Neural Reduced Potential via Persistent Homology

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Abstract

Constructing reduced models of gradient systems from high-dimensional data is challenging because image-based latent spaces typically require high dimensions and lack robustness. We propose a framework integrating persistent homology with neural-reduced potential modeling. Time-series images are transformed into persistent diagrams (PDs), vectorized, and encoded by an autoencoder, while a V_{NN}–an architecture inspired by Hamiltonian neural networks–learns the reduced potential. When 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 using topological descriptors for interpretable and efficient data-driven modeling of physical systems.

1 Introduction

Many natural phenomena–including 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 based on 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 because spatiotemporal patterns are high dimensional and complex.

Recent machine-learning studies have addressed this problem. Chen et al. [Chen et al., 2022] demonstrated that neural networks can extract hidden variables from experiments, and Tsuji et al. [Tsuji et al., 2023] proposed a Neural Reduced Potential inspired by Hamiltonian neural networks [Greydanus et al.] to learn potential functions from image sequences. While effective, such image-based embeddings typically require high-dimensional latents and lack robustness when high predictive accuracy is needed. In addition, applying neural network models becomes challenging when the image size is large.

Topological data analysis (TDA), particularly persistent homology, is an alternative method for capturing multiscale structures through persistent diagrams (PDs). Mototake et al. [Mototake et al., 2023] demonstrated that PDs yield robust descriptors of magnetic domain formation that are correlated with physical parameters.

In this study, we integrate these approaches and propose a framework that learns a Neural Reduced Potential from the topological representations of data. Time-series images were transformed into PDs, vectorized, and encoded using an autoencoder, and in this latent topological space, the V_{NN} approximates the reduced potential. Application to magnetic domain dynamics modeled by time

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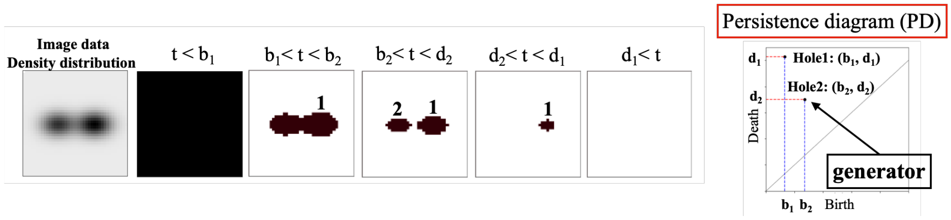
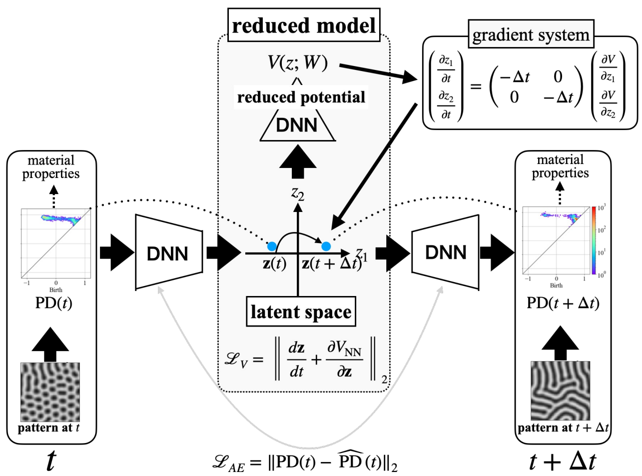


Figure 1: Illustration of persistent homology for topological data analysis. (Left) Example of a two-dimensional density distribution and the evolution of connected components and holes as the threshold t increases. The labels b_i and d_i denote the birth and death times of features. (Right) The birth 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.



$$\begin{pmatrix} \frac{\partial z_1}{\partial t} \\ \frac{\partial z_2}{\partial t} \end{pmatrix} = \begin{pmatrix} -\Delta t & 0 \\ 0 & -\Delta t \end{pmatrix} \begin{pmatrix} \frac{\partial V}{\partial z_1} \\ \frac{\partial V}{\partial z_2} \end{pmatrix}$$

$$\mathscr{L}_V = \left\| \frac{d\mathbf{z}}{dt} + \frac{\partial V_{\mathrm{NN}}}{\partial \mathbf{z}} \right\|_2$$

$$\mathscr{L}_{AE} = \|\mathrm{PD}(t) - \widehat{\mathrm{PD}}(t)\|_2$$

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.

dependent Ginzburg–Landau equation, our method reproduces the gradient behavior and yields smoother, lower-dimensional latent dynamics than direct image-based encodings.

Our contributions are as follows: (a) integration of persistent homology with neural-reduced potential modeling, enabling potential learning from robust topological descriptors. (b) Validation of magnetic domain simulations to achieve continuous latent dynamics with respect to physical parameters. (c) Demonstration that PD-based representations improve interpretability, that is, low-dimensionality, and cause naturally reduced coordinates compared to conventional image-based approaches.

2 Topological data analysis

Topological Data Analysis (TDA) provides a mathematical framework for extracting 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 the threshold parameter changes [Zomorodian and Carlsson, 2005]. This enables us to detect multiscale structures in data that are invariant to continuous deformations and robust against noise.

In this study, each snapshot of the physical pattern (e.g., magnetic domain configuration) was first mapped onto a PD. As illustrated in Fig. 1, the procedure is as follows: (i) the original data (grayscale density fields or point clouds) are embedded into a filtration by gradually varying a threshold parameter, and (ii) at each threshold, connected components, and holes emerged or disappeared; and (iii) the birth and death times of these features were recorded as points on the 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 typically associated with fluctuations.

The obtained PDs summarized both the global and local geometric information of the pattern in a compact representation. Previous work has demonstrated that PD-based features retain sufficient information to infer the control parameters of underlying dynamical models and to classify pattern states in a physically meaningful manner [Mototake et al., 2023, Obayashi and Hiraoka, 2018]. In this framework, the PDs are further vectorized into finite-dimensional feature vectors [Adams et al., 2017, Bubenik, 2015], which are used as inputs to the autoencoder, as described in Section 3. This facilitates the construction of a reduced potential function V_{NN} in 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 expected to follow gradient systems. The framework further validates whether the obtained model is consistent with the observed phenomena and incorporates useful properties.

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

Next, the vectorized PDs were processed using 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 considered as the state of the system in a topological latent space, that is $z_t = \boldsymbol{u}_t$.

Subsequently, as shown in Fig. 2, the reduced potential function V_{NN} was modeled in this latent space. Our approach was inspired by HNNs [Greydanus et al.], which demonstrate that neural architectures can recover energy functions (Hamiltonians) directly from raw time-series data of dynamical systems. Similarly, the V_{NN} is trained to approximate the potential function of the 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 results section, to verify whether the V_{NN} captured the gradient information of the phenomenon, the trajectories perturbed based on the gradients of the V_{NN} were 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 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. Note that the goal is not to predict system dynamics directly from observations, but to derive 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.

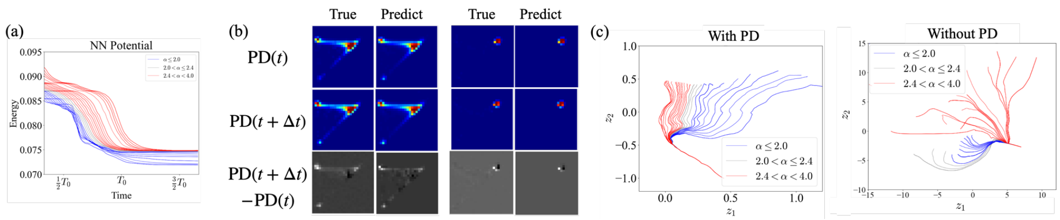


Figure 3: Results of the proposed framework. (a) Neural Reduced Potential V_{NN} decreases monotonically with time for all values of anisotropy α, demonstrating that the model correctly learns a gradient system. (b) Reconstruction and prediction of PDs: the autoencoder successfully reconstructs the PDs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

4 Demonstration

The effectiveness of the proposed method was validated using simulation data of magnetic domain pattern dynamics in magnetic materials. Magnetic materials are important industrial materials widely used in devices, such as motors and hard-disk magnetic heads. Understanding the energy landscape underlying the domain pattern dynamics is crucial for assessing their performance and functionality. Potential function of the magnetic domain pattern dynamics is 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 the magnetic domain formation. However, it remains high-dimensional, as 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 in this study were generated following [Kudo et al., 2007]. A saturated 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 is 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 PD, which encodes the multi-scale topological features of the domain patterns. The PDs were vectorized and passed through an autoencoder (AE) to obtain the latent representation z_t. This latent vector, together with physical parameters, such as anisotropy α and external field $h(t)$, serves as input to the V_{NN}. Consequently, 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 over time for all anisotropy α, indicating that the network successfully captures the structure of a gradient system. (b) The reconstructed and predicted persistent diagrams closely match the ground truth, demonstrating that the latent representation preserves essential topological information and that V_{NN} governs their temporal evolution. (c) Compared to 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 latent representations.

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

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