Variational Autoencoders for Learning Nonlinear Dynamics of Physical Systems

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Abstract

We develop **data-driven methods for incorporating physical information** for priors to learn parsimonious representations of **nonlinear systems** arising from parameterized PDEs and mechanics.

Our approach is based on **Variational Autoencoders (VAEs)** for learning from observations **nonlinear state space models**. We incorporate geometric and topological priors through general **manifold latent space representations.**

We give results for **low dimensional representations** for the **nonlinear Burgers equation** and **constrained mechanical systems.**

Acknowledgements

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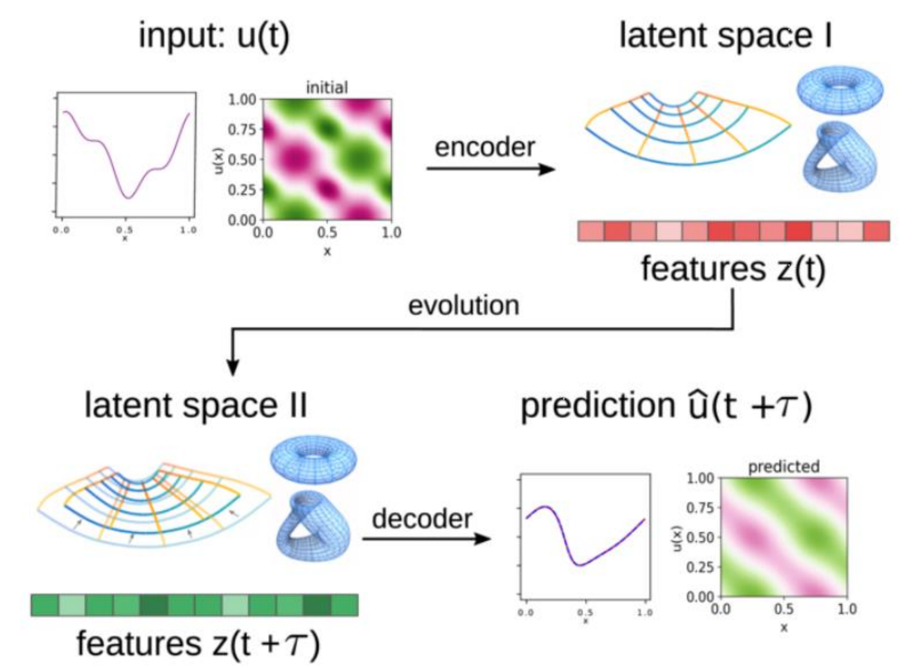
Latent Variable Representations Geometric / Topologic Priors



Manifold Latent Spaces

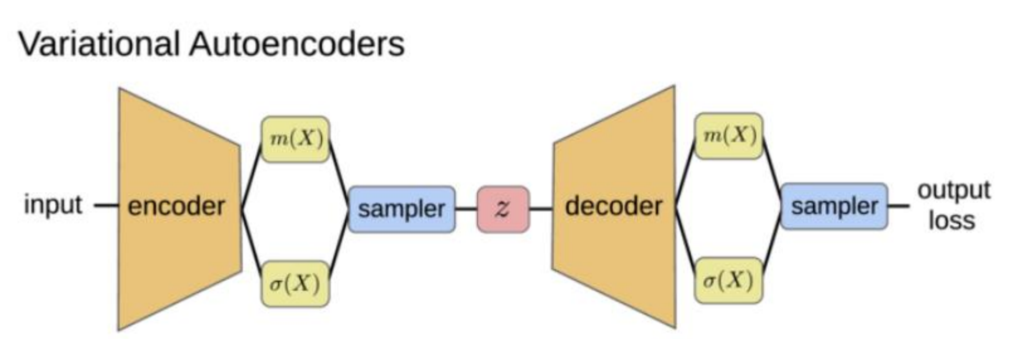
$$\mathbf{z} \in \mathcal{M} \subset \mathbb{R}^{2m} \quad \mathbf{z} = \mathcal{E}_\phi(\mathbf{x}) = \Lambda(\tilde{\mathcal{E}}_\phi(\mathbf{x})) = \Lambda(\mathbf{w}), \quad \mathbf{w} = \tilde{\mathcal{E}}_\phi(\mathbf{x})$$

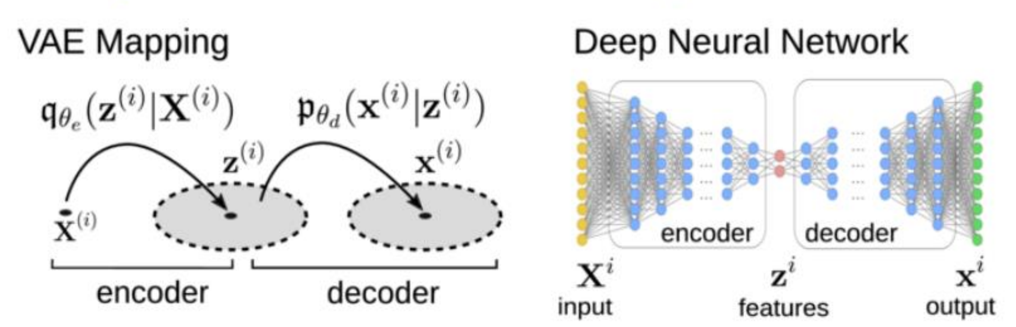
(learnable encoder map class)

Point-cloud representation of manifold: (implicit map to manifold)

$$z^* = \arg\min_{z \in \mathcal{M}} \frac{1}{2}\|w - z\|_2^2 \longrightarrow \Lambda(\mathbf{w}) := \mathbf{z}^*$$ (see paper for details)

Variational Autoencoders for Dynamics





Variational Autoencoder (VAE) Framework:

Probabilistic Autoencoders (PAE): map X → x, encoder θ_e , decoder θ_d
Motivation: Maximum Likelihood Estimation (MLE) with ELBO approximation.

$$\theta^* = \arg\min_{\theta_e,\theta_d} -\mathcal{L}^B(\theta_e,\theta_d,\theta_\ell;\mathbf{X}^{(i)},\mathbf{x}^{(i)}),$$ (loss function)

$$\mathcal{L}^B = \mathcal{L}_{RE} + \mathcal{L}_{KL} + \mathcal{L}_{RR},$$ (ELBO + regularizations)

$$\mathcal{L}_{RE} = E_{\mathfrak{q}_{\theta_e}(\mathbf{z}|\mathbf{X}^{(i)})}\left[\log \mathfrak{p}_{\theta_d}(\mathbf{x}^{(i)}|\mathbf{z}')\right]$$ (reconstruction error)

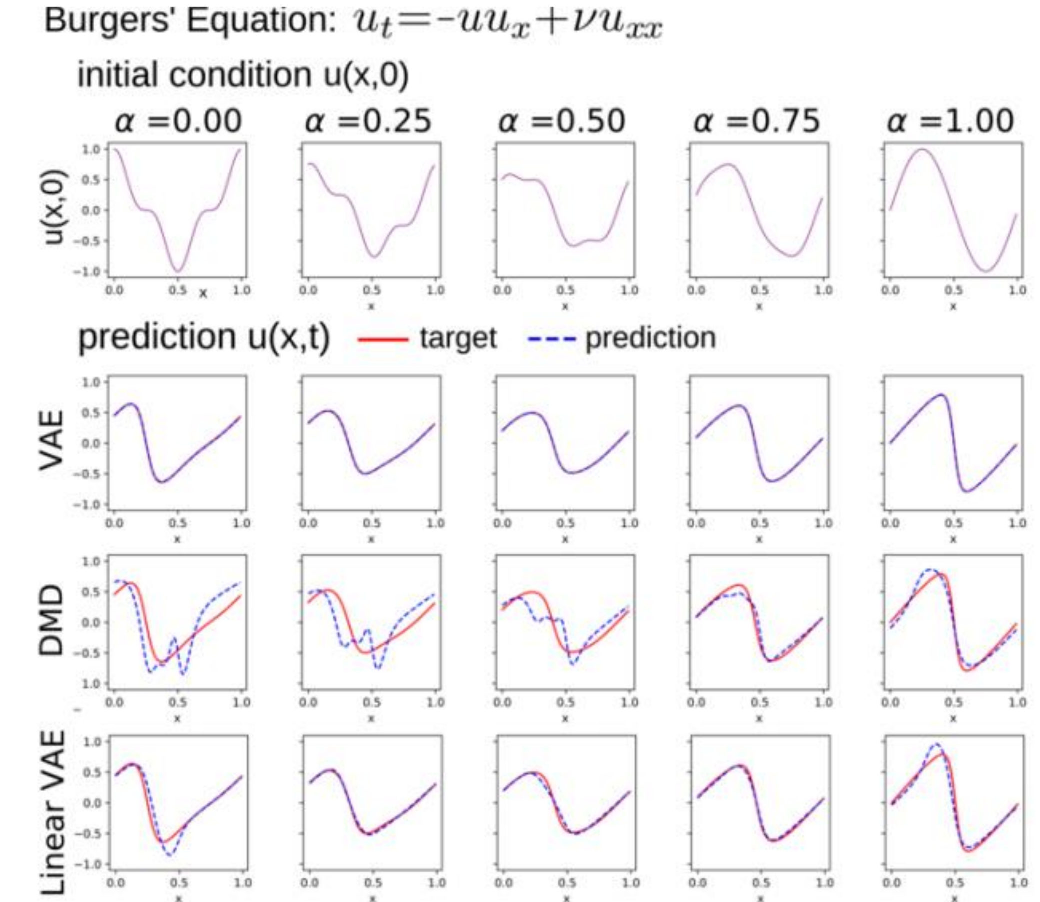
$$\mathcal{L}_{KL} = -\beta\mathcal{D}_{KL}\left(\mathfrak{q}_{\theta_e}(\mathbf{z}|\mathbf{X}^{(i)}) \,\|\, \tilde{\mathfrak{p}}_{\theta_d}(\mathbf{z})\right)$$ (KL-divergence w/ prior)

$$\mathcal{L}_{RR} = \gamma E_{\mathfrak{q}_{\theta_e}(\mathbf{z}'|\mathbf{x}^{(i)})}\left[\log \mathfrak{p}_{\theta_d}(\mathbf{x}^{(i)}|\mathbf{z}')\right].$$ (reconstruction regularization)

Deep Neural Networks (DNNs) trained within Stochastic Gradient Descent (SGD) in PyTorch.

Nonlinear Dimension Reduction (Burgers PDE)

Burgers' Equation: $u_t = -uu_x + \nu u_{xx}$



$$\mathcal{U}_1 = \{u \,|\, u(x,t;\alpha) = \alpha\sin(2\pi x) + (1-\alpha)\cos^3(2\pi x)\}$$

Cole-Hopf (CH) Transformation $\phi_t = \nu\phi_{xx}$

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

$$u(x,t) = \mathcal{CH}^{-1}[\phi] = -2\nu\frac{\partial}{\partial x}\ln\phi(x,t).$$

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

$$\hat{\phi}_k(0) = \mathcal{F}_k[\phi(x,0)]$$ (Fourier Transform)

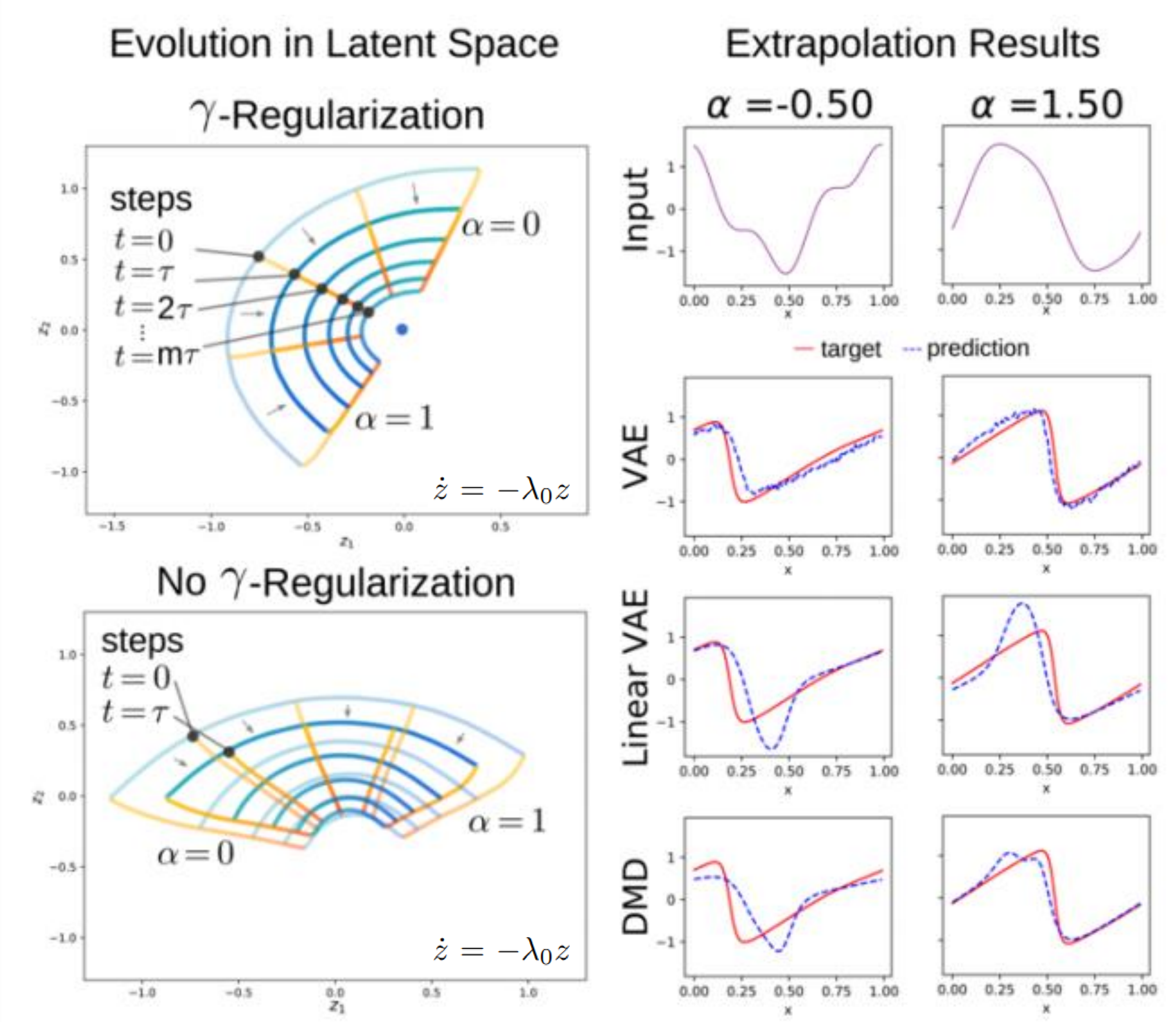
CH Reduction

$$u(x,t) = \mathcal{CH}^{-1}[\phi(x,t)]$$

$$\hat{\phi}(0) = \mathcal{F}[\mathcal{CH}[u(x,0)]]$$

truncate the series for $\phi(x,t)$

Nonlinear Dynamics Representations



Reconstruction Accuracy:

Method	Dim	0.25s	0.50s	0.75s	1.00s
VAE Nonlinear	2	**4.44e-3**	**5.54e-3**	**6.30e-3**	**7.26e-3**
VAE Linear	2	9.79e-2	1.21e-1	1.17e-1	1.23e-1
DMD	3	2.21e-1	1.79e-1	1.56e-1	1.49e-1
POD	3	3.24e-1	4.28e-1	4.87e-1	5.41e-1
Cole-Hopf-2	2	5.18e-1	4.17e-1	3.40e-1	1.33e-1
Cole-Hopf-4	4	5.78e-1	6.33e-2	9.14e-3	1.58e-3
Cole-Hopf-6	6	1.48e-1	2.55e-3	9.25e-5	7.47e-6

γ	0.00s	0.25s	0.50s	0.75s	1.00s
0.00	1.600e-01	6.906e-03	1.715e-01	3.566e-01	5.551e-01
0.50	1.383e-02	1.209e-02	1.013e-02	9.756e-03	1.070e-02
2.00	1.337e-02	1.303e-02	9.202e-03	8.878e-03	1.118e-02

β	0.00s	0.25s	0.50s	0.75s	1.00s
0.00	1.292e-02	1.173e-02	1.073e-02	1.062e-02	1.114e-02
0.50	1.190e-02	1.126e-02	1.072e-02	1.153e-02	1.274e-02
1.00	1.289e-02	1.193e-02	7.903e-03	7.883e-03	9.705e-03
4.00	1.836e-02	1.677e-02	8.987e-03	8.395e-03	8.894e-03

Methods:
Dynamic Mode Decomposition (DMD)
Principle Orthogonal Decomposition (POD)
Variational Autoencoder (VAE)

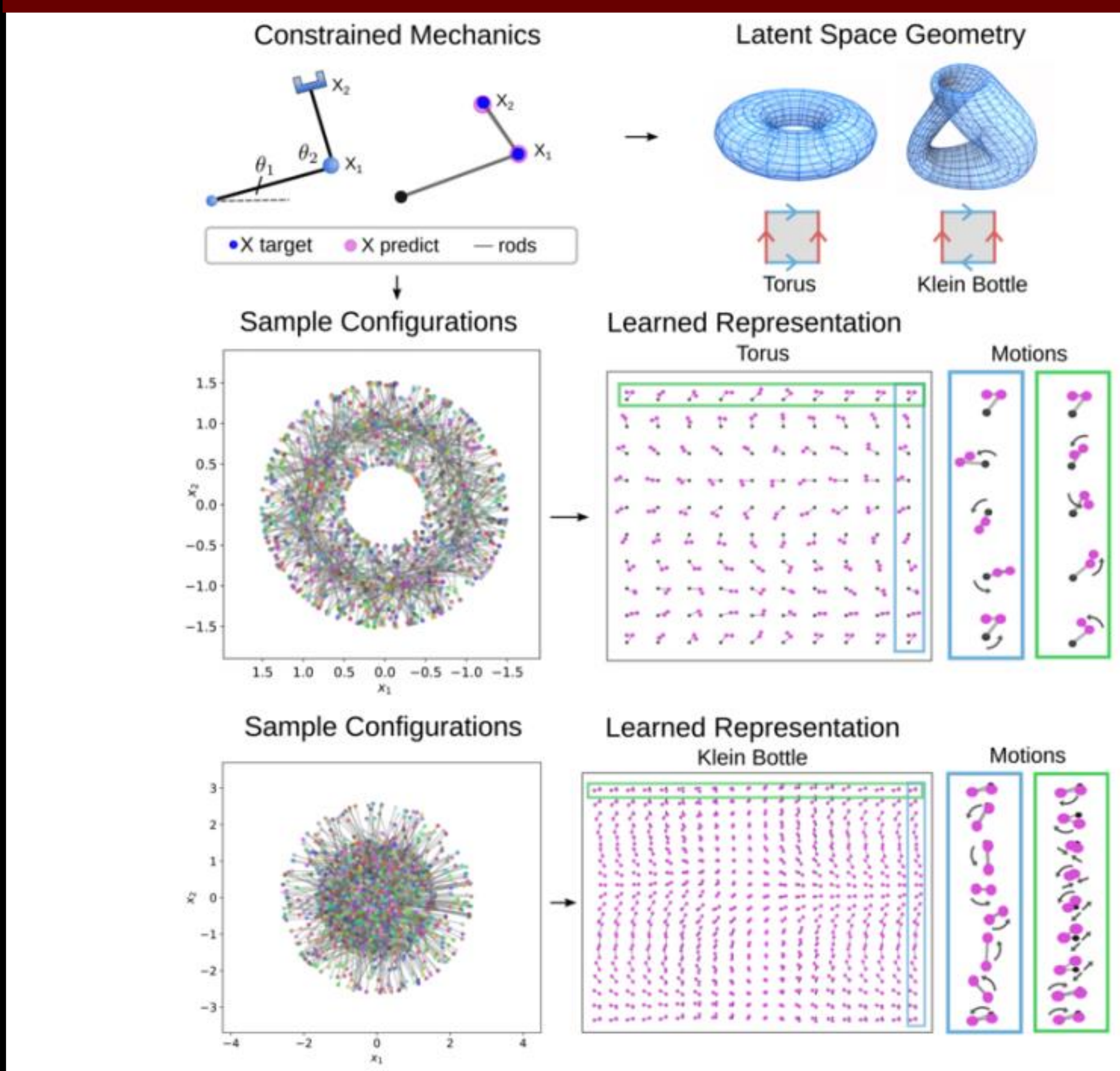
Nonlinear approximation vs linear in reconstruction accuracy.

Learned Representations: VAE gives semi-circle arcs in latent space.

Extrapolation: VAE prediction capabilities in parameters and in time.

γ - **Reconstruction Regularization:** helps align for multi-step predictions.

Constrained Mechanical Systems



Reconstruction Accuracy:

Torus	epoch			
method	1000	2000	3000	final
VAE 2-Manifold	**6.6087e-02**	**6.6564e-02**	**6.6465e-02**	**6.6015e-02**
VAE $\mathbb{R}^2$	1.6540e-01	1.2931e-01	9.9903e-02	8.0648e-02
VAE $\mathbb{R}^4$	8.0006e-02	7.6302e-02	7.5875e-02	7.5626e-02
VAE $\mathbb{R}^{10}$	8.3411e-02	8.4569e-02	8.4673e-02	8.4143e-02
with noise σ	0.01	0.05	0.1	0.5
VAE 2-Manifold	**6.7099e-02**	**8.0608e-02**	**1.1198e-01**	**4.1988e-01**
VAE $\mathbb{R}^2$	8.5879e-02	9.7220e-02	1.2867e-01	4.5063e-01
VAE $\mathbb{R}^4$	7.6347e-02	9.0536e-02	1.2649e-01	4.9187e-01
VAE $\mathbb{R}^{10}$	8.4780e-02	1.0094e-01	1.3946e-01	5.2050e-01
Klein Bottle	epoch			
method	1000	2000	3000	final
VAE 2-Manifold	**5.7734e-02**	**5.7559e-02**	**5.7469e-02**	**5.7435e-02**
VAE $\mathbb{R}^2$	1.1802e-01	9.0728e-02	8.0578e-02	7.1026e-02
VAE $\mathbb{R}^4$	6.9057e-02	6.5593e-02	6.4047e-02	6.3771e-02
VAE $\mathbb{R}^{10}$	6.8899e-02	6.9802e-02	7.0953e-02	6.8871e-02
with noise σ	0.01	0.05	0.1	0.5
VAE 2-Manifold	**5.9816e-02**	**6.9934e-02**	**9.6493e-02**	**4.0121e-01**
VAE $\mathbb{R}^2$	1.0120e-01	1.0932e-01	1.3154e-01	4.8837e-01
VAE $\mathbb{R}^4$	6.3885e-02	7.6096e-02	1.0354e-01	4.5769e-01
VAE $\mathbb{R}^{10}$	7.4587e-02	8.8233e-02	1.2082e-01	4.8182e-01

Learned Representations: Constrained mechanical systems (torus / klein bottle examples).

Manifold Latent Space (prior): Enhances training efficiency, robustness to noise, accuracy.

Papers

Variational Autoencoders for Learning Nonlinear Dynamics of Physical Systems, R. Lopez, and P. J. Atzberger, http://arxiv.org/abs/2012.03448

Importance of the Mathematical Foundations of Machine Learning Methods for Scientific and Engineering Applications, P. J. Atzberger, http://arxiv.org/abs/1808.02213

More Information:
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