Symplectic Neural Gaussian Processes for Meta-learning Hamiltonian Dynamics

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Abstract

We propose a meta-learning method for modeling Hamiltonian dynamics from a limited number of data. Although Hamiltonian neural networks have been successfully used for modeling dynamics that obey the energy conservation law, they require many data to achieve high performance. The proposed method meta-learns our neural network-based model using datasets in various dynamical systems, such that our model can predict vector fields of unseen systems. In our model, a system representation is inferred from given small data using an encoder network. Then, the system-specific vector field is predicted by modeling the Hamiltonian using a Gaussian process (GP) with neural network-based mean and kernel functions that depend on the inferred system representation. This GP-based Hamiltonian allows us to analytically obtain predictions that are adapted to small data while imposing the constraint of the conservation law. The neural networks are shared across systems, which enables us to learn knowledge from multiple systems, and use it for unseen systems. In our experiments, we demonstrate that the proposed method outperforms existing methods for predicting dynamics from a small number of observations in target systems.

1 Introduction

Modeling the dynamics of physical systems given time-series data is important in various fields, such as physics [Braun and Kivshar, 1998], biology [Daniels and Nemenman, 2015], and engineering [Leonessa *et al.*, 2001]. Neural networks have been widely used for modeling the dynamics due to its high representation learning capability [Chen *et al.*, 2018; Che *et al.*, 2018]. By incorporating inductive biases, we can learn underlying behaviors beyond the given data [Haussler, 1988; Baxter, 2000; Chang and Zeng, 2023; Chang *et al.*, 2023]. Hamiltonian neural networks (HNNs) [Greydanus *et al.*, 2019; Mattheakis *et al.*, 2022; Chen *et al.*, 2022b] incorporate an inductive bias of physics, where the total energy of the system is conserved. HNNs have been shown to be effective in learning Hamiltonian dynamics from data [Finzi *et al.*, 2020; Zhong *et al.*, 2020; Chen *et al.*, 2020; Chen *et al.*, 2021; Tong *et al.*, 2021; Tanaka *et al.*, 2022]. However, they require a large amount of data for training. In real-world applications, preparing sufficient data incurs a high cost and is time-consuming.

In this paper, we propose a meta-learning method for modeling Hamiltonian dynamics from a limited number of data. The proposed method meta-learns our neural network-based model using meta-training datasets in various dynamical systems, such that it can model unseen systems given small data. Figure 1 illustrates our problem setting.

The meta-learning framework is formulated as a bilevel optimization, where the inner optimization corresponds to the adaptation of the system-specific components in our model, and the outer optimization corresponds to the estimation of the system-shared components. We model a system-specific Hamiltonian using a Gaussian process (GP), by which we can incorporate the inductive bias of the energy conservation law. By this GP framework, we can analytically obtain a vector field that is adapted to given small data in the inner optimization. This enables effective backpropagation through the inner optimization, which is required for each outer optimization iteration.

In system-specific GPs for Hamiltonian, we use neural network-based mean and kernel functions that depend on a system representation. The system representation is obtained using an encoder network from given small data. Using the system representation yields a system-specific vector field. With the neural networks, we can flexibly model various vector fields. The neural networks are shared across all systems, by which we can learn common knowledge in multiple systems, and use the knowledge for newly given systems. We call our model the symplectic neural Gaussian process (SNGP) since our neural network-based GP incorporates the symplectic structure for the energy conservation law. The neural network parameters are trained by minimizing the expected test error of vector fields when a few data are given, which is calculated using meta-training datasets by an episodic training framework [Finn *et al.*, 2017].

The main contributions of this paper are as follows: 1) We propose a neural network-based GP model for modeling Hamiltonian dynamics that obeys the conservation law, where the adaptation to given data can be performed in a closed form. 2) We develop a meta-learning procedure for our model

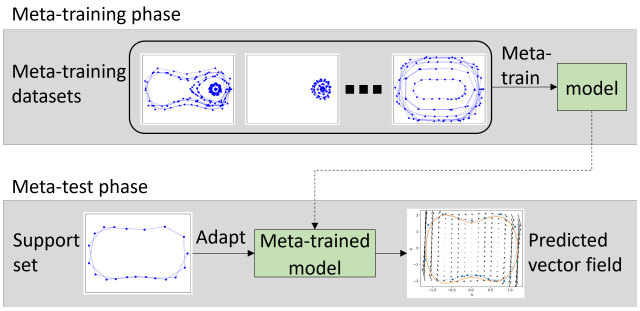


Figure 1: Problem setting. In the meta-training phase, we are given meta-training datasets, which contain time-series data in various dynamical systems. The Hamiltonians are different across systems. Our model is meta-trained with the meta-training datasets. In the meta-test phase, we are given a support set, which contains a small number of time-series data in an unseen system with an unknown Hamiltonian. Our meta-trained model is adapted by the support set, and predicts the vector field, which can be used for forecasting dynamics. The systems in the meta-training and meta-test phases are different but related, e.g., pendulums with different lengths.

to improve the expected test predictive performance on vector fields. 3) We empirically demonstrate that the proposed method performs well in modeling Hamiltonian dynamics with a limited number of data.

2 Related Work

Meta-learning has been successfully used for improving the prediction performance on unseen tasks with few data by learning to learn from various tasks [Finn *et al.*, 2017; Vinyals *et al.*, 2016; Snell *et al.*, 2017; Rothfuss *et al.*, 2021; Psaros *et al.*, 2022; Chen *et al.*, 2022a]. However, these existing methods are not for Hamiltonian dynamics except for [Lee *et al.*, 2021]. [Lee *et al.*, 2021] proposed to meta-learn HNNs using gradient-based methods [Finn *et al.*, 2017; Raghu *et al.*, 2020], which require iterative optimization procedures for adaptation. The backpropagation through such procedures is costly in terms of memory, and the total number of iterations must be kept small [Finn *et al.*, 2017]. On the other hand, the proposed method can perform adaptation in a closed form with GPs. The effectiveness of closed-form adaptation has been shown in meta-learning for classification and regression tasks [Bertinetto *et al.*, 2018; Fortuin *et al.*, 2019; Patacchiola *et al.*, 2020; Iwata and Tanaka, 2022]. Although GPs have been used for modeling Hamiltonian [Rath *et al.*, 2021; Tanaka *et al.*, 2022], these methods cannot perform meta-learning. The proposed method enables meta-learning by effectively integrating the GP-based Hamiltonian in neural networks. Our model is related to neural processes (NPs) [Garnelo *et al.*, 2018] as both use neural networks for task (system) representation inference and for prediction with inferred task representations. However, since NP prediction is based on fully parametric models, they are less flexible in adapting to given data than GPs. In contrast, our GP-based model enables swift adaptation by explicitly solving an optimization problem for adaptation.

3 Preliminaries: Hamiltonian Mechanics

In the Hamiltonian system, the continuous-time evolution is described in phase space, which is the product space of generalized coordinates $\mathbf{x}^{\mathrm{q}} = (x_1^{\mathrm{q}}, \ldots, x_M^{\mathrm{q}})$ and generalized momenta $\mathbf{x}^{\mathrm{p}} = (x_1^{\mathrm{p}}, \ldots, x_M^{\mathrm{p}})$, where M is the degree of freedom. Let $\mathbf{x} = (\mathbf{x}^{\mathrm{q}}, \mathbf{x}^{\mathrm{p}}) \in \mathbb{R}^J$, be a state of the system, where $J = 2M$. The system's evolution is determined by Hamiltonian $H(\mathbf{x}) : \mathbb{R}^J \to \mathbb{R}$, which denotes the system's total energy. In particular, the dynamics of a Hamiltonian system with additive dissipative terms is given by

$$\frac{d\mathbf{x}}{dt} = (\mathbf{A} - \mathbf{R})\nabla H(\mathbf{x}) \equiv f(\mathbf{x}), \text{ where } \mathbf{A} = \begin{pmatrix} \mathbf{O} & \mathbf{I} \\ -\mathbf{I} & \mathbf{O} \end{pmatrix}, \tag{1}$$

where $\nabla H(\mathbf{x})$ is the gradient of the Hamiltonian with respect to state $\mathbf{x}$, $\mathbf{A} \in \mathbb{R}^{J \times J}$ is a skew-symmetric matrix, $\mathbf{R} \in \mathbb{R}^{J \times J}$ is a positive semi-definite dissipation matrix, $\mathbf{I}$ is the identity matrix, and $\mathbf{O}$ is the zero matrix. The dynamics of this system conserves the total energy when $\mathbf{R} = \mathbf{O}$. An example of the dissipation matrix is $\mathbf{R} = \mathrm{diag}(0, \ldots, 0, r_1, \ldots, r_M)$, representing a dissipative system with friction coefficient $r_m \geq 0$. Eq. (1) defines the time derivatives of the state by function $f(\mathbf{x}) : \mathbb{R}^J \to \mathbb{R}^J$, which is a special kind of vector field that has a symplectic geometric structure (called Hamiltonian vector field or symplectic gradient).

The Hamiltonian neural network (HNN) is a representative method for modeling the dynamics that obeys Hamiltonian mechanics without manually designed Hamiltonians. In HNNs, a Hamiltonian is modeled by a neural network, and the dynamics is derived using Eq. (1) as follows,

$$\hat{f}_{\mathrm{HNN}}(\mathbf{x}) = (\mathbf{A} - \mathbf{R})\nabla \mathrm{NN}(\mathbf{x}), \tag{2}$$

where NN is a neural network. The gradient of the neural network is calculated with automatic differentiation [Paszke *et al.*, 2019]. The parameters of the HNN are estimated by minimizing the error between observed and predicted vector fields, $\| \mathbf{f} - \hat{f}_{\mathrm{HNN}}(\mathbf{x}) \|^2$.

4 Proposed Method

4.1 Problem Formulation

In the meta-training phase, we are given time-series datasets of D dynamical systems, $\{\mathcal{D}_d\}_{d=1}^D$, where $\mathcal{D}_d = \{\{(\mathbf{x}_{dbn}, \mathbf{f}_{dbn})\}_{n=1}^{N_{db}}\}_{b=1}^{B_d}$ is B_d sequences in the dth system, $\mathbf{x}_{dbn} \in \mathbb{R}^J$ is the nth state of the rth sequence, $\mathbf{f}_{dbn} \in \mathbb{R}^J$ is its time derivative, and N_{rd} is the number of observations. In the meta-test phase, we are given a small number of time-series data $\mathcal{S} = \{\{(\mathbf{x}_{bn}^{\mathrm{S}}, \mathbf{f}_{bn}^{\mathrm{S}})\}_{n=1}^{N^{\mathrm{S}}}\}_{b=1}^{B^{\mathrm{S}}}$, which are called a support set, in an unseen system, which is different from the meta-training systems. Our aim is to predict the vector fields, which are the time derivatives of the system's states, and to forecast the time-series in such meta-test systems, as shown in Figure 1. We assume that all systems obey Hamiltonian dynamics with additive dissipation, although the Hamiltonians are unknown, and the Hamiltonians are different across systems. When analytic time derivatives are unavailable, we obtain them by calculating their finite difference approximation from the sequences of the states.

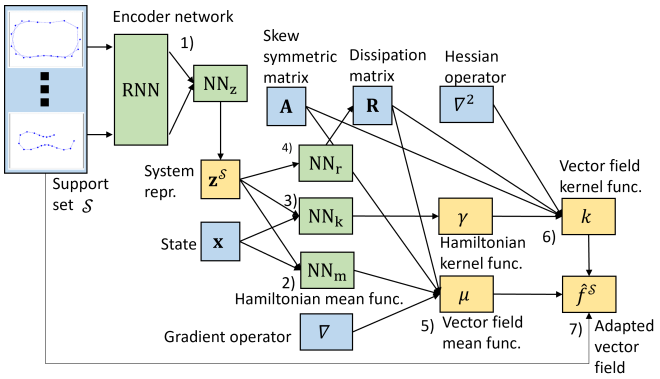


Figure 2: Our symplectic neural Gaussian process model. 1) Sequences in support set $\mathcal{S}$ is transformed to system representation $\mathbf{z}^{\mathcal{S}}$ by encoder network based on RNN and neural network $\mathrm{NN_z}$ in Eq. (3). 2) Mean function of GP for Hamiltonian is modeled by neural network $\mathrm{NN_m}$ that takes system representation $\mathbf{z}^{\mathcal{S}}$ as input in Eq. (4). 3) Kernel function of GP for Hamiltonian is modeled by RBF kernel γ, where input is transformed by neural network $\mathrm{NN_k}$ with system representation $\mathbf{z}^{\mathcal{S}}$ in Eq. (5). 4) When the system is dissipative, dissipation matrix $\mathbf{R}$ is obtained using neural network $\mathrm{NN_r}$ using system representation $\mathbf{z}^{\mathcal{S}}$ in Eq. (6); when it is conservative, $\mathbf{R} = \mathbf{O}$. 5) Mean function of GP for vector field is obtained from that for Hamiltonian using skew-symmetric and dissipation matrices, $\mathbf{A}$ and $\mathbf{R}$, and gradient operator ∇, in Eq. (8). 6) Kernel function of GP for vector field is obtained from that for Hamiltonian using skew-symmetric and dissipation matrices, $\mathbf{A}$ and $\mathbf{R}$, and Hessian operator ∇^2, in Eq. (9). 7) Vector field $\hat{f}^{\mathcal{S}}$ adapted to support set $\mathcal{S}$ is obtained by posterior mean of GP for vector field in Eq. (10). Blue boxes are given data or operators. Green boxes are neural networks shared across all systems. Yellow boxes are system-specific variables or functions obtained by our model.

4.2 Symplectic Neural Gaussian Process Model

Our symplectic neural Gaussian process (SNGP) model gives system-specific vector field $\hat{f}^{\mathcal{S}}(\mathbf{x})$ that obey Hamiltonian dynamics given support set $\mathcal{S}$. We use superscript $\mathcal{S}$ when the function or variable depends on support set $\mathcal{S}$. Figure 2 illustrates our model.

First, we obtain system representation $\mathbf{z}^{\mathcal{S}} \in \mathbb{R}^{K_\mathrm{z}}$ from support set $\mathcal{S}$ using the following encoder network,

$$\mathbf{z}^{\mathcal{S}} = \mathrm{NN_z}\left(\frac{1}{R^{\mathrm{S}}}\sum_{b=1}^{B^{\mathrm{S}}} \mathrm{RNN}\left(([\mathbf{x}_{bn}^{\mathrm{S}}, \mathbf{f}_{bn}^{\mathrm{S}}])_{n=1}^{N^{\mathrm{S}}}\right)\right), \quad (3)$$

where RNN is a recurrent neural network (RNN), $\mathrm{NN_z}$ is a feed-forward neural network, and $[\cdot,\cdot]$ represents the vector concatenation. With the RNN, we can extract information on the dynamics in each sequence with arbitrary lengths. The encoder network is a permutation invariant neural network [Che *et al.*, 2018], which can handle an arbitrary number of sequences, and which can obtain a system representation that does not depend on the order of sequences. Here, we assume the time-series are regularly sampled. In the case of irregularly-sampled time series, we can additionally input the timestamp to the RNN as in [Che *et al.*, 2018], $[\mathbf{x}_{bn}^{\mathrm{S}}, \mathbf{f}_{bn}^{\mathrm{S}}, t_{bn}^{\mathrm{S}}]$, instead of $[\mathbf{x}_{bn}^{\mathrm{S}}, \mathbf{f}_{bn}^{\mathrm{S}}]$, where t_{bn}^{S} is the nth timestamp of the rth sequence.

Next, we model system-specific Hamiltonian $H^{\mathcal{S}}$ by the following GP with deep kernels [Wilson *et al.*, 2016],

$$H^{\mathcal{S}}(\mathbf{x}) \sim \mathrm{GP}\left(\mathrm{NN_m}([\mathbf{x}, \mathbf{z}^{\mathcal{S}}]), \gamma(\mathbf{x}, \mathbf{x}', \mathbf{z}^{\mathcal{S}})\right), \quad (4)$$

where $\mathrm{NN_m} : \mathbb{R}^{J+K_\mathrm{z}} \to \mathbb{R}$ is a mean function based on a feed-forward neural network, γ is a deep kernel function based on the RBF kernel,

$$\begin{aligned}&\gamma(\mathbf{x}, \mathbf{x}', \mathbf{z}^{\mathcal{S}})\\ &= \alpha \exp\left(-\frac{\eta}{2} \parallel \mathrm{NN_k}([\mathbf{x}, \mathbf{z}^{\mathcal{S}}]) - \mathrm{NN_k}([\mathbf{x}', \mathbf{z}^{\mathcal{S}}]) \parallel^2\right)\\ &+ \beta\delta(\mathbf{x}, \mathbf{x}'),\end{aligned} \quad (5)$$

$\alpha, \beta, \eta \in \mathbb{R}_+$ are the kernel parameters, $\mathrm{NN_k} : \mathbb{R}^{J+K_\mathrm{z}} \to \mathbb{R}^{K_\mathrm{g}}$ is a feed-forward neural network, and $\delta(\mathbf{x}, \mathbf{x}') = 1$ if $\mathbf{x}$ and $\mathbf{x}'$ are identical, and zero otherwise. With system representation $\mathbf{z}^{\mathcal{S}}$ for the input of neural networks, $\mathrm{NN_m}$ and $\mathrm{NN_k}$, we can make their outputs depend on support set $\mathcal{S}$. With deep kernels, we can flexibly transform states such that the GP can model the Hamiltonian appropriately. When the system is dissipative, elements in the dissipation matrix $\mathbf{r} = (r_1, \ldots, r_M)$ is obtained from system representation $\mathbf{z}^{\mathcal{S}}$ as follows,

$$\mathbf{r} = \mathrm{NN_r}(\mathbf{z}^{\mathcal{S}}), \quad (6)$$

where $\mathrm{NN_r} : \mathbb{R}^{K_\mathrm{z}} \to \mathbb{R}^M$ is a feed-forward neural network. Neural networks, RNN, $\mathrm{NN_z}$, $\mathrm{NN_m}$, and $\mathrm{NN_k}$, are shared across different systems, which enables us to learn knowledge that is useful across systems, and use it for unseen systems.

Since $(\mathbf{A} - \mathbf{R})\nabla$ is a linear operator, and a GP with linear transformation is again a GP [Rath *et al.*, 2021], system-specific vector field $f^{\mathcal{S}}(\mathbf{x}) = (\mathbf{A} - \mathbf{R})\nabla H^{\mathcal{S}}(\mathbf{x})$ is represented by the following a multi-output GP using Eqs. (1,4),

$$f^{\mathcal{S}}(\mathbf{x}) \sim \mathrm{GP}\left(\mu(\mathbf{x}, \mathbf{z}^{\mathcal{S}}), k(\mathbf{x}, \mathbf{x}', \mathbf{z}^{\mathcal{S}})\right), \quad (7)$$

where

$$\mu(\mathbf{x}, \mathbf{z}^{\mathcal{S}}) = (\mathbf{A} - \mathbf{R})\nabla \mathrm{NN_m}([\mathbf{x}, \mathbf{z}^{\mathcal{S}}]) \in \mathbb{R}^J, \quad (8)$$

$$k(\mathbf{x}, \mathbf{x}', \mathbf{z}^{\mathcal{S}}) = (\mathbf{A} - \mathbf{R})\nabla^2(\mathbf{A} - \mathbf{R})\gamma(\mathbf{x}, \mathbf{x}', \mathbf{z}^{\mathcal{S}}) \in \mathbb{R}^{J\times J}, \quad (9)$$

and ∇^2 is the Hessian operator. The gradient and Hessian operators are calculated with automatic differentiation [Paszke *et al.*, 2019; He and Zou, 2021]. By using the GP with deep kernels, we can model a system-specific vector field that obey Hamiltonian dynamics.

Since the prior distribution of the vector field is a GP in Eq. (7), the predictive value of the vector field adapted to support set $\mathcal{S}$, which is the posterior mean of the GP, is given by

$$\hat{f}^{\mathcal{S}}(\mathbf{x}) = \mu(\mathbf{x}, \mathbf{z}^{\mathcal{S}}) + \mathbf{k}^\top \mathbf{K}^{-1}(\mathbf{f}^{\mathrm{S}} - \mathbf{m}), \quad (10)$$

where $\mathbf{K} \in \mathbb{R}^{B^{\mathrm{S}}N^{\mathrm{S}}J \times B^{\mathrm{S}}N^{\mathrm{S}}J}$ is the kernel matrix evaluated between states in the support set, $\mathbf{K}_{bN^{\mathrm{S}}+n, b'N^{\mathrm{S}}+n'} = k(\mathbf{x}_{bn}^{\mathrm{S}}, \mathbf{x}_{b'n'}^{\mathrm{S}}, \mathbf{z}^{\mathcal{S}})$, $\mathbf{k} = ((k(\mathbf{x}, \mathbf{x}_{bn}, \mathbf{z}^{\mathcal{S}}))_{n=1}^{N^{\mathrm{S}}})_{b=1}^{B^{\mathrm{S}}} \in \mathbb{R}^{B^{\mathrm{S}}N^{\mathrm{S}}J\times J}$ is the kernels evaluated between state $\mathbf{x}$ and states in the support set, $\mathbf{f}^{\mathrm{S}} = ((\mathbf{f}_{bn}^{\mathrm{S}}))_{n=1}^{N^{\mathrm{S}}})_{b=1}^{B^{\mathrm{S}}} \in \mathbb{R}^{B^{\mathrm{S}}N^{\mathrm{S}}J}$

is the observed vector fields of the support set, and $\mathbf{m} = (\mu(\mathbf{x}^{\mathrm{S}}_{bn}))^{N^{\mathrm{S}}}_{n=1})^{B^{\mathrm{S}}}_{b=1} \in \mathbb{R}^{B^{\mathrm{S}}N^{\mathrm{S}}J}$ is the predicted vector fields of the support set by mean function μ.

Eq. (10) minimizes the mean squared error on the support set with a regularizer [Vovk, 2013]. An advantage of our model is that the predictive value given the support set is analytically calculated without iterative optimization, by which we can minimize the expected test error effectively based on a stochastic gradient descent method in our meta-learning framework.

4.3 Meta-learning

The system-shared parameters $\boldsymbol{\theta}$ in the SNGP are parameters in neural networks, RNN, $\mathrm{NN_z}$, $\mathrm{NN_m}$, $\mathrm{NN_k}$, $\mathrm{NN_r}$, and kernel parameters, α, β, η. We train them by minimizing the expected test mean squared error using an episodic training framework [Ravi and Larochelle, 2017],

$$\hat{\boldsymbol{\Theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, \mathbb{E}_d \mathbb{E}_{\mathcal{S},\mathcal{Q}\sim\mathcal{D}_t} \left[\frac{1}{N^{\mathrm{Q}}} \sum_{(\mathbf{x},\mathbf{f})\in\mathcal{Q}} \| \mathbf{f} - \hat{f}^{\mathcal{S}}(\mathbf{x}) \|^2 \right], \tag{11}$$

where $\mathbb{E}_d$ represents the expectation over systems, and $\mathbb{E}_{\mathcal{S},\mathcal{Q}\sim\mathcal{D}_d}$ represents the expectation over support and query sets that are generated from meta-training dataset $\mathcal{D}_d$ in the dth system. Query set $\mathcal{Q} = \{\{(\mathbf{x}^{\mathrm{Q}}_{bn}, \mathbf{f}^{\mathrm{Q}}_{bn})\}^{N^{\mathrm{Q}}}_{n=1}\}^{B^{\mathrm{Q}}}_{b=1}$ is a time-series data set that is different from the support set used for adapting GP, by which we can evaluate the test error. Minimizing our meta-learning loss in Eq. (11) is a bilevel optimization problem. In the inner optimization, a system-specific prediction model is adapted to the support set based on the GP framework as described in Section 4.2. In the outer optimization, system-shared parameters are estimated by minimizing the error on the query set when the system-specific prediction model obtained in the inner optimization is used.

Algorithm 1 shows the meta-training procedure of the proposed model. The expectation in Eq. (11) is approximated by the Monte Carlo method in Lines 3–5, where a system, support and query instances are randomly sampled from the meta-training datasets. In Line 7, the inner optimization is performed, which corresponds to obtaining the posterior mean of the GP in Eq. (10). When the distributions of systems are the same between meta-training and meta-test phases, and a sufficient number of meta-training datasets are given, the expected error in the meta-test phase is improved by the minimization in Eq. (11).

The computational complexity of calculating the test error for a query set is $O((B^{\mathrm{S}}N^{\mathrm{S}}J)^3)$ since we need the inverse of the kernel matrix whose size is $B^{\mathrm{S}}N^{\mathrm{S}}J \times B^{\mathrm{S}}N^{\mathrm{S}}J$. In few-shot settings, which is our focus, the number of support instances $B^{\mathrm{S}}N^{\mathrm{S}}$ is small, and the proposed method can meta-learn our model efficiently.

Algorithm 1 Meta-learning procedure of our SNGP model.

Input: Meta-training data $\mathcal{D}$, number of support sequences B^{S}, number of support observations N^{S}, number of query sequences B^{Q}, number of query observations N^{Q}
Output: Trained model parameters $\boldsymbol{\theta}$

1: Initialize model parameters $\boldsymbol{\theta}$.
2: **while** End condition is satisfied **do**
3: Randomly select system index d from $\{1, \cdots, D\}$.
4: Randomly sample B^{S} sequences with N^{S} observations for support set $\mathcal{S}$ from $\mathcal{D}_d$.
5: Randomly sample B^{Q} sequences with N^{Q} observations for query set $\mathcal{Q}$ from $\mathcal{D}_d$ such that there is no overlap between the support and query sequences.
6: Calculate system representation $\mathbf{z}^{\mathcal{S}}$ using Eq. (3).
7: Calculate predictive vector field values $\hat{f}^{\mathcal{S}}(\mathbf{x})$ adapted to support set $\mathcal{S}$ using Eq. (10).
8: Calculate test error $\frac{1}{N^{\mathrm{Q}}} \sum_{(\mathbf{x},\mathbf{f})\in\mathcal{Q}} \| \mathbf{f} - \hat{f}^{\mathcal{S}}(\mathbf{x}) \|^2$.
9: Update system-shared parameters $\boldsymbol{\theta}$ using the gradient of the test error by a stochastic gradient method.
10: **end while**

5 Expriments

5.1 Data

We used six types of dynamical systems: mass-spring, pendulum, and Duffing systems without friction, and those with friction. In each type, physical parameters were different across systems as in [Lee *et al.*, 2021].

The Hamiltonian of the one-dimensional mass-spring system without friction is given by $H(\mathbf{x}) = \frac{1}{2}kx^{\mathrm{q}2} + \frac{x^{\mathrm{p}2}}{2m}$, where k is the spring constant, and m is the mass constant. For each system, $k \in [5, 6]$ and $m \in [0.5, 1.5]$ were determined uniformly randomly within their given range. The initial coordinates for each sequence were determined uniformly randomly from $[1, 2]$.

The Hamiltonian of the pendulum system without friction with a single degree of freedom is $H(\mathbf{x}) = mg\ell(1 - \cos(x^{\mathrm{q}})) + \frac{x^{\mathrm{p}2}}{2m\ell^2}$, where g is the gravitational constant, m is the mass constant, and ℓ is the length of the pendulum. Length $\ell \in [0.5, 1.5]$ was determined uniformly randomly for each system. and $g = 9.8$ and $m = 1$ were fixed for all systems. The initial coordinates were determined uniformly randomly from $[1, \pi]$.

The Hamiltonian of the Duffing system without friction is $H(\mathbf{x}) = \frac{1}{2}x^{\mathrm{p}2} + \frac{\alpha}{4}x^{\mathrm{q}4} + \frac{\beta}{2}x^{\mathrm{q}2}$, where $\beta = [-10, 0]$ was determined uniformly randomly for each system, and $\alpha = 10$ was fixed. The initial coordinates were randomly determined from $[0.5, 1.5]$. In systems with friction, the friction coefficient was uniformly randomly determined in $[0, 1]$.

In all systems, a state is a two-dimensional vector, $\mathbf{x} = (x^{\mathrm{q}}, x^{\mathrm{p}}) \in \mathbb{R}^2$, or $M = 2$. and the initial momentum was set to zero. For each system, 30 sequences of the states were sampled at a frequency of five Hz for four seconds with additive Gaussian noise with standard deviation 10^{-2}. For each type, five systems were used for meta-training, three for meta-validation, and six for meta-test. The number of support sequences was $\{1, 3, 5\}$, and the number of query sequences was 10. The time derivatives were obtained by the central finite difference approximation. The experiments were conducted ten times by resampling the meta-training, meta-validation, and meta-test systems.

For the evaluation measurement, we used the test mean

squared errors of the predicted trajectories of the query sets in the meta-test systems given the initial states. To obtain trajectories, we integrated models with the fourth-order Runge-Kutta integrator in `scipy.integrate.solve_ivp` with error tolerance to 10^{-12} [Dormand and Prince, 1980].

5.2 Compared Methods

We compared the proposed method (Ours) with the following methods: Hamiltonian neural process (HNP), meta-learning Hamiltonian neural network (MHNN) [Lee *et al.*, 2021], meta-learning Gaussian process (MGP) [Iwata and Tanaka, 2022], neural process (NP) [Garnelo *et al.*, 2018], meta-learning neural network (MNN), Symplectic Gaussian process (SGP) [Rath *et al.*, 2021], Hamiltonian neural network (HNN) [Greydanus *et al.*, 2019], neural network (NN), and Gaussian process (GP). Ours, HNP, HHNN, MGP, NP, and MNN are meta-learning methods that give system-adapted models by training with multiple meta-training systems. Ours, HNP, MHNN, HGP, and HNN use the inductive bias of the conservation law with Hamiltonian.

With neural process-based methods (HNP and NP), system representations were obtained by Eq. (3) as the same with the proposed method. HNP used a neural network for modeling Hamiltonian $H(\mathbf{x})$, and NP used it for modeling vector field $f(\mathbf{x})$, where the system representation and the state were taken as the input. HNP corresponds to the proposed method without adaptation with GPs. MHNN and MNN used model-agnostic meta-learning (MAML) [Finn *et al.*, 2017] for meta-learning, where MHNN used a Hamiltonian neural network, and MNN used a feed-forward neural network for their models. MGP used a GP with deep kernel for modeling the vector field, where the GP was adapted for each system, and the deep kernel was shared across systems. SGP used a GP with the Gaussian kernel for modeling the Hamiltonian. In HNN and NN, a neural network was shared across all systems, and trained using the meta-training datasets. In GP, a GP with the Gaussian kernel was adapted for each system.

5.3 Settings

For obtaining system representation in Eq. (3), we used the bidirectional LSTM [Graves and Graves, 2012] for RNN with 32 hidden units, where the sequence of the states was used for input. For NN_z and NN_k, we used three-layered feed-forward neural networks with 32 hidden and output units. For NN_m, we used four-layered feed-forward neural networks with 32 hidden units. For the activation function, we used the hyperbolic tangent. We optimized our models using Adam [Kingma and Ba, 2015] with learning rate 10^{-3}, and batch dataset size four. The meta-validation datasets were used for early stopping, for which the maximum number of meta-training epochs was 5,000.

In the compared methods, we used the same neural network architectures and training procedures as the proposed method. In MAML-based methods (MHNN and MNN), we used learning rate 10^{-2} and five epochs for inner optimization. For neural networks in HNP, MHNN, NP, HNN, and NN, we used four-layered feed-forward neural networks. In MGP, HGP, and GP, kernel parameters of RBF kernels were optimized using the meta-training datasets.

We implemented all methods with PyTorch [Paszke *et al.*, 2019]. For gradient and Hessian operators in Eqs. (8,9), we used functorch [He and Zou, 2021].

5.4 Results

Table 1 shows the test mean squared errors of trajectories. In all cases, the proposed method achieved the lowest error. The test error by HNP was high since the system adaptation is modeled only by neural networks. On the other hand, the proposed method performs the system adaptation by minimizing the training error, which leads to better performance. Since MHNN uses an iterative optimization with a small number of steps for system adaptation, it was difficult to adapt to various systems. In contrast, the proposed method can obtain a solution of the inner optimization in a closed form using GPs. MGP, NP, MNN, NN and GP do not use the inductive bias on the Hamiltonian systems. Therefore, the performance of these methods was low. Since HNN and NN use the same models for all systems, they cannot handle the difference among systems, and resulted in their high error. Since GP modeled the vector field for each system, its performance was low, especially when the number of support sequences was small. The proposed method achieved better performance with a small number of support sequences using knowledge in other systems with different Hamiltonians by sharing neural networks.

Figure 3 shows the predicted trajectories on the Duffing without friction system with one support sequence per system. The proposed method successfully estimated system-specific vector fields and trajectories. The methods that model the Hamiltonian, i.e., the proposed method, HNP, MNN, HGP, and HNN, estimated the vector field that obeyed the conservation law. On the other hand, the other methods estimated diverging or decaying vector fields, even though it was a conservation system. These results indicate the effectiveness of modeling the Hamiltonian.

Figure 4 shows the test mean squared errors with different numbers of meta-training systems. As the number of the meta-training systems increased, the error decreased. This result indicates that the proposed method improved the performance by using knowledge in different systems.

Table 2 shows the test mean squared errors in ablation study. Removing system representations, neural network-based mean functions, and neural network-based kernel functions decreased the performance. This result indicates that the system-shared neural networks in our model is important for meta-learning to share knowledge across different dynamical systems. Note that all methods in Table 2 are newly proposed in this paper, and our model can adapt to each system based on the GP framework even without system representations.

Additional experimental results, such as the errors of predicted vector fields, the errors of predicted total energies, computational time for meta-training, and computational time for predicting vector fields, are shown in the supplementary material. In most of the cases, the proposed method outperformed the compared methods for predicting vector fields. The proposed method achieved low errors in all cases for predicting total energies. In the other methods, predicted total energies were sometimes diverged from the ground truth,

(a) Mass-spring without friction

N^{S}	Ours	HNP	MHNN	MGP	NP	MNN	HGP	HNN	NN	GP
1	**0.638**	1.543	2.783	3.962	1.502	**1.067**	1.687	5.209	3.390	2.892
3	**0.669**	1.809	3.969	1.856	1.688	**1.145**	1.250	5.209	3.390	1.367
5	**0.649**	1.497	3.265	1.500	1.696	1.304	**0.879**	5.209	3.390	1.083

(b) Mass-spring with friction

N^{S}	Ours	HNP	MHNN	MGP	NP	MNN	HGP	HNN	NN	GP
1	**0.217**	**5.994**	0.757	1.834	**0.454**	0.493	0.834	1.043	1.068	1.341
3	**0.183**	**6.302**	0.738	0.606	0.504	0.446	0.511	1.043	1.068	0.527
5	**0.192**	**6.269**	0.721	0.418	0.587	0.454	0.451	1.043	1.068	0.370

(c) Pendulum without friction

N^{S}	Ours	HNP	MHNN	MGP	NP	MNN	HGP	HNN	NN	GP
1	**0.723**	1.542	9.312	4.317	2.055	3.844	8.556	7.468	4.469	7.339
3	**0.708**	1.715	10.864	0.997	2.190	3.778	1.522	7.468	4.469	2.899
5	**0.499**	1.772	9.805	0.817	2.167	3.931	**0.569**	7.468	4.469	1.565

(d) Pendulum with friction

N^{S}	Ours	HNP	MHNN	MGP	NP	MNN	HGP	HNN	NN	GP
1	**1.053**	35.484	3.007	1.708	1.832	**1.323**	4.664	3.738	3.034	2.753
3	**0.660**	34.132	2.642	**0.634**	1.717	1.141	2.127	3.738	3.034	1.190
5	**0.561**	35.520	2.500	**0.540**	1.513	1.095	2.050	3.738	3.034	0.769

(e) Duffing without friction

N^{S}	Ours	HNP	MHNN	MGP	NP	MNN	HGP	HNN	NN	GP
1	**1.384**	**1.574**	**2.776**	6.663	**1.338**	**2.067**	2.968	2.195	2.158	2.402
3	**1.306**	**1.503**	2.354	5.421	**1.186**	**1.657**	1.819	2.195	2.158	2.140
5	**1.251**	**1.350**	2.276	6.826	**1.318**	1.654	1.526	2.195	2.158	2.013

(f) Duffing with friction

N^{S}	Ours	HNP	MHNN	MGP	NP	MNN	HGP	HNN	NN	GP
1	**0.333**	20.328	0.752	1.093	0.575	0.706	1.277	0.804	1.070	0.951
3	**0.347**	21.369	0.645	1.130	0.502	0.650	**0.523**	0.804	1.070	0.708
5	**0.327**	22.780	0.628	1.117	0.586	0.654	**0.438**	0.804	1.070	0.656

Table 1: Test mean squared errors of trajectories with different numbers of support sequences N^{S}. Values in bold typeface are not statistically significantly different at the 5% level from the best performing method in each row according to a paired t-test.

Ours	w/o-$\mathbf{z}^{S}$	w/o-NN_{m}	w/o-NN_{k}
0.650	0.684	0.826	0.852

Table 2: Ablation studies of our model: test mean squared errors of trajectories averaged over all cases. 'w/o-$\mathbf{z}^{S}$' is the proposed method without system representations. 'w/o-NN_{m}' is the proposed method without neural network-based mean functions, where zero mean functions are used. 'w/o-NN_{k}' is the proposed method without neural network-based kernel functions, where state $\mathbf{x}$ is directly inputted into RBF kernels.

which resulted in high variance of their errors. The proposed method took a longer time than HNP, MGP, and HGP since it contains them as components. The meta-training time by the proposed method was shorter than MAML-based methods (MHNN and MNN) since the MAML-based methods need iterative optimization for system adaptation. The inference time by the proposed method was short for predicting vector fields given meta-trained models.

6 Conclusion

We proposed a neural network-based meta-learning method that effectively extracts common knowledge from data in multiple dynamical systems. The proposed method can learn dynamics that exactly conserves the total energy by modeling Hamiltonian, where a system-specific Hamiltonian adapted to given data is obtained in a closed form using GPs. Our experiments demonstrate that the proposed method achieves better performance than the existing methods with a small number of training data.

Although our results are encouraging as a data-efficient method for modeling Hamiltonian systems, there are some limitations to overcome. First, we plan to apply our method to systems with a larger number of states by improving computational efficiency using random Fourier features for GPs [Tanaka *et al.*, 2022]. Second, we will improve data efficiency of the proposed method further by using constrained HNNs [Finzi *et al.*, 2020] and graph neural networks [Thangamuthu *et al.*, 2022]. Third, we would like to extend our method to find state spaces by combining with Hamiltonian generative networks [Toth *et al.*, 2020].

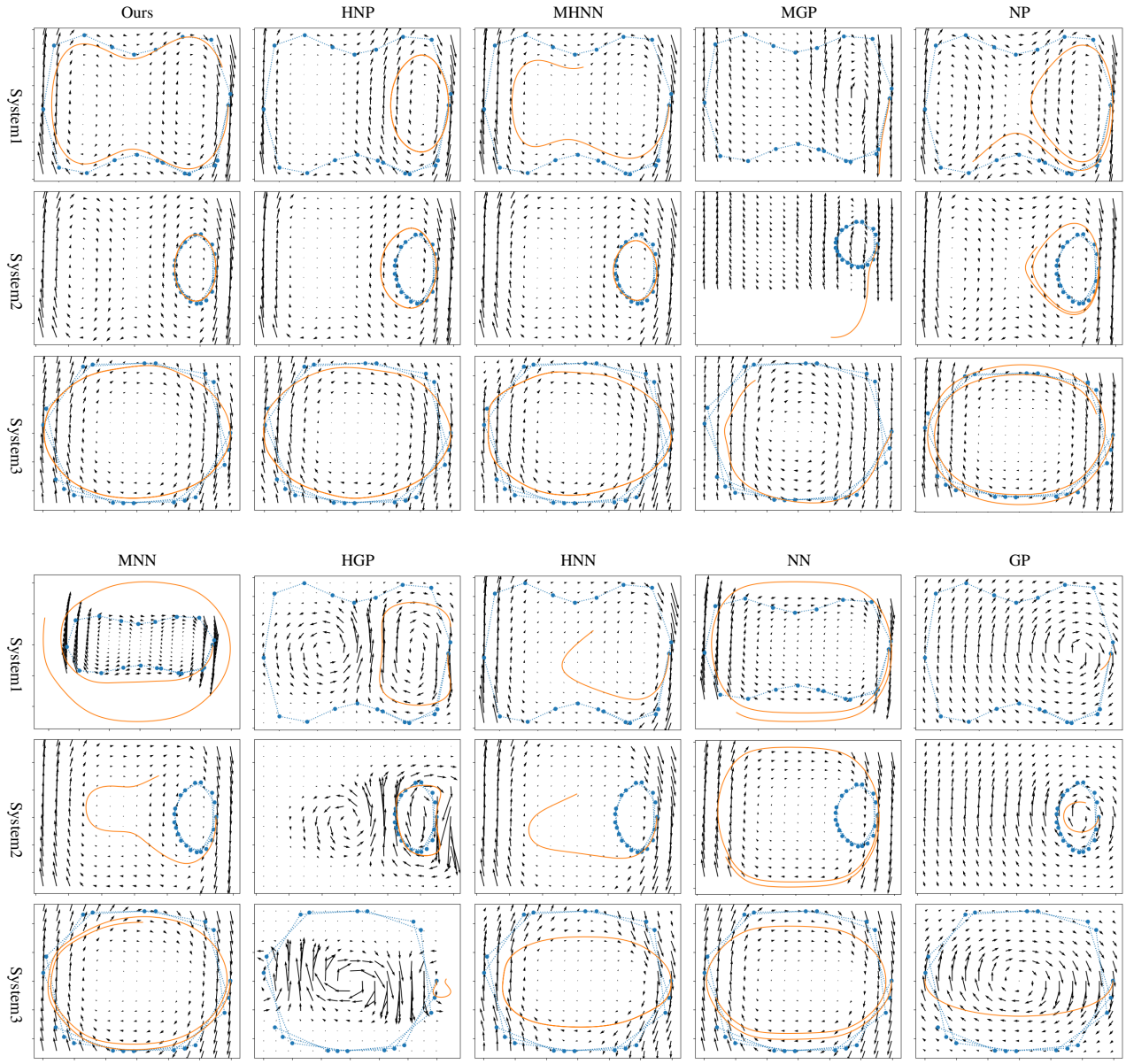
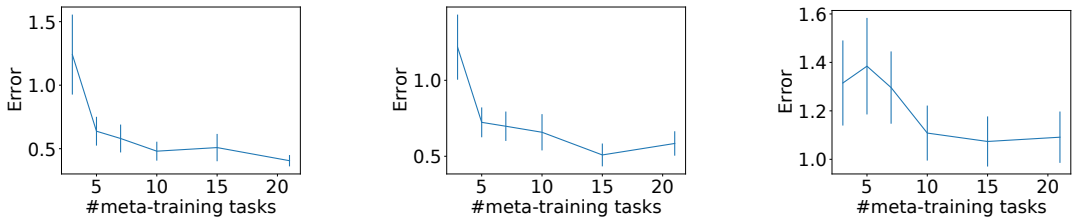


Figure 3: Predicted trajectories in a state space, and estimated vector fields in three meta-test datasets with one support sequence per system. Systems 1, 2, and 3 are Duffing without friction with different physical parameters. Blue circles are states on true trajectories, orange lines are the predicted trajectories, and black arrows are the predicted vector field.



(a) Mass-spring (b) Pendulum (c) Duffing

Figure 4: Test mean squared errors of trajectories with different numbers of meta-training systems on (a) Mass-spring, (b) Pendulum, and (c) Duffing systems without friction. Error bars show the standard errors.

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