Imperial College London

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Disentangled Generative Models for Robust Prediction of System Dynamics

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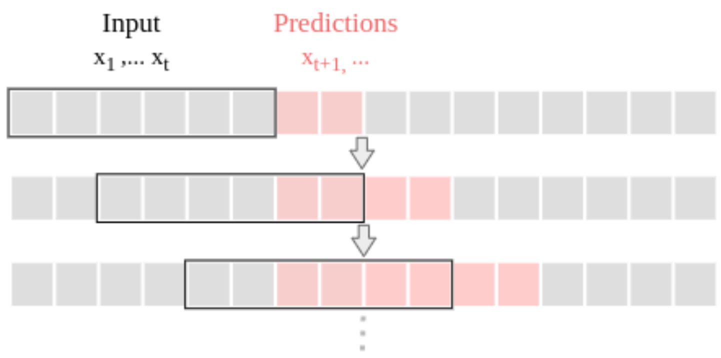
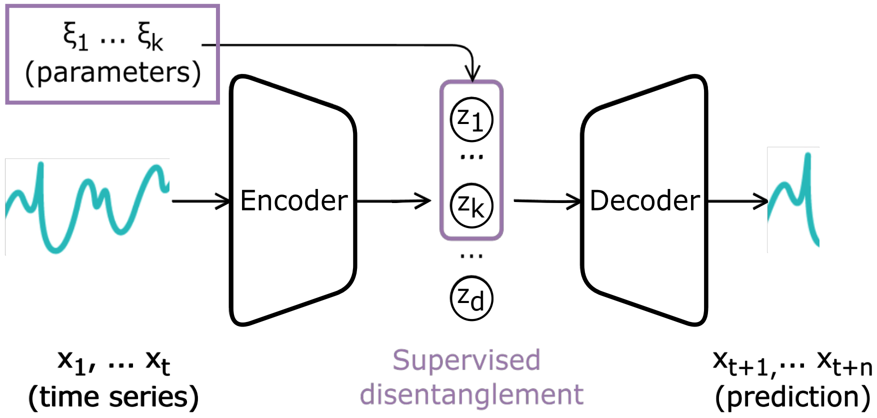
Dynamical systems modelling

- Differential Equations (ODEs/PDEs)
- Data-driven prediction using neural networks
  - Long-term accuracy
  - OOD Robustness



Disentangling parameters from dynamics



Deterministic system with observation noise

$$P(x_{>t};x_{<t},\xi)\sim f(x_{<t},\xi)+\epsilon$$

$$P(x_{>t};z)\sim Dec(z)+\epsilon \quad \Rightarrow \quad P(x_{>t};z_{<t},z_{\xi})\sim Dec(z_{<t},z_{\xi})+\epsilon$$

VAE

SD-VAE

Training SD-VAE

Supervised disentanglement as constrained optimization

$$z_i = \xi_i$$

Under KKT conditions constraint becomes a regularizer

$$\mathcal{L}_{\boldsymbol{\xi}}(\mathbf{z}_{1:N_\xi}, \boldsymbol{\xi}) = \|\mathbf{z}_{1:N_\xi} - \boldsymbol{\xi}\|_2^2$$

SD-VAE objective: Combination of beta-VAE ELBO and regularizer

$$\mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{Q_\phi(\mathbf{z}|\mathbf{x})}\left[\log P_\theta(\mathbf{x} \mid \mathbf{z}) + \delta \mathcal{L}_{\boldsymbol{\xi}}(\mathbf{z}_{1:N_{\boldsymbol{\xi}}}, \boldsymbol{\xi})\right] - \beta D_{KL}\left(Q_\phi(\mathbf{z} \mid \mathbf{x}) || P(\mathbf{z})\right)\right]$$

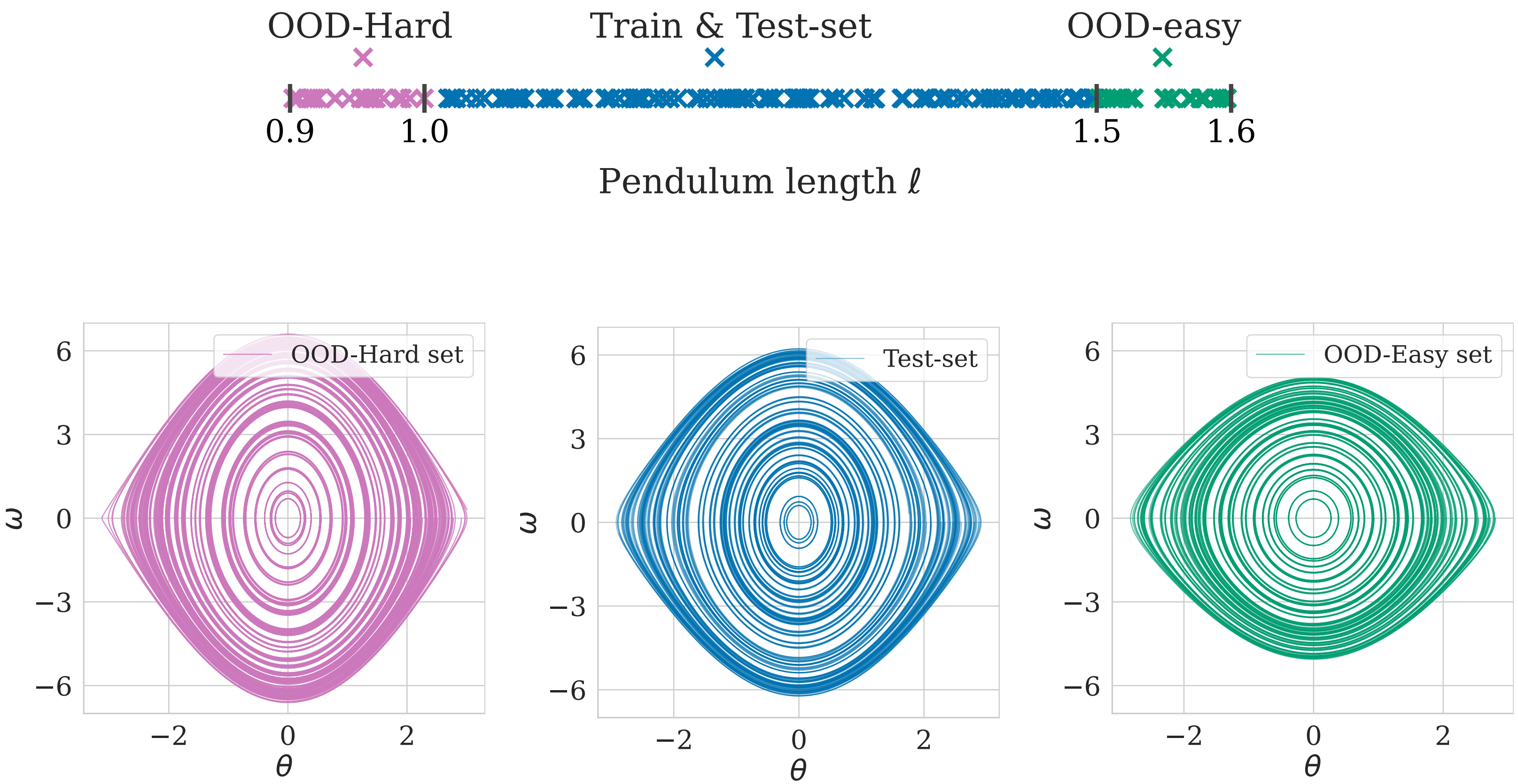
Datasets

Dynamical Systems

- Pendulum
- Lotka-Volterra
- 3-body system

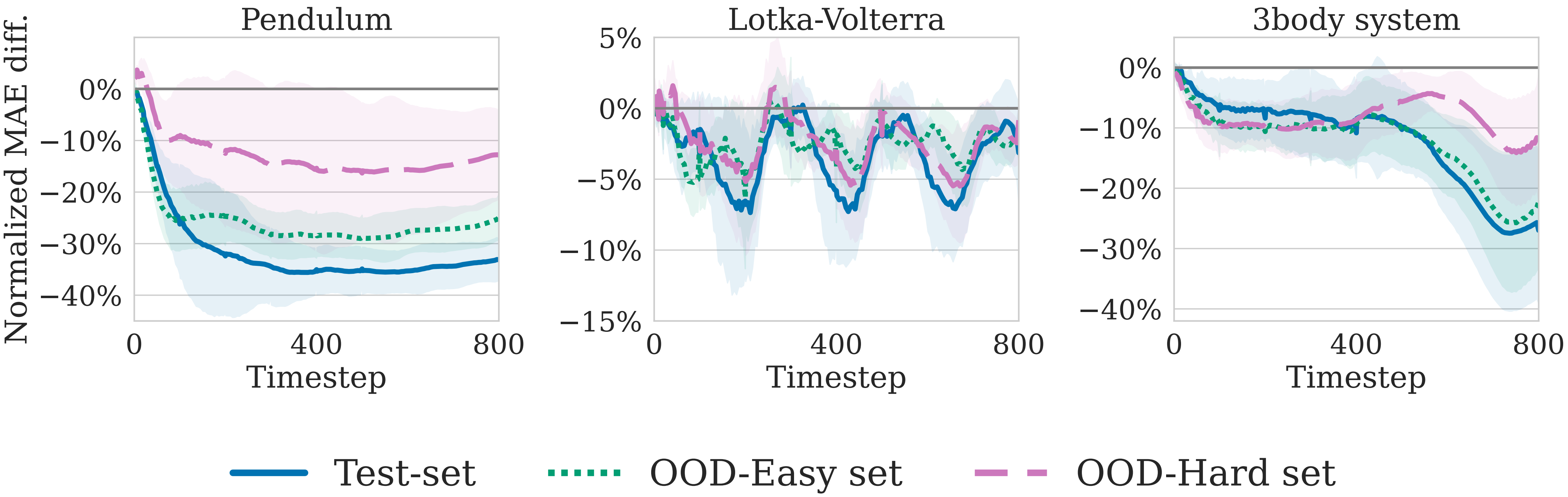
Datasets

- Train / Test set
- Two OOD Test sets
  - OOD-Easy
  - OOD-Hard



Prediction error

Error reduction of SD-VAE vs VAE

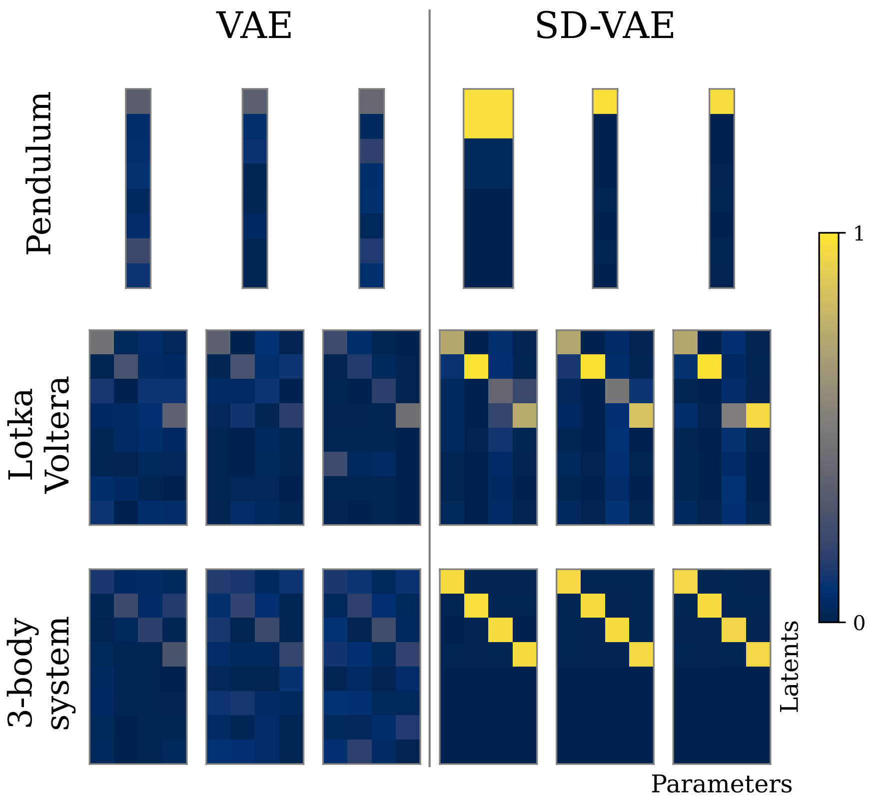


Disentangled representations

Disentanglement Metrics

	Pendulum		Lotka-Volterra		3 body system	
	VAE	SD-VAE	VAE	SD-VAE	VAE	SD-VAE
Disentanglement	-	-	0.27	**0.53**	0.20	**0.90**
Completeness	0.17	**0.90**	0.20	**0.57**	0.13	**0.90**
Informativeness	0.94	**0.99**	**1.00**	**1.00**	**1.00**	**1.00**
SAP	0.03	**0.87**	0.04	**0.21**	0.01	**0.67**
MIG	0.01	**0.17**	0.00	**0.03**	0.00	**0.08**

Predictive power of latents



Thank you!