbol{u}^0\|_2}\Big\|\frac{\boldsymbol{u}^1 - \boldsymbol{u}^0}{\Delta t}\Big\|_2 &= \lim_{\Delta t \to 0} \frac{1}{\|\boldsymbol{u}^0\|_2}\Big\|\frac{\sum_{i=1}^n c_i \boldsymbol{v}_i e^{\lambda_i \Delta t} - \sum_{i=1}^n c_i \boldsymbol{v}_i}{\Delta t}\Big\|_2 \\
&= \frac{1}{\|\boldsymbol{u}^0\|_2}\Big\|\sum_{i=1}^n c_i \lambda_i \boldsymbol{v}_i\Big\|_2 \\
&= \big(\sum_{i=1}^n \frac{c_i^2}{\sum_{s=1}^n c_s^2}\lambda_i^2\big)^{1/2}.
\end{aligned} \tag{13}$$

We let $\ell_i \triangleq \frac{c_i^2}{\sum_{s=1}^n c_s^2} \geq 0$ and have $\sum_{i=1}^n \ell_i = 1$. □

## C SUPPLEMENTARY RESULTS

In this section we provide some supplementary results to the experiments of the main text.

Figure 9 gives a comparison of the predicted trajectories of the billiard model, and this is a supplement to Figure 4. Again, we see that SANN recovers visually the same trajectories as the reference. For the three-body problem, Figure 10 and Figure 11 show the orbits of three particles learned by different methods, and these results are a supplement to Figure 6. We can see that HNN and SRNN diverge from the orbits after a period of time while SANN produces orbits that are nearly identical to the orbits of the reference and the energy is roughly conserved.

Figure 12 displays the comparison of SAI and SI with time, and these results are a supplement to Figure 7. These four examples in Figure 12 support that the SAI keeps the same trend as SI and achieves the peak at the same time as SI does.

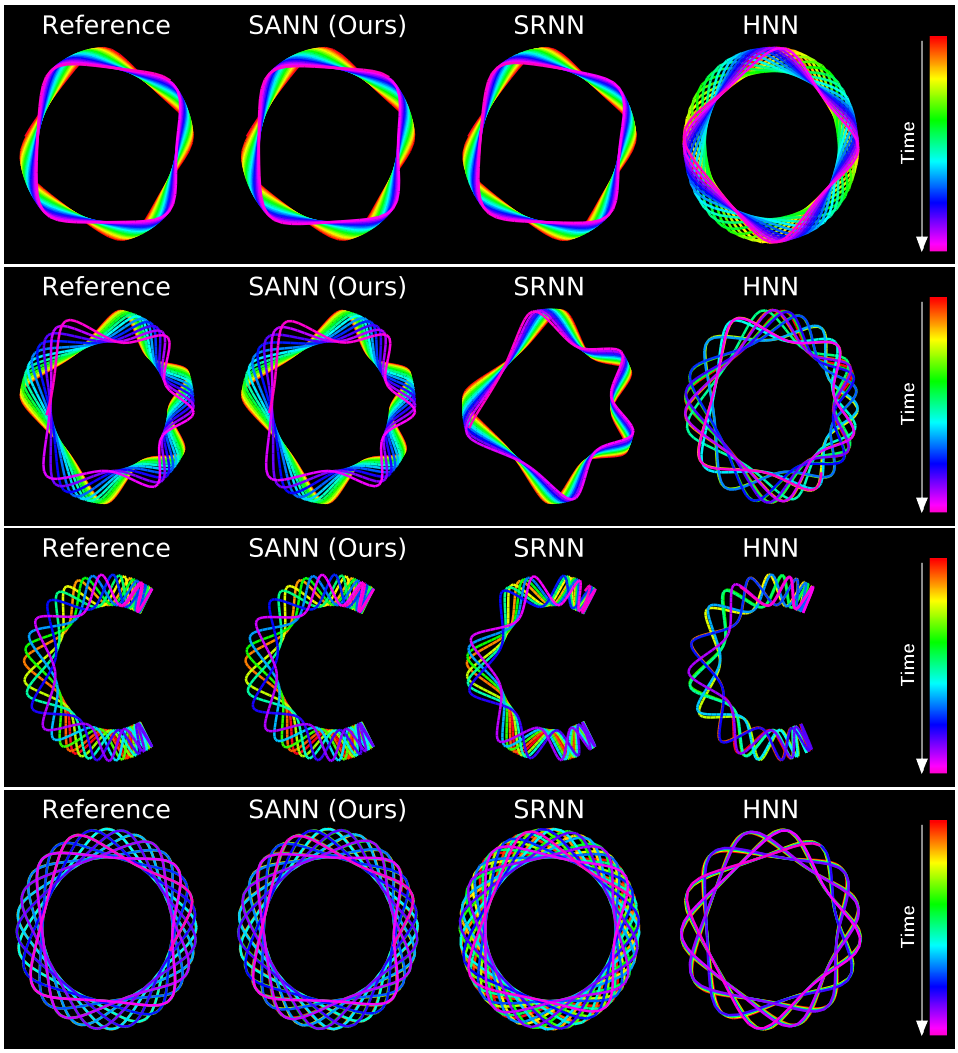


Figure 9: (Supplement to Fig. 4) Comparison of billiard orbits simulated using the Hamiltonian learned by different methods.

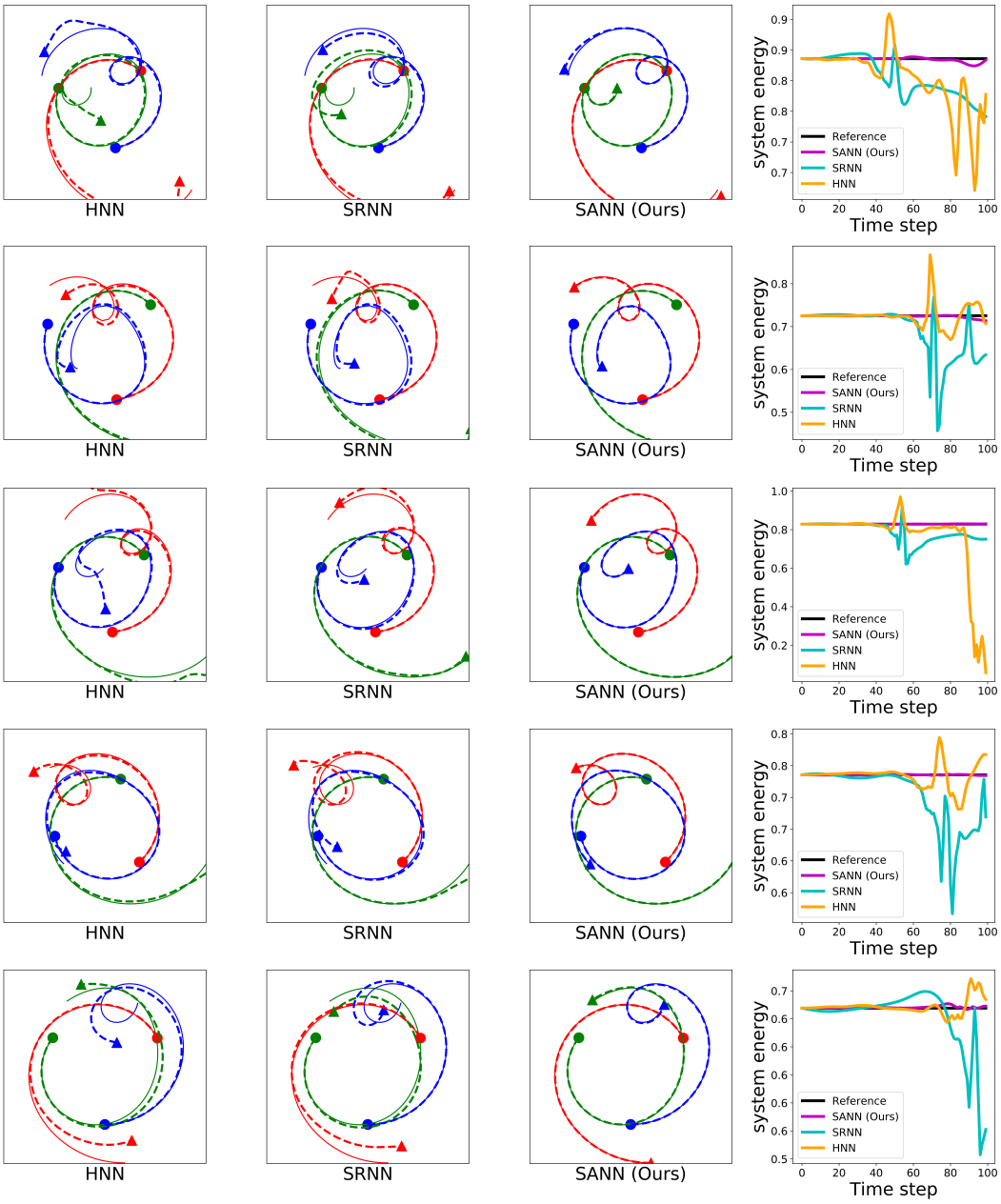


Figure 10: (Supplement to Fig. 6) The first three columns show the comparison of the reference orbits (solid curves) and the orbits learned by different method (dotted curves). ● is the initial position, and ▶ is the direction.

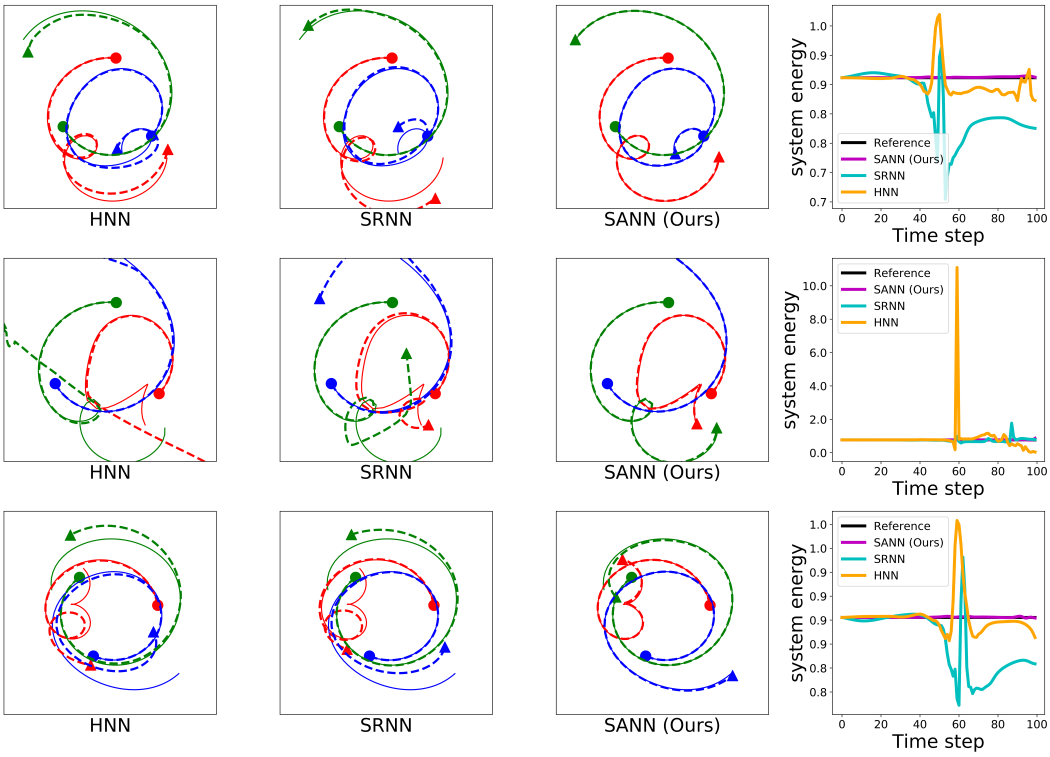


Figure 11: (Supplement to Fig. 6) The first three columns show the comparison of the reference orbits (solid curves) and the orbits learned by different methods (dotted curves). • is the initial position, and ▶ is the direction.

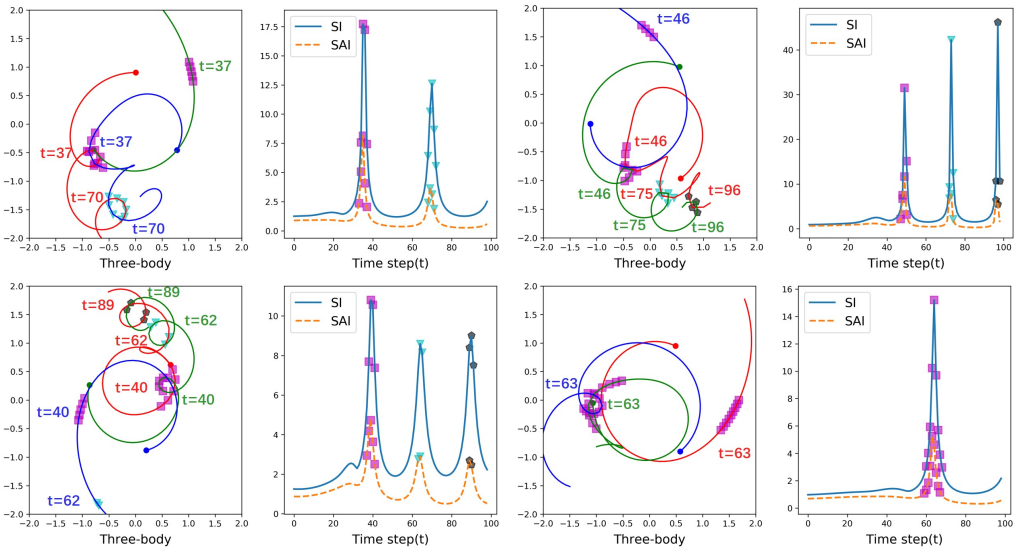


Figure 12: (Supplement to Fig. 7) Comparison of SAI and SI with time. The color markers refers to the occurrence of the stiffness phenomena, and the same color corresponds to the same time period. The trends of SAI and SI are consistent.

## D NOISY DATA

In this section we evaluate our method on the noisy training data on Billiard model. We add the Gaussian noise with different noise levels (standard deviation) to the clean training data. Figures 13 and 14 respectively show the MSE and relative energy error with time under noisy data with different noise level. We can see that all the learned dynamical systems become unstable and the energy gets nonconserved. We see that HNN, SRNN, and SANN have difficulty in learning the chaotic dynamics when the data is disturbed by noise.

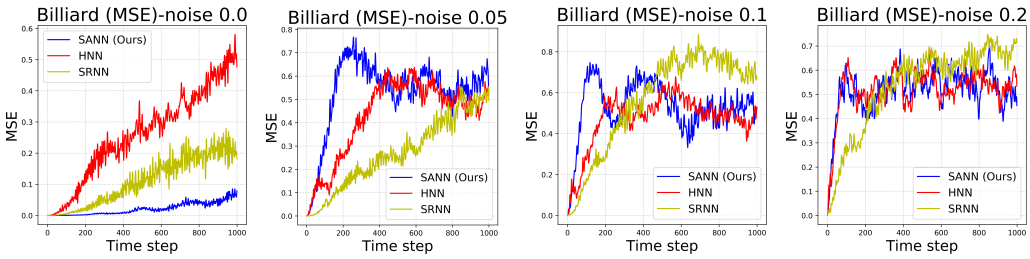


Figure 13: Comparison of MSE of the learned dynamical systems under noisy data with different noise levels.

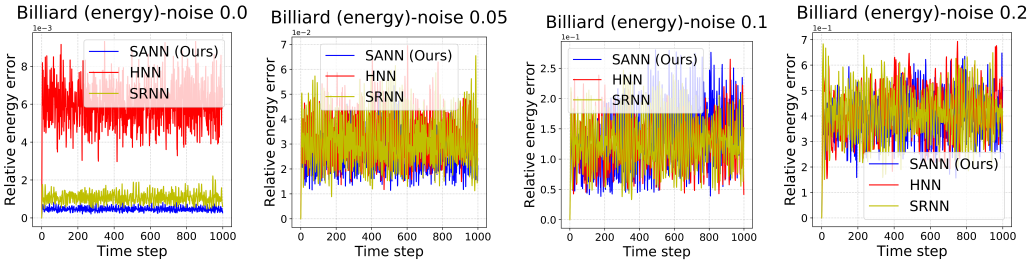


Figure 14: Comparison of relative energy error of the learned dynamical systems under noisy data with different noise levels.