Neural Reduced Potential via Persistent Homology

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Abstract

Constructing reduced models of gradient systems from high-dimensional data is challenging, as image-based latent spaces often require high dimensions and lack robustness. We propose a framework that integrates persistent homology with Neural Reduced Potential modeling. Time-series images are transformed into persistent diagrams (PDs), vectorized, and encoded by an autoencoder, and a neural network V_{NN}, inspired by Hamiltonian neural networks, learns the reduced potential. Applied to magnetic domain dynamics modeled by the time-dependent Ginzburg–Landau equation, our method reproduces gradient behavior, accurately reconstructs and predicts PD evolution, and yields smooth, low-dimensional latent dynamics with respect to anisotropy. These results demonstrate the advantage of topological descriptors for interpretable and efficient data-driven modeling of physical systems.

1 Introduction

Many natural phenomena, such as crystal growth Kobayashi [1993], Steinbach [2009], biological pattern formation Turing [1952], and magnetic domain dynamics Jagla [2004, 2005], Kudo et al. [2007], can be described as gradient systems that evolve according to the gradient of a potential function. Classic formulations include the Cahn–Hilliard Cahn and Hilliard [1958] and time-dependent Ginzburg–Landau equations Landau and Ginzburg [1950], as well as related effective theories Tomonaga [1950], Bohm and Pines [1951]. However, deriving interpretable reduced models directly from data remains challenging, since spatiotemporal patterns are high-dimensional and complex.

Recent machine learning studies have addressed this problem. Chen et al. Chen et al. [2022] showed that neural networks can extract hidden variables from experiments, and Tsuji et al. Tsuji et al. [2023] proposed the *Neural Reduced Potential*, inspired by Hamiltonian neural networks Greydanus et al. [2019], to learn potential functions from image sequences. While effective, such image-based embeddings often require high-dimensional latents and lack robustness when we realize high prediction ability. Also, it is difficult to apply neuralnetwork model when the size of images are large.

Topological data analysis (TDA), particularly persistent homology, provides an alternative by capturing multi-scale structures through persistent diagrams (PDs). Mototake et al. Mototake et al. [2023] demonstrated that PDs yield robust descriptors of magnetic domain formation correlated with physical parameters.

In this work, we combine these approaches and propose a framework that learns a Neural Reduced Potential on topological representations of data. Time-series images are first transformed into PDs, vectorized, and encoded by an autoencoder. In this latent topological space, a neural network V_{NN} approximates the reduced potential. Applied to magnetic domain dynamics modeled by the time-dependent Ginzburg–Landau equation, our method reproduces gradient behavior and yields smoother, lower-dimensional latent dynamics than direct image-based encodings.

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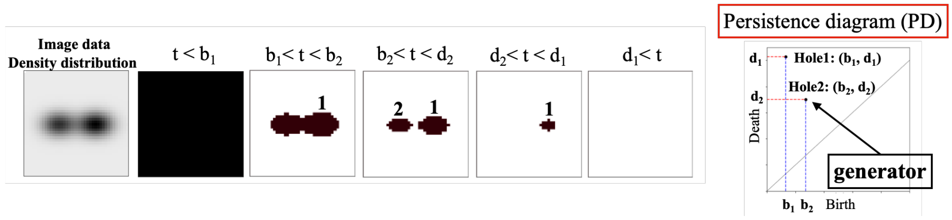

Figure 1: Illustration of persistent homology for topological data analysis. (Left) Example of a two-dimensional density distribution and the evolution of connected components and holes as the threshold t increases. The labels b_i and d_i denote the birth and death times of features. (Right) The birth and death times are summarized in a persistent diagram (PD), where each point (b_i, d_i) corresponds to the lifetime of a topological feature.

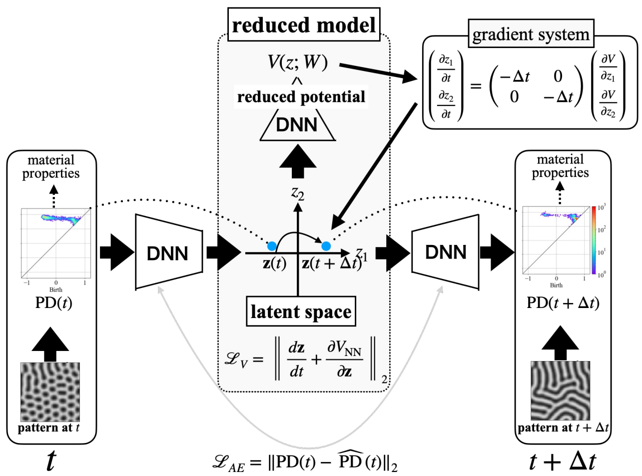

Figure 2: Overview of the proposed framework. Time-series image data of physical patterns are first transformed into persistent diagrams (PDs) that capture multi-scale topological features. The PDs are then embedded into a latent space via an autoencoder. In this latent space, a neural network V_{NN}, inspired by Hamiltonian neural networks (HNN), is trained to approximate the reduced potential function of the gradient system.

Our contributions are as follows: (a) Integration of persistent homology with Neural Reduced Potential modeling, enabling potentials to be learned from robust topological descriptors. (b) Validation on magnetic domain simulations, achieving continuous latent dynamics with respect to physical parameters. (c) Demonstration that PD-based representations improve interpretability, that is low-dimensionality, and lead the natural reduced coordinate over conventional image-based approaches.

2 topological data analysis

Topological Data Analysis (TDA) provides a mathematical framework to extract structural information from complex spatiotemporal data Edelsbrunner et al. [2002], Ghrist [2008]. In particular, persistent homology characterizes the birth and death of topological features, such as connected components or loops, as a threshold parameter changes Zomorodian and Carlsson [2005]. This allows us to detect multi-scale structures in data that are invariant to continuous deformations and robust against noise.

In the present study, each snapshot of the physical pattern (e.g., magnetic domain configurations) is first mapped into a persistent diagram (PD). As illustrated in Fig. 1, the procedure can be understood as follows: (i) the original data (either grayscale density fields or point clouds) are embedded into a filtration by gradually varying a threshold parameter, (ii) at each threshold, connected components and holes emerge or disappear, and (iii) the birth and death times of these features are recorded as points on a two-dimensional PD. Each point (b_i, d_i) in the PD represents the lifetime of a topological feature, with long-lived points corresponding to robust structures and short-lived points often associated with fluctuations.

The obtained PDs summarize both global and local geometric information of the pattern in a compact representation. Previous work has shown that PD-based features retain sufficient information to infer control parameters of underlying dynamical models and to classify pattern states in a physically meaningful way Mototake et al. [2023], Obayashi and Hiraoka [2018]. In this framework, PDs are further vectorized into finite-dimensional feature vectors Adams et al. [2017], Bubenik [2015], which are then used as inputs to the autoencoder described in Sec. 3. This enables the subsequent construction of a reduced potential function V_{NN} on a latent topological space, combining the robustness and interpretability of TDA with the expressive power of neural networks.

3 Proposed framework

In this study, we propose a framework that estimates the reduced potential function from topological data representations of unknown phenomena that are expected to follow gradient systems. The framework further validates whether the obtained model is consistent with the observed phenomena and incorporates its useful properties.

An overview of the proposed framework is presented in Fig. 2. In this framework, as shown in Fig. 2, the first step is to transform raw time-series image data into topological descriptors. For each snapshot of the system, persistent diagrams (PDs) are computed using persistent homology, which captures the birth and death of topological features (e.g., connected components, loops, voids) across multiple spatial scales. The obtained PDs are then vectorized into a finite-dimensional representation suitable for neural network training.

Next, the vectorized PDs are processed by an autoencoder (AE) Hinton and Salakhutdinov [2006] to construct a latent space representation of the system. The AE consists of an encoder E, which maps the vectorized PD at time t into a reduced vector z_t, and a decoder D, which reconstructs the PD from z_t: $E(\mathrm{PD}_t) = z_t, \quad D(z_t) = \widehat{\mathrm{PD}}_t$. The AE is trained to minimize the reconstruction loss $\mathcal{L}_{AE} = \|\mathrm{PD} - \widehat{\mathrm{PD}}\|_2$. Thus, the reduced vector z_t obtained from the AE is regarded as the state of the system in a topological latent space, i.e., $z_t = \boldsymbol{u}_t$.

Subsequently, as shown in Fig. 2, the reduced potential function V_{NN} is modeled in this latent space. Here, our approach is inspired by Hamiltonian neural networks (HNN) Greydanus et al. [2019], which demonstrated that neural architectures can recover energy functions (Hamiltonians) directly from raw time-series data of dynamical systems. In a similar spirit, V_{NN} is trained to approximate the potential function of gradient systems in the PD-based latent space, thereby serving as a *Neural Reduced Potential*.

In gradient systems, the following relationship holds:

$$\frac{d\boldsymbol{u}}{dt} = -\frac{\partial V}{\partial \boldsymbol{u}}, \tag{1}$$

where $\boldsymbol{u}$ is the system state, t is time, and V is the potential function. Equation (1) implies that by moving $\boldsymbol{u}$ in the direction of $-\frac{\partial V}{\partial \boldsymbol{u}}$, the temporal evolution of the system can be described. Therefore, as shown in the result section, to verify whether V_{NN} captures the gradient information of the phenomenon, the trajectories perturbed according to the gradients of V_{NN} are compared with the true evolution of the topological descriptors.

To train V_{NN}, we minimize the following loss: $\mathcal{L}_V = \left\| \frac{dz}{dt} + \frac{\partial V_{\mathrm{NN}}}{\partial z} \right\|_2$, where $\frac{dz}{dt}$ is estimated from the temporal changes in the PD-based latent vectors. The entire network is optimized using a combined objective: $\mathcal{L}_{all} = \mathcal{L}_{AE} + \lambda \mathcal{L}_V$, where $\lambda = 0.1$ in this study. It should be emphasized that the goal is not to predict system dynamics directly from observations, but to obtain a potential function that reflects the underlying topological structure of the phenomenon. Accordingly, the input to V_{NN} includes both the latent representation z and relevant physical parameters of the system.

4 Demonstration

In this study, the effectiveness of the proposed method was validated by applying the framework to simulation data of magnetic domain pattern dynamics in magnetic materials. Magnetic materials

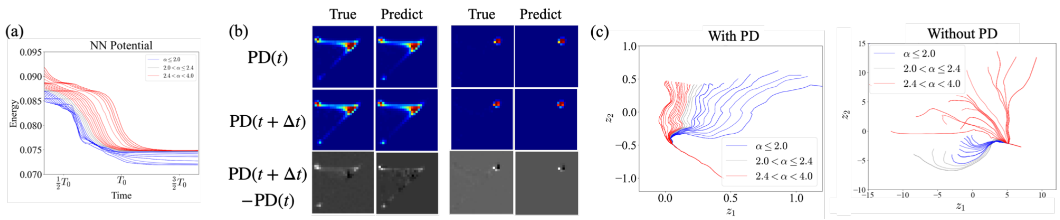

Figure 3: Results of the proposed framework. (a) Neural Reduced Potential V_{NN} decreases monotonically with time for all values of anisotropy α, demonstrating that the model correctly learns a gradient system. (b) Reconstruction and prediction of persistent diagrams (PDs): the autoencoder successfully reconstructs the PDs and their temporal changes are well reproduced by trajectories updated with $-\nabla_z V_{\mathrm{NN}}$. (c) Comparison of latent dynamics with and without PD input. The proposed method (*with PD*) produces smooth, continuous trajectories with respect to α, whereas the conventional approach (*without PD*) fails to capture such transitions in two dimensions.

are important industrial materials that are widely used in devices such as motors and hard-disk magnetic heads. Understanding the energy landscape underlying domain pattern dynamics is crucial for assessing their performance and functionality. The potential function of the magnetic domain pattern dynamics is often modeled as: $\frac{\partial \phi(\boldsymbol{r})}{\partial t} = -\frac{\delta H}{\delta \phi(\boldsymbol{r})}$, using the time-dependent Ginzburg–Landau (TDGL) equation Landau and Ginzburg [1950], where

$$H = \alpha\lambda(\boldsymbol{r}) \int d\boldsymbol{r} \left(-\frac{\phi(\boldsymbol{r})^2}{2} + \frac{\phi(\boldsymbol{r})^4}{4} \right) + \beta \int d\boldsymbol{r} \frac{|\nabla \phi(\boldsymbol{r})|^2}{2} + \gamma \int d\boldsymbol{r} d\boldsymbol{r}' \frac{\phi(\boldsymbol{r})\phi(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|^3} - h(t) \int d\boldsymbol{r}\, \phi(\boldsymbol{r}).$$

The TDGL equation is a two-dimensional model that effectively describes magnetic domain formation. However, it is still high-dimensional, since the system is represented by the scalar field $\phi(\boldsymbol{r}) : \mathbb{R}^2 \to \mathbb{R}$, where $\phi(\boldsymbol{r})$ denotes the average of the spin components in grid cells. The resulting patterns can be complex, and extracting interpretable descriptors directly from this field remains challenging. Therefore, in this study, we attempted to derive interpretable descriptors through the *Neural Reduced Potential* obtained from persistent homology applied to the TDGL simulation data.

The simulation data used here were generated following Kudo et al. [2007]. A saturation magnetic field h_{init} was applied, and a constant decay rate v was assumed for the external magnetic field $h(t)$. Thus, $h(t) = h_{init} - vt \quad (t < T_0)$ and $h(t) = 0 \quad (t \geq T_0)$, where $T_0 = h_{init}/v$ is the time when the external field vanishes. The simulation was performed until $t = 2T_0$. The parameters were set as $v = 10^{-2}$, $\beta = 2.0$ (neighboring spin interaction), $\gamma = 2.0/\pi$ (dipolar interaction), $\lambda(\boldsymbol{r}) \sim \mathcal{N}(0, 0.3^2)$, $h_{init} = 1.5$, and the anisotropy parameter α was varied in the range $[1.0, 4.0]$.

In the demonstration, each spin configuration $\phi(\boldsymbol{r})$ generated by the TDGL model was first converted into a persistent diagram (PD), which encodes the multi-scale topological features of the domain patterns. The PDs were then vectorized and passed through the autoencoder (AE) to obtain the latent representation z_t. This latent vector, together with physical parameters such as anisotropy α and external field $h(t)$, was used as input to the neural network V_{NN}. In this way, the proposed framework learns a reduced potential function that reflects both the topological structure and physical properties of the domain dynamics.

5 Results and Discussion

Fig. 3 summarizes the main results. (a) The Neural Reduced Potential decreases monotonically with time for all anisotropy α, indicating that the network successfully learns the structure of a gradient system. (b) The reconstructed and predicted persistent diagrams closely match the ground truth, showing that the latent representation retains essential topological information and that V_{NN} governs their temporal evolution. (c) Compared with the conventional approach (*without PD*), the proposed method (*with PD*) yields smooth latent trajectories that vary continuously with α, whereas the conventional method fails to capture this transition in two dimensions. This suggests that incorporating PDs enables lower-dimensional, more interpretable latent representations, consistent with prior work that required higher-dimensional latents.

Overall, these results demonstrate that topological descriptors provide a robust basis for constructing reduced potentials, improving both interpretability and efficiency in modeling gradient systems.

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