THE UNIVERSITY OF CHICAGO
DATA SCIENCE INSTITUTE

APS March Meeting

AI in Science
A program of SCHMIDT FUTURES

Training Machine Learning Emulators

to Preserve Invariant Measures of Chaotic Attractors



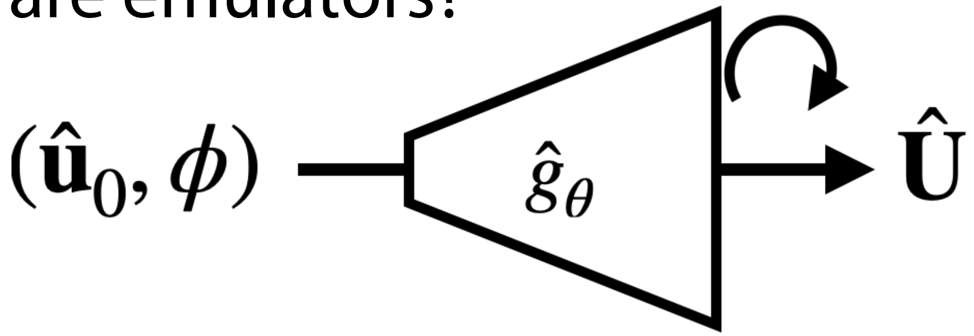

Ruoxi Jiang*, ***Peter Y. Lu****, Elena Orlova, Rebecca Willett

APS March Meeting 2024

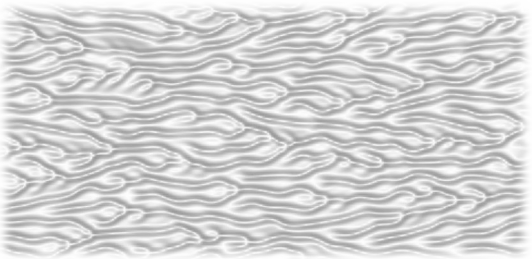
March 7, 2024

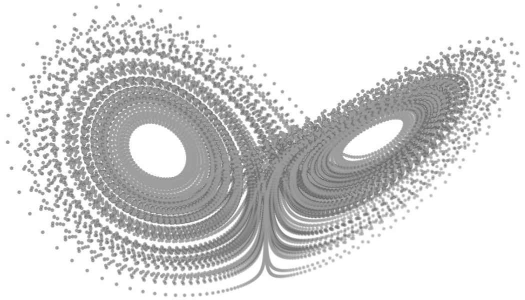
NeurIPS 2023

Introduction: What are emulators?

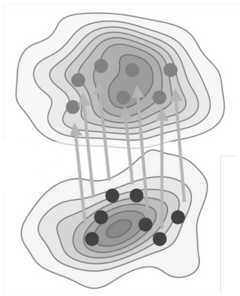


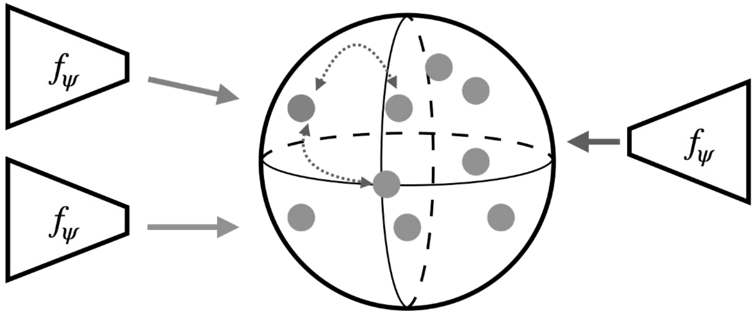
Problem: Why is it difficult to train emulators for chaos?





New Methods: How do we train emulators to capture chaos?





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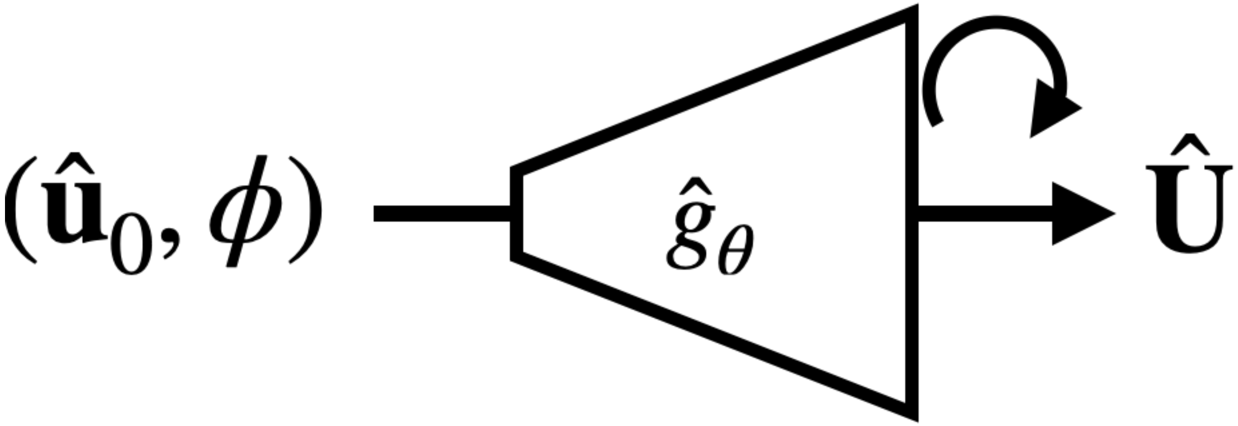

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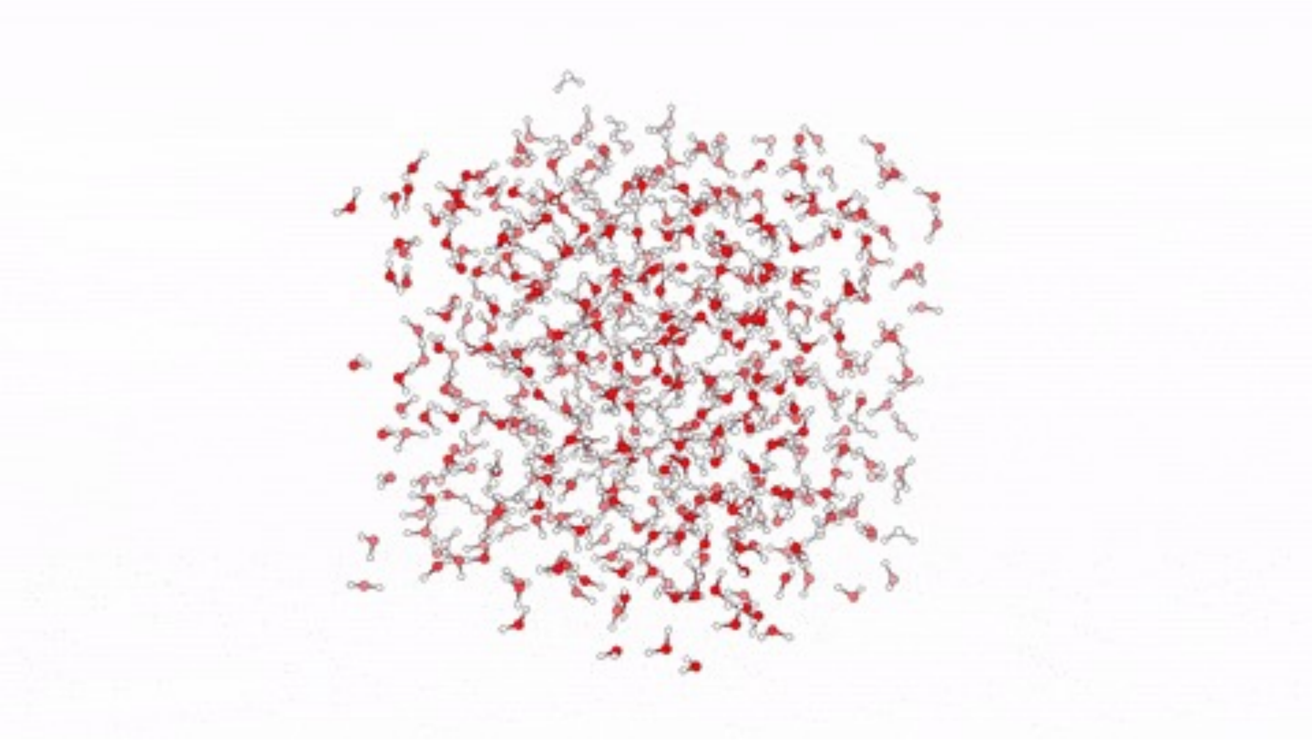
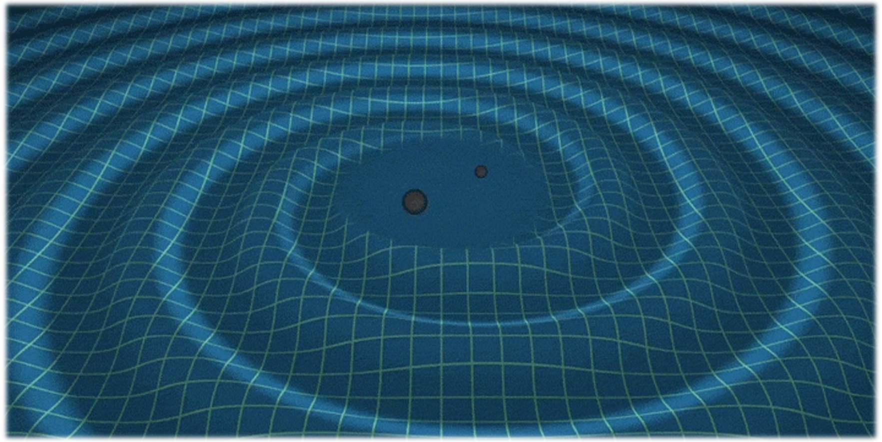
Dynamical Systems

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = G(\mathbf{u}, \phi)$$





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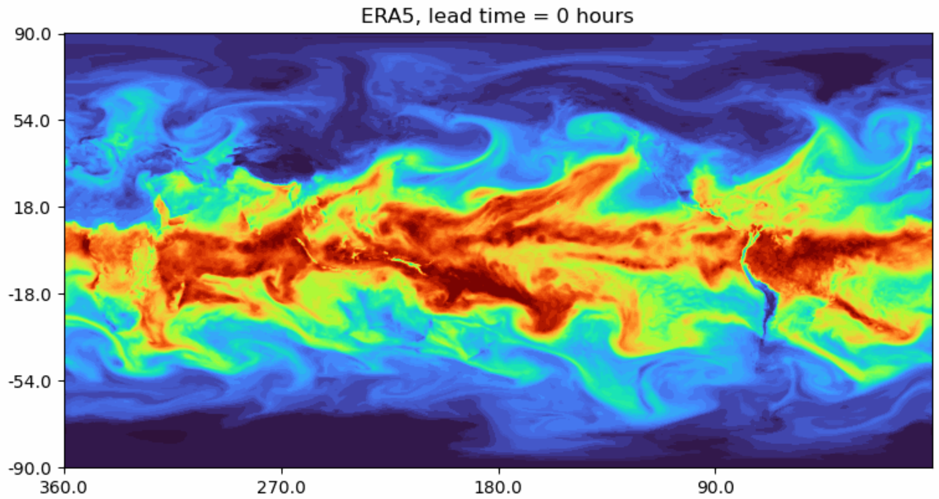

https://github.com/NVlabs/FourCastNet

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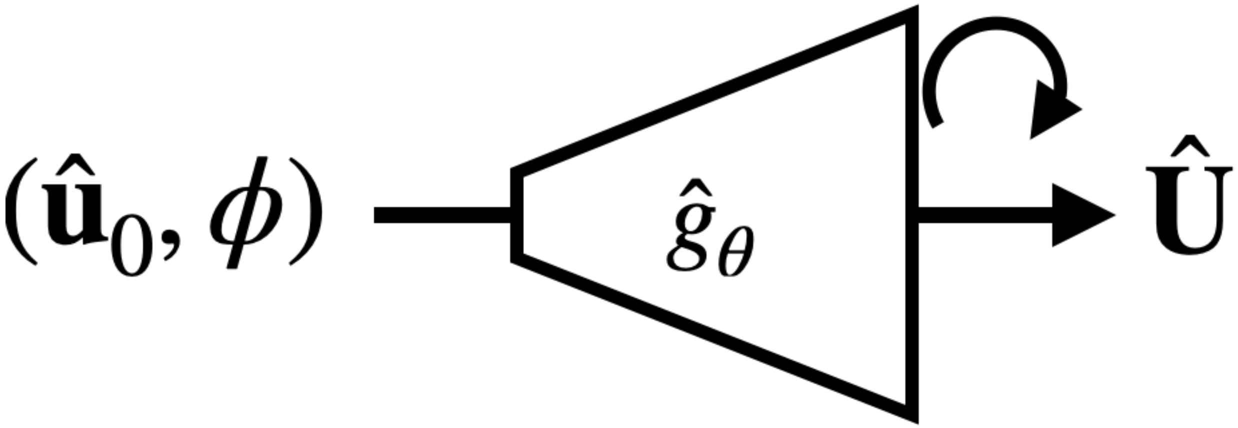
Machine Learning Emulators

Emulators are machine learning models trained to **simulate physical systems**.

Emulators often consist of a **physics-informed architecture** trained on **observed or simulated data**.



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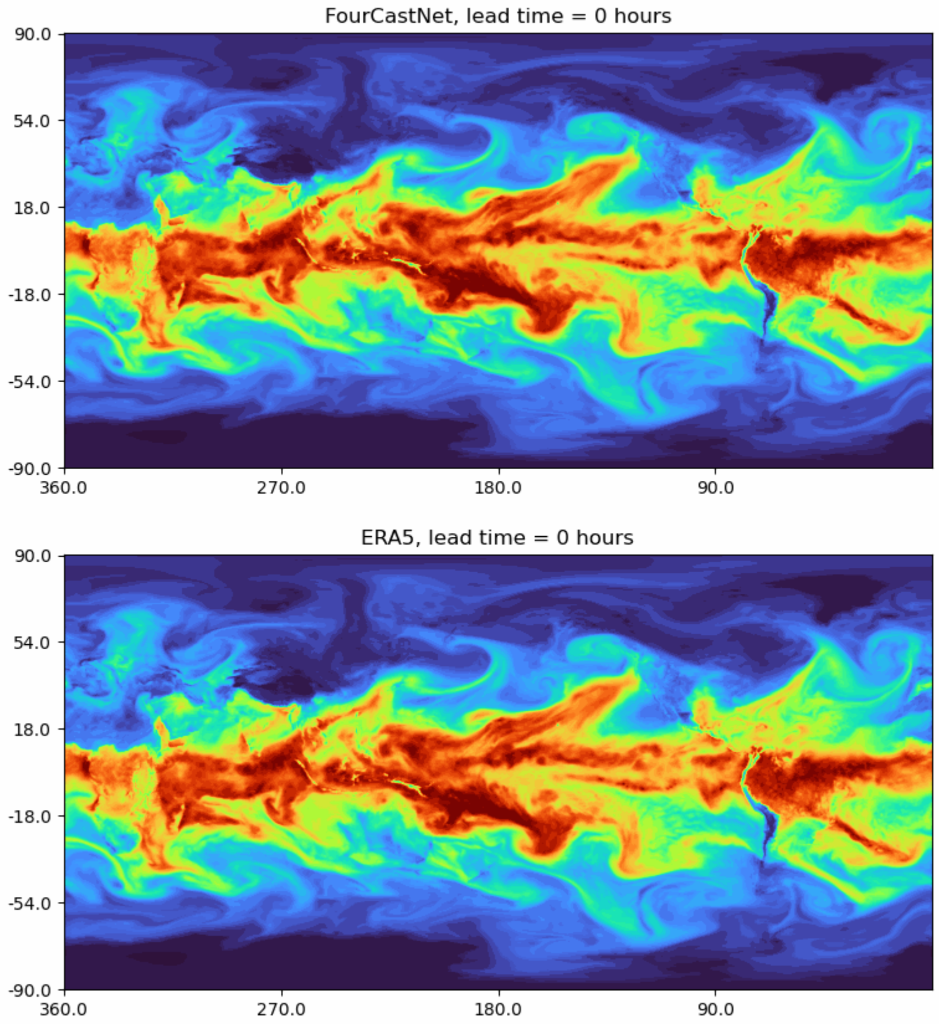

Pathak et al. arXiv:2202.11214

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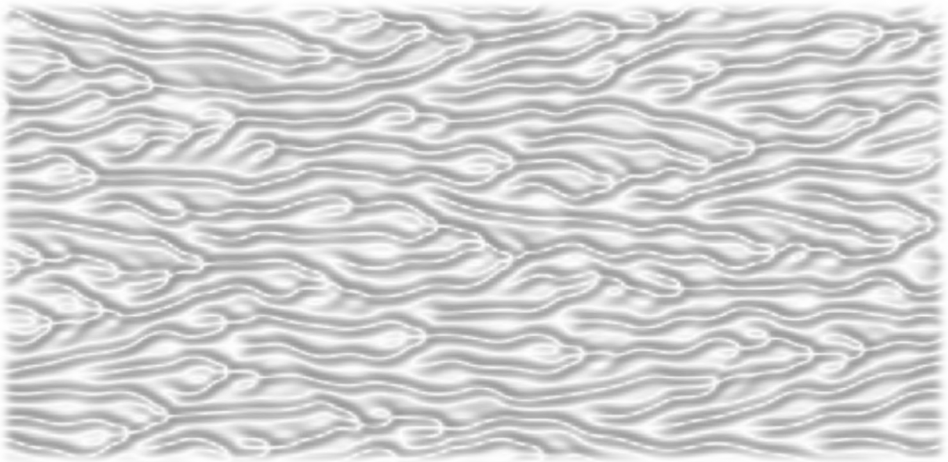
Machine Learning Emulators

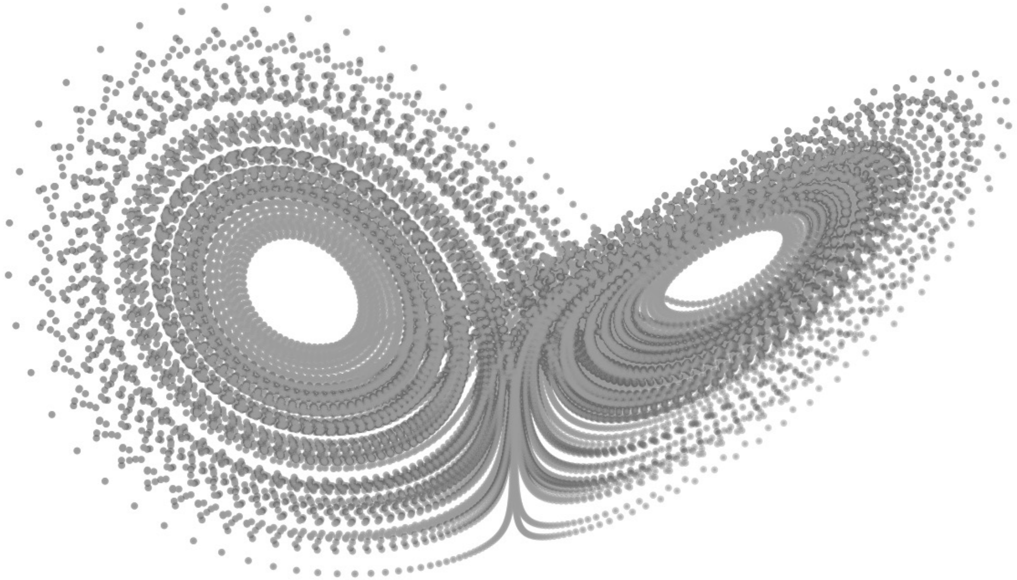
Accelerate expensive numerical simulations:
fast predictions, fast sampling for uncertainty quantification

Improve existing physical models using data:
more accurate predictions, better scientific understanding

Solve inverse problems (simulation-based inference):
parameter estimation, state reconstruction

Why is it difficult to train emulators for chaos?





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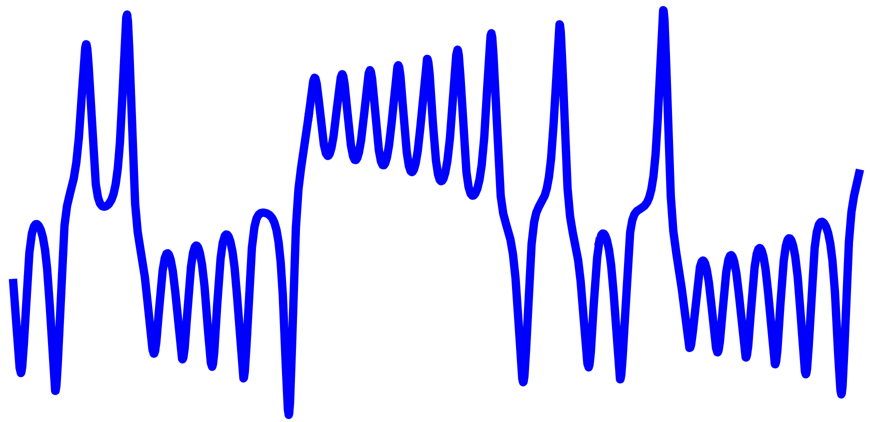
Chaotic Dynamics

A key feature of chaos is **sensitivity to initial conditions**.

Simple example: Lorenz-63



Time ⟶

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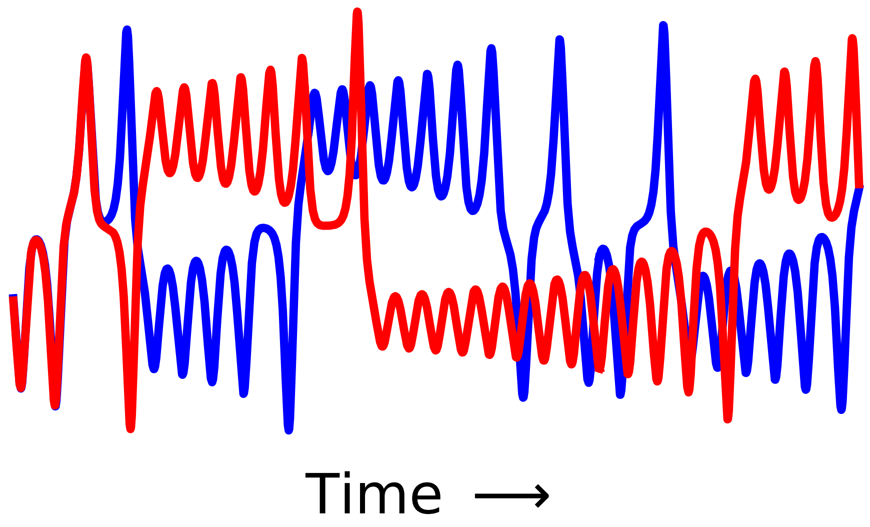

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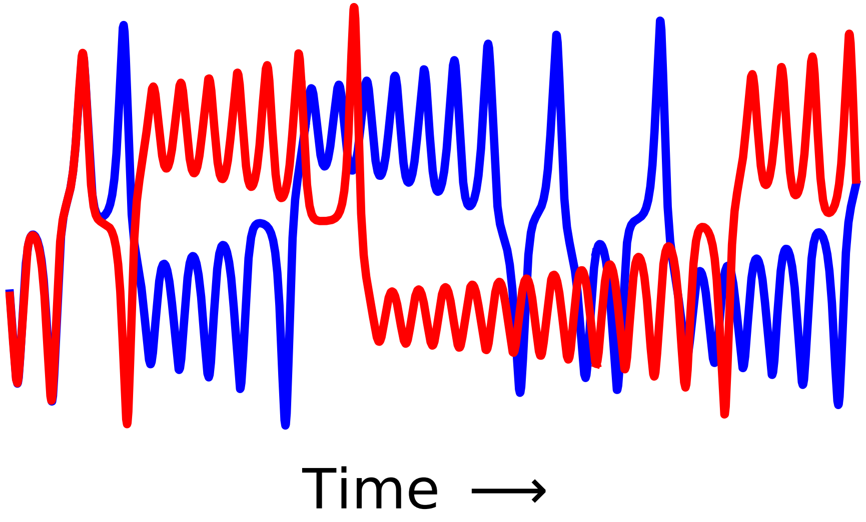

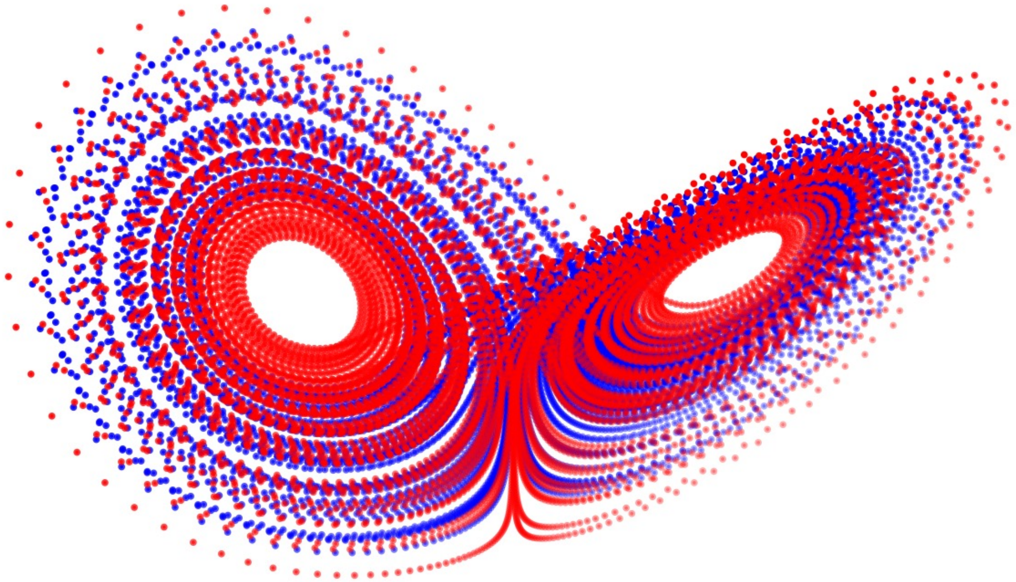

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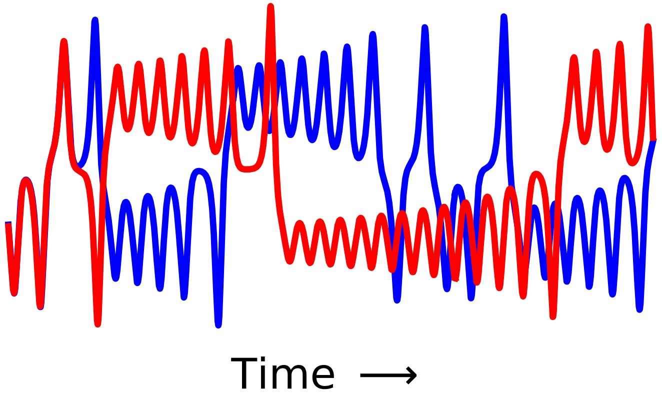
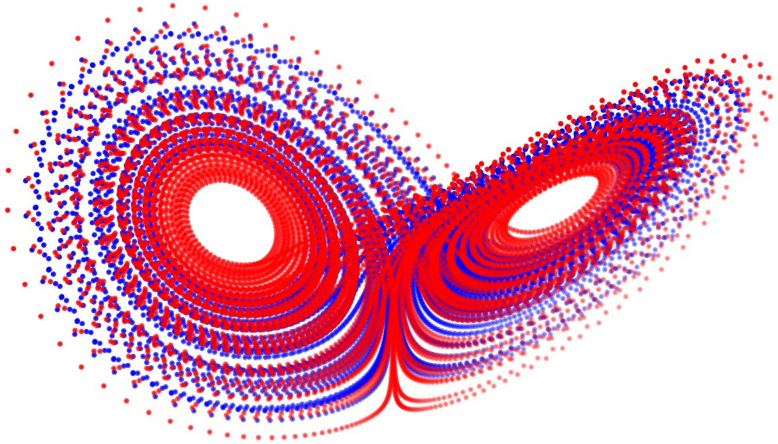
Chaotic Dynamics & Noise

Training emulators for chaotic dynamics is hard because **chaos is fundamentally unpredictable**.

Noise makes this worse due to **sensitivity to initial conditions**.

→ Instead of short-term forecasts, focus on **long-term statistics**.





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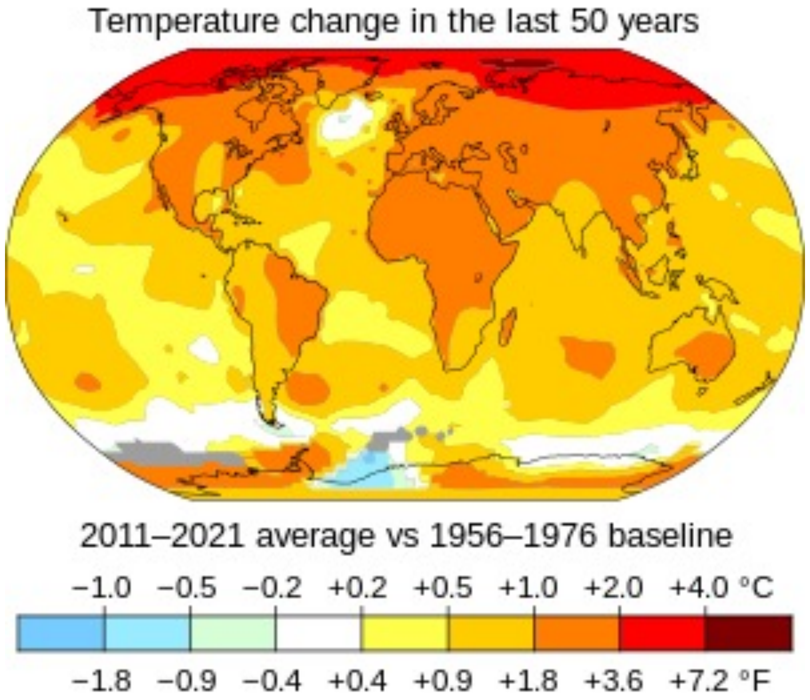
Modeling Chaos: Forecasting vs. Statistics

Example:
Weather vs. Climate

https://www.bbc.com/news/world-us-canada-47071683



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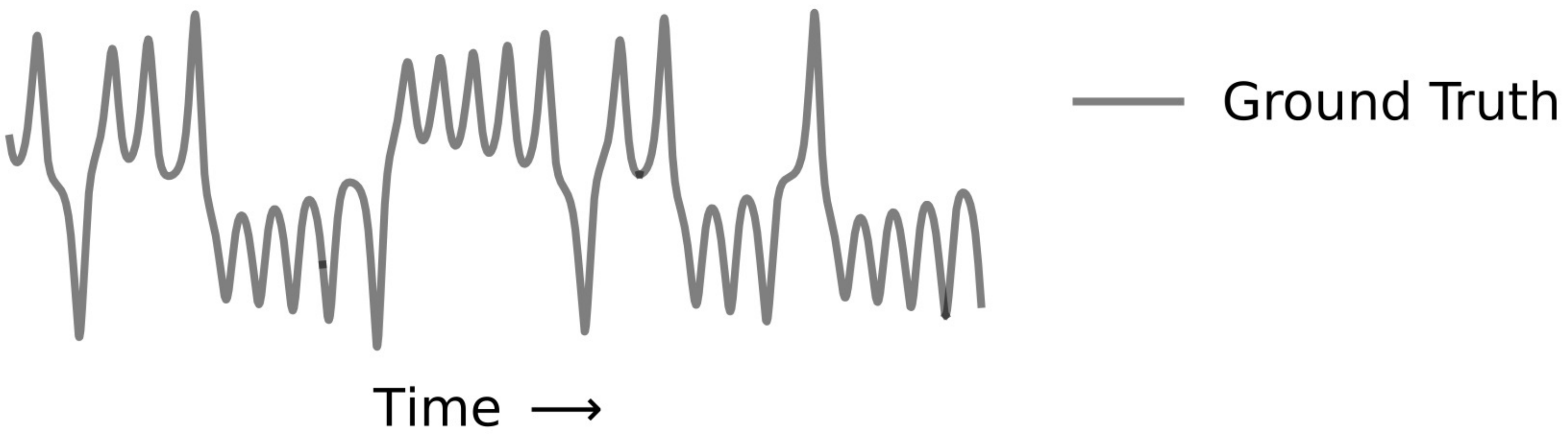
Modeling Chaos: Forecasting vs. Statistics

Accurate short-term forecasting

≠

Correct long-term statistics!



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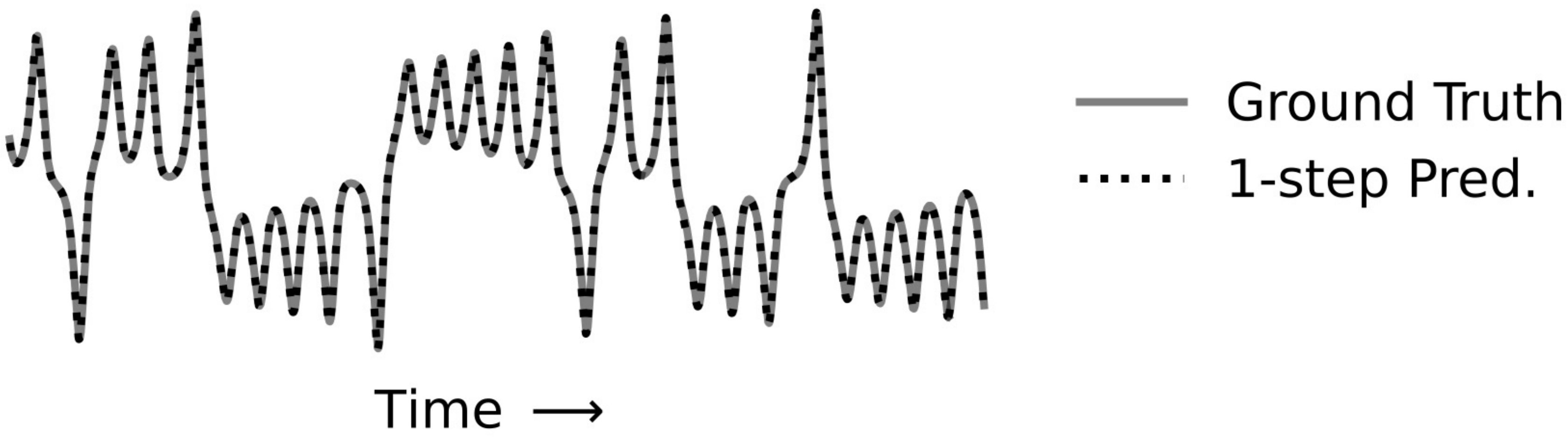

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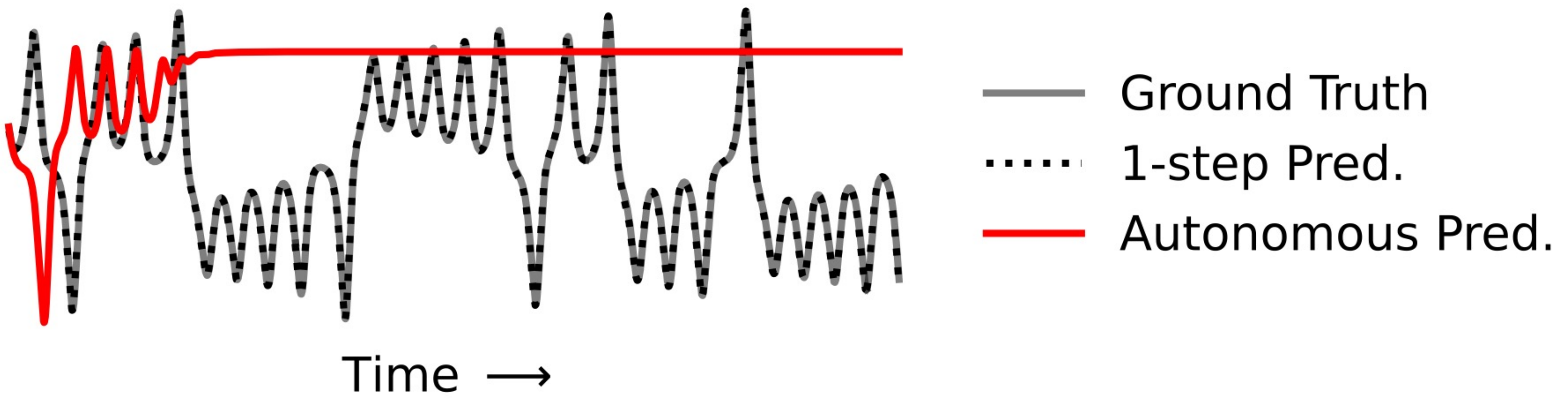

Modeling Chaos: Forecasting vs. Statistics

Accurate short-term forecasting

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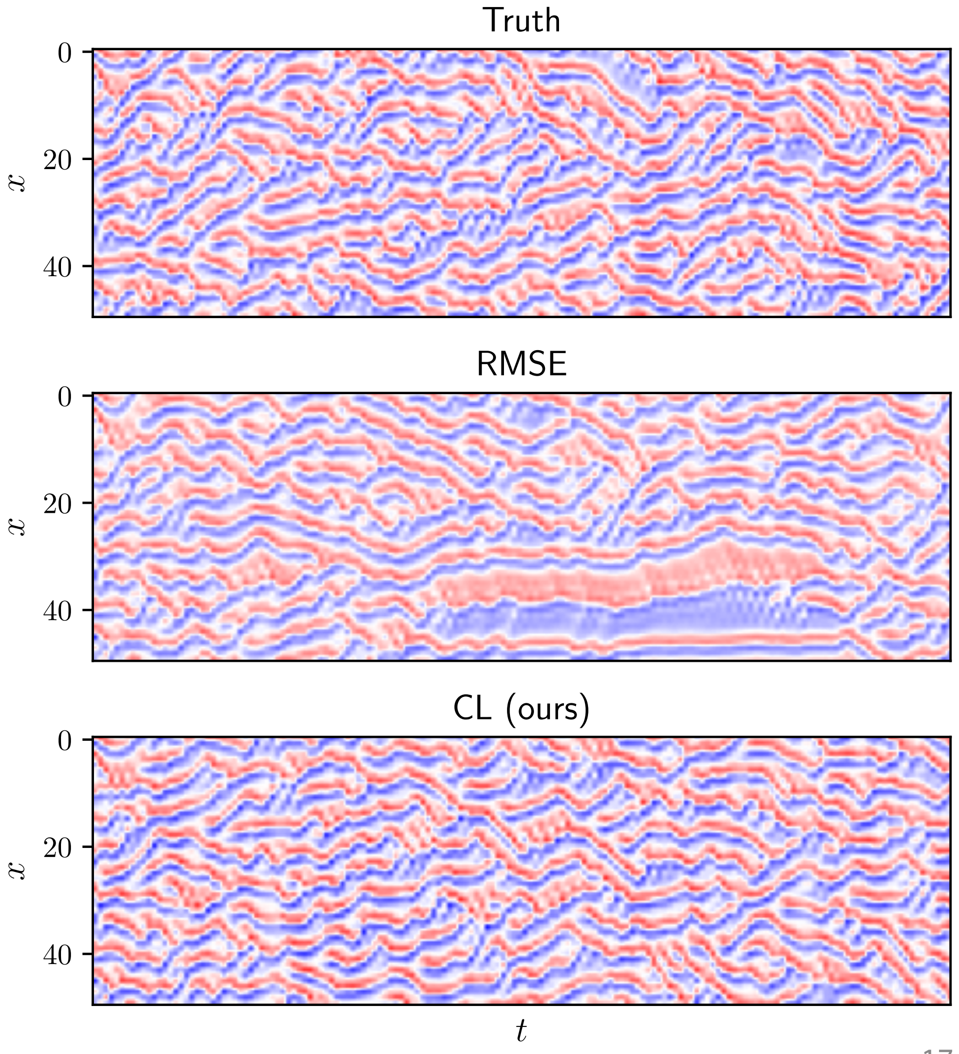
Correct long-term statistics!

Preview of results on noisy data:

Training on short-term *RMSE*

vs.

Training using *invariant statistics*



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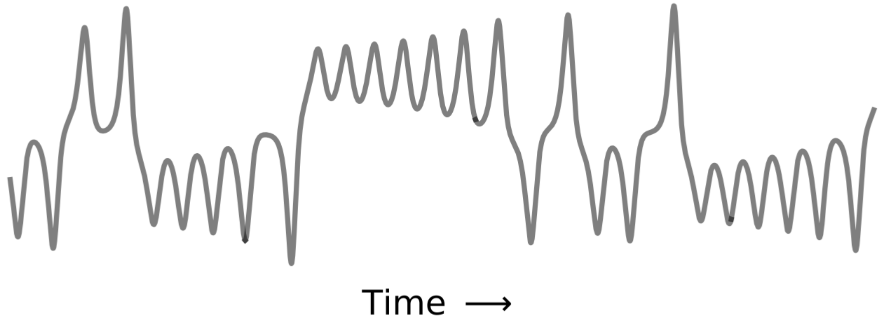
Effect of Noise on Error Metrics

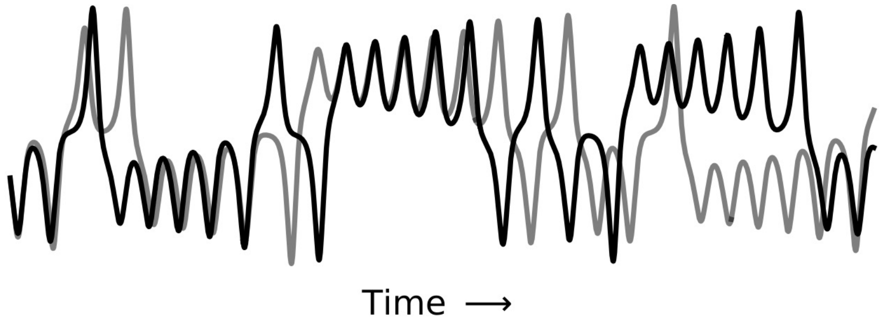
Original trajectory

$$U_G(u_0)$$



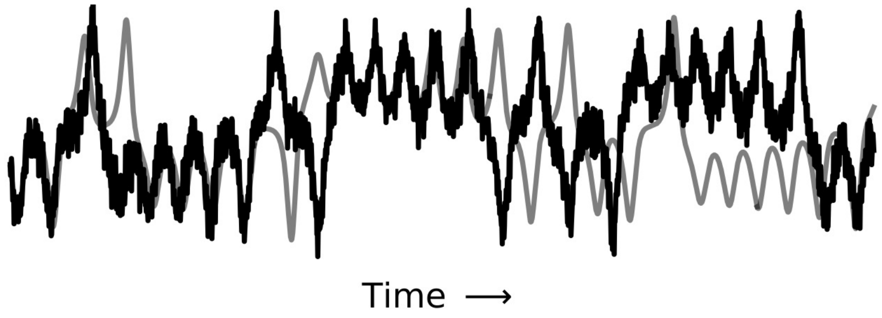
Noisy initial conditions

$$U_G(u_0 + \eta)$$



Noisy IC & measurements

$$U_G(u_0 + \eta) + \eta$$



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Effect of Noise on Error Metrics

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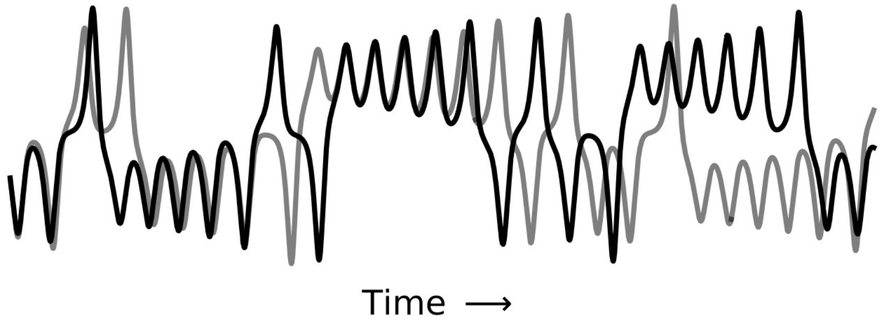
How does increasing noise η affect error metrics?

Noisy initial conditions

$$U_G(u_0 + \eta)$$



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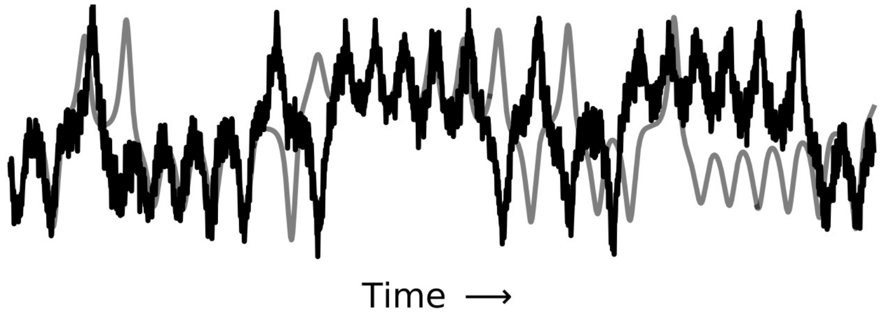

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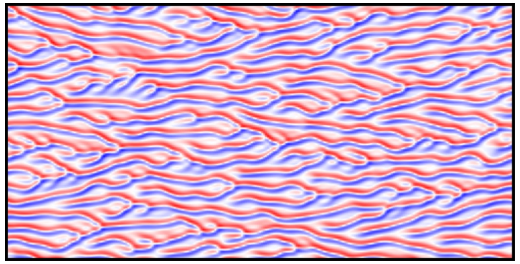

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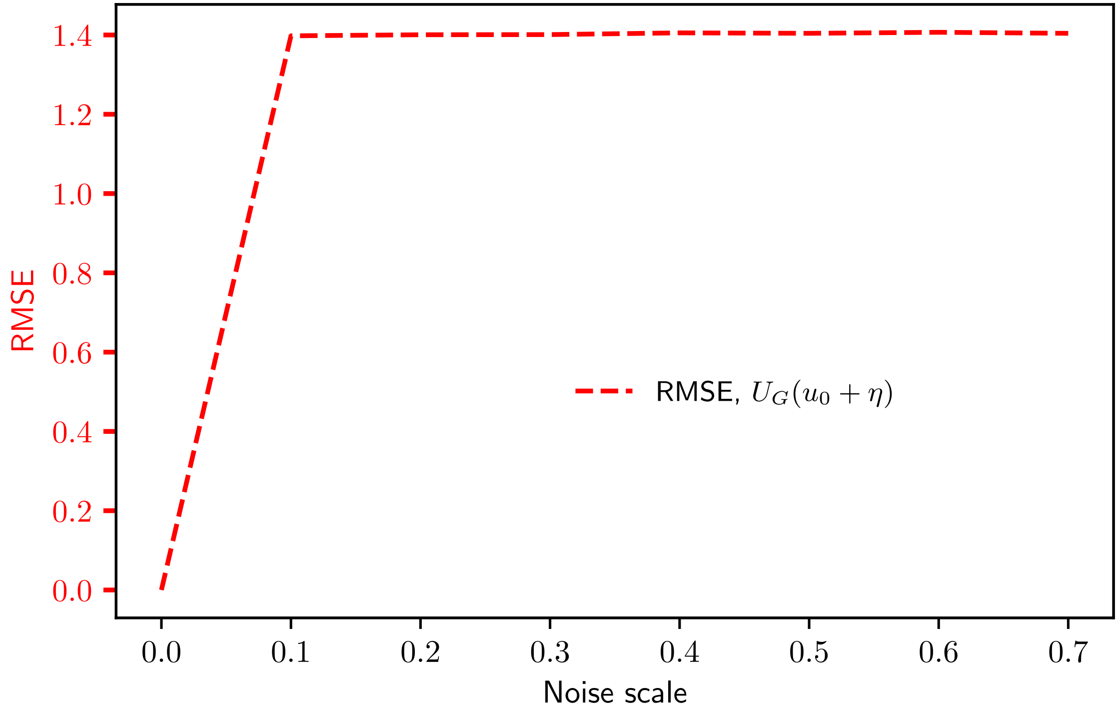

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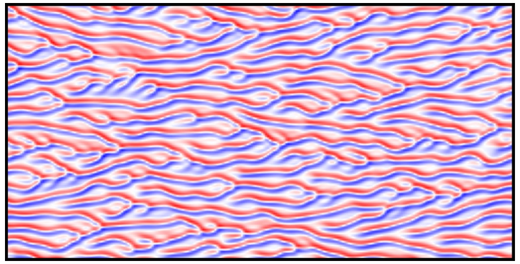

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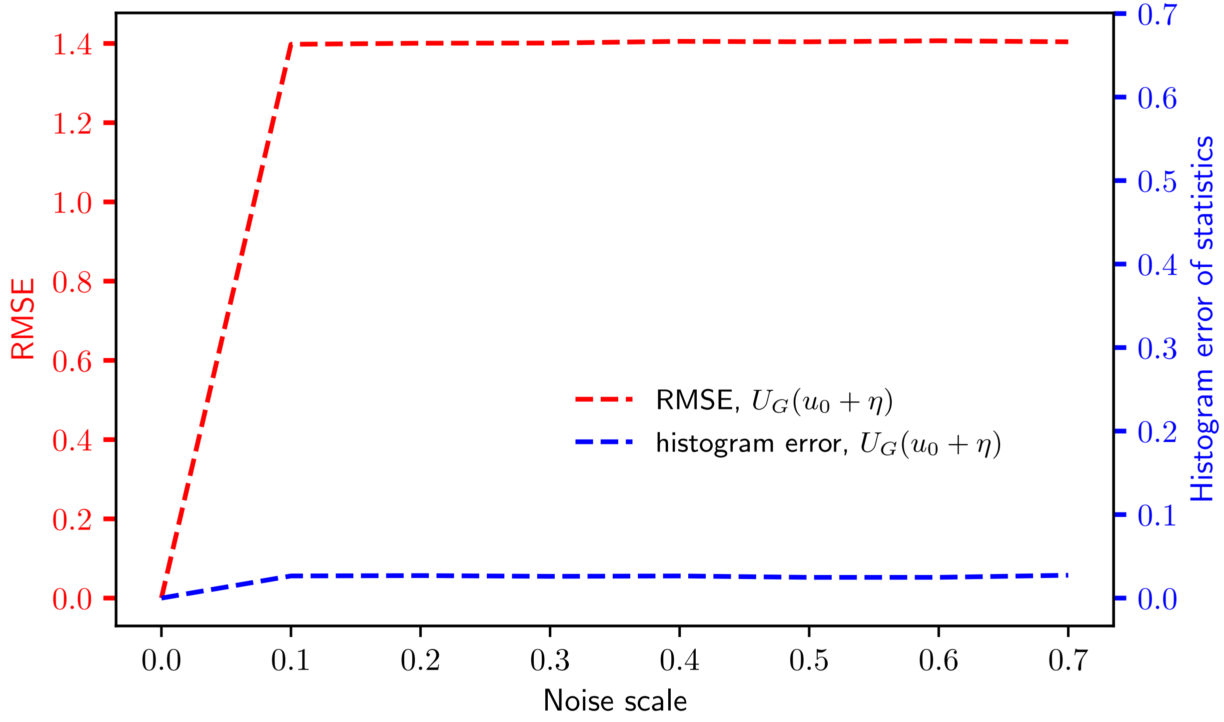

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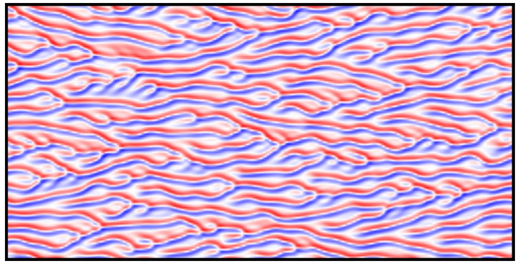

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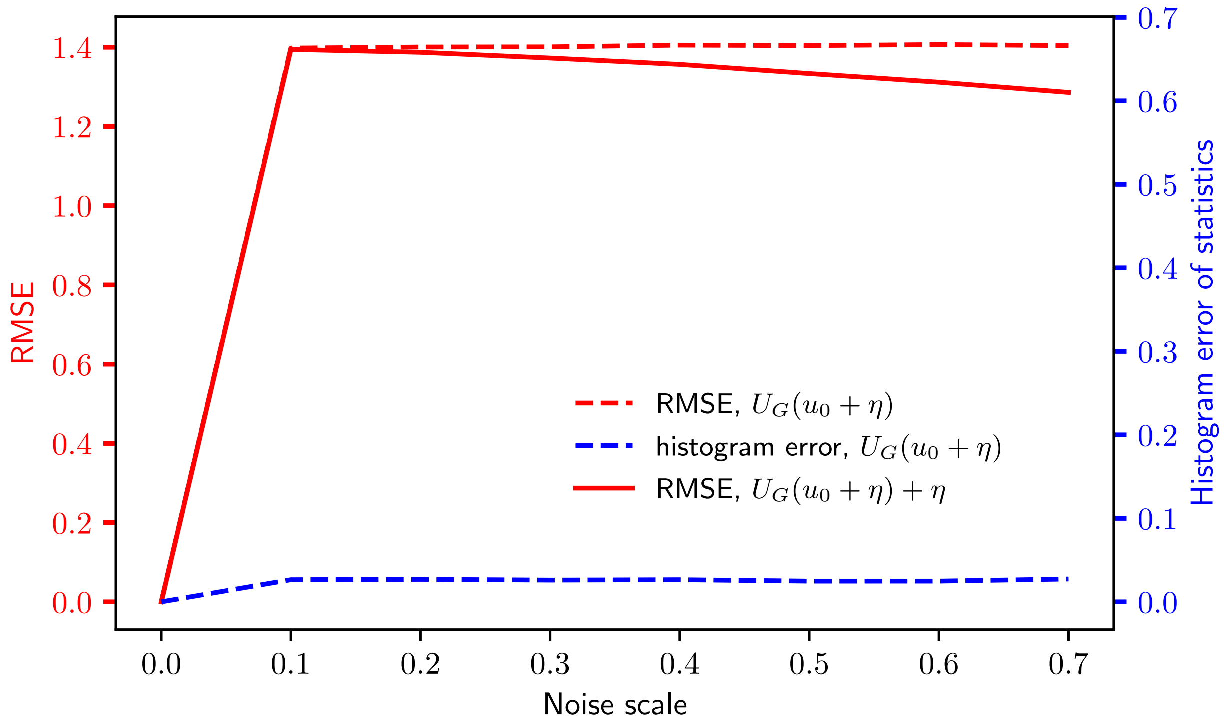

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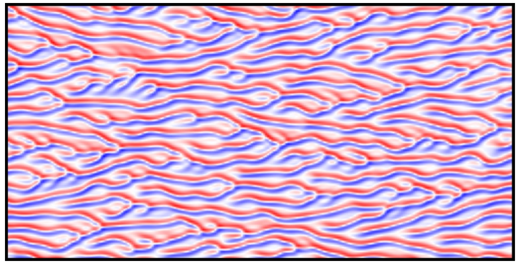

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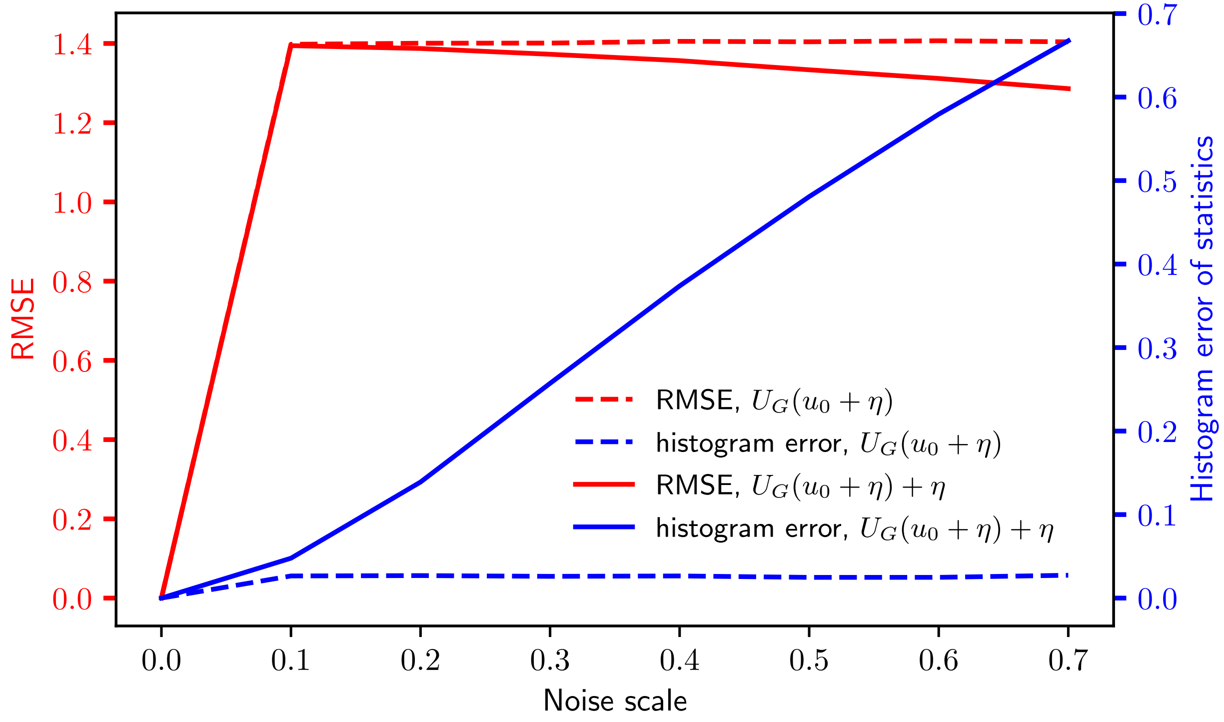

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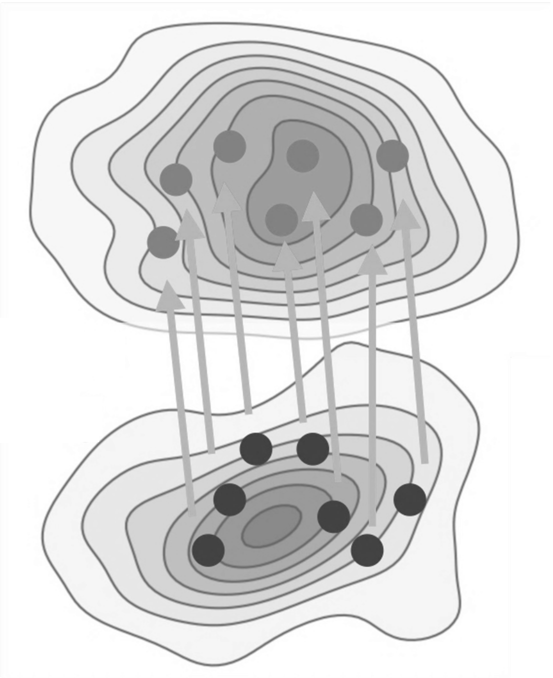
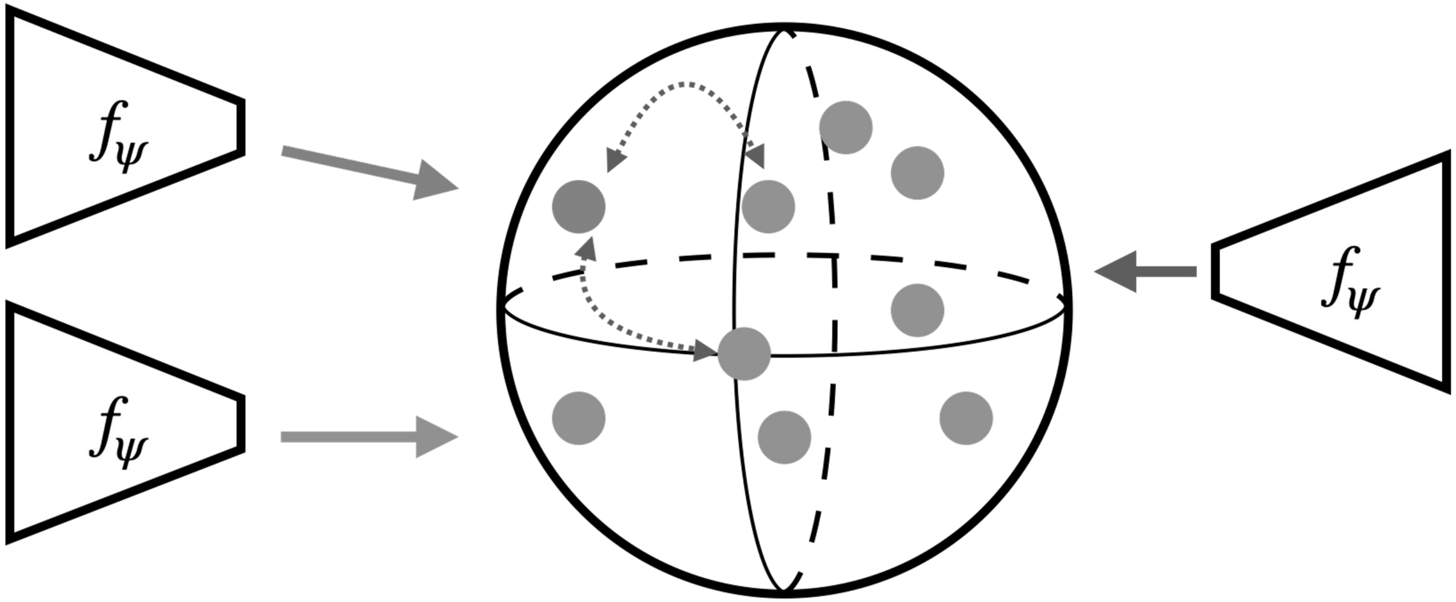
How do we train emulators to capture chaos?





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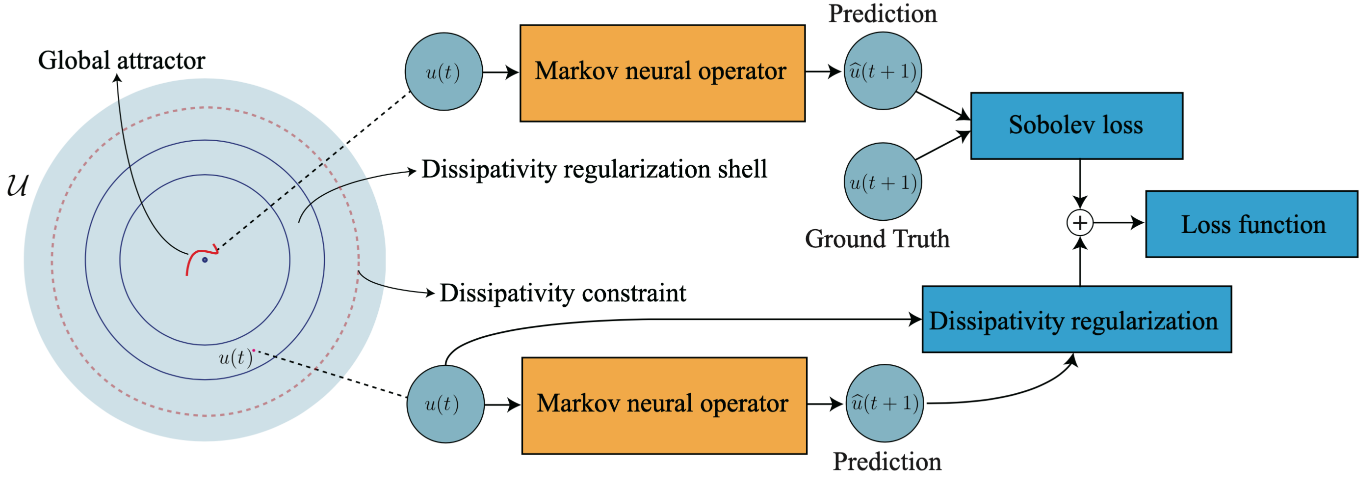
Recent Work

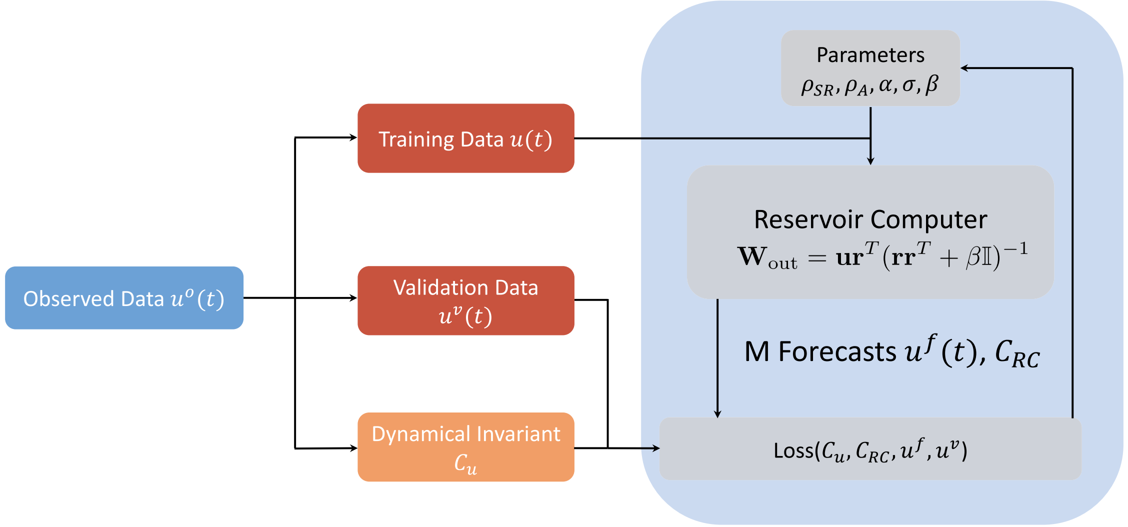
Zongyi Li et al. NeurIPS 2022

proposed Sobolev norm and dissipative regularization.



Jason A. Platt et al. Chaos (2023)

proposed enforcing dynamical invariants in reservoir computers.



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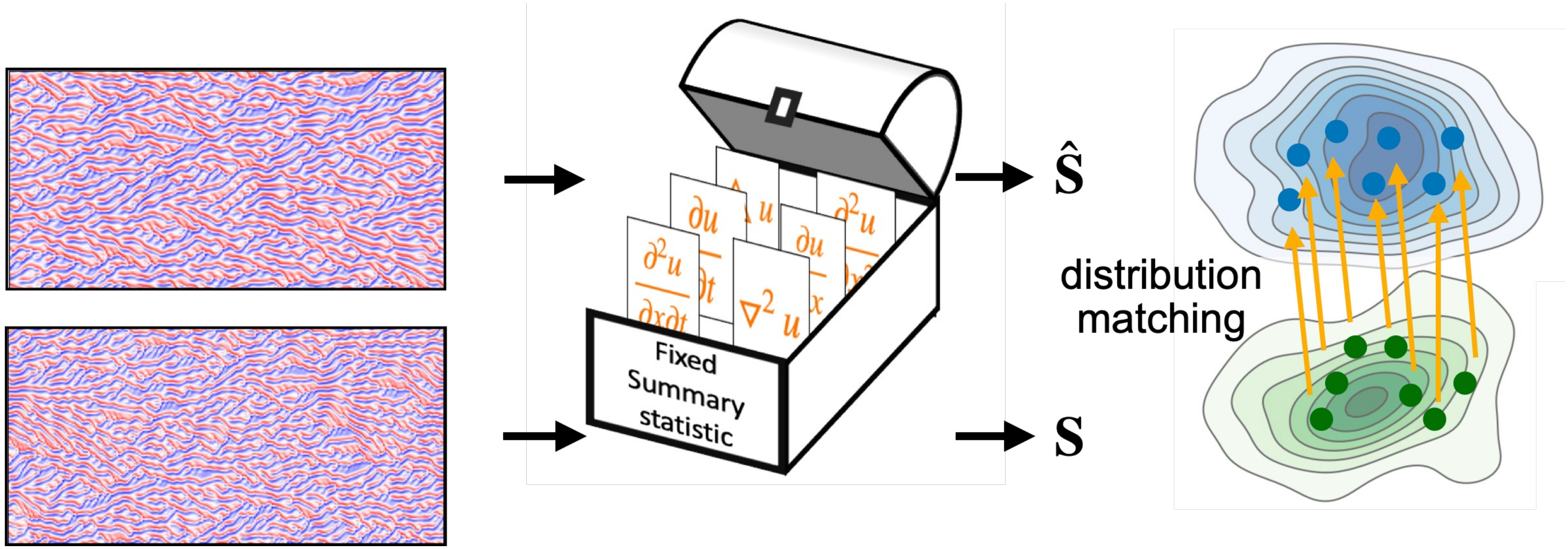
Using Known Summary Statistics

For **high-dimensional problems**, we cannot explicitly match the attractor measure.

Using Known Summary Statistics

For **high-dimensional problems**, we cannot explicitly match the attractor measure.

Instead, we can use **Sinkhorn divergence** (~ Wasserstein **optimal transport** distance) to match **known summary statistics**.



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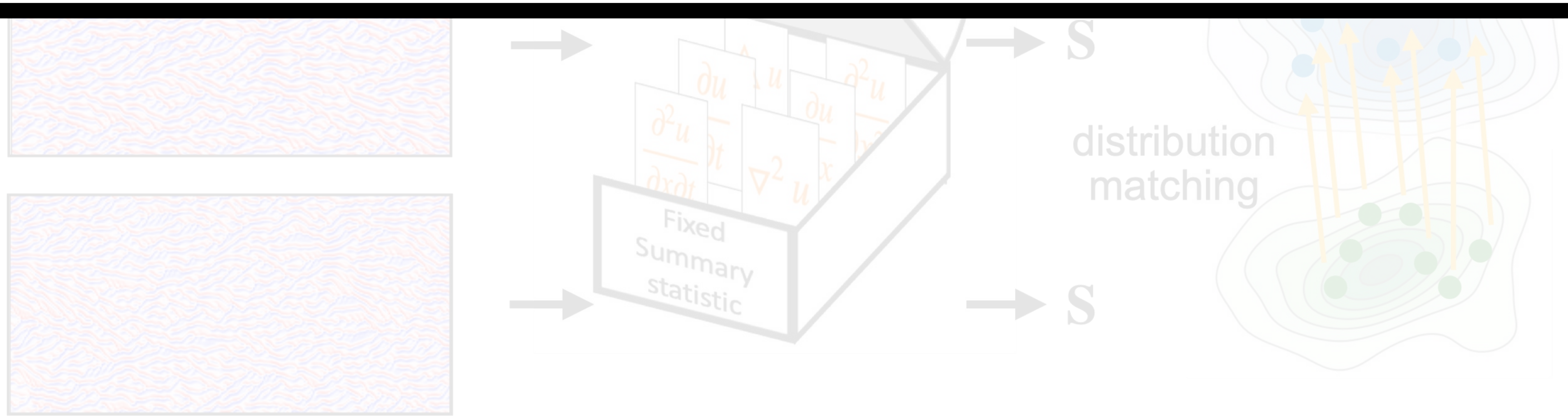
Instead **nal**

transp

What if we don't know the relevant statistics?



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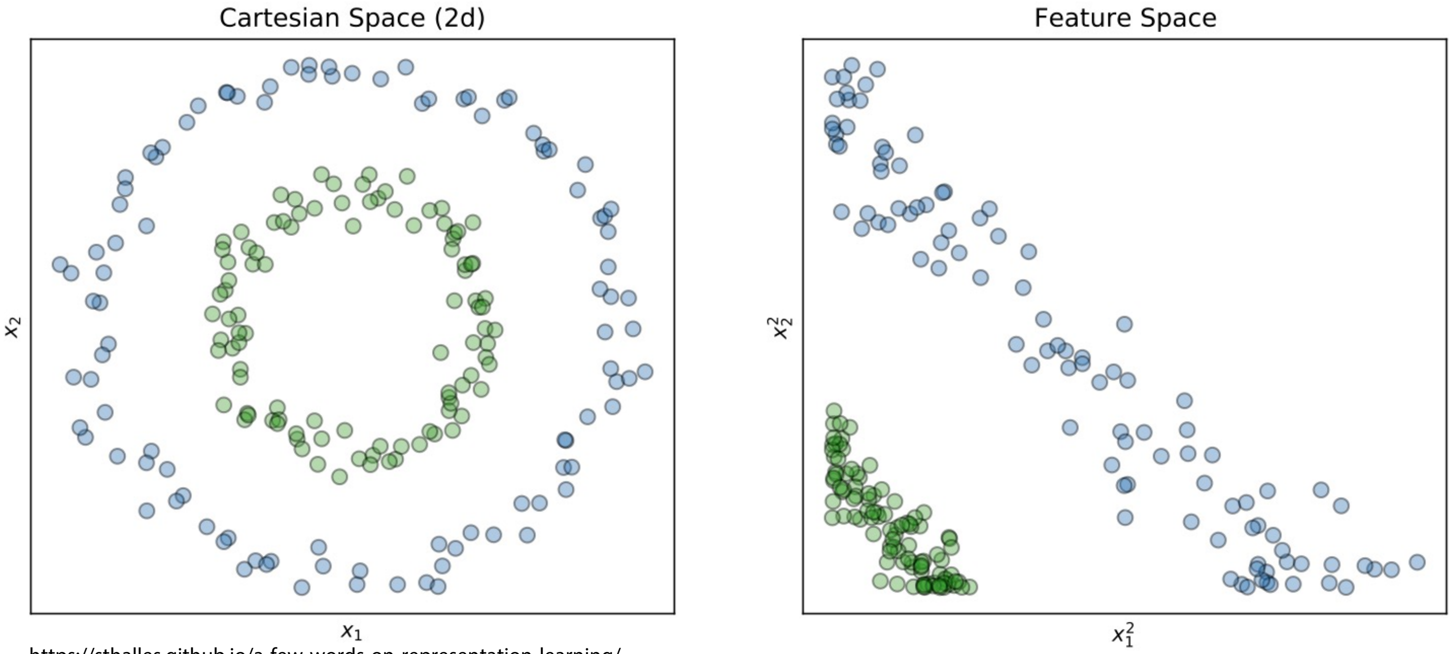
Representation Learning

What if we don't know the relevant statistics?

Representation learning aims to automatically discover **representations** or **features** that characterize a dataset.

- Useful for **dimensionality reduction**, **downstream tasks**, and sometimes **interpretability**.



https://sthalles.github.io/a-few-words-on-representation-learning/

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- Useful for **dimensionality reduction**, **downstream tasks**, and sometimes **interpretability**.

Scientists have always been doing representation learning!

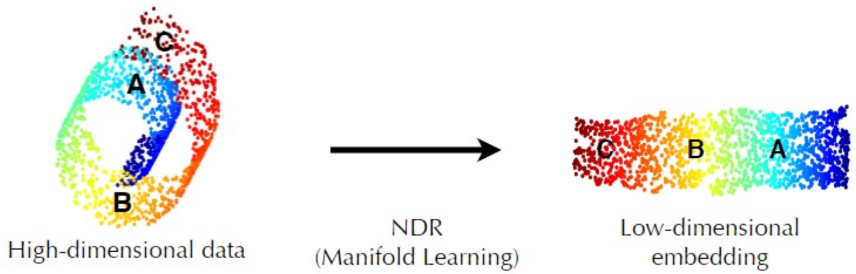
- The world is inherently high-dimensional.
- What we call **"scientific understanding"** is a low-dimensional description.

Representation Learning

What if we don't know the relevant statistics?

Classical Manifold Learning (*popular for data visualization*)

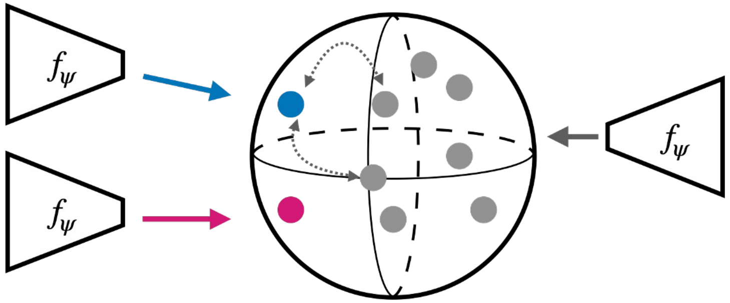
- PCA, MDS, Isomap, t-SNE, UMAP, LLE
- Diffusion maps, Laplacian eigenmaps



Unsupervised/Self-Supervised Learning

(*popular in computer vision & natural language processing*)

- Autoencoders, variational autoencoders
- Contrastive learning, CLIP



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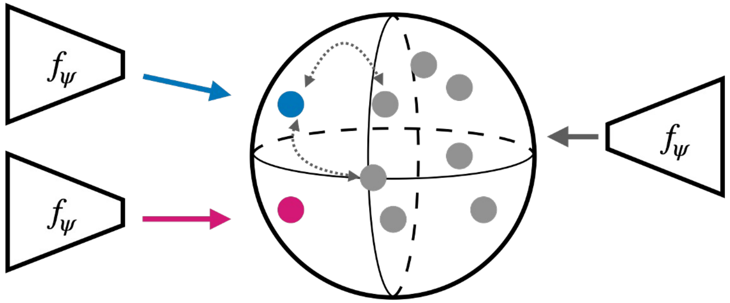

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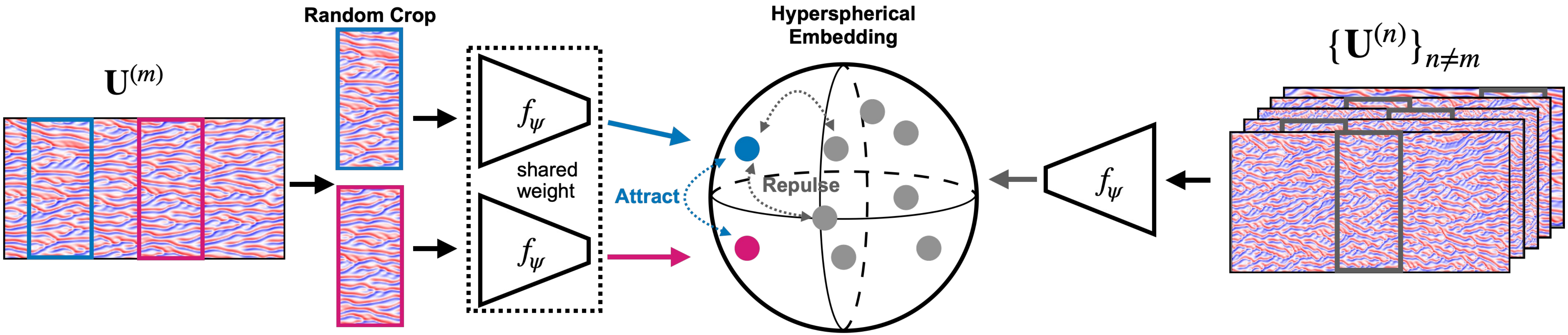
Learning Invariant Statistics from Data

Without prior knowledge, we can use **contrastive learning** in a multi-environment setting to learn **relevant invariant statistics**.



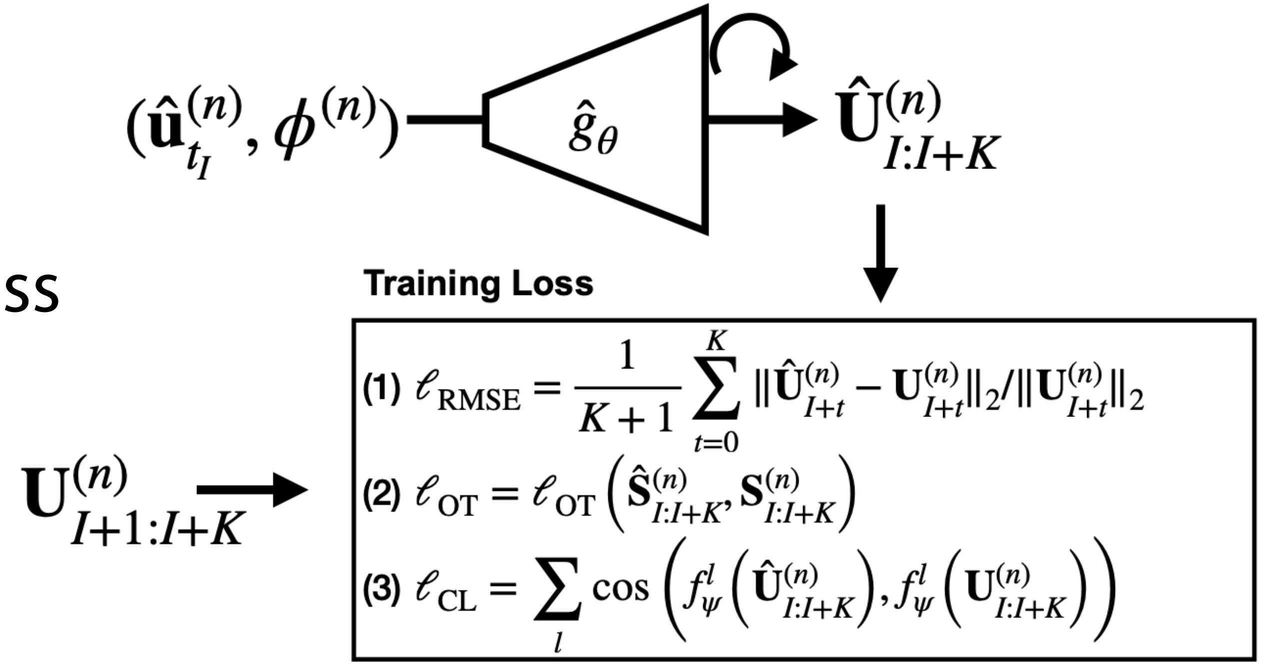
Training Emulators on Chaotic Dynamics

Optimal Transport (OT):

1. Choose summary statistics via expert knowledge
2. Train w/ RMSE + OT Sinkhorn loss

Contrastive Learning (CL):

1. Learn invariant statistics via contrastive learning
2. Train w/ RMSE + CL feature loss



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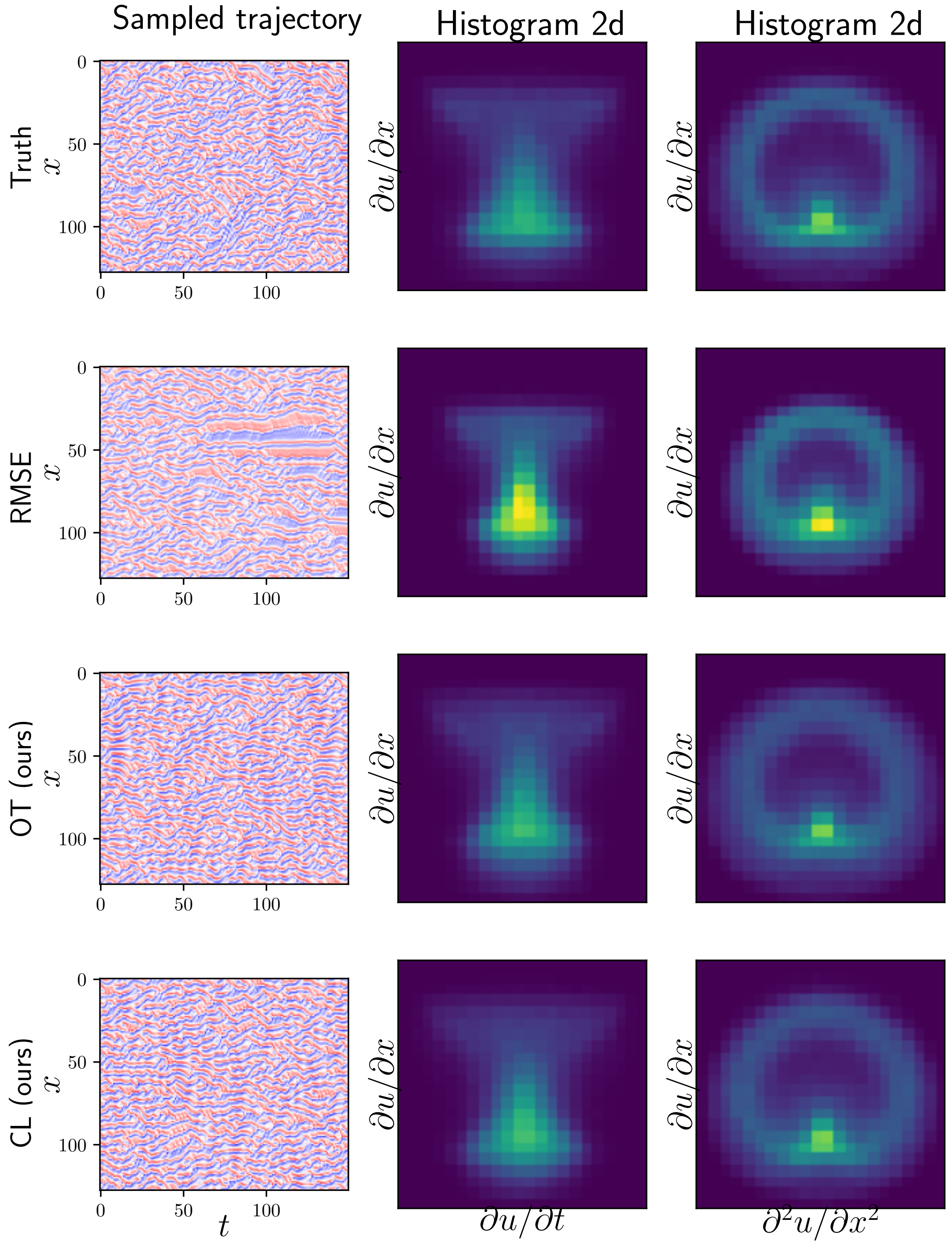
Emulator Evaluation: Kuramoto–Sivashinsky

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - \phi\frac{\partial^2 u}{\partial x^2} - \frac{\partial^4 u}{\partial x^4}$$



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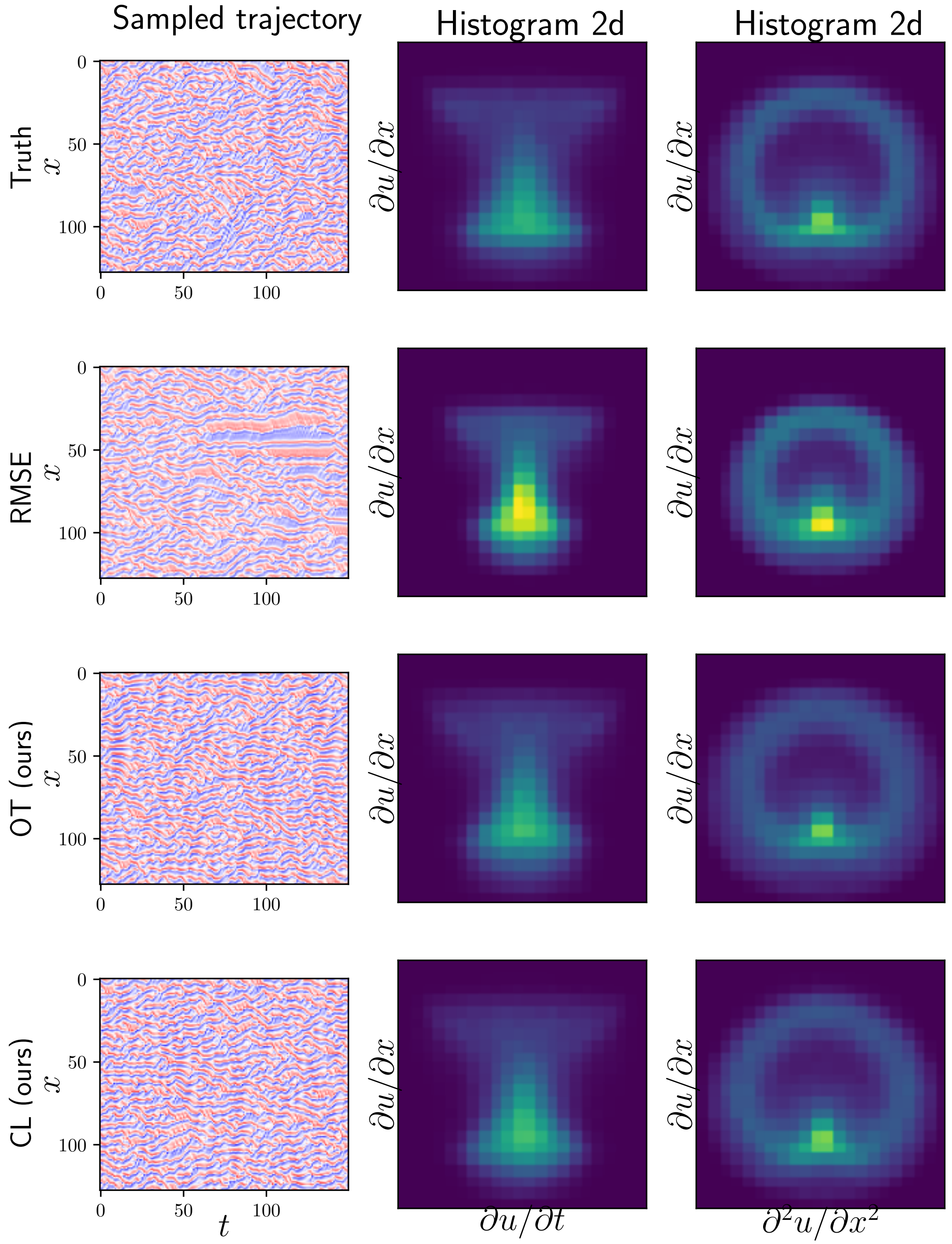
Training	Histogram Error ↓
ℓ_{RMSE}	0.390 (0.325, 0.556)
$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	**0.172** (0.146, 0.197)
$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	0.193 (0.148, 0.247)



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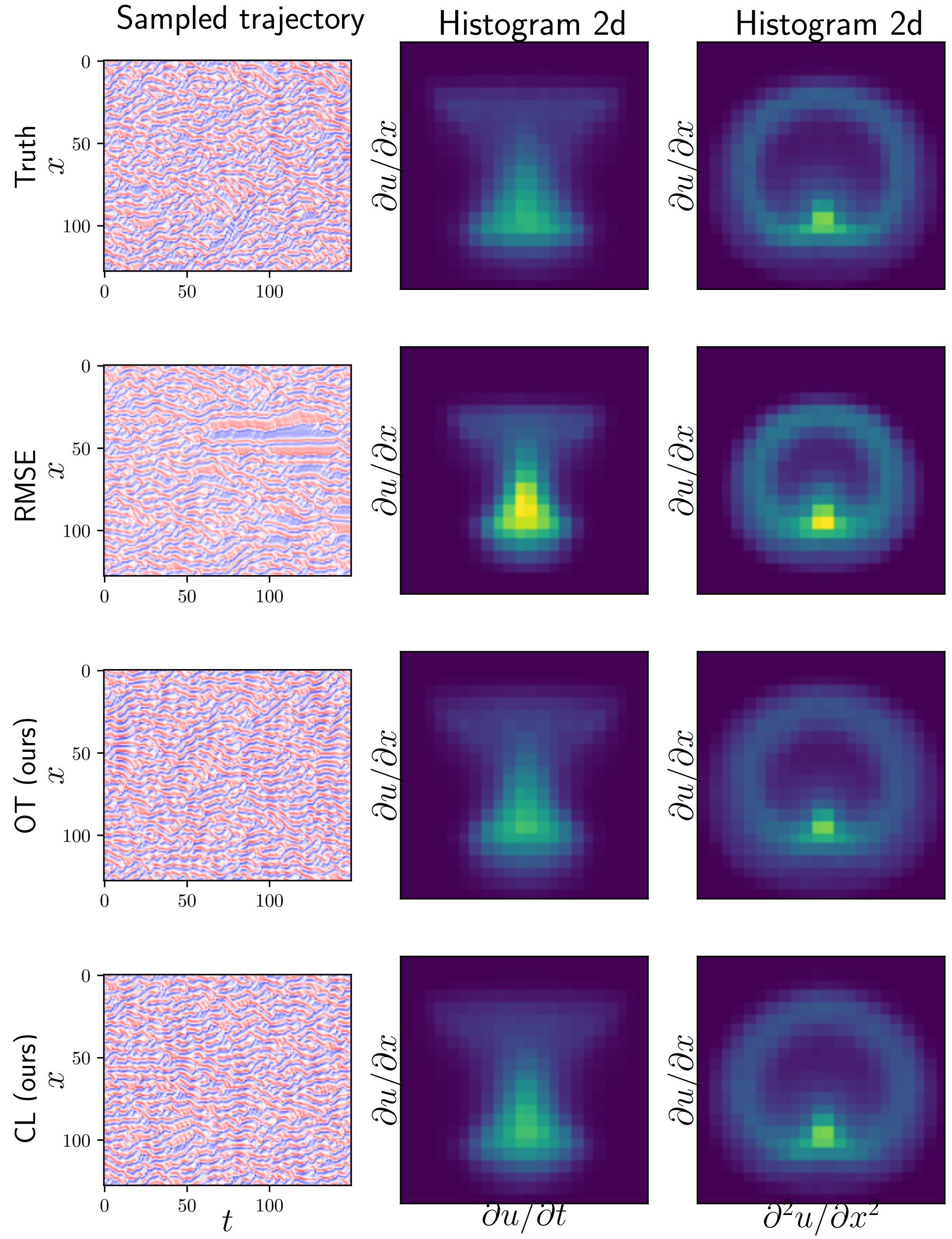
- We see significant improvements on statistical properties for noisy data.
- Again, contrastive learning requires **no prior knowledge**!



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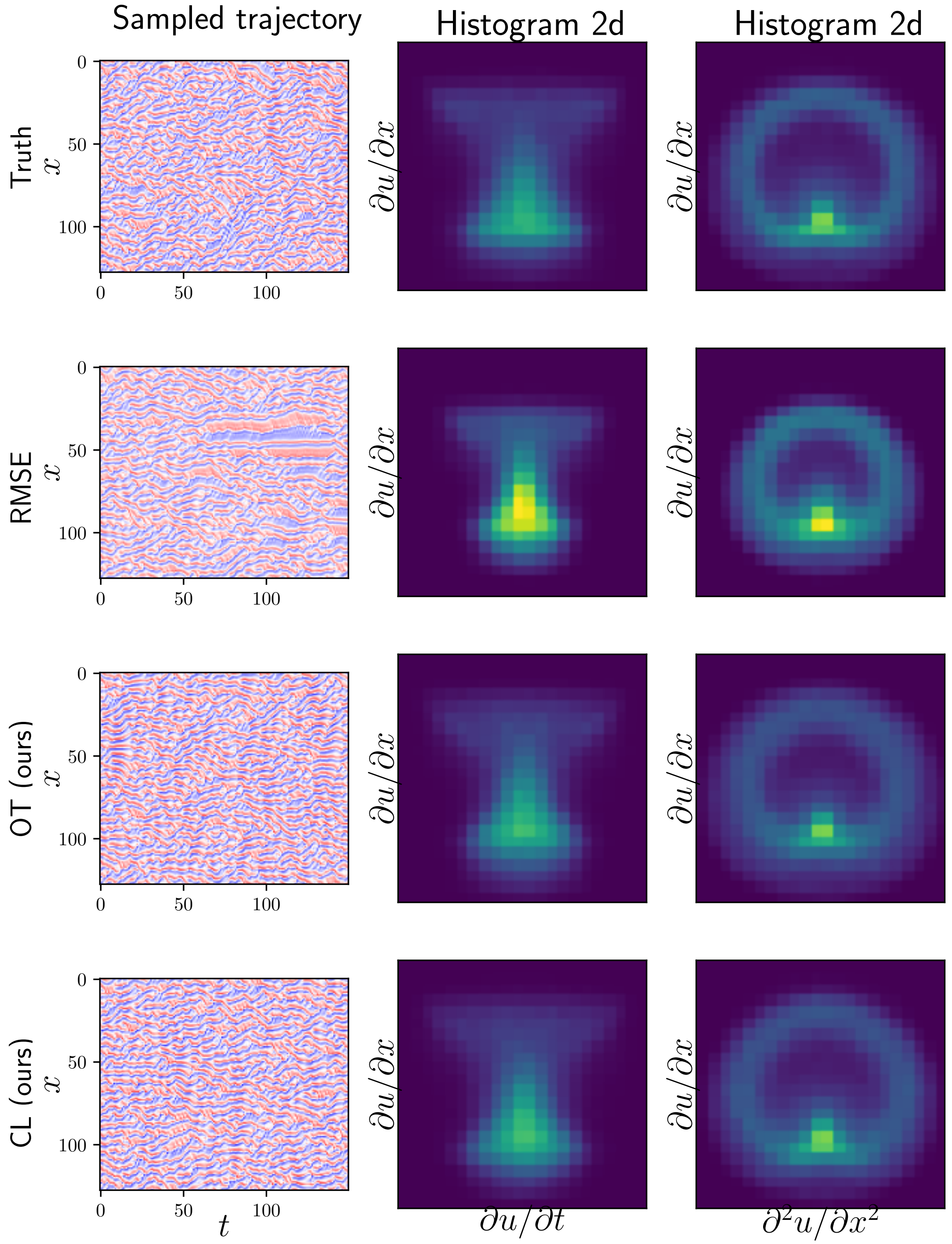
Training	Energy Spec. Error ↓
ℓ_{RMSE}	0.290 (0.225, 0.402)
$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	0.211 (0.188, 0.250)
$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	**0.176** (0.130, 0.245)

- We see significant improvements on statistical properties for noisy data.
- Again, contrastive learning requires **no prior knowledge**!



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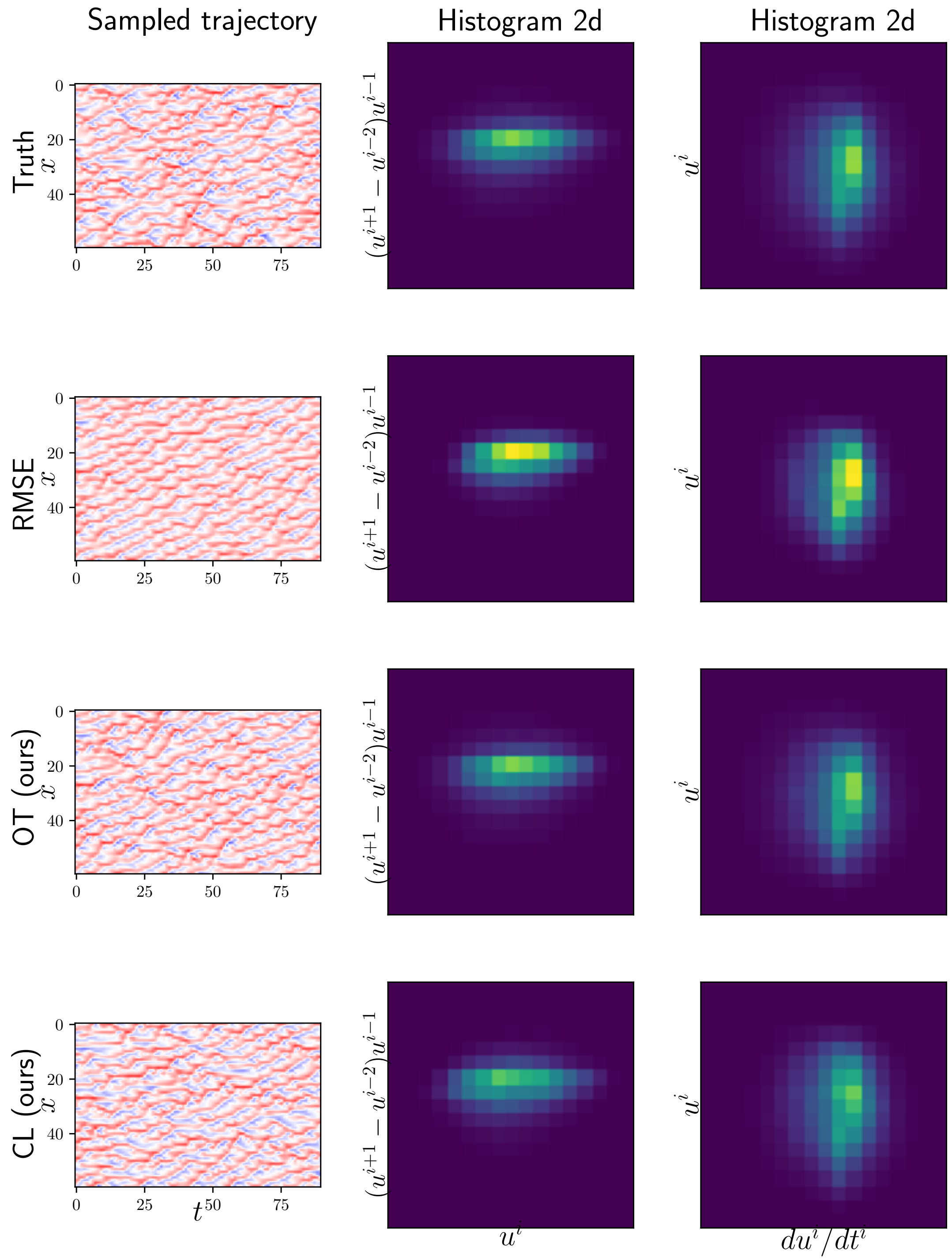
Emulator Evaluation: Lorenz 96

$$\frac{du_i}{dt} = (u_{i+1} - u_{i-2})u_{i-1} - u_i + F$$

r	Training	Histogram Error ↓
0.1	ℓ_{RMSE}	0.056 (0.051, 0.062)
	$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	**0.029** (0.027, 0.032)
	$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	0.033 (0.029, 0.037)
0.2	ℓ_{RMSE}	0.130 (0.118, 0.142)
	$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	**0.039** (0.035, 0.042)
	$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	0.073 (0.066, 0.080)
0.3	ℓ_{RMSE}	0.215 (0.204, 0.234)
	$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	**0.057** (0.052, 0.064)
	$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	0.132 (0.111, 0.151)



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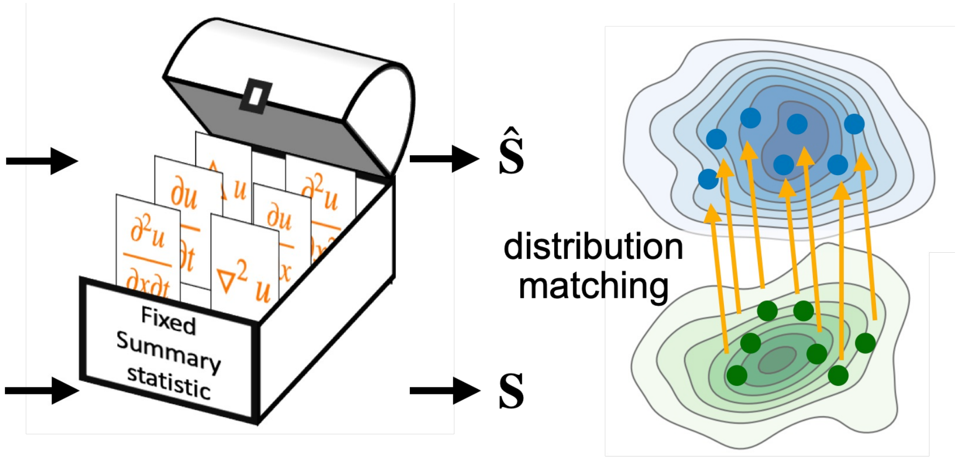
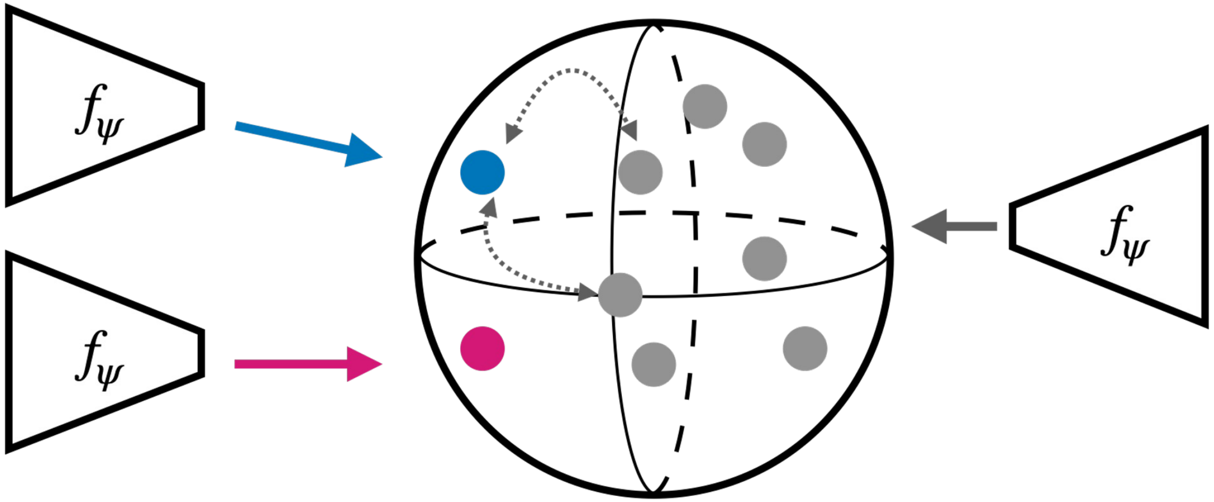
Training Emulators for Chaos:
Summary

We train emulators to match the statistics of **high-dimensional, spatiotemporal chaotic attractors**.

Our approach performs significantly better in the **high noise regime**.

Contrastive representation learning can identify relevant statistics **without prior knowledge**.





Training Emulators for Chaos:
Future Directions

Applications:

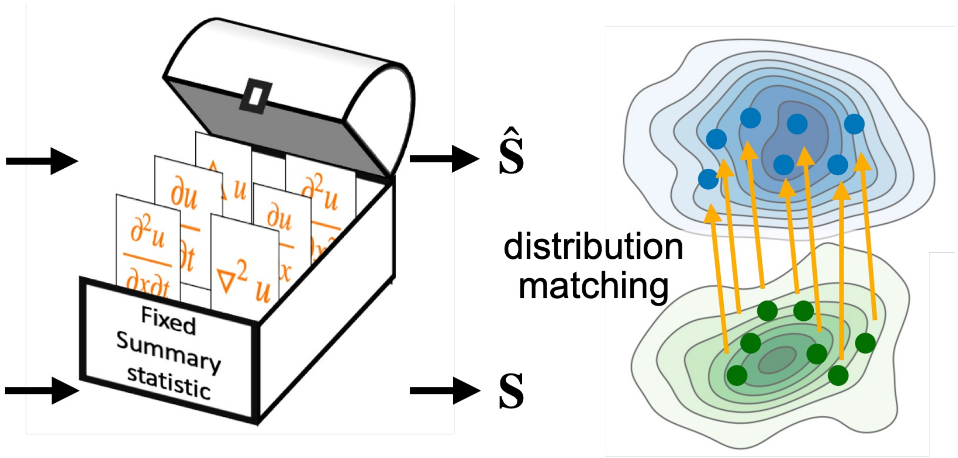
- Fluid turbulence
- Weather/climate modeling

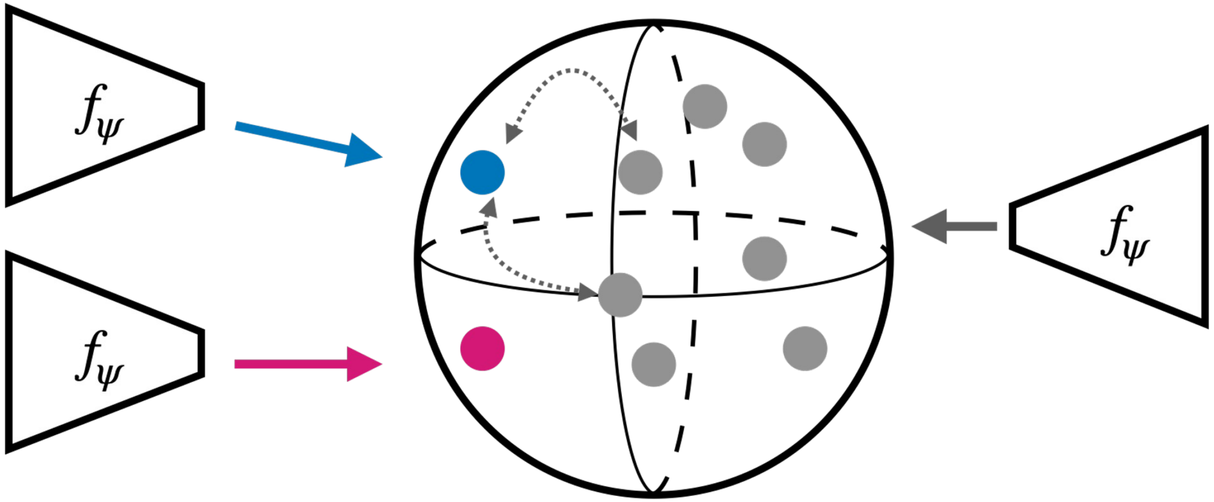
Extensions:

- Transient dynamics
- Stochastic dynamics

Interpretability:

- What are the learned statistics?
- Can we improve interpretability?





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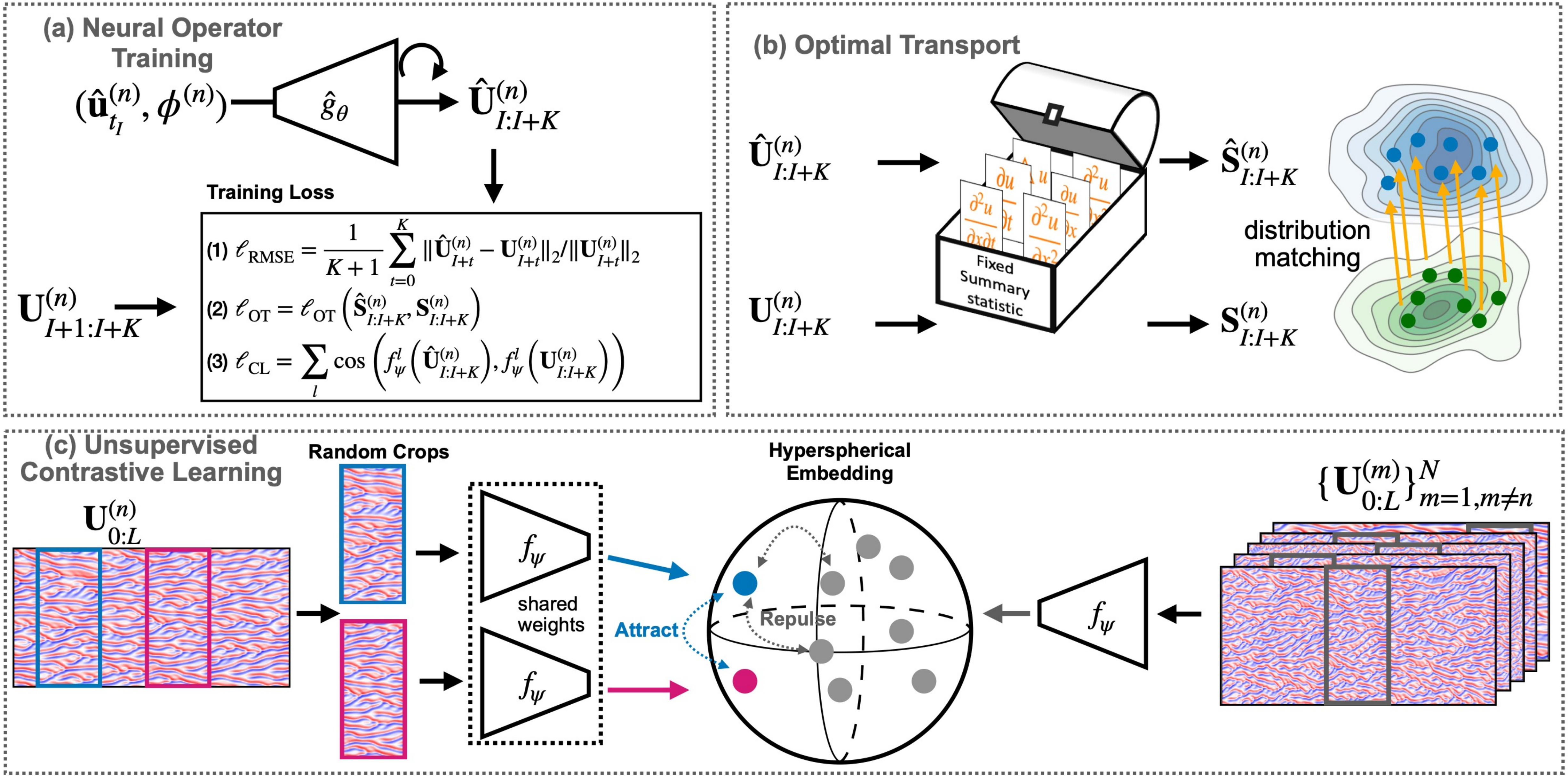

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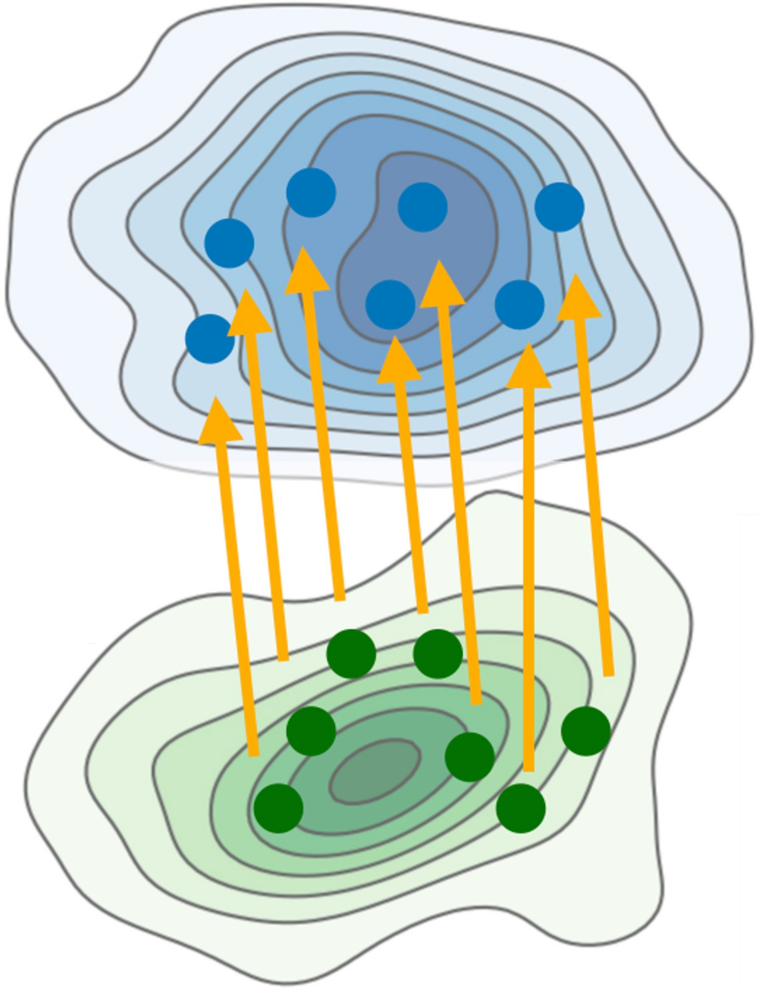
Wasserstein Distance

$$\frac{1}{2}W(\mathbf{S},\hat{\mathbf{S}})^2 := \min_{T\in\Pi}\sum_{i,j} T_{ij}C_{ij}$$

$$C_{ij} = \tfrac{1}{2}\|\mathbf{s}_i - \hat{\mathbf{s}}_j\|^2$$

$$\forall i,j, T_{ij} \geq 0, \textstyle\sum_j T_{ij} = 1, \text{ and } \textstyle\sum_i T_{ij} = 1$$

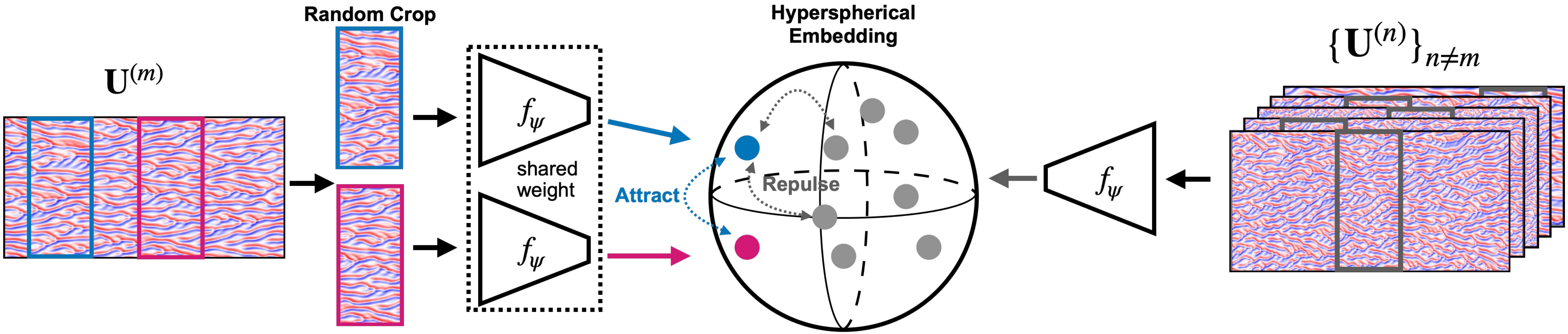


Entropy-regularized Wasserstein distance:

$$\frac{1}{2}W^{\gamma}(\mathbf{S},\hat{\mathbf{S}})^2 := \min_{T\in\Pi}\sum_{i,j} T_{ij}C_{ij} - \gamma\, h(T)$$

$$h(T) = -\textstyle\sum_{i,j} T_{ij}\log T_{ij}$$

Contrastive Learning: InfoNCE Loss



$$\ell_{\mathrm{InfoNCE}}(\psi;\tau) := \mathop{\mathbb{E}}_{\substack{n\in\{1,\dots,N\}\\ I,J\in\{0,\dots,L-K\}}}\left[-\log\left(\frac{\exp\left(\langle f_\psi(\mathbf{U}^{(n)}_{I:I+K}), f_\psi(\mathbf{U}^{(n)}_{J:J+K})\rangle/\tau\right)}{\mathop{\mathbb{E}}_{\substack{m\neq n\\ H\in\{0,\dots,L-K\}}}\left[\exp\left(\langle f_\psi(\mathbf{U}^{(n)}_{I:I+K}), f_\psi(\mathbf{U}^{(m)}_{H:H+K})\rangle/\tau\right)\right]}\right)\right]$$

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Full Results: Kuramoto–Sivashinsky

Training	Histogram Error ↓	Energy Spec. Error ↓	Leading LE Error ↓
ℓ_{RMSE}	0.390 (0.325, 0.556)	0.290 (0.225, 0.402)	0.101 (0.069, 0.122)
$\ell_{\text{Sobolev}} + \ell_{\text{dissipative}}$	0.427 (0.289, 0.616)	0.237 (0.204, 0.315)	**0.023** (0.012, 0.047)
$\ell_{\text{MMD}} + \ell_{\text{RMSE}}$	0.245 (0.218, 0.334)	0.216 (0.186, 0.272)	0.101 (0.058, 0.125)
$\ell_{\text{OT}} + \ell_{\text{RMSE}}$	**0.172** (0.146, 0.197)	0.211 (0.188, 0.250)	**0.094** (0.041, 0.127)
$\ell_{\text{CL}} + \ell_{\text{RMSE}}$	0.193 (0.148, 0.247)	**0.176** (0.130, 0.245)	0.108 (0.068, 0.132)

Training	Histogram Error ↓	Energy Spec. Error↓	Leading LE Error ↓
ℓ_{RMSE} ($\sigma_b = 0.1$)	**0.390** (0.326, 0.556)	**0.290** (0.226, 0.402)	**0.098** (0.069, 0.127)
ℓ_{RMSE} ($\sigma_b = 0.5$)	1.011 (0.788, 1.264)	0.493 (0.379, 0.623)	**0.098** (0.041, 0.427)
ℓ_{RMSE}	**0.390** (0.325, 0.556)	**0.290** (0.225, 0.402)	0.101 (0.069, 0.122)

Full Results: Lorenz 96

r	Training	Histogram Error ↓	Energy Spec. Error ↓	Leading LE Error ↓	FD Error ↓
	ℓ_{RMSE}	0.056 (0.051, 0.062)	0.083 (0.078, 0.090)	**0.013** (0.006, 0.021)	1.566 (0.797, 2.309)
0.1	$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	**0.029** (0.027, 0.032)	**0.058** (0.052, 0.064)	0.050 (0.040, 0.059)	1.424 (0.646, 2.315)
	$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	0.033 (0.029, 0.037)	**0.058** (0.049, 0.065)	0.065 (0.058, 0.073)	**1.042** (0.522, 1.685)
	ℓ_{RMSE}	0.130 (0.118, 0.142)	0.182 (0.172, 0.188)	0.170 (0.156, 0.191)	2.481 (1.428, 3.807)
0.2	$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	**0.039** (0.035, 0.042)	**0.086** (0.079, 0.095)	0.016 (0.006, 0.030)	2.403 (1.433, 3.768)
	$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	0.073 (0.066, 0.080)	0.131 (0.117, 0.149)	**0.012** (0.006, 0.018)	**1.681** (0.656, 2.682)
	ℓ_{RMSE}	0.215 (0.204, 0.234)	0.291 (0.280, 0.305)	0.440 (0.425, 0.463)	3.580 (2.333, 4.866)
0.3	$\ell_{\mathrm{OT}} + \ell_{\mathrm{RMSE}}$	**0.057** (0.052, 0.064)	**0.123** (0.116, 0.135)	0.084 (0.062, 0.134)	3.453 (2.457, 4.782)
	$\ell_{\mathrm{CL}} + \ell_{\mathrm{RMSE}}$	0.132 (0.111, 0.151)	0.241 (0.208, 0.285)	**0.064** (0.045, 0.091)	**1.894** (0.942, 3.108)

Training statistics	Histogram Error ↓	Energy Spec. Error ↓	Leading LE Error ↓	FD Error ↓
$\mathbf{S}$ (full)	**0.057** (0.052, 0.064)	**0.123** (0.116, 0.135)	0.084 (0.062, 0.134)	3.453 (2.457, 4.782)
$\mathbf{S}_1$ (partial)	0.090 (0.084, 0.098)	0.198 (0.189, 0.208)	0.263 (0.217, 0.323)	3.992 (2.543, 5.440)
$\mathbf{S}_2$ (minimum)	0.221 (0.210, 0.234)	0.221 (0.210, 0.230)	0.276 (0.258, 0.291)	**3.204** (2.037, 4.679)

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