Time-Reversal Symmetric ODE Network

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Abstract

Time-reversal symmetry, which requires that the dynamics of a system should not change with the reversal of time axis, is a fundamental property that frequently holds in classical and quantum mechanics. In this paper, we propose a novel loss function that measures how well our ordinary differential equation (ODE) networks comply with this time-reversal symmetry; it is formally defined by the discrepancy in the time evolution of ODE networks between forward and backward dynamics. Then, we design a new framework, which we name as Time-Reversal Symmetric ODE Networks (TRS-ODENs), that can learn the dynamics of physical systems more sample-efficiently by learning with the proposed loss function. We evaluate TRS-ODENs on several classical dynamics, and find they can learn the desired time evolution from observed noisy and complex trajectories. We also show that, even for systems that do not possess the full time-reversal symmetry, TRS-ODENs can achieve better predictive errors over baselines.

1 Introduction

Recent advances in artificial intelligence allow researchers to recover laws of physics and predict dynamics of physical systems from observed data by utilizing machine learning techniques, e.g., evolutionary algorithms [35, 28], sparse optimizations [33, 4], Gaussian process regressions [38, 8], and neural networks [18, 1, 15, 42, 32]. Among various models, the neural networks are considered as one of the most powerful tools to model complicated physical phenomena, owing to their remarkable ability to approximate arbitrary functions [17]. One notable aspect of the observations in physical systems is that they manifest some fundamental properties including conservation or invariance [14, 2]. However, it is not straightforward for neural networks to learn and model the embedded physical properties from observed data only. Consequently, they often overfit to short-term training trajectories and fail to predict the long-term behaviors of complex dynamical systems [15, 42].

To overcome these issues, it is important to introduce appropriate inductive biases based on knowledge of physics, dynamics and their properties [42, 32]. Common approaches to incorporate physics-based inductive bias include modifying neural network architectures [36, 37] or introducing regularization terms based on specialized knowledge of physics and natural sciences [29, 27]. These methods demonstrate impressive performance on their target problems, but such a problem-specific model cannot generalize across domains. As for more general approaches, the authors in [6, 5] propose the ordinary differential equation (ODE) networks, which view the neural networks as parameterized ODE functions. They are shown to be able to represent the vast majority of dynamical systems with higher precision over vanilla recurrent neural networks and their variants [6, 5], but are still unable to learn underlying physics such as the law of conservation [15]. Recent works [15, 42, 32, 7, 40] apply the Hamiltonian mechanics to ODE networks, and succeed in enforcing the energy conservation as well as the accurate time evolution of classical conservative systems. However, these Hamiltonian ODE networks have inherent limitations that they cannot be applied to non-conservative systems, since the Hamiltonian structures require to strictly conserve the total energy [15].

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To address such limitations of existing works on modeling classical dynamics, we introduce a physics-inspired, general, and flexible inductive bias, symmetries. It is at the heart of the physics: the laws of physics are invariant under certain transformations in space and time coordinates, thus show the universality [12, 26]. For example, the classical dynamics possess the time-reversal symmetry, which means the classical equations of motion should not change under the transformation of time reversal: $t \mapsto -t$ [22, 30] (see Figure 1). Therefore, if the target underlying physics being approximated has some symmetries, it is natural that the approximated physics using neural networks should also comply with these properties. Motivated by this, we feed the symmetry as an additional information to help neural networks learn the physical systems more efficiently.

Specifically, we focus on the time-reversal symmetry of classical dynamics described above, due to its simplicity and popularity. We propose a new ODE learning framework, which we refer to as Time-Reversal Symmetry ODE Network (TRS-ODEN), that utilize the time-reversal symmetry as a regularizer in training ODE networks, by unifying recent studies of ODE networks [7] and classical symmetry theory for ODE systems [22]. Our scheme can be easily implemented with a small modification of codes for conventional ODE networks, and is also compatible with extensions of ODE networks, such as Hamiltonian ODE networks [42, 32, 7]. It can be used to predict many branches of physical systems, because the isolated classical and quantum dynamics exhibit the perfect time-reversal symmetry [22, 31]. Moreover, even for the case when the full time-reversal symmetry are broken [22], e.g., in the presence of interaction with environments through friction or energy transfer, we also show that TRS-ODENs are beneficial to learn such system by annealing the strength of the proposed regularizer appropriately. This flexibility with regard to the target problem is the main advantage of the proposed framework, in contrast to prior methods, e.g., only for suitable explicitly conservative systems [15]. In summary, our contribution is threefold:

- We propose a novel loss function that measures the discrepancy in the time evolution of ODE networks between forward and backward dynamics, thus estimate whether the ODE networks are time-reversal symmetric or not.
- We show ODE networks with the proposed loss, coined TRS-ODENs, achieve better predictive error than baselines, e.g., from 50.81 to 10.85 for non-linear oscillators.
- We validate even for time-irreversible systems, the proposed framework still works well compared to baselines, e.g., from 3.68 to 0.12 in terms of error for damped oscillators.

2 Background and Setup

2.1 Predicting dynamical systems

In a dynamical system, its states evolve over time according to the governing time-dependent differential equations. The state is a vector in the phase space, which consists of all possible positions and momenta of all particles in the system. If one knows the governing differential equation and initial state of the system, the future state is predictable by solving the equation analytically or numerically.
On the other hand, if one does not know the exact governing equation, but has some state trajectories of the system, one can try to model the dynamical system, e.g., by using neural networks. More specifically, one can build a neural network whose input is current state (or trajectory) and the output is the next state, from the perspective of the sequence prediction. However, such a method may overfit to short-term training trajectories and fail to predict the long-term behaviors [42]. It is also not straightforward to predict the continuous-time dynamics, because neural network models typically assume the discrete time-step between states [15].

Neural ODE and its applications [6, 5, 15, 42, 32, 7, 40], alias ODE networks (ODENs), tackle these issues by learning the governing equations, rather than the state transitions directly. Moreover, some of them use special ODE functions such as Hamilton’s equations to incorporate physical properties to neural network structurally [15, 42, 32, 7, 40]. In the rest of this section, we briefly review ODENs and Hamiltonian ODE networks (HODENs), which are closely related to our work.

### 2.2 ODE networks (ODENs) for learning and predicting dynamics

We consider dynamics of state $x$ in phase space $\Omega (= \mathbb{R}^{2n},$ in classical dynamics) given by:

$$\frac{dx}{dt} = f(x) \quad \text{for } t \in \mathbb{R}, \quad x \in \Omega, \quad f : \Omega \rightarrow T\Omega. \tag{1}$$

The continuous time evolution between arbitrary two time points $t_i$ and $t_{i+1}$ by (1) is equal to:

$$x(t_{i+1}) = x(t_i) + \int_{t_i}^{t_{i+1}} f(x)dt. \tag{2}$$

The recent works [42, 32, 6, 7] propose the ODENs, which represent the ODE functions $f$ in (1) by neural networks and learn the unknown dynamics from data. For ODENs, fully-differentiable numerical ODE solvers are required to train the black-box ODE functions, e.g., Runge-Kutta method [11] or symplectic integrators such as leapfrog method [23]. With an ODE solver, say $\text{Solve}$, one can obtain the estimate time evolution by ODENs:

$$\hat{x}(t_{i+1}) = \text{Solve}\{\hat{x}(t_i), f_\theta, \Delta t_i\}, \quad \hat{x}(t_0) = x(t_0), \tag{3}$$

where $f_\theta$ is a $\theta$-parameterized neural network, $\hat{x}(t_i)$ is a prediction of $x(t_i)$ using ODENs, $\Delta t_i = t_{i+1} - t_i$ is a time-step, and $x(t_0)$ is a given initial value. Given observed trajectory $x(t_1), \ldots, x(t_T)$, ODENs can learn the dynamics by minimizing the mean-squared lose function $L_{\text{ODE}} \equiv \sum_{i=0}^{T-1} \|\text{Solve}\{\hat{x}(t_i), f_\theta, \Delta t_i\} - x(t_{i+1})\|^2$. 

### 2.3 Hamiltonian ODE networks (HODENs)

The Hamiltonian mechanics describes the phase space equations of motion for conservative systems by following two first-order ODEs called Hamilton’s equations [14]:

$$\frac{dq}{dt} = \nabla_p \mathcal{H}(q, p), \quad \frac{dp}{dt} = -\nabla_q \mathcal{H}(q, p), \tag{4}$$

where $q \in \mathbb{R}^n$, $p \in \mathbb{R}^n$, and $\mathcal{H} : \mathbb{R}^{2n} \mapsto \mathbb{R}$ are positions, momenta, and Hamiltonian of the system, respectively. Recent works [42, 32, 7] apply the Hamilton’s equations to ODENs, by parameterizing the Hamiltonian as $H_\theta$, and replacing $f_\theta(q, p)$ to the gradients of $H_\theta$ with respect to inputs $(p, q)$ according to (4). Thus, the time evolution of HODENs is equal to:

$$(q(t_{i+1}), p(t_{i+1})) = \text{Solve}\{(q(t_i), p(t_i)), (\nabla_p H_\theta, -\nabla_q H_\theta), \Delta t_i\}. \tag{5}$$

HODENs shows better predictive performance for conservation systems. Furthermore, they can lean the underlying law of conservation of energy automatically, because they fully exploit the nature of the Hamiltonian mechanics [15]. However, a fundamental limitation of HODENs is that they do not work properly for the non-conservative systems [15], because they always conserve the energy.

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For Hamiltonian as an example, $x = (q, p)$, where $q \in \mathbb{R}^n$ and $p \in \mathbb{R}^n$ are positions and momenta.
3 Time-Reversal Symmetry Inductive Bias for ODENs

3.1 Target problems

Before introducing the time-reversal symmetry, we briefly explain two perspectives of the classical dynamical systems: \textit{conservative} and \textit{reversible}. The former is the system that its Hamiltonian does not depend on time explicitly, i.e., $\partial \mathcal{H}/\partial t = 0$. The latter is the system that possesses the time-reversal symmetry, whose mathematical details will be discussed in the following section.

\textbf{Conservative and reversible systems.} All conservative systems that their Hamiltonians satisfy $\mathcal{H}(q, p) = \mathcal{H}(q, -p)$ are also reversible \cite{22}. It means that many kinds of classical dynamics are both conservative and reversible\(^2\). For these systems, both Hamiltonian and time-reversal symmetry inductive biases are appropriate. Furthermore, combining two inductive biases can improve the sample efficiency of a learning scheme.

\textbf{Non-conservative and reversible systems.} It is noteworthy that reversible systems are not necessarily conservative systems. Some examples about non-conservative but reversible systems can be found in \cite{22, 30}. Clearly, baselines such as HODENs that enforce conservative property would break down in this environment. On the other hand, our scheme, named TRS-ODEN, presented in Section 3.3 would accurately model the dynamics of given data by exploiting time-reversal symmetry.

\textbf{Non-conservative and irreversible systems.} Under interactions with environments, the dynamical systems become non-conservative and often irreversible\(^3\). Depending on the intensity of such interactions, the Hamiltonian or time-reversal symmetry inductive bias can be beneficial or harmful. HODENs strictly enforce the conservation, thus they are not suitable for this \cite{15}. On the other hand, TRS-ODENs are more flexible, since they use the inductive bias as a form of regularizer, which is easily controlled via hyper-parameter tuning \cite{34}.

3.2 Time-reversal symmetry in dynamics

First-order ODE systems (1) are said to be \textit{time-reversal symmetric} if there is an invertible transformation $R: \Omega \mapsto \Omega$, that reverses the direction of time:

$$\frac{dR(x)}{dt} = -f(R(x)), \quad (6)$$

where $R$ is called \textit{reversing operator} \cite{22}. Comparing (1) and (6), one can find that the equation is invariant under the transformations of phase space $R$ and time-reversal $t \mapsto -t$. For notational simplicity, let’s introduce a time evolution operator $U_t : \Omega \mapsto \Omega$ for (1) as follows \cite{22}:

$$U_t : x(t) \mapsto U_t(x(t)) = x(t + \Delta t), \quad (7)$$

for arbitrary $t, \Delta t \in \mathbb{R}$. Then, in terms of the time evolution operator (7), (6) imply:

$$R \circ U_t = U_{-t} \circ R, \quad (8)$$

which means that \textit{the reversing of the forward time evolution of an arbitrary state should be equal to the backward time evolution of the reversed state} (see Figure 1).

In classical dynamics, generally, even-order and odd-order derivatives with respect to $t$ are respectively preserved and reversed under $R$ \cite{22, 30}. For example, consider a conservative and reversible Hamiltonian $\mathcal{H}(q, p) = \mathcal{H}(q, -p)$, as mentioned in Section 3.1. Because $q$ and $p$ are respectively zeroth and first order derivatives with respect to $t$, $R$ is simply given by $R(q, p) = (q, -p)$. In this case, one can easily check the Hamilton’s equations (4) are invariant under $R$ and $t \mapsto -t$.

3.3 Time-reversal symmetry ODE networks (TRS-ODENs)

Inspired from ODENs (3) and time-reversal symmetry (8), here we propose a novel \textit{time-reversal symmetry loss function}. First, the backward time evolution of the reversed state for ODENs can be obtained as follows:

$$x_R(t_{i+1}) = \text{Solve} \{ \dot{x}_R(t_i), f_R, -\Delta t_i \}, \quad x_R(t_0) = R(x(t_0)). \quad (9)$$

\(^2\)Note that the most basic definition of the Hamiltonian is the sum of kinetic and potential energy, i.e., $\mathcal{H}(q, p) = p^2/2 + V(q)$ (if we omit the mass) \cite{14}, which possess $\mathcal{H}(q, p) = \mathcal{H}(q, -p)$ naturally.

\(^3\)Let’s consider a damped pendulum. They are irreversible since one can distinguish the motion of the pendulum in forward (amplitude increases) and that in backward directions (amplitude decreases).
Then, using (3) and (9), we define the time-reversal symmetry loss $\mathcal{L}_{\text{TRS}}$ as an ODEN version of (8):

$$
\mathcal{L}_{\text{TRS}} \equiv \sum_{i=0}^{T-1} \| R(\text{Solve}(\dot{x}(t_i), f_\theta, \Delta t_i)) - \text{Solve}(\dot{x}(t_i), f_\theta, -\Delta t_i) \|^2_2. 
$$

(10)

Finally, we define the TRS-ODEN as a class of ODENs whose loss function $\mathcal{L}_{\text{TRS-ODEN}}$ is given by the sum of standard ODEN error $\mathcal{L}_{\text{ODE}}$ and time-reversal symmetry regularizer $\mathcal{L}_{\text{TRS}}$ as follows:

$$
\mathcal{L}_{\text{TRS-ODEN}}(x(t), \dot{x}(t), \ddot{x}(t), R, \theta) \equiv \mathcal{L}_{\text{ODE}}(x(t), \dot{x}(t), \theta) + \lambda \cdot \mathcal{L}_{\text{TRS}}(\dot{x}(t), \ddot{x}(t), R, \theta),
$$

(11)

where $\lambda \geq 0$ is a hyper-parameter. It is noteworthy that $\lambda$ can also be a function of time $t$. This is owing to the heuristic that although the target dynamics do not possess the full time-reversal symmetry over time, they can be partially reversible when the symmetry breaking terms become negligible at certain time points.

4 Experiments

4.1 Setups

**Default model setting.** We compare three models: vanilla ODENs, HODENs, and TRS-ODENs. A single neural network $f_\theta(q, p)$ is used for ODENs and TRS-ODENs, while HODENs consist of two neural networks $K_\theta(q)$ and $V_\theta(q)$, i.e., separable $H_\theta(q) = K_\theta(q) + V_\theta(q)$. We use the leapfrog integrator for $\text{Solve}$, following the recent work [7]. The maximum allowed value of trajectory length at training phase is set to 10. If training trajectories are longer than 10, we divide them properly. We train models by using the Adam [19] with initial learning rate of $2 \times 10^{-4}$ during 5,000 epochs. We use the full-batch training because the training sample sizes are quite small.

**Performance metric.** As primary performance metrics, we use the mean-squared error (MSE) between test ground truths and models’ predictive phase space trajectories as well as total energies$^4$ (see Table 1 for summary). The predictive trajectories are obtained by recursively solving (3) or (5), thus errors accumulate and diverge over time if the models do not learn the accurate time evolution.

**Default data generation method.** In this paper, we focus on the Duffing oscillators [21], which are generalized equations of motion for oscillating systems and given by$^5$:

$$
\frac{dq}{dt} = p, \quad \frac{dp}{dt} = -\alpha q - \beta q^3 - \gamma p + \delta \cos(t),
$$

(12)

where $\alpha$, $\beta$, $\gamma$, and $\delta$ are scalar parameters that determine the linear stiffness, non-linear stiffness, damping, and driving force terms, respectively. For non-zero parameters, Duffing oscillators are neither conservative nor reversible. Furthermore, they often exhibit chaotic behaviors [21]. However, the characteristics of Duffing oscillator can be changed greatly by adjusting parameters. Thus, by this single coupled equations, we can simulate several dynamical systems mentioned in Section 3.1.

We generate 50 trajectories each for training and test sets. For each trajectory, The initial state $(q(t_0), p(t_0))$ is uniformly sampled from $[0, 2, 1]$. The length of training and test trajectories are 30 and 200, respectively, while the time-step is fixed at 0.1, i.e., $\Delta t_i = 0.1$ for all $i$. Thus, we can evaluate whether the models can mimic the untrained long-term dynamics. We add Gaussian noise $0.1n, n \sim \mathcal{N}(0, 1)$ to training set. We use fourth order Runge-Kutta method to get trajectories.

4.2 Conservative and reversible systems

First, we evaluate our proposed method for conservative and reversible systems, where we demonstrate that TRS-ODENs are comparable with or even outperform HODENs. Moreover, we confirm combining HODENs and time-reversal symmetry loss can lead further improvement for these systems.

**Experiment 1: Simple oscillator.** For a toy example, we choose simple oscillators, i.e., $\alpha = 1$ and $\beta = \gamma = \delta = 0$. We use single hidden layer neural networks consists of 1,000 hidden units and tanh activations for all models. Figure 2 (a-b) show that TRS-ODENs with $\lambda = 10$ outperform both ODENs and HODENs. For qualitative analysis, we plot a test trajectory and its total energy (see Figure 2 (c-h)). It shows the TRS-ODENs lean the energy conservation as well as accurate dynamics.

$^4$They can be calculated from trajectories. For example, a total energy of simple oscillator is $q^2 + p^2$.

$^5$Typically, Duffing oscillator is given by a second order ODE $\ddot{x} + \alpha x + \beta \dot{x}^3 + \gamma x = \delta \cos(t)$. We separate this equation from the perspective of the pseudo-phase space, although they are not in canonical coordinates.
Experiment II: Non-linear oscillator. As a more interesting problem, we choose the undamped and unforced non-linear oscillator, i.e., $\alpha = -1$, $\beta = 1$, and $\gamma = \delta = 0$. We use neural networks consist of two hidden layers with 100 units and $\tanh$ activations.

In this experiment, TRS-ODENs outperform HODENs in terms of the trajectory MSE, and vice-versa for total energy MSE (see Figure 3 (a-b)). For qualitative analysis, we sample five trajectories and their energy values (see Figure 3 (c-h)). It shows HODENs fail to lean time evolution especially near the origin point, while TRS-ODENs shows undesirable peaks in energy. This room for improvement leads us to combining the HODENs and TRS-ODENs, the Time-Reversal Symmetric Hamiltonian ODE Networks (TRS-HODENs).\(^6\) After estimation, We find that TRS-HODENs can achieve almost same performance as HODEN in terms of energy MSE, and clearly outperform baselines for trajectory MSE (see Figure 3 (a-b) and 4 (a-b)). Furthermore, we evaluate the sample efficiency and find that the combination of two inductive bias improves the learning process more reliable (see Figure 4 (c)).

4.3 Non-conservative and reversible systems

Second, we evaluate proposed framework for non-conservative and reversible systems. To avoid getting some trivial results, we try to model the chaotic systems using TRS-ODENs.

\(^{6}\)It can be obtained straightforwardly by combining (5) and (8), similar to (9-10).
Figure 4: (a-b) Sampled five (a) trajectories and (b) their total energies in the case of TRS-HODENs. (c) Test trajectory MSE vs. the number of training samples across the models. The means and error bars of MSE are calculated from results of five different test sets, each consist of 50 trajectories.

Figure 5: Summary of Experiment III. (a-b) Test (a) trajectory MSE (b) and energy MSE across the models. (c-h) Sampled five trajectories and their total energies for (c-d) ODENs, (e-f) HODENs, and (g-h) TRS-ODENs.

Experiment III: Forced non-linear oscillator. We set $\alpha = -0.2$, $\beta = 0.2$, $\gamma = 0$, and $\delta = 0.15$ for system parameters. Due to the periodic driving force $\delta \cos t$, the systems are non-autonomous. Therefore, we use a tuple $(q, p, t)$ as an input of the neural networks for this experiment. Hyper-parameters of neural networks are same as them for Experiment II, except for $\lambda$: $\lambda \in \{0.5, 1.5\}$ is estimated in here. We generate 200 and 50 trajectories whose lengths are 50 and 100, respectively, for train and test sets in this experiment, considering the complexity of the target system.

We find that TRS-ODENs clearly outperform their baselines with significant margin in both trajectory and energy MSE metrics (see Figure 5 (a-b)). From Figure 5 (c-h), one can check the dynamics predicted by ODENs or HODENs diverge as times passes, while TRS-ODENs shows reliable long-term behaviors. As a result, the total energy of TRS-ODENs follow the ground truth reasonably, while that estimated by baselines soar explosively in $t > 8$.

4.4 Non-conservative and irreversible systems

Finally, we validate our proposed framework for non-conservative and irreversible damped systems. HODENs cannot learn this system because of their strong tendency to conserve the energy, as previously reported in [15]. We demonstrate TRS-ODENs can learn this system flexibly.

Experiment IV: Damped oscillator. We simulate damped oscillators by setting the system parameters as follows: $\alpha = 1$, $\beta = 0$, $\gamma = 0.1$, $\delta = 0$. In this experiment, we assume the time-reversal symmetry tends to hold as $t \to \infty$, thus evaluate the time-dependent $\lambda$ approach. This assumption is quite reasonable for various dissipative irreversible systems, because their irreversibility is typically originated from the (odd powers of) $p^2$ in their governing ODEs, e.g., $\gamma p$ in (12). Since dissipative systems lose their kinetic energy as time passes, i.e., $p \to 0$ as $t \to \infty$, we can design $\lambda$ as a

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7In [15, 7], the authors say for HODENs, time dependency should be modeled separately from them. However, we use time-dependent HODENs in here to prevent large modifications of HODENs for fair comparison.

8It is because of the definition of the classical reversing operator $R(q, p) = (q, -p)$. 

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Figure 6: Summary of Experiment IV. (a-b) Test (a) trajectory MSE and (b) energy MSE across the models. (c-h) Sampled trajectory and its total energy for (c-d) ODENs, (e-f) HODENs, and (g-h) TRS-ODENs.

Table 1: Summary of test MSEs across all experiments. All MSE values are multiplied by $10^2$.

| Metric  | Model     | Experiment I | Experiment II | Experiment III | Experiment IV |
|---------|-----------|--------------|---------------|----------------|---------------|
| Traj.   | ODEN      | 4.05 ± 2.66  | 50.81 ± 26.80 | 39.21 ± 21.19  | 1.28 ± 0.82   |
|         | HODEN     | 0.84 ± 0.37  | 17.40 ± 17.74 | 24.09 ± 14.29  | 3.68 ± 2.19   |
|         | TRS-ODEN  | **0.31 ± 0.19** | 13.78 ± 14.86 | **6.50 ± 5.59** | **0.12 ± 0.06** |
|         | TRS-HODEN | N/A          | 10.85 ± 12.62 | N/A            | N/A           |
| Energy  | ODEN      | 9.04 ± 10.14 | 6.14 ± 9.13   | 242.06 ± 204.59 | 1.04 ± 1.17   |
|         | HODEN     | 0.08 ± 0.09  | **0.22 ± 0.17** | 80.50 ± 128.94 | 8.26 ± 9.60   |
|         | TRS-ODEN  | **0.07 ± 0.09** | 0.53 ± 0.75   | **1.52 ± 3.20** | **0.03 ± 0.03** |
|         | TRS-HODEN | N/A          | 0.29 ± 0.18   | N/A            | N/A           |

It is shown that the TRS-ODENs can outperform ODENs and HODENs, except for $\lambda = 1$ case (see Figure 6 (a-b)). Especially, $\lambda = 0.5t$ case shows great predictability in both time evolution and total energy of the damped system, while ODENs lose their energy too excessively and HODENs conserve their energy too strictly (see Figure 6 (c-h)). We believe it is owing to the balance between physics-based inductive bias and data-driven learning process.

5 Conclusion

Introducing physics-based inductive bias for neural networks is actively studied. e.g., ODE [6], Hamiltonian [15, 32, 40, 42, 7], and other domain knowledge [36, 37, 27, 29]. We have proposed a simple yet effective approach to incorporate the time-reversal symmetry into ODEN, coined TRS-ODEN, which is not shown in previous works. The proposed method can learn the dynamical system accurately and efficiently. We have validated our proposed framework with various experiments including non-conservative and irreversible systems.

There are some papers discuss the use of symmetry for neural networks. For example, the rotational or reflection symmetries are frequently used in computer vision tasks [13, 10, 41]. Some researchers have focused on finding symmetries using neural networks, especially in theoretical physics [9, 25, 3]. Among them, [3, 25] are closely related to our work because they discuss the method of searching a canonical transformation that satisfies the symplectic symmetry of Hamiltonian systems. Combining these approaches, i.e., finding symmetry, with our proposed framework, i.e., exploiting symmetry, would be an interesting direction for future work.
Broader Impact

In this paper, we introduce a neural network model that regularized by a physics-originated inductive bias, the symmetry. Our proposed model can be used to identify and predict unknown dynamics of physical systems. In what follows, we summarize the expected broader impacts of our research from two perspectives.

Use for current real world applications. Predicting dynamics plays a important role in various practical applications, e.g., robotic manipulation [16], autonomous driving [24], and other trajectory planning tasks. For these tasks, the predictive models should be highly reliable to prevent human and material losses due to accidents. Our propose model have a potential to satisfy this high standard on reliability, considering its robustness and efficiency (see Figure 4 (c) as an example).

First step for fundamental inductive bias. According to the CPT theorem in quantum field theory, the CPT symmetry, which means the invariance under the combined transformation of charge conjugate (C), parity transformation (P), and time reversal (T), exactly holds for all phenomena of physics [20]. Thus, the CPT symmetry is a fundamental rule of nature: that means, it is a fundamental inductive bias of deep learning models for natural science. However, this symmetry-based bias has been unnoticed previously. We study one of the fundamental symmetry, the time-reversal symmetry in classical mechanics, as a proof-of-concept in this paper. We expect our finding can encourage researchers to focus on the fundamental bias of nature and extend the research from classical to quantum, and from time-reversal symmetry to CPT symmetry. Our work would also contribute to bring together experts in physics and deep learning in order to stimulate interaction and to begin exploring how deep learning can shed light on physics.

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Supplementary Material:
Time-Reversal Symmetric ODE Network

A Time-reversal symmetry loss for non-autonomous systems

Here, we consider the time-reversal symmetry of non-autonomous ODE systems, i.e., systems that depend on time \( t \) explicitly as follows:

\[
\frac{dx}{dt} = f(x, t). \tag{S1}
\]

This non-autonomous systems are said to be time-reversal symmetric if there is a reversing operator \( R_a : (x, t) \mapsto (R(x), -t + a) \) which satisfies [22]:

\[
\frac{dR(x)}{dt} = -f(R(x), -t + a), \tag{S2}
\]

for some \( a \in \mathbb{R} \). It means that we should consider the time \( t \) itself carefully, as well as the direction of time, unlike the autonomous case (6-10) in the main paper. For example, consider forced non-linear oscillators estimated in Experiment III (Section 4.3 in the main paper):

\[
\frac{dq}{dt} = p, \quad \frac{dp}{dt} = -\alpha q - \beta |q|^3 + \delta \cos(\omega t + \phi). \tag{S3}
\]

(S3) is time-reversal symmetric under \( R_{-2\phi/\omega} : (q, p, t) \mapsto (q, -p, -t - 2\phi/\omega) \).

The forward time evolution of non-autonomous ODENs is given by:

\[
\tilde{x}(t_{i+1}) = \text{Solve}\{\tilde{x}(t_i), t_i, f_\theta, \Delta t_i\}, \quad \tilde{x}(t_0) = x(t_0). \tag{S4}
\]

On the other hand, the backward time evolution is equal to:

\[
\tilde{x}_R(t_{i+1}) = \text{Solve}\{\tilde{x}_R(t_i), \tau_i, f_\theta, -\Delta t_i\}, \quad \tilde{x}_R(t_0) = R_a(\tilde{x}(t_0)), \tag{S5}
\]

where \( \tau_i = -t_i + a \). As a result, the time-reversal symmetry loss of autonomous ODE systems is given by:

\[
L_{\text{TRS}} \equiv \sum_{i=0}^{T-1} \|R(\text{Solve}\{\tilde{x}(t_i), t_i, f_\theta, \Delta t_i\}) - \text{Solve}\{\tilde{x}_R(t_i), \tau_i, f_\theta, \tau_i, -\Delta t_i\}\|^2. \tag{S6}
\]

B Reasoning on the improvement made by TRS-HODENs

As mentioned in Section 3.1 in the main paper, the Hamiltonian \( \mathcal{H} \) of conservative and reversible systems satisfies \( \mathcal{H}(q, p) = \mathcal{H}(q, -p) \). With this symmetry property, we analyze the reason of improvement made by TRS-HODENs over HODENs in Experiment II (Section 4.2 in the main paper). Note that the ground truth Hamiltonian of non-linear oscillator tested in Experiment II is described as:

\[
\mathcal{H}(q, p) = \frac{p^2}{2} + \alpha |q|^2 + \beta |q|^4, \quad \mathcal{H}(q, -p) = \mathcal{H}(q, -p). \tag{S7}
\]

We find that the time-reversal symmetry loss helps the learned \( \theta \)-parameterized Hamiltonian \( \mathcal{H}_\theta(q, p) \) possess the above property thanks to the symmetry under the momentum-reversing operator \( R(q, p) = (q, -p) \). To show this, we calculate \( \mathcal{H}_\theta(q, p) = \mathcal{H}_\theta(q, -p) \) for HODEN and
C Predicting stable centers and homoclinic orbits of non-linear oscillators

The non-linear oscillator systems in Experiment II have two stable centers at $(1, 0)$, $(-1, 0)$, and saddle point at $(0, 0)$ (see Figure S2 (a)). Clearly, at the stable centers, states do not evolve with time at all, i.e., the equilibrium states. At the saddle point, there are two interesting trajectories, that appear to start and end at the same saddle point. These trajectories are called homoclinic orbits [39]. Note that the homoclinic orbits lie on $q > 0$ and $q < 0$ respectively start from $(\epsilon, \epsilon)$ and $(-\epsilon, -\epsilon)$, for some small positive constants $\epsilon$.

Here, we estimate whether the learned dynamics can represent the special trajectories originated from these critical points well. To do this, we generate trajectories, whose initial states are given by the centers or saddle point\(^9\), by using the models trained in Experiment II: ODENs, HODENs, and TRS-HODENs.

\(^9\)We use $10^{-8}$ and $10^{-2}$ instead of 0 and $\epsilon$, respectively, considering numerical stability.
Figure S3: The critical phase space trajectories obtained from (a) ODENs, (b) HODENs, (c) TRS-ODENs, and (d) TRS-HODENs.

Table S1: Summary of phase space trajectory and total energy MSEs evaluated in Section C. All MSE values are multiplied by $10^2$.

| Model          | ODEN         | HODEN        | TRS-ODEN     | TRS-HODEN    |
|----------------|--------------|--------------|--------------|--------------|
| MSE (Traj.)    | $14.28 \pm 10.47$ | $15.26 \pm 25.15$ | $3.88 \pm 5.92$ | $2.03 \pm 2.17$ |
| MSE (Energy)   | $9.31 \pm 16.11$ | $0.32 \pm 0.53$ | $0.52 \pm 0.78$ | $0.21 \pm 0.21$ |

TRS-ODENs ($\lambda = 10$), and TRS-HODENs ($\lambda = 10$). Figure S3 demonstrates the generated phase space trajectories. For ODENs, they cannot achieve the accurate time evolution at all. HODENs show relatively reasonable behaviors, but they predict the same direction of homoclinic orbits for $(\epsilon, \epsilon)$ and $(-\epsilon, -\epsilon)$. Also, periodic motions near the stable centers are observed for HODENs. TRS-ODENs and TRS-HODENs show two separated homoclinic orbits, clearly. Moreover, TRS-HODENs show stable equilibrium behaviors at the center points. In summary, TRS-HODENs can predict physically-consistent behaviors even for critical points. We summarize the phase space trajectory and total energy MSE metrics in Table S1.