GD-VAEs: Geometric Dynamic Variational Autoencoders for Learning Nonlinear Dynamics and Dimension Reductions

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Abstract

We develop data-driven methods incorporating geometric and topological information to learn parsimonious representations of nonlinear dynamics from observations. We develop approaches for learning nonlinear state space models of the dynamics for general manifold latent spaces using training strategies related to Variational Autoencoders (VAEs). Our methods are referred to as Geometric Dynamic (GD) Variational Autoencoders (GD-VAEs). We learn encoders and decoders for the system states and evolution based on deep neural network architectures that include general Multilayer Perceptrons (MLPs), Convolutional Neural Networks (CNNs), and Transpose CNNs (T-CNNs). Motivated by problems arising in parameterized PDEs and physics, we investigate the performance of our methods on tasks for learning low dimensional representations of the nonlinear Burgers equations, constrained mechanical systems, and spatial fields of reaction-diffusion systems. GD-VAEs provide methods for obtaining representations for use in diverse learning tasks involving dynamics.

Keywords: variational autoencoders, dimension reduction, dynamical systems, scientific machine learning

1. Introduction

The general problem of learning dynamical models from a time series of observations has a long history spanning many fields [60; 78; 18; 39] including in dynamical systems [10; 78; 80; 56; 59; 61; 35; 22; 26], control [11; 60; 71; 74], statistics [1; 57; 29], and machine learning [18; 39; 53; 69; 5; 87; 54]. Referred to as system identification in control and engineering, many approaches have been developed starting with linear dynamical systems (LDS). These include the Kalman Filter and extensions [44; 25; 31; 83; 85], Proper Orthogonal Decomposition (POD) [15; 58], and more recently Dynamic Mode Decomposition (DMD) [74; 51; 82] and Koopman Operator approaches [59; 23; 48]. These successful and widely-used approaches rely on assumptions about the model structure, most commonly, that a time-invariant LDS provides a good local approximation or that noise is Gaussian.

There also has been research on more general nonlinear system identification [1; 76; 18; 39; 77; 56; 57; 60]. Nonlinear systems pose many open challenges and fewer unified approaches given the rich behaviors of nonlinear dynamics. For classes of systems and specific application domains, methods have been developed which make different levels of assumptions about the underlying structure of the dynamics. Methods for learning nonlinear dynamics include the NARX and NOE approaches with function approximators based on neural networks and other models classes [60; 78], sparse symbolic dictionary methods that are linear-in-parameters such as SINDy [11; 75; 78], and dynamic
Bayesian networks (DBNs), such as Hidden Markov Chains (HMMs) and Hidden-Physics Models [69; 63; 73; 7; 49; 29].

A central challenge in learning non-linear dynamics is to obtain representations not only capable of reproducing similar outputs as observed directly in the training data set but to infer structures that can provide stable more long-term extrapolation capabilities over multiple future steps and input states. In this work, we develop learning methods aiming to obtain robust non-linear models by providing ways to incorporate more structure and information about the underlying system related to smoothness, periodicity, topology, physical principles, and other constraints. We focus particularly on developing Probabilistic Autoencoders (PAEs) that incorporate noise-based regularizations and priors to learn lower dimensional representations from observations. This provides the basis of nonlinear state space models for prediction. We develop methods for incorporating into such representations geometric and topological information about the system. This facilitates capturing qualitative features of the dynamics to enhance robustness and to aid in interpretability of results. We demonstrate and perform investigations of our methods to obtain models for reductions of parameterized PDEs, constrained mechanical systems, and reaction-diffusion systems.

2. Learning Nonlinear Dynamics with Variational Autoencoders (VAEs)

We develop data-driven approaches based on a Variational Autoencoder (VAE) framework [46]. We learn from observation data a set of lower dimensional representations that are used to make predictions for the dynamics. In practice, data can include experimental measurements, large-scale computational simulations, or solutions of complicated dynamical systems for which we seek reduced models. Reductions aid in gaining insights for a class of inputs or physical regimes into the underlying mechanisms generating the observed behaviors. Reduced descriptions are also helpful in many optimization problems in design and in development of controllers [60].

Standard autoencoders can result in encodings of observations $x$ that yield unstructured scattered disconnected coding points $z$ representing the system features. VAEs provide probabilistic encoders and decoders where noise provides regularizations that promote more connected encodings, smoother dependence on inputs, and more disentangled feature components [46]. As we shall discuss, we also introduce other regularizations into our methods to help aid in interpretation of the learned latent representations.

Figure 1: **Learning Nonlinear Dynamics with Encoders and Decoders.** Data-driven methods are developed for learning robust models to predict from $u(x, t)$ the non-linear evolution to $u(x, t + \tau)$ for PDEs and other dynamical systems. Probabilistic Autoencoders (PAEs) are utilized to learn representations $z$ of $u(x, t)$ in low dimensional latent spaces with prescribed geometric and topological properties. The model makes predictions using learnable maps that (i) encode an input $u(x, t) \in \mathcal{U}$ as $z(t)$ in latent space (left), (ii) evolve the representation $z(t) \rightarrow z(t + \tau)$ (middle), (iii) decode the representation $z(t + \tau)$ to predict $\hat{u}(x, t + \tau)$ (right).
We learn VAE predictors using a Maximum Likelihood Estimation (MLE) approach for the Log Likelihood (LL) $L_{LL} = \log(p_\theta(X, x))$. For dynamics of $u(s)$, let $X = u(t)$ and $x = u(t + \tau)$. We base $p_\theta$ on the autoencoder framework in Figure 1 and 2. We use variational inference to approximate the LL by the Evidence Lower Bound (ELBO) [9]. We train a model with parameters $\theta$ using encoders and decoders based on minimizing the loss function

$$
\theta^* = \arg\min_{\theta_e, \theta_d} -\mathcal{L}^B(\theta_e, \theta_d; \mathcal{X}^{(i)}, \mathcal{X}^{(i)}), \quad \mathcal{L}^B = \mathcal{L}_{RE} + \mathcal{L}_{KL} + \mathcal{L}_{RR},
$$

where

$$
\mathcal{L}_{RE} = E_{q_{\theta_e}(z|\mathcal{X}^{(i)})} \left[ \log p_{\theta_d}(\mathcal{X}^{(i)}|z') \right], \quad \mathcal{L}_{KL} = -\beta D_{KL} (q_{\theta_e}(z|\mathcal{X}^{(i)}) \parallel p_{\theta_d}(z)),
$$

$$
\mathcal{L}_{RR} = \gamma E_{q_{\theta_e}(z|\mathcal{X}^{(i)})} \left[ \log p_{\theta_d}(\mathcal{X}^{(i)}|z') \right].
$$

The $q_{\theta_e}$ denotes the encoding probability distribution and $p_{\theta_d}$ the decoding probability distribution. The loss $\ell = -\mathcal{L}^B$ in equation 1 provides a regularized form of MLE. The term $\mathcal{L}^B$ approximates the likelihood for the encoder-decoder model can be decomposed into the following three terms (i) $\mathcal{L}_{RR}$ is the log likelihood of reconstructing samples, (ii) $\mathcal{L}_{RE}$ is the log likelihood of predicting samples after a single time step, and (iii) $\mathcal{L}_{KL}$ is a regularization term associated with VAEs.

**Figure 2: Variational Autoencoder (VAE) Framework.** Encoders and decoders based on the VAE framework [46] are used to learn representations of the nonlinear dynamics. Deep Neural Networks (DNNs) are trained (i) to serve as feature extractors to represent functions $u(x, t)$ and their evolution in a low dimensional latent space as $z(t)$ (probabilistic encoder $\sim q_{\theta_e}$), and (ii) to serve as approximators that can construct predictions $u(x, t+\tau)$ using features $z(t+\tau)$ (probabilistic decoder $\sim p_{\theta_d}$).

The terms $\mathcal{L}_{RE}$ and $\mathcal{L}_{KL}$ arise from the ELBO variational bound $L_{LL} \geq \mathcal{L}_{RE} + \mathcal{L}_{KL}$ when $\beta = 1$, [9]. This provides a way to estimate the log likelihood that the encoder-decoder reproduce the observed data sample pairs $(\mathcal{X}^{(i)}, \mathcal{X}^{(i)})$ using the codes $z'$ and $z$. Here, we include a latent-space mapping $z' = f_{\theta_e}(z)$ which is parameterized by $\theta_e$. This describes either the parameters associated with a prescribed mapping or for a class of maps these parameters can be learned during training. The latent-space mapping can be used to characterize the evolution of the system or
further processing of features. The $X^{(i)}$ is the input and $x^{(i)}$ is the output prediction. For the case of dynamical systems, we take $X^{(i)} \sim u^{(i)}(t)$ a sample of the initial state function $u^{(i)}(t)$ and the output $x^{(i)} \sim u^{(i)}(t+\tau)$ the predicted state function $u^{(i)}(t+\tau)$. We discuss the specific distributions used in more detail below.

The $L_{KL}$ term involves the Kullback-Leibler Divergence [50; 21] acting similar to a Bayesian prior on latent space to regularize the encoder conditional probability distribution $p_\theta(z|X)$ so that for each sample this distribution is similar to $p_{\theta_d}$. We take $p_{\theta_d} = \eta(0,\sigma_d^2)$ a multi-variate Gaussian with independent components. This serves (i) to disentangle the features from each other to promote independence, (ii) provide a reference scale and localization for the encodings $z$, and (iii) promote parsimonious codes utilizing smaller dimensions than $d$ when possible.

The $L_{RR}$ term gives a regularization that promotes retaining information in $z$ so the encoder-decoder pair can reconstruct functions. As we shall discuss, this also promotes organization of the latent space for consistency over multi-step predictions and aids in model interpretability.

We use for the specific encoder probability distributions conditional Gaussians $z \sim q_{\theta_e}(z|x^{(i)}) = a(X^{(i)},x^{(i)}) + \eta(0,\sigma_e^2)$ where $\eta$ is a Gaussian with variance $\sigma_e^2$, (i.e. $E^X(z) = a$, $\text{Var}^X(z) = \sigma_e^2$). One can think of the learnable mean function $a$ in the VAE as corresponding to a typical encoder $a(X^{(i)},x^{(i)};\theta_e) = a(x^{(i)};\theta_e)$ and the variance function $\sigma_e^2 = \sigma_e^2(\theta_e)$ as providing control of a noise source to further regularize the encoding. The $a$ can be represented by a deep neural network. Among other properties, the use of this approach with noise promotes connectedness of the ensemble of latent space codes, see Figure 2 (lower-left). For the VAE decoder distribution, we take $x \sim p_{\theta_d}(x|z^{(i)}) = b(z^{(i)}) + \eta(0,\sigma_d^2)$. The learnable mean function $b(z^{(i)};\theta_d)$ corresponds to a typical decoder and the variance function $\sigma_e^2 = \sigma_e^2(\theta_d)$ controls the source of regularizing noise. In practice, while the variances are learnable for many problems it can be useful to treat the $\sigma_e$ as hyper-parameters. We discuss some ways to use learning these parameters to extract geometric structure in Appendix C.

The terms to be learned in the VAE framework are $(a,\sigma_e, f_{\theta_e}, b,\sigma_d)$ which are parameterized by $\theta = (\theta_e, \theta_d, \theta_f)$. We learn predictors for the dynamics by training over samples of evolution pairs $\{(u_n^i, u_{n+1}^i)\}_{i=1}^m$ where $i$ denotes the sample index and $u_n^i = u^i(t_n)$ with $t_n = t_0 + n\tau$ for a time-scale $\tau$. To make predictions, the learned models use the following stages: (i) extract from $u(t)$ the features $z(t)$, (ii) evolve $z(t) \rightarrow z(t+\tau)$, (iii) predict using $z(t+\tau)$ the $\hat{u}(t+\tau)$, summarized in Figure 1. By composition of the latent evolution map the model makes multi-step predictions of the dynamics.

3. Learning with Manifold Latent Spaces having General Geometries and Topologies

For many systems, parsimonious representations can be obtained by working with non-euclidean manifold latent spaces, such as a torus for doubly periodic systems or even non-orientable manifolds, such as a klein bottle as arises in imaging and perception studies [13]. For this purpose, we learn encoders $E$ over a family of mappings to a prescribed manifold $M$ of the form

$$z = \mathcal{E}_\phi(x) = \Lambda(\tilde{\mathcal{E}}_\phi(x)) = \Lambda(w), \text{ where } w = \tilde{\mathcal{E}}_\phi(x).$$

(2)

The $\mathcal{E}_\phi$ is a candidate encoder to the manifold when the parameters are $\phi$, see equation 3.

To generate a family of maps over which we can learn in practice, we use that a smooth closed manifold $M$ of dimension $m$ can be embedded within $\mathbb{R}^{2m}$, as supported by the Whitney Embedding Theorem [86]. We obtain a family of maps to the manifold by constructing maps in two steps using equation 2. In the first step, we use an unconstrained encoder $\tilde{\mathcal{E}}$ from $x$ to a point $w$ in the embedding space. In the second step, we use a map $\Lambda$ that projects a point $w \in \mathbb{R}^{2m}$ to a point $z \in M \subset \mathbb{R}^{2m}$ within the embedded manifold. In this way, $\tilde{\mathcal{E}}$ can be any learnable mapping from $\mathbb{R}^n$ to $\mathbb{R}^{2m}$ for which there are many model classes including neural networks. To obtain a particular manifold
Figure 3: Learnable Mappings for Manifold Latent Spaces. We develop methods for using manifold latent space representations having general geometries and topologies through projection maps. For inter-operability with widely used trainable mappings, such as neural networks, we use a strategy of mapping inputs first to a point \( \tilde{E}_\phi(x) \in \mathbb{R}^N \) for the embedding space which is then projected to a point in the manifold \( \Lambda(w) \in \mathcal{M} \subset \mathbb{R}^N \). This provides trainable mappings for general manifold latent spaces. In practice, we can represent the manifold and compute projections based on general point cloud representations, analytic descriptions, product spaces, or other approaches.

map, the \( \tilde{E} \) only needs to learn an equivalent mapping from \( x \) to \( w \), where \( w \) is in the appropriate equivalence class \( Q_z \) of a target point \( z \) on the manifold, \( w \in Q_z = \{ w \mid \Lambda(w) = z \} \). Here, we accomplish this in practice two ways: (i) we provide an analytic mapping \( \Lambda \) to \( \mathcal{M} \), (ii) we provide a high resolution point-cloud representation of the target manifold along with local gradients and use for \( \Lambda \) a quantized or interpolated mapping to the nearest point on \( \mathcal{M} \). We provide more details of our methods below and in Appendix A.

In practice, we can view the projection map \( z = \Lambda(w) \) to the manifold as the solution of the optimization problem

\[
\mathbf{z}^* = \arg \min_{z \in \mathcal{M}} \frac{1}{2} \|w - z\|^2_2.
\]  

(3)

We can always express patches of a smooth manifold using local coordinate charts \( z = \sigma^k(u) \) for \( u \in \mathcal{U} \subset \mathbb{R}^m \). For example, we could use in practice a local Monge-Gauge quadratic fit to a point cloud representation of the manifold, as in [33]. We can express \( \mathbf{z}^* = \sigma^k(u^*) \) for some chart \( k^* \) for solution of equation 3. In terms of the collection of coordinate charts \( \mathcal{U}^k \) and local parameterizations \( \{\sigma^k(u)\} \), we can express this as

\[
\mathbf{u}^*,k^* = \arg \min_{k,u \in \mathcal{U}^k} \Phi_k(u, w), \text{ where } \Phi_k(u, w) = \frac{1}{2} \|w - \sigma^k(u)\|^2_2.
\]  

(4)

The \( w \) is the input and \( \mathbf{u}^*,k^* \) is the solution of equation 4. This gives the coordinate-based representation \( \mathbf{z}^* = \sigma^k(u^*) = \Lambda(w) \). For smooth parameterizations \( \sigma(u) \), the optimal solutions \( \mathbf{u}^*(w) \) satisfies from the optimization procedure the following implicit equation

\[
G(u^*, w) := \nabla_u \Phi_k(u^*, w) = 0.
\]  

(5)
During learning with backpropogation, we need to be able to compute the gradient

$$\nabla_\phi z^* = \nabla_\phi \sigma^k(\mathbf{u}^*) = \nabla_\phi \Lambda \left( \tilde{E}_\phi(\mathbf{x}) \right) = \nabla_w \Lambda(\mathbf{w}) \nabla_\phi \tilde{E}_\phi,$$

where $\mathbf{w} = \tilde{E}_\phi$. If we approach training models using directly the expressions of equation 6, we would need ways to compute both the gradients $\nabla_\phi \tilde{E}_\phi$ and $\nabla_w \Lambda(\mathbf{w})$. While the gradients $\nabla_\phi \tilde{E}_\phi$ can be obtained readily for many model classes, such as neural networks using backpropogation, the gradients $\nabla_w \Lambda(\mathbf{w})$ pose additional challenges. If $\Lambda$ can be expressed analytically then backpropagation techniques in principle may still be employed directly. However, in practice $\Lambda$ will often result from a numerical solution of the optimization problem in equation 3 using equation 4. We show how in this setting alternative approaches can be used to obtain the gradient $\nabla_\phi z^* = \nabla_\phi \Lambda \left( \tilde{E}_\phi(\mathbf{x}) \right)$.

To obtain gradients $\nabla_\phi z^*$, we derive expressions by considering variations $\mathbf{w} = \mathbf{w}(\gamma)$, $\phi = \phi(\gamma)$ for a scalar parameter $\gamma$. For example, this can be motivated by taking $\mathbf{w}(\gamma) = \tilde{E}_\phi(\mathbf{x}(\gamma))$ and $\phi = \phi(\gamma)$ for some path $(\mathbf{x}(\gamma), \phi(\gamma))$ in the input and parameter space $(\mathbf{x}, \phi) \in \mathcal{X} \times \mathcal{P}$. We can obtain the needed gradients by determining the variations of $\mathbf{u}^* = \mathbf{u}^*(\gamma)$ obtained from equation 4. This follows since $\mathbf{z}^* = \sigma^k(\mathbf{u}^*)$ and $\nabla_\phi \mathbf{z}^* = \nabla_\mathbf{u} \sigma^k(\mathbf{u}^*) \nabla_\phi \mathbf{u}^*$. The $\nabla_\mathbf{u} \sigma^k(\mathbf{u}^*)$ often can be readily obtained numerically or from backpropagation.

From equation 5, this allows us to express the gradients using the Implicit Function Theorem as

$$0 = \frac{d}{d\gamma} G(\mathbf{u}^*(\gamma), \mathbf{w}(\gamma)) = \nabla_\mathbf{u} G \frac{d\mathbf{u}^*}{d\gamma} + \nabla_\mathbf{w} G \frac{d\mathbf{w}}{d\gamma}. \tag{7}$$

The term typically posing the most significant computational challenge is $d\mathbf{u}^*/d\gamma$ since $\mathbf{u}^*$ is obtained numerically from the optimization problem in equation 4. We solve for it using the expression in equation 7 to obtain

$$\frac{d\mathbf{u}^*}{d\gamma} = -\left[ \nabla_\mathbf{u} G \right]^{-1} \nabla_\mathbf{w} G \frac{d\mathbf{w}}{d\gamma}. \tag{8}$$

This only requires that we can evaluate for a given $(\mathbf{u}, \mathbf{w})$ the local gradients $\nabla_\mathbf{u} G$, $\nabla_\mathbf{w} G$, $d\mathbf{w}/d\gamma$, and that $\nabla_\mathbf{u} G$ is invertible. Computationally, this only requires us to find numerically the solution $\mathbf{u}^*$ and evaluate numerically the expression in equation 8 for a given $(\mathbf{u}^*, \mathbf{w})$. This allows us to avoid needing to compute directly $\nabla_\mathbf{w} \Lambda(\mathbf{w})$. This provides an alternative practical approach for computing $\nabla_\phi \mathbf{z}^*$ useful in training models.

For learning via backpropogation, we use these results to assemble the needed gradients for our manifold encoder maps $\tilde{E}_\phi = \Lambda(\tilde{E}_\phi(\mathbf{x}))$ as follows. Using $\mathbf{w} = \tilde{E}_\phi(\mathbf{x})$, we first find numerically the closest point in the manifold $\mathbf{z}^* \in \mathcal{M}$ and represent it as $\mathbf{z}^* = \sigma(\mathbf{u}^*) = \sigma^k(\mathbf{u}^*)$ for some chart $k^*$. Next, using this chart we compute the gradients using that

$$G = \nabla_\mathbf{u} \Phi(\mathbf{u}, \mathbf{w}) = -(\mathbf{w} - \sigma(\mathbf{u}))^T \nabla_\mathbf{u} \sigma(\mathbf{u}). \tag{9}$$

We take in equation 9 a column vector convention with $\nabla_\mathbf{u} \sigma(\mathbf{u}) = [\sigma_{u_1} | \ldots | \sigma_{u_k}]$. We next compute

$$\nabla_\mathbf{u} G = \nabla_{\mathbf{uu}} \Phi = \nabla_{\mathbf{u}} \sigma^T \nabla_{\mathbf{u}} \sigma - (\mathbf{w} - \sigma(\mathbf{u}))^T \nabla_{\mathbf{uu}} \sigma(\mathbf{u}) \tag{10}$$

and

$$\nabla_\mathbf{w} G = \nabla_{\mathbf{ww}} \Phi = -I \nabla_{\mathbf{u}} \sigma(\mathbf{u}). \tag{11}$$

From equations 10 and 11, the gradients $\nabla_\mathbf{u} G$, $\nabla_\mathbf{w} G$, and using equation 8, we compute $\nabla_\phi \mathbf{z}^*$. This allows us to learn VAEs with latent spaces for $\mathbf{z}$ with general specified topologies and controllable geometric structures. We provide additional details in Appendix A.
We refer to our learning framework for learning dynamics on latent spaces having general geometries as Geometric Dynamic Variational Autoencoders (GD-VAEs). In contrast to $\mathbb{R}^n$ which is typically used as the latent space, the topologies of sphere, torus, klein bottle are intrinsically different and can provide ways to reduce the dimensionality or provide novel types of latent representations. This also allows for new types of priors to be used, such as uniform distributions on compact manifolds or prior distributions with other properties arising from the geometry, such as periodicity. As we shall discuss in more detail, additional latent space structure can also help in learning more robust representations and reduce sensitivity to noise. Manifold latent spaces provide ways when geometric information is known to help unburden the encoder and decoder from having also to learn the embedding geometry as part of the learning task. We can also reduce the subset of points and number of dimensions on which encoders/decoders must learn. This also can further enhance statistical power of the training data and stability. Among other possible advantages, our introduced methods for working with manifold latent spaces allow for more parsimonious representations and smaller dimensions aiding in identifiability and interpretability of the learned models. We discuss below this further in the context of specific applications of GD-VAEs.

4. Related Work

Many variants of autoencoders have been developed for making predictions of sequential data, including those based on Recurrent Neural Networks (RNNs) with LSTMs and GRUs [38; 32; 19]. While RNNs provide a rich approximation class for sequential data, they pose for dynamical systems challenges for interpretability and for training to obtain predictions stable over many steps with robustness against noise in the training data set. Autoencoders have also been combined with symbolic dictionary learning for latent dynamics in [14] providing some advantages for interpretability and robustness, but require specification in advance of a sufficiently expressive dictionary. Neural networks incorporating physical information have also been developed with some imposing stability conditions during training [62; 3; 81; 53; 81; 4; 27]. The work of [20] investigates combining RNNs with VAEs to obtain more robust models for sequential data and considered tasks related to processing speech and handwriting.

In our work we learn dynamical models making use of VAEs to obtain probabilistic encoders and decoders between euclidean and more general manifold latent spaces to provide additional regularizations to help promote parsimoniousness, disentanglement of features, robustness, and interpretability. Prior VAE methods used for dynamical systems include [34; 64; 54; 30; 16; 64; 70]. These works use primarily euclidean latent spaces and consider applications including human motion capture and ODE systems. Approaches for incorporating topological information into latent variable representations include the early works by Kohonen on Self-Organizing Maps (SOMs) [47] and Bishop on Generative Topographical Maps (GTMs) based on density networks providing a generative approach [8]. More recently, VAE methods using non-euclidean latent spaces include [42; 43; 28; 17; 54; 24; 2]. These incorporate the role of geometry by augmenting the prior distribution $\tilde{p}_\theta(z)$ on latent space to bias toward a manifold. In the recent work [66], an explicit projection procedure is introduced, but in the special case of a few manifolds having an analytic projection map. We also introduced methods for more general manifolds methods in our proceedings paper [54].

In our work, we develop further methods for more general latent space representations, including non-orientable manifolds, and applications to parameterized PDEs, constrained mechanical systems, and reaction-diffusion systems. We introduce more general methods for non-euclidean latent spaces in terms of point-cloud representations of the manifold along with local gradient information that can be utilized within general back-propogation frameworks. This also allows for the case of manifolds that are non-orientable and having complex shapes. Our methods provide flexible ways to design and control both the topology and the geometry of the latent spaces. We investigate the roles of latent space geometry, non-linearities, and noise-based regularizations by making comparisons with other data-driven methods. We also consider additional types of regularizations for learning
dynamical models facilitating multi-step predictions and more interpretable state space models. In our work, we show how the introduced data-driven methods can be used to obtain representations for constrained mechanical systems and reduced models for non-linear PDEs, including Burgers equations and reaction-diffusion systems.

5. Results

We report on the performance of the methods. We consider examples that include learning the dynamics of the non-linear Burger’s PDEs and reaction-diffusion PDEs. We also investigate learning representations for constrained mechanical systems. We consider the roles of manifold latent spaces having different dimensions, topology, and geometry.

5.1 Burgers’ Equation of Fluid Mechanics: Learning Nonlinear PDE Dynamics

We consider the nonlinear viscous Burgers’ equation

\[ u_t = -uu_x + \nu u_{xx}, \]  

where \( \nu \) is the viscosity [6; 40]. We consider periodic boundary conditions on \( \Omega = [0, 1] \). Burgers equation is motivated as a mechanistic model for the fluid mechanics of advective transport and shocks, and serves as a widely used benchmark for analysis and computational methods.

The nonlinear Cole-Hopf Transform \( CH \) can be used to relate Burgers equation to the linear Diffusion equation \( \phi_t = \nu \phi_{xx} \) [40]. This provides a representation of the solution \( u \)

\[ \phi(x, t) = CH[u] = \exp\left( -\frac{1}{2\nu} \int_0^x u(x', t) dx' \right), \quad u(x, t) = CH^{-1}[\phi] = -2\nu \frac{\partial}{\partial x} \ln \phi(x, t). \]  

This can be represented by the Fourier expansion

\[ \phi(x, t) = \sum_{k=-\infty}^{\infty} \hat{\phi}_k(0) \exp(-4\pi^2k^2\nu t) \cdot \exp(i2\pi kx). \]

The \( \hat{\phi}_k(0) = F_k[\phi(x, 0)] \) and \( \phi(x, t) = F^{-1}[\{\hat{\phi}_k(0) \exp(-4\pi^2k^2\nu t)\}] \) with \( F \) the Fourier transform. This provides an analytic representation of the solution of the viscous Burgers equation \( u(x, t) = CH^{-1}[\phi(x, t)] \) where \( \phi(0) = F[CH[u(x, 0)]] \). In general, for nonlinear PDEs with initial conditions within a class of functions \( \mathcal{U} \), we aim to learn models that provide predictions \( u(t + \tau) = S_\tau u(t) \) approximating the evolution operator \( S_\tau \) over time-scale \( \tau \). For the Burgers equation, the \( CH \) provides in principle an analytic way to obtain a reduced order model by truncating the Fourier expansion to \( |k| \leq n_f/2 \). This provides for the Burgers equation a benchmark model against which to compare our learned models. For general PDEs comparable analytic representations are not usually available. In addition, for many problems arising in practice, we are interested primarily in how the system behaves for a limited class of initial conditions and parameters. The aim then becomes to find a reduced model that predicts well the outcomes for these circumstances. We show how data-driven approaches can be developed for this purpose.

We develop VAE methods for learning reduced order models for the responses of nonlinear Burgers Equation when the initial conditions are from a collection of functions \( \mathcal{U} \). We consider in particular \( \mathcal{U} = \mathcal{U}_1 = \{ u \mid u(x, t; \alpha) = \alpha \sin(2\pi x) + (1 - \alpha) \cos(2\pi x) \} \). We remark that while the initial conditions are a linear combination of two functions, this relation does not hold for the solutions given the non-linear dynamics of the Burgers’ PDE. We learn VAE models that extract from \( u(x, t) \) latent variables \( z(t) \) to predict \( u(x, t + \tau) \). Given the non-uniqueness of representations and to promote interpretability of the model, we introduce the inductive bias that the evolution dynamics in latent space for \( z \) is linear of the form \( \dot{z} = -\lambda_0 z \), giving exponential decay rate \( \lambda_0 \). For discrete times,
we take \( z_{n+1} = f_{\theta}(z_n) = \exp(-\lambda_0 \tau) \cdot z_n \), where \( \theta = (\lambda_0) \). We treated \( \lambda_0 \) as a hyperparameter in our studies with \( \exp(-\lambda_0 \tau) = 0.75 \), but this could also be learned if additional criteria is introduced for the latent-space representations. The exponential decay is used to influence how the dynamical information is represented in latent space and also helps ensure dynamical stability for predictions. For the encoders and decoders, we consider general nonlinear mappings which are represented by deep neural networks. We train the model on the pairs \((u(x, t), u(x, t+\tau))\) by drawing \( m \) samples of \( u'(x, t_i) \in S_t U \) which generates the evolved state under Burgers equation \( u'(x, t_i+\tau) \) over time-scale \( \tau \). We perform VAE studies with parameters \( \nu = 2 \times 10^{-2}, \tau = 2.5 \times 10^{-1} \) with VAE Deep Neural Networks (DNNs) with layer sizes (in)-400-400-(out), ReLU activations, and \( \gamma = 0.5, \beta = 1 \), and initial standard deviations \( \sigma_d = \sigma_e = 4 \times 10^{-3} \). We show results of our VAE model predictions in Figure 4 and Table 1.

**Figure 4:** **Burgers’ Equation: Prediction of Dynamics.** We consider responses for initial conditions \( \mathcal{U}_1 = \{ u \mid u(x, t; \alpha) = \alpha \sin(2\pi x) + (1 - \alpha) \cos^3(2\pi x) \} \). Predictions are made for the evolution \( u \) over the time-scale \( \tau \) satisfying equation 12 with initial conditions in \( \mathcal{U}_1 \). We find our nonlinear VAE methods are able to learn with 2 latent dimensions the dynamics with errors < 1%. Methods such as DMD [74; 82] with 3 modes which are only able to use a single linear space to approximate the initial conditions and prediction encounter challenges in approximating the nonlinear evolution. We find our linear VAE method with 2 modes provides some improvements, by allowing for using different linear spaces for representing the input and output functions, but at the cost of additional computations. Results are summarized in Table 1.
Figure 5: Burgers’ Equation: Latent Space Representations and Extrapolation Predictions. We show the latent space representation $z$ of the dynamics for the input functions $u(\cdot,t;\alpha) \in U_1$. VAE organizes for $u$ the learned representations $z(\alpha,t)$ in parameter $\alpha$ (blue-green) into circular arcs that are concentric in the time parameter $t$, (yellow-orange) (left). The reconstruction regularization with $\gamma$ aligns subsequent time-steps of the dynamics in latent space facilitating multi-step predictions. The learned VAE model exhibits a level of extrapolation to predict dynamics even for some inputs $u \notin U_1$ beyond the training data set (right).

We show the importance of the non-linear approximation properties of our VAE methods in capturing system behaviors by making comparisons with Dynamic Mode Decomposition (DMD) [74; 82], Proper Orthogonal Decomposition (POD) [15], and a linear variant of our VAE approach. Recent CNN-AEs have also studied related advantages of non-linear approximations [53]. Some distinctions in our work is the use of VAEs to further regularize AEs and using topological latent spaces to facilitate further capturing of structure. The DMD and POD are widely used and successful approaches that aim to find an optimal linear space on which to project the dynamics and learn a linear evolution law for system behaviors. DMD and POD have been successful in obtaining models for many applications, including steady-state fluid mechanics and transport problems [82; 74]. However, given their inherent linear approximations they can encounter well-known challenges related to translational and rotational invariances, as arise in advective phenomena and other settings [10]. Our comparison studies can be found in Table 1.

We also considered how our VAE methods performed when adjusting the parameter $\gamma$ for the strength of the reconstruction regularization. The reconstruction regularization has a significant influence on how the VAE organizes representations in latent space and the accuracy of predictions of the dynamics, especially over multiple steps, see Figure 5 and Table 2. The regularization serves
We start by considering Burgers’ equations with initial conditions parameterized periodically as

\[ u_\alpha(x, t = 0) = \begin{bmatrix} \cos(2\pi \alpha) \\ \sin(2\pi \alpha) \end{bmatrix} \cdot \begin{bmatrix} \cos(2\pi x) \\ \sin(2\pi x) \end{bmatrix}, \quad \alpha \in [0, 1]. \quad (14) \]

We consider solutions with \( x, t \in [0, 1] \). Since the boundary conditions are periodic \( u(0, t) = u(1, t) \), the initial conditions parameterized by \( \alpha \) effectively shift relative to one another and we have the

<table>
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<td>7.41e-06 ± 0.0e-00</td>
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</table>

Table 1: Burgers’ Equation: Prediction Accuracy. The reconstruction \( L^1 \)-relative errors in predicting \( u(x, t) \) and standard error over 5 training trials. We compare our VAE methods, Dynamic Model Decomposition (DMD), and Proper Orthogonal Decomposition (POD), and reduction by Cole-Hopf (CH), over multiple-steps and number of latent dimensions (Dim).

<table>
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<th>( \gamma )</th>
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<td>5.55e-03 ± 4.9e-04</td>
<td>8.52e-03 ± 1.1e-03</td>
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Table 2: Burgers’ Equation: Prediction Accuracy and Regularizations. The reconstruction \( L^1 \)-relative errors and standard error over 5 training trials. We show prediction of \( u(x, t) \) varying the strength of the reconstruction regularization \( \gamma \) in equation 1.
topology of a circle. We also consider initial conditions parameterized doubly-periodic as

\[
\begin{bmatrix}
\cos(\alpha_1) \\
\sin(\alpha_1) \\
\cos(\alpha_2) \\
\sin(\alpha_2)
\end{bmatrix} \cdot 
\begin{bmatrix}
\cos(2\pi x) \\
\sin(2\pi x) \\
\cos(4\pi x) \\
\sin(4\pi x)
\end{bmatrix}, \quad \alpha_1, \alpha_2 \in [0, 2\pi].
\] (15)

This corresponds to the topology of a torus. We can project our solutions onto the Clifford Torus given by the product space \( S^1 \times S^1 \subset \mathbb{R}^4 \), where \( S^1 \) is the circle space \([45; 84]\). For example representations of latent spaces, see Figure 6. In each case, we seek representations that disentangle the temporal and common state information of the collection of solutions \( \{u_\alpha\} \) or \( \{u_{\alpha_1, \alpha_2}\} \).

Figure 6: GD-VAE Manifold Latent Spaces for Periodic and Doubly-Periodic Systems.

For time-dependent PDE solutions it is natural to consider latent spaces with cylinder-like shapes. In the cylinder topology the infinite axis corresponds to time and the other dimensions to the state of the system. When the parameters are periodic this gives responses with topology of a cylinder, which can be represented as a product-space \( \mathcal{B} \times \mathbb{R} \) where \( \mathcal{B} \) is the base-space. For a single periodic parameter the base-space \( \mathcal{B} \) is a circle, giving cylinder shown on (left). For two doubly-periodic parameters it is natural to consider for responses a torus for the base-space \( \mathcal{B} \). This can be represented in \( \mathbb{R}^3 \) or for visualization as shown on the (right). A Clifford Torus \( S^1 \times S^1 \subset \mathbb{R}^4 \) also can be used in practice for \( \mathcal{B} \) during training.

In principle for the periodic case, one analytic way the family of solutions \( \{u_\alpha\} \) could be encoded continuously is to use the \( \mathbb{R}^2 \) latent space with mapping

\[
u_\alpha(x, t) \rightarrow (t \cos(2\pi \alpha), t \sin(2\pi \alpha)).
\] (16)

This is similar to projecting a cone-shaped manifold in three dimensions to the two dimensional plane. In practice, the rather particular structure of this representation, which entangles the time and configuration state information, makes it difficult to learn during training, see Appendix B. Also, while such encodings may be useful for some problems, learning models that disentangle time and the configuration state information into separate dimensions in the latent space often results in simpler manifold structures and more interpretable results. We seek representations of the form

\[
u_\alpha(x, t) \rightarrow (f(\alpha), t),
\]

where we have a non-time-dependent mapping \( f \) that captures state information. Due to the potential non-trivial topology of the \( \alpha \) latent variable, if working only with Euclidean latent spaces a continuous encoder that disentangles time must map to a sufficiently larger number of dimensions.
to embed the manifold to preserve the topology. In the periodic case, this would be to at least three
dimensions. An example of such an analytic mapping to 
\[ u_\alpha(x, t) \rightarrow (\cos(2\pi \alpha), \sin(2\pi \alpha), t) \].

This mapping corresponds in a latent space having a cylinder topology. Similarly, for the doubly-
periodic family \( \{u_{\alpha_1, \alpha_2}\} \) the state information can be mapped in principle to a torus by \( f(\alpha) \). This would yield the disentangled embedding \( u_\alpha(x, t) \rightarrow (f(\alpha), t) \) with \( \alpha = (\alpha_1, \alpha_2) \). The torus can be represented in principle in \( \mathbb{R}^3 \) or as a product space \( S^1 \times S^1 \) where \( S^1 \) is the circle space. This latter representation is referred to as the Clifford Torus [45; 84]. This gives the latent space with 
\[ B \times \mathbb{R} \]
represented in principle in \( \mathbb{R}^3 \) or as a product space \( S^1 \times S^1 \) where \( S^1 \) is the circle space. This gives the latent space with the cylinder topology \( B \times \mathbb{R} \), where \( B \) is the base-space. For periodic case the \( B = S^1 \) is a circle and for the doubly-periodic case the \( B = S^1 \times S^1 \) is a torus.

We demonstrate how our methods can be used in practice to learn representations for the dynamics of the Burgers’ Equation solutions for latent spaces having specified topologies. We use a few approaches to leverage the prior geometric information about the system and to regulate how the model organizes the latent representations. This includes (i) specifying an explicit time-evolution map to disentangle time by requiring \( f_{ev}(z) = z + \Delta t e_n \in \mathbb{R}^n \), where \( \Delta t \) is the discrete time step and \( e_n = (0, \ldots, 0, 1) \) is the \( n^{th}\)-standard basis vector. We also use (ii) projection of the representation to a manifold structure, here we project the first \( n-1 \) dimensions to impose the topology as discussed in Section 3. In this way, we can introduce inductive biases for general initial conditions leveraging topologic and geometric knowledge to regulate the latent representations toward having desirable properties. This includes biasing toward disentangling time from the other state information captured in the latent state space representations.

For our example of the Burger’s Equations 12 with the periodic initial conditions in equation 14, we train using \( 10^4 \) solutions sampled uniformly over \( \alpha \) and time \( t \). The samples are corrupted with a Gaussian noise having standard deviation \( \sigma = 0.02 \). We train GD-VAEs using our framework discussed in Section 2. The neural networks have the architecture with number of layers for encoders (in)-400-400-(latent-space) and decoders (latent-space)-400-400-(out). The layers have a bias except for the last layer and ReLU activation functions [32; 52]. The numerical solutions of the Burgers equation 12 are sampled as \( u(x_k, t) = u_k \) with \( x_k \) at \( n = 100 \) points giving (in)=(out)=n=100. We also perform trainings representing the encoder variance with a trainable deep neural network, and set decoder variance such that log likelihood can be viewed as a Mean Square Error (MSE) loss with weight \( 10^{-4} \).

We predict the future evolution of the solutions of the Burger’s Equation over multiple steps using equation 2. We investigate the \( L^1 \)-accuracy of the learned GD-VAE predictions relative to the numerical solutions. We compare the GD-VAE with more conventional VAE methods that do not utilize topological information. We also make comparisons with standard Autoencoders (AEs) with and without utilizing topological information and our projection approaches in Section 3. We refer in the notation to our geometric projection as \( g\text{-projection} \). We show our results in Table 3.

We find our GD-VAE methods are able to learn parsimoneous disentangled representations that achieve a comparable reconstruction accuracy to standard VAE and AE provided these latter methods use enough dimensions. Reconstruction accuracy alone is only one way to measure the quality of the latent-space representations. Topological considerations play a significant role. When using too few dimensions, we see the standard AE and VAE methods can struggle to learn a suitable representation, see Figure 7. As we discuss in more detail in Appendix B, this arises since the autoencoders involve continuous maps that are unable to accomodate the topology injectively. For periodic systems this can result in rapid looping back behaviors approximating a discontinuity which results in scattered latent space points, see Figure 14. For additional discussions of the role of latent topology and training behaviors see Appendix B.

For longer-time multi-step predictions, we find our geometric projections can help with stability of the predictions arising from composition of the learned maps. We find both GD-VAEs and AEs
with $g$-projection have enhanced stability when compared to standard AEs for multi-step predictions. We find at time $t = 1.00s$, the AE+$g$-projection still is able to make accurate predictions, while the standard AE incurs significant errors, see Table 3. This arises from the geometric constraints reducing the number of dimensions and the "volume" of the subset of points in the latent space over which the encoder and decoders must learn correct mappings for responses. The geometric projection also serves to enhance the statistical power of the training data given more opportunities for common overlap of cases. In contrast, for multi-step predictions by general autoencoder maps new latent-space codes can arise during compositions that are far from those encountered in the training set resulting in unknown behaviors for the dynamic predictions. While in some cases there is comparable $L^1$-reconstruction errors to AEs with $g$-projection, the VAEs give better overall representations and more reliable training since the noise regularizations result in smoother organization of the latent codes with less local sensitivity in the encoder-decoder maps relative to the AEs. The geometric projections developed for GD-VAEs provide further benefits for stability by constraining the latent-space dynamics to be confined within a closed manifold which further enhances the multi-step predictions, see results for $t = 1.00s$ in Table 3.

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Table 3: Burgers’ Equations for Periodic and Doubly-Periodic Parameterized PDEs: $L^1$-Prediction Accuracy. The $L^1$-relative errors and standard error over 5 training trials. We train using the GD-VAEs framework discussed in Sections 2 and 3. We make comparisons to more conventional Variational Autoencoders (VAEs) and standard Autoencoders (AEs). The AE-(g-projection) method refers to the case where we combine using a standard AE (non-variational) and project the latent codes using our geometric projection approach developed in Section 3.
Figure 7: **Learned Latent Spaces for Burgers’ Equations.** The methods learn different three dimensional latent space representations for the non-linear dynamics. The GD-VAE method learns a model that encodes state information of the solutions on a circle which is aligned temporally (left). This allows for a representation of the evolution dynamics in the latent space following a simple contour in the direction of the Latent Dimension 3. While VAE without using a geometric prior learns an embedding having cylindrical topology the latent representation is geometrically distorted (left-middle). The AE+$g$-projection is found to learn a latent space representation with disentangled time and state information and with encodings that are aligned temporally (right-middle). The AE without using a geometric prior learns an arbitrary embedding that entangles the temporal and state information (right). The general AE representations also do not have a preferred scale nor an alignment with the coordinate origin relative to the GD-VAE methods. The $g$-projection approach is discussed in more detail in Section 3.
5.4 Constrained Mechanical Systems: Learning with General Manifold Latent Spaces

We learn from observations representations for constrained mechanical systems using manifold latent spaces of general shape $M$. The arm mechanism has configurations $x = (x_1, x_2) \in \mathbb{R}^4$ (left). For rigid segments, the motions are constrained to be on a manifold (torus) $M \subset \mathbb{R}^4$. For extendable segments, we can also consider more exotic constraints, such as requiring $x_1, x_2$ to be on a klein bottle in $\mathbb{R}^4$ (middle). Results of our GD-VAE methods for learned representations for motions under these constraints are shown. GD-VAE learns the segment length constraint and two nearly decoupled coordinates for the torus data set that mimic the roles of angles (right-top). GD-VAE learns for the klein bottle data set two segment motions to generate configurations (right-bottom).

We consider physical systems with constrained mechanics, such as the arm mechanism for reaching for objects in Figure 8. The observations are taken to be the two locations $x_1, x_2 \in \mathbb{R}^2$ giving $x = (x_1, x_2) \in \mathbb{R}^4$. When the segments are constrained these configurations lie on a manifold embedded in $\mathbb{R}^4$. When the segments are constrained to be rigid this results in a torus. We can also allow the segments to extend and consider more exotic constraints such as the two points $x_1, x_2$ must be on a klein bottle in $\mathbb{R}^4$. Related situations arise in other areas of imaging and mechanics, such as in pose estimation and in studies of visual perception \cite{65; 13; 72}.

For the arm mechanics, we can use this prior knowledge to construct a torus latent space represented by the product space of two circles $S^1 \times S^1$. To obtain a learnable class of manifold encoders, we use the family of maps $E_\theta = \Lambda(\hat{E}_\theta(x))$, with $\hat{E}_\theta(x)$ into $\mathbb{R}^4$ and $\Lambda(w) = \Lambda(w_1, w_2, w_3, w_4) = (z_1, z_2, z_3, z_4) = z$, where $(z_1, z_2) = (w_1, w_2)/\|(w_1, w_2)\|$, $(z_3, z_4) = (w_3, w_4)/\|(w_3, w_4)\|$, see Section 3. For the case of klein bottle constraints, we use our point-cloud representation of the non-orientable manifold with the parameterized embedding in $\mathbb{R}^4$

\[
\begin{align*}
  z_1 &= (a + b \cos(u_2)) \cos(u_1) \\
  z_2 &= (a + b \cos(u_2)) \sin(u_1) \\
  z_3 &= b \sin(u_2) \cos \left( \frac{u_1}{2} \right) \\
  z_4 &= b \sin(u_2) \sin \left( \frac{u_1}{2} \right),
\end{align*}
\]
with \( u_1, u_2 \in [0, 2\pi] \). The \( \Lambda(w) \) is taken to be the map to the nearest point of the manifold \( \mathcal{M} \), which we compute numerically along with the needed gradients for backpropagation as discussed in Section 3.

Our GD-VAE methods are trained with encoder and decoder DNN’s having layers of sizes (in)-100-500-100-(out) with Leaky-ReLU activations with \( s = 1e-6 \) with results reported in Figure 8. These results demonstrate how we can learn smooth representations for constrained mechanical systems for both orientable and non-orientable manifold latent spaces. For both the torus and klein bottle latent spaces, we see smooth representations are learned for generating the configurations. For the latent torus manifold, the representation is comparable to the two angular degrees of freedom. This shows our GD-VAE approaches can be used as unsupervised learning methods for constrained mechanical systems to learn representations in manifold latent spaces with general topology and orientability.

5.5 Reaction-Diffusion PDEs in 2D: Learning Latent Space Representations for Spatially Distributed Dynamics

![Figure 9: Brusselator Dynamics: Concentration Fields \( u \) and \( v \).](image)

We show the dynamics of the concentration fields \( u(x, t) \) and \( v(x, t) \) of the reaction-diffusion PDEs in equation 17 with initial conditions for \( \alpha = 0.0 \) in equation 18. Shown is the evolution of the concentration fields \( u, v \) from left to right starting at time \( t = 60\Delta t \) to time \( t = 140\Delta t \). After a transient the concentration field dynamics approach a limit cycle having approximately periodic dynamics.

We show how our GD-VAEs can be used to learn features for representing the states and dynamic evolution of spatially extended reaction-diffusion systems, see Figure 9. Consider the system

\[
\frac{\partial u}{\partial t} = D_1 \Delta u + f(u, v), \quad \frac{\partial v}{\partial t} = D_2 \Delta v + g(u, v).
\]  

(17)

The \( u = u(x, t) \) and \( v(x, t) \) give the spatially distributed concentration of each chemical species at time \( t \) with \( x \in \mathbb{R}^2 \). We consider the case with periodic boundary conditions with \( x \in [0, L] \times [0, L] \). We develop learning methods for investigating the Brusselator system [68; 67], which is known to have regimes exhibiting limit cycles [79; 36; 37]. This indicates after an initial transient the orbit associated with the dynamics will approach localizing near a subset of states having a geometric structure topologically similar to a circle. We show how GD-VAE can utilize this topological information to construct latent spaces for encoding states of the system. The Brusselator [68; 67] has
Lopez and Atzberger

reactions with $f(u, v) = a - (1+b)u + vu^2$ and $g(u, v) = bu - vu^2$. We take throughout the diffusivity $D_1 = 1, D_2 = 0.1$ and reaction rates $a = 1, b = 3$.

We consider initial conditions for the concentration fields $u$ and $v$ parameterized by $\alpha \in [0, 1]$ given by

\begin{align*}
u(x, y) &= \alpha \sin(2\pi x/L_x) + (1 - \alpha) \cos^3(2\pi x/L_x) \\
v(x, y) &= \alpha \sin(2\pi y/L_y) + (1 - \alpha) \cos^3(2\pi y/L_y). \quad (19)
\end{align*}

We remark that while the initial conditions are given by a linear combination of functions the resulting solutions do not satisfy this relation given the non-linear dynamics of the reaction-diffusion system. The chemical fields evolve under periodic boundary conditions within a box length $L_x = L_y = 64$. We use second order Central-Differences to estimate the spatial derivatives and Backward-Euler method for the temporal evolution [41; 12] (py-pde python package [88] is used for numerical calculations). For the discretization, we space the grid points with $\Delta x = 1.0$ and use a time-step of $\Delta t = 10^{-3}$.

![Figure 10: GD-VAE Convolutional Neural Network Architecture.](image)

For spatially extended fields $u, v$, we use architectures based on Convolutional Neural Networks (CNNs) consisting of the following processing steps. For the encoder, we extract features from the spatial fields using Convolutional Neural Networks (CNNs) which are fed into dense Multilayer Perceptrons (MLPs). The encoder serves to map the spatial fields $u, v$ to codes $z$ in a manifold latent space having prescribed topology using our methods discussed in Section 3. For the decoder, we use MLPs that feed into Transpose Convolutional Neural Networks (T-CNNs) that serve to reconstruct from $z$ the spatial fields $u, v$. We learn the encoders and decoders using our GD-VAE training framework discussed in Section 2.

We show how our GD-VAE methods can be used for solutions to learn a parsimonious disentangled representations in a manifold latent space. The dynamics consists of a brief transient followed by close approach to a limit cycle. For the dynamics after the transient, we encode the temporal and state information using a cylindrical topology. While a preliminary application of Principle Component Analysis (PCA) in a sufficiently large number of dimensions can be used to identify the transient and the period of the limit cycle, it does not provide a well-organized or parsimonious representation of the dynamics. Using from PCA the top three singular vectors, we show the entangled embedding in Figure 11.

We use GD-VAE methods to learn a more organized encoding for representing the states and system dynamics. For this purpose, we develop encoders based on Convolutional Neural Networks (CNNs) and Multilayer Perceptrons (MLPs) to map from spatial concentration fields $u, v$ to latent codes $z$. The encoder serves to map the spatial fields $u, v$ to codes $z$ in a manifold latent space having prescribed topology using our methods discussed in Section 3. We develop decoders based on
Figure 11: Embeddings for Brusselator Reaction-Diffusion Dynamics. A Principle Component Analysis (PCA) embedding is compared to GD-VAE embeddings for solutions of the PDEs in equation 17. While the PCA embedding provides some information on the transient and limit cycle behaviors, the latent space representation entangles the temporal and state information, (left). The GD-VAE allows for learning a more organized and parsimonious embedding for the dynamics where state information is captured by \((z_1, z_2)\) and time by \(z_3\), (right).

using MLPs that control Transpose Convolutional Neural Networks (T-CNNs) to map from latent codes \(z\) to construct spatial concentration fields \(u, v\), see Figure 10.

We specify a manifold latent space having the geometry of a cylinder \(M = B \times \mathbb{R}\) with \(B = S^1\) and axis in the \(z_3\)-direction. We prescribe on this latent space the dynamics having the rotational evolution

\[
\mathbf{z}(t + \Delta t) = \begin{bmatrix} \cos(\omega \Delta t) & -\sin(\omega \Delta t) & 0 \\ \sin(\omega \Delta t) & \cos(\omega \Delta t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{z}(t). \tag{20}
\]

This is expressed in terms of an embedding in \(\mathbb{R}^3\). The \(\omega\) gives the angular velocity. This serves to regularize how the encoding of the reaction-diffusion system is organized in latent space.

The GD-VAE then is tasked with learning the encoding and decoding mappings for the reaction-diffusion concentration fields \(u, v\) to representations that are well-organized for capturing and predicting the reaction-diffusion system states and dynamics. This organization allows for making multi-step predictions from the latent space. Throughout our empirical studies, we use the angular velocity \(\omega = 0.282\) determined from the preliminary PCA analysis. In principle, such parameters also can be learned as part of the training of the GD-VAE. We use an architecture with CNNs having four layers each of which has (in-channels, out-channels, kernel-size, stride, padding) with parameters as follows respectively \((2,10,3,3,1), (10,20,3,3,1),(20,40,2,2,1),(40,100,5,1,0)\). Each layer was followed by a ReLU activation, except for the last layer which is fed into the MLPs. The MLPs have an architecture with layer sizes 100-(latent-space-embed) where latent-space-embed=3. The \(g\)-projection is then applied to the output of the MLPs to map to the manifold latent space \(M\) using our methods discussed in Section 3. For the decoder, we use MLPs with layer sizes (latent-space-embed)-100. We use T-CNNs having four layers each of which has (in-channels, out-channels, kernel-size, stride, padding) with parameters \((100, 40, 5, 1, 0), (40, 20, 2, 2, 1), (20, 10, 3, 3, 1), (10, 2, 3, 3, 1)\). All layers have a bias and ReLU activations except for the last layer.
We use our GD-VAE methods for learning representations and for predicting the evolution dynamics of the reaction-diffusion system. A few predictions of GD-VAE in comparison with numerical solutions of the PDE for the concentration fields are shown in Figure 12. We characterize the accuracy of the predictions and reconstructions using $L_1$-relative errors. We report results of our methods for multi-step predictions in Table 4.

Figure 12: Brusselator: GD-VAE Prediction of Concentration Fields $u$ and $v$. We show initial concentrations of two chemical species with spatial distribution given by the fields $u$ and $v$ (left). We consider how these evolve after undergoing reaction and diffusion processes according to the PDEs in equation 17. We show the GD-VAE predictions for the spatial fields $u,v$ with those of the numerical solutions of the PDEs (right). We show the cases for $\alpha = 0.0$ and $\alpha = 0.5$ starting at $t = 15s$ and predicting the concentration fields $u,v$ at time $t = 17s$. The $L^1$-relative errors of predictions are given in Table 4.

<table>
<thead>
<tr>
<th>Method</th>
<th>Dim</th>
<th>0.00s</th>
<th>2.00s</th>
<th>4.00s</th>
<th>6.00s</th>
<th>8.00s</th>
</tr>
</thead>
<tbody>
<tr>
<td>GD-VAE</td>
<td>3</td>
<td>3.16e-02 ± 5.4e-03</td>
<td>2.87e-02 ± 3.8e-03</td>
<td>3.63e-02 ± 7.0e-03</td>
<td>3.77e-02 ± 6.8e-03</td>
<td>3.56e-02 ± 8.3e-03</td>
</tr>
<tr>
<td>VAE-3D</td>
<td>3</td>
<td>2.61e-02 ± 2.9e-03</td>
<td>2.36e-02 ± 2.4e-03</td>
<td>2.08e-01 ± 1.8e-01</td>
<td>2.61e-01 ± 2.3e-01</td>
<td>2.16e-01 ± 1.9e-01</td>
</tr>
<tr>
<td>AE (g-projection)</td>
<td>3</td>
<td>2.96e-02 ± 3.5e-03</td>
<td>2.75e-02 ± 2.8e-03</td>
<td>3.91e-02 ± 9.7e-03</td>
<td>4.25e-02 ± 1.2e-02</td>
<td>2.99e-02 ± 2.5e-03</td>
</tr>
<tr>
<td>AE (no projection)</td>
<td>3</td>
<td>2.36e-02 ± 1.8e-03</td>
<td>2.19e-02 ± 1.5e-03</td>
<td>3.49e-01 ± 3.2e-01</td>
<td>1.88e-01 ± 1.6e-01</td>
<td>1.55e-01 ± 1.3e-01</td>
</tr>
</tbody>
</table>

Table 4: Brusselator: $L^1$-Prediction Accuracy. The reconstruction $L_1$-relative errors and standard error over 5 training trials. We compare the GD-VAE approach with other methods for learning latent space representations for the reaction-diffusion dynamics. We consider the relative error of predictions when receiving the concentration field at time $t_1$ and making a prediction of the concentration field at time $t_1 + \tau$. We investigate the multi-step predictions up to time-scale $\tau = 8.00s$. This involves a composition of the single-step predictions over multiple steps for dynamics that has gone entirely through at least one period of the limit cycle. We see the geometric structure in the latent space greatly enhances the stability and resulting accuracy of predictions.

We find that GD-VAEs are able to learn representations in the manifold latent spaces capable of making good predictions of the dynamics. The manifold latent space is particularly advantageous for multi-step predictions by helping to constrain the encodings promoting more robust learning over a lower dimensional space and smaller subset of points. In this geometric setting, learning only needs to be performed over the subset of points on the manifold enhancing the statistical power of the training data. This also simplifies the type of encoder and decoder response functions that need to be learned relative to learning in a higher dimensional space $\mathbb{R}^n$. In addition, during multi-
step predictions we see the geometric constraints also enhance stability. This arises from the latent space dynamics always being confined within the manifold. As a result, it is less likely for a one-step update to map to a code in parts of the latent space that are far from instances already explored and characterized during the training. The lower dimension of the geometric latent space also provides similar benefits with encoding points more concentrated providing more statistical power in learning a model for the local responses of the underlying reaction-diffusion system. The more organized representations are also more amenable to interpretation. These results indicate some of the ways our GD-VAE approaches can be used to leverage qualitative information about the dynamics both to enhance learning and to gain insights into system dynamics. The methods provide practical ways to learn parsimonious representations capable of providing quantitatively accurate predictions for high-dimensional dynamical systems having latent low-dimensional structures. The GD-VAEs can be used to obtain representations for learning tasks for diverse types of dynamical systems.

6. Software Package

We have developed a python package for the introduced GD-VAE methods. This includes implementations of our Geometric Projections (g-projection) methods with custom backpropagation approaches for modular training, Variational Autoencoder (VAE) training methods, and related examples. The package can be quick installed using `pip install gd-vae-pytorch`. For additional information on ways to download, install, and examples see [http://atzberger.org/](http://atzberger.org/).

7. Conclusions

We introduce GD-VAEs for learning representations of nonlinear dynamics on latent spaces having general geometry and topology. By accommodating general topologies, our methods facilitate obtaining more parsimonious representations of nonlinear dynamical systems and enhancing training of encoders and decoders by restricting responses to smaller subsets of latent codes and on lower dimensional spaces. We characterized how our methods perform in practice for learning representations for the nonlinear dynamics of PDEs arising in physics, including Burgers’ equations and reaction-diffusion systems, and for constrained mechanical systems. Our introduced methods for incorporating geometric and topological information present opportunities to simplify model representations, aid in interpretability, and enhance robustness of predictions in data-driven learning methods. The GD-VAEs can be used to obtain representations for use with diverse types of learning tasks involving dynamics.

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Appendix

A. Backpropogation of Encoders for Non-Euclidean Latent Spaces given by General Manifolds

We develop methods for using backpropogation to learn encoder maps from $\mathbb{R}^d$ to general manifolds $\mathcal{M}$. We perform learning using the family of manifold encoder maps of the form $E_\theta = \Lambda(\tilde{E}_\theta(x))$. This allows for use of latent spaces having general topologies and geometries. We represent the manifold as an embedding $\mathcal{M} \subset \mathbb{R}^{2m}$ and computationally use point-cloud representations along with local gradient information, see Figure 13 and 3. To allow for $E_\theta$ to be learnable, we develop approaches for incorporating our maps into general backpropogation frameworks.

Figure 13: Learnable Mappings to Manifold Surfaces. We develop methods based on point cloud representations embedded in $\mathbb{R}^n$ for learning latent manifold representations having general geometries and topologies.

For a manifold $\mathcal{M}$ of dimension $m$, we can represent it by an embedding within $\mathbb{R}^{2m}$, as supported by the Whitney Embedding Theorem [86]. We let $z = \Lambda(w)$ be a mapping $w \in \mathbb{R}^{2m}$ to points on the manifold $z \in \mathcal{M}$. This allows for learning within the family of manifold encoders $w = \tilde{E}_\theta(x)$ any function from $\mathbb{R}^d$ to $\mathbb{R}^{2m}$. This facilitates use of deep neural networks and other function classes. In practice, we shall take $z = \Lambda(w)$ to map to the nearest location on the manifold. We can express this as the optimization problem

$$z^* = \arg\min_{z \in \mathcal{M}} \frac{1}{2} \|w - z\|^2_2.$$

We can always express a smooth manifold using local coordinate charts $\sigma^k(u)$, for example, by using a local Monge-Gauge quadratic fit to the point cloud [33]. We can express $z^* = \sigma^k(u^*)$ for some chart $k^*$. In terms of the coordinate charts $\{U_k\}$ and local parameterizations $\{\sigma^k(u)\}$ we can express this as

$$u^*, k^* = \arg\min_{k, u \in U_k} \frac{1}{2} \|w - \sigma^k(u)\|^2_2,$$

where $\Phi_k(u, w) = \frac{1}{2} \|w - \sigma^k(u)\|^2_2$. The $w$ is the input and $u^*, k^*$ is the solution sought. For smooth parameterizations, the optimal solution satisfies

$$G = \nabla u^* \Phi_{k^*}(u^*, w) = 0.$$

During learning we need gradients $\nabla_y \Lambda(w) = \nabla_y z$ when $w$ is varied characterizing variations of points on the manifold $z = \Lambda(w)$. We derive these expressions by considering variations $w = w(\gamma)$ for a scalar parameter $\gamma$. We can obtain the needed gradients by determining the variations of $u^* = u^*(\gamma)$. We can express these gradients using the Implicit Function Theorem as

$$0 = \frac{d}{d\gamma} G(u^*(\gamma), w(\gamma)) = \nabla_u G \frac{du^*}{d\gamma} + \nabla_w G \frac{dw}{d\gamma}.$$
This implies
\[ \frac{du^*}{d\gamma} = - [\nabla_u G]^{-1} \nabla_w G \frac{dw}{d\gamma}. \]
As long as we can evaluate at \( u \) these local gradients \( \nabla_u G, \nabla_w G, dw/d\gamma \), we only need to determine computationally the solution \( u^* \). For the backpropogation framework, we use these to assemble the needed gradients for our manifold encoder maps \( \mathcal{E}_\theta = \Lambda(\tilde{\mathcal{E}}_\theta(x)) \) as follows.

We first find numerically the closest point in the manifold \( z^* \in \mathcal{M} \) and represent it as \( z^* = \sigma(u^*) = \sigma^k(u^*) \) for some chart \( k \). In this chart, the gradients can be expressed as
\[ G = \nabla_u \Phi(u, w) = -(w - \sigma(u))^T \nabla_u \sigma(u). \]
We take here a column vector convention with \( \nabla_u \sigma(u) = [\sigma_{u_1}, \ldots, \sigma_{u_k}] \). We next compute
\[ \nabla_u G = \nabla_{uu} \Phi = \nabla_u \sigma^T \nabla_u \sigma - (w - \sigma(u))^T \nabla_{uu} \sigma(u) \]
and
\[ \nabla_w G = \nabla_{w,u} \Phi = -I \nabla_u \sigma(u). \]
For implementation it is useful to express this in more detail component-wise as
\[ [G]_i = - \sum_k (w_k - \sigma_k(u)) \partial_{u_i} \sigma_k(u), \]
with
\[ [\nabla_u G]_{i,j} = [\nabla_{uu} \Phi]_{i,j} = \sum_k \partial_{u_i} \sigma_k(u) \partial_{u_j} \sigma_k(u) \]
\[ = - \sum_k (w_k - \sigma_k(u)) \partial_{u_i} \sigma_k(u) \]
[\nabla_w G]_{i,j} = [\nabla_{w,u} \Phi]_{i,j} = - \sum_k \partial_{w_i} w_k \partial_{u_j} \sigma_k(u) = - \partial_{u_i} \sigma_j(u). \]
The final gradient is given by
\[ \frac{d\Lambda(w)}{d\gamma} = \frac{dz^*}{d\gamma} = \nabla_u \sigma \frac{du^*}{d\gamma} = - \nabla_u \sigma [\nabla_u G]^{-1} \nabla_w G \frac{dw}{d\gamma}. \]

In summary, once we determine the point \( z^* = \Lambda(w) \) we need only evaluate the above expressions to obtain the needed gradient for learning via backpropogation
\[ \nabla_{\theta} \mathcal{E}_\theta(x) = \nabla_w \Lambda(w) \nabla_{\theta} \tilde{\mathcal{E}}_\theta(x), \ w = \tilde{\mathcal{E}}_\theta(x). \]
The \( \nabla_{\theta} \Lambda \) is determined by \( d\Lambda(w)/d\gamma \) using \( \gamma = w_1, \ldots, w_n \). In practice, the \( \tilde{\mathcal{E}}_\theta(x) \) is represented by a deep neural network from \( \mathbb{R}^d \) to \( \mathbb{R}^{2m} \). In this way, we can learn general encoder mappings \( \mathcal{E}_\theta(x) \) from \( x \in \mathbb{R}^d \) to general manifolds \( \mathcal{M} \).

**B. Role of Latent Space Geometry in Training**

In practice, the encodings that organize the data in a manner convenient for representing the dynamic evolution can be challenging to learn in data-driven methods. In cases where the embedding space is too low dimensional or incompatible with the intrinsic topology this is further compounded. To illustrate some of the issues that arise, we consider a dynamical system with a periodic parameterization using as our example the Burgers’ equation in equation 12 discussed in Section 5.1.
Lopez and Atzberger

Figure 14: **Latent Space with Incompatible Geometry** We show a typical behavior encountered during training for dynamical systems having periodic parameterization $\alpha \in [0, 1]$ when using a latent space representation based on $\mathbb{R}^2$. While for a finite duration of time $t \in [0, T]$ there are in principle embeddings for such dynamics into $\mathbb{R}^2$ as in equation 16, these can be difficult to find during training, and further not possible to disentangle time and state configurations into separate dimensions. From the periodicity of inputs and the continuity of the encoder a typical behavior instead is for most states to be mapped to a patch and for the mapping to incur a penalty by rapidly loop back over only a small subset of inputs, here for responses for $\alpha \sim 0.85$. The continuous function approximates what would have been a discontinuity (right). This rapid variation of the encoder results in states being mapped to a scattered set of codes which provide a poor representation for the dynamics. This is exhibited by the long spirals that show segments of the dynamics over time and how the states are mapped to the latent codes for $\alpha \sim 0.85$, (left). Our GD-VAEs provide approaches to avoid this issue by allowing for general manifold latent spaces which maintain low dimension while accommodating such topology.

For this data set, it is natural to consider representing the system state and the dynamics using the geometry of a cylinder. In principle, it is possible to obtain a representation of the dynamics if restricted over a finite duration of time using only a two dimensional euclidean space $\mathbb{R}^2$ as in equation 16. This is similar to a projection of a cone-shaped manifold in three dimensions projected to the two dimensional plane.

However, in practice this can be difficult to work with since there is an inherent tension during training between the periodicity and the natural ways the typical encoders will operate. This arises from the continuity of the encoder model class used in training that maps from the dynamical system solutions to the $\mathbb{R}^2$ latent space. We find that training proceeds initially by mapping a collection of states to a smooth patch of codes in the latent space. As a consequence of continuity, the encoder for the states associated with system responses for $\alpha$ and $\alpha' \equiv \alpha \pm 1.0 \mod 1.0$ need to map to similar codes. This results in an encoder that exhibits for a subset of states an extreme sensitivity to inputs that results in rapidly varying the code to loop back to accommodate the periodicity, see $\alpha = \lim \uparrow 0.85$ and $\alpha' = \lim \downarrow 0.85$ in Figure 14. Again, the issue arises since the states must map continuously to the latent space for all encoders encountered during training. Unless the map happens already to form a circle or other periodic structure in $\mathbb{R}^2$ there will be a subset of points that arise with rapid variation. This results in a subset of points having a poor encoding with states mapped to codes scattered in the latent space. This provides a poor basis for representing and predicting the system dynamics. When encoding over time we see disorganized fragments, connected again by transitions having rapid variations. We show this typical behavior observed during such training in Figure 14. This indicates the importance of choosing a latent space with either a sufficiently large
number of dimensions or which has a topology that is compatible with the data set. Our GD-VAE approach allows for keeping the latent space dimensionality small by allowing for accommodating general topologies in the latent space using our methods in Section 3.

C. Identifying Latent Geometric Structures using VAE Covariance $\sigma_e^2$

The VAE training can be performed with a learnable covariable structure $\sigma_e^2 = [\sigma_{e,ij}]$, see equation 1. In VAE the $KL$-divergence regularization term is typically used to drive the encoding points to match a standard Gaussian distribution or other prior. The coding-point distribution arises from a combination of the scattering of the coding of points from the encoded training data points and from the Gaussian noise controlled by the variance $\sigma_e^2$, see equation 1. Consider covariance $\sigma_e^2 = \text{diag}(\sigma^2_{e,i})$, where $\sigma^2_{e,i} = \sigma^2_{e,ii}$. If components of $\sigma^2_{e,i}$ are held fixed to be a small value then the coding-point distribution can only arise from scattering of the encoding points. However, if $\sigma^2_{e,i}$ is learnable, then the encoder can map to a narrow distribution in some of the coding points with the Gaussian noise with variance $\sigma^2_{e,i}$ compensating to satisfy the $KL$-regularization term.

![Figure 15: Extracting Latent Geometric Structure using Learned VAE Variances.](image)

We use the $\sigma_{e,i}$ and $\mu_{e,i}$ of VAEs to further extract geometric information from data and to perform reductions similar to [55]. By looking at mini-batches of data, we can compute two statistics (i) the mean of the variance (mov) $q_{i,\text{mov}}$ and (ii) the variance of the mean (vom) $q_{i,\text{vom}}$, see equations 21 and 22. We show results for Burgers’ Equation with embedding in an unconstrained 10 dimensional space. We see the most relevant feature dimensions are the ones with $q_{i,\text{vom}}$ large and $q_{i,\text{mov}}$ small (left). This yields a reduced three dimensional embedding with a good representation for the state information using $z_1, z_9$ coordinates (middle). In contrast, using two arbitrary dimensions such as coordinates $z_1, z_2$ yields a poor representation which is entangled and mapped to small scales (right). This provides further ways to extract geometric information from the data and representations of latent structures.

We have found in practice in some cases this can be used to identify geometric structure within the data. We perform the embedding into a higher dimensional space than is needed, we find smaller values of $\sigma_e$ correlate with encoding to a lower dimensional manifold structure, similar to [55]. We show how this can be used in practice to find reduced embeddings. By looking at mini-batches of data with $N_b$ samples, we can compute two statistics (i) the mean of the variance (mov)

$$q_{i,\text{mov}} = \frac{1}{N_b} \sum_{\ell=1}^{N_b} \sigma^2_{e,i}(x^{(\ell)}),$$

(21)
and (ii) the variance of the mean (vom)

$$q_{i,vom} = \frac{1}{N_b} \sum_{\ell=1}^{N_b} \mu_{e,i}^2(x^{(\ell)}) - \bar{\mu}_{e,i}^2,$$

(22)

where \(\bar{\mu}_{e,i} = \frac{1}{N_b} \sum_{\ell=1}^{N_b} \mu_{e,i}(x^{(\ell)})\).

When allowing the variance to be trainable, we can compute \(q_{i,vom}\) and \(q_{i,mov}\) to help identify important feature directions in latent space. We show results for training the Burgers’ Equation embedding the cylinder topology case of Section 5.3 in Figure 15. We see important feature components of the encoded data have the characteristic signature of having a large \(q_{i,vom}\) and a small \(q_{i,mov}\). If we reduce the encoding to just these components, we can obtain a lower dimensional embedding for the data. We find this emebedding have a cylindrical geometric structure providing a good latent space representation of the system state information. In contrast, if we were to choose any two arbitrary latent code dimensions, such as \(z_1, z_2\) we obtain a poor entangled representation, see Figure 15. This allows for using information from the \(\sigma_{e,i}\) and \(\mu_{e,i}\) to further extract geometric structure from data. This can be used to formulate latent manifold spaces for use with our GD-VAE approaches.
References


