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Multimodal Teacher Forcing for Reconstructing Nonlinear Dynamical Systems

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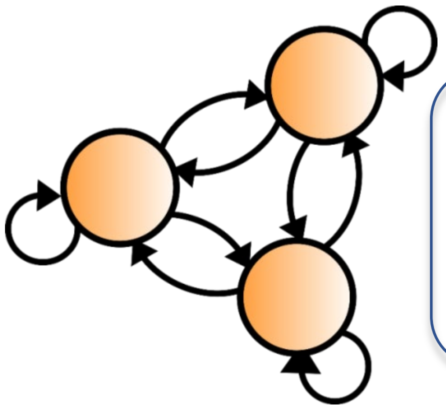
When Machine Learning meets Dynamical Systems: Theory and Application

Dynamical Systems Reconstructions (DSR)

Unknown DS

$$\dot{x}_1 = s(x_2 - x_1)$$
$$\dot{x}_2 = rx_1 - x_2 - x_1x_3$$
$$\dot{x}_3 = x_1x_2 - bx_3$$

Inference

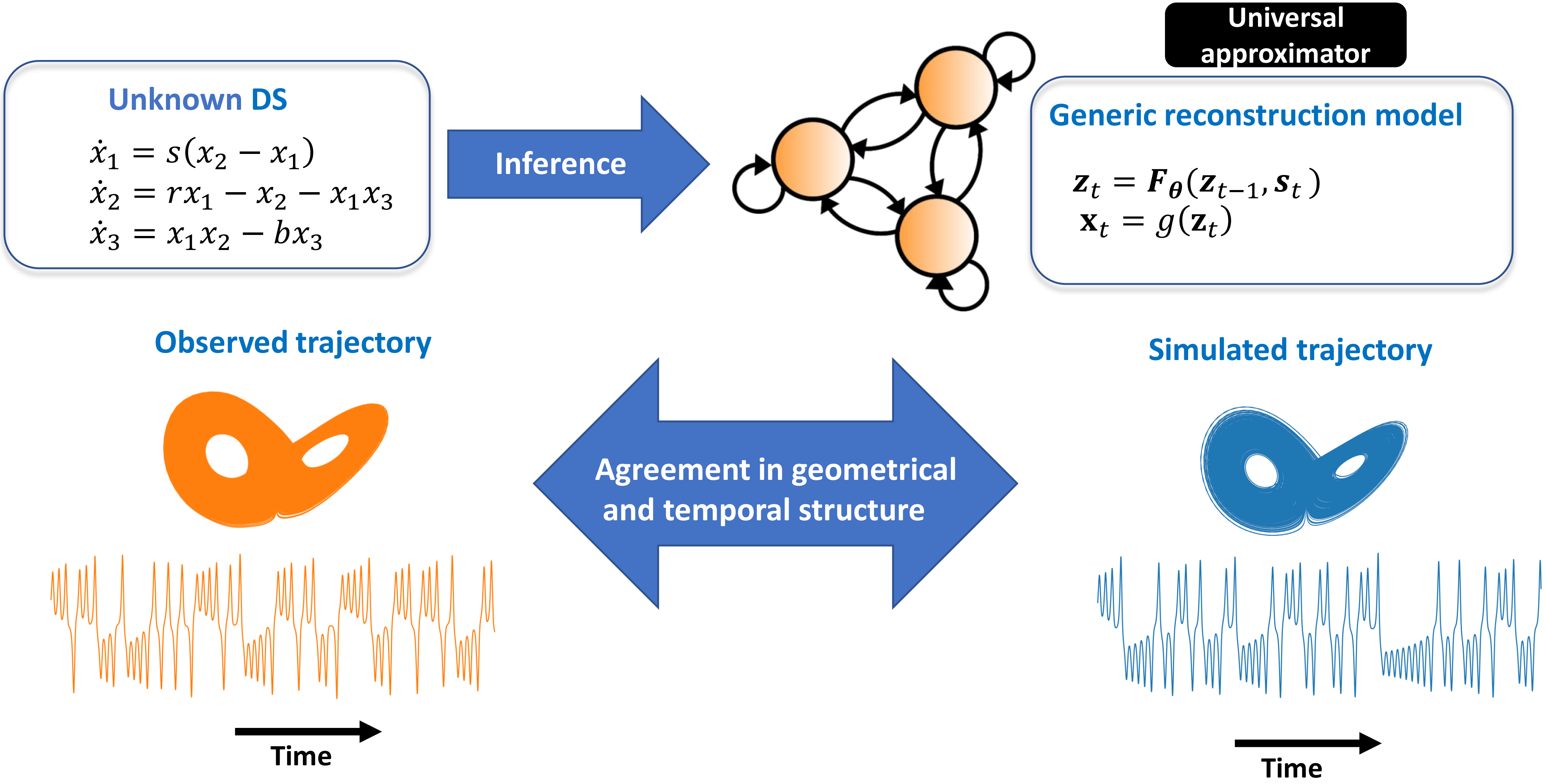


Universal approximator

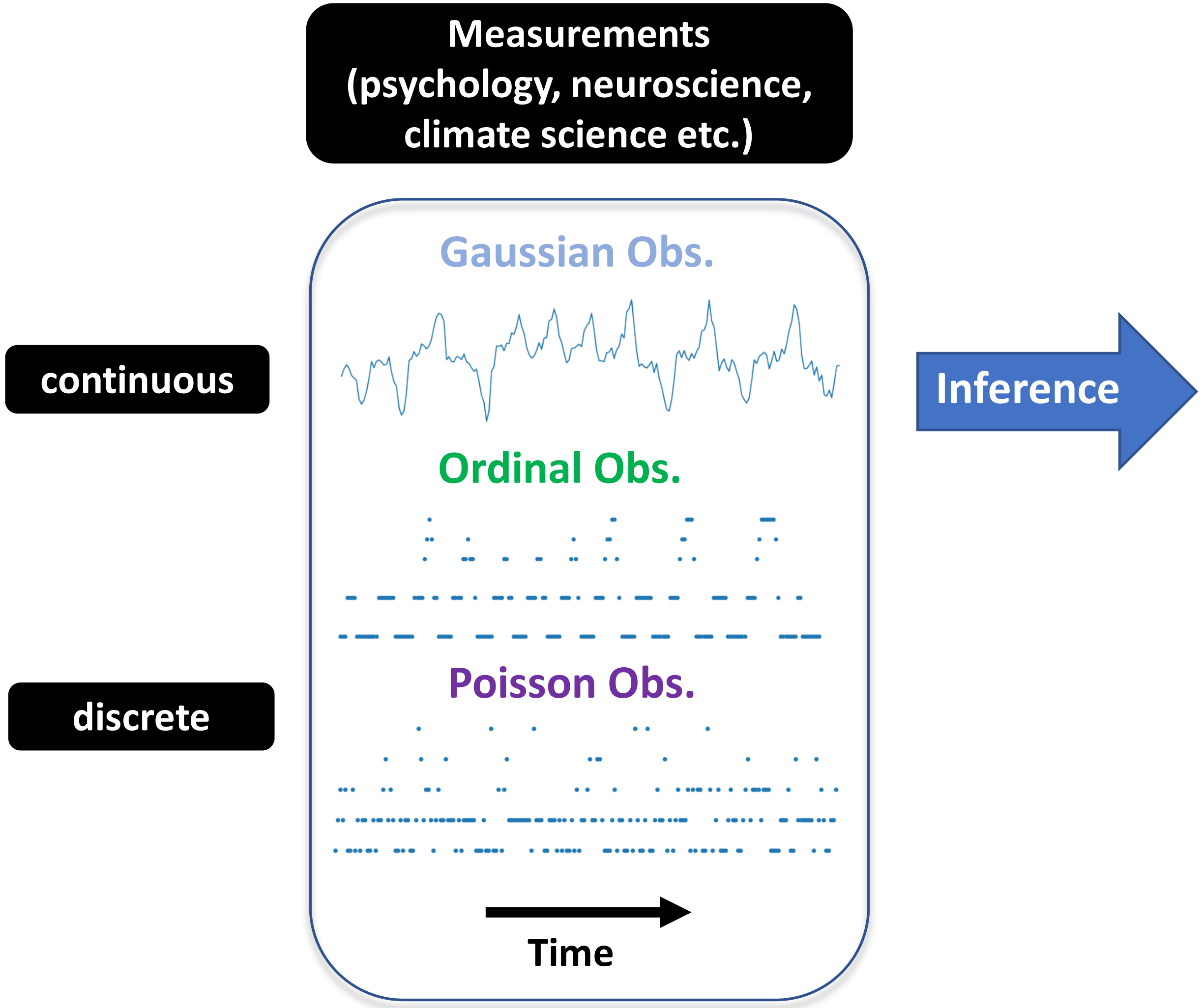
Generic reconstruction model

$$\boldsymbol{z}_t = \boldsymbol{F}_{\boldsymbol{\theta}}(\boldsymbol{z}_{t-1}, \boldsymbol{s}_t)$$
$$\mathbf{x}_t = g(\mathbf{z}_t)$$

Dynamical Systems Reconstructions (DSR)



DSR from Multimodal Time Series

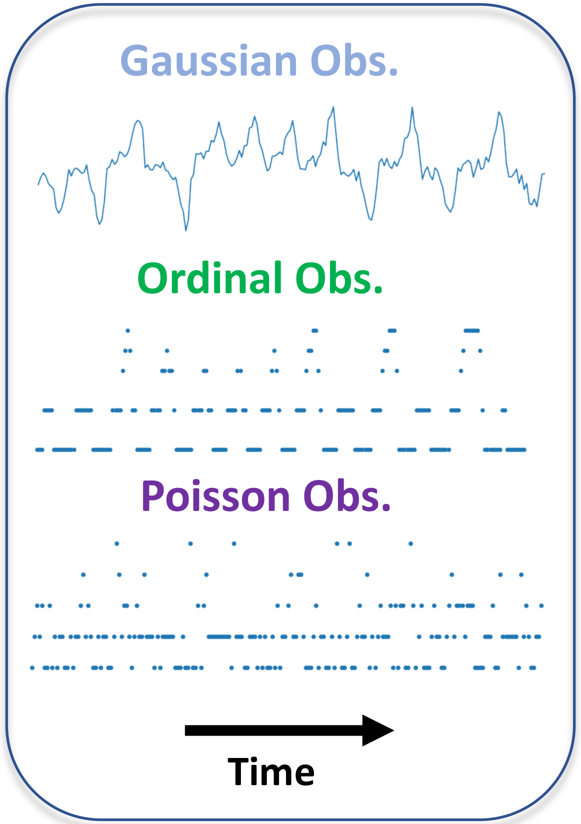


DSR from Multimodal Time Series

Measurements (psychology, neuroscience, climate science etc.)

continuous

discrete



Inference

$$\cdots \; z_{t-1} \rightarrow z_t \rightarrow z_{t+1} \; \cdots$$

dendPLRNN (Brenner, Hess et al., ICML 2022)

Math. tractability

$$\boldsymbol{z}_t = \boldsymbol{A}\boldsymbol{z}_{t-1} + \boldsymbol{W}\phi(\boldsymbol{z}_{t-1}) + \boldsymbol{h}$$

$$\phi(\boldsymbol{z}_{t-1}) = \sum_{b=1}^{B} \alpha_b \max(0, \boldsymbol{z}_{t-1} - \boldsymbol{h}_b)$$

Different distributional assumptions

Gaussian Obs.

$$\boldsymbol{x}_t | \boldsymbol{z}_t \sim \mathcal{N}(\mathbf{B}\boldsymbol{z}_t, \boldsymbol{\Gamma})$$

Ordinal Obs.

$$\boldsymbol{o}_t | \boldsymbol{z}_t \sim \text{Ordinal}(\beta \boldsymbol{z}_t, \epsilon)$$

Poisson Obs.

$$\boldsymbol{p}_t | \boldsymbol{z}_t \sim \text{Poisson}(\lambda(\boldsymbol{z}_t))$$

Challenges of DSR

Challenge

Chaotic dynamics

↓

Divergent loss gradients
(Mikhaeil, Monfared&Durstewitz, NeurIPS 2022)

Theorem 2. *Suppose that an RNN $F_{\boldsymbol{\theta}} \in \mathcal{R}$ (parameterized by $\boldsymbol{\theta}$) has a chaotic attractor Γ^* with $\mathcal{B}_{\Gamma^*}$ as its basin of attraction. Then, for almost every orbit with $\boldsymbol{z}_1 \in \mathcal{B}_{\Gamma^*}$, (i) the Jacobians connecting temporally distal states $\boldsymbol{z}_T$ and $\boldsymbol{z}_t$ ($T \gg t$), $\frac{\partial \boldsymbol{z}_T}{\partial \boldsymbol{z}_t}$, will exponentially explode for $T \to \infty$, and (ii) the tangent vector $\frac{\partial \boldsymbol{z}_T}{\partial \boldsymbol{\theta}}$ and so the gradients of the loss function, $\frac{\partial \mathcal{L}_T}{\partial \boldsymbol{\theta}}$, will diverge as $T \to \infty$.*

Challenges of DSR

Challenge

Chaotic dynamics

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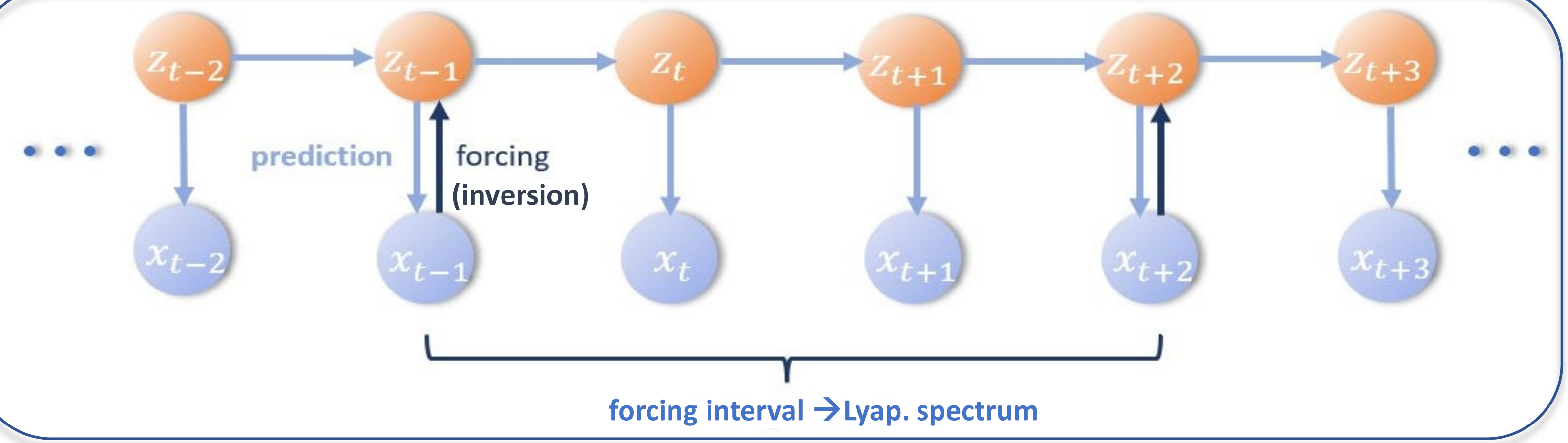
Theorem 2. *Suppose that an RNN $F_{\theta} \in \mathcal{R}$ (parameterized by θ) has a chaotic attractor Γ^* with $\mathcal{B}_{\Gamma^*}$ as its basin of attraction. Then, for almost every orbit with $z_1 \in \mathcal{B}_{\Gamma^*}$, (i) the Jacobians connecting temporally distal states z_T and z_t $(T \gg t)$, $\frac{\partial z_T}{\partial z_t}$, will exponentially explode for $T \to \infty$, and (ii) the tangent vector $\frac{\partial z_T}{\partial \theta}$ and so the gradients of the loss function, $\frac{\partial \mathcal{L}_T}{\partial \theta}$, will diverge as $T \to \infty$.*

Proposed Solution

Sparse teacher forcing (TF)

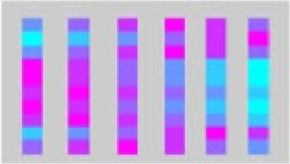


SOTA performance for DSR on unimodal normal data (Brenner, Hess et al., ICML 2022)

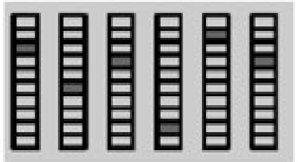
Multimodal Variational Autoencoders

Observations

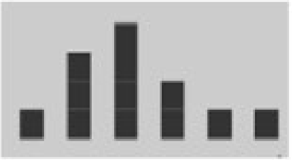
Gaussian Obs.



Ordinal Obs.



Poisson Obs.



$$\boldsymbol{Y} = \{\{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_T\}; \{\boldsymbol{o}_1, \cdots, \boldsymbol{o}_T\}; \{\boldsymbol{c}_1, \cdots, \boldsymbol{c}_T\}\}$$

Encoder (CNN)

Approximate posterior

$$q_{\phi}(\tilde{\boldsymbol{Z}}|\boldsymbol{Y}) = \mathcal{N}(\boldsymbol{\mu}_{\phi}(\boldsymbol{Y}), \boldsymbol{\Sigma}_{\phi}(\boldsymbol{Y}))$$

Decoder

Observation Models

$$\boldsymbol{x}_t \mid \tilde{\boldsymbol{z}}_t \sim \mathcal{N}(\boldsymbol{B}\tilde{\boldsymbol{z}}_t, \boldsymbol{\Gamma})$$

$$\boldsymbol{o}_t \mid \tilde{\boldsymbol{z}}_t \sim \mathrm{Ordinal}(\boldsymbol{\beta}\tilde{\boldsymbol{z}}_t, \epsilon)$$

$$\boldsymbol{c}_t \mid \tilde{\boldsymbol{z}}_t \sim \mathrm{Poisson}(\lambda(\tilde{\boldsymbol{z}}_t))$$

ELBO Loss

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}; \boldsymbol{Y}) = -\mathbb{E}_{q_{\phi}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{Y}|\tilde{\boldsymbol{Z}}) + \log p_{\boldsymbol{\theta}}(\tilde{\boldsymbol{Z}})] - \mathbb{H}_{q_{\phi}}(\tilde{\boldsymbol{Z}} \mid \boldsymbol{Y})$$

Data Likelihoods

$$\log p_{\boldsymbol{\theta}}(\boldsymbol{Y}|\tilde{\boldsymbol{Z}}) = \sum_{t=1}^{T} (\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\tilde{\boldsymbol{z}}_t) + \log p_{\boldsymbol{\theta}}(\boldsymbol{o}_t|\tilde{\boldsymbol{z}}_t) + \log p_{\boldsymbol{\theta}}(\boldsymbol{c}_t|\tilde{\boldsymbol{z}}_t))$$

Multimodal Teacher Forcing (MVAE-TF)

$$\mathcal{L} = \mathcal{L}_{MVAE} + \mathcal{L}_{con} + \mathcal{L}_{PLRNN}$$

MVAE Loss

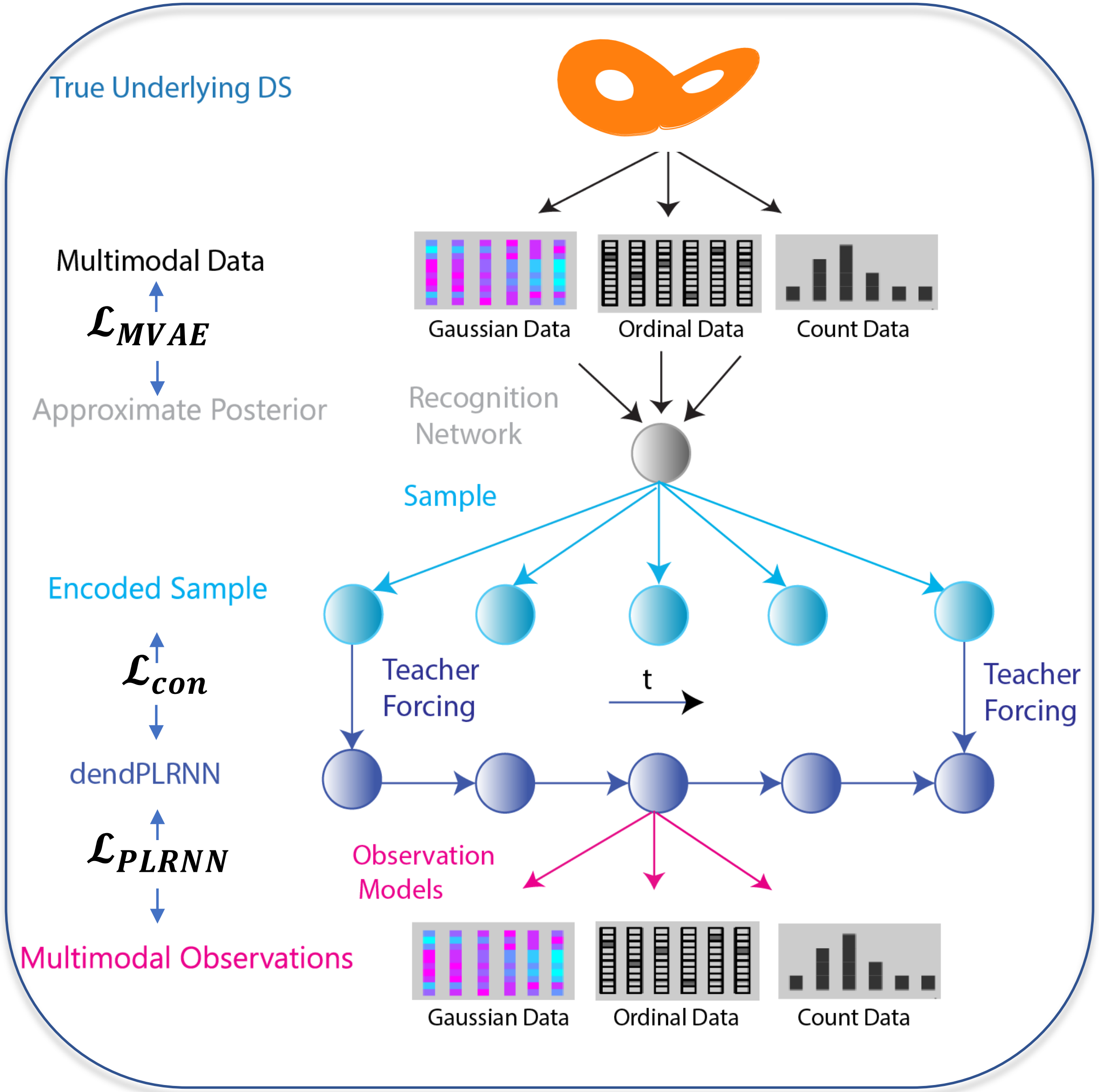
$$\mathcal{L}_{MVAE} = -\mathbb{E}_{q_\phi}[\log p_{\boldsymbol{\theta}}(\boldsymbol{Y}|\tilde{\boldsymbol{Z}}) - \mathbb{H}_{q_\phi}(\tilde{\boldsymbol{Z}} \mid \boldsymbol{Y})$$

Consistency Loss between MVAE and PLRNN

$$\mathcal{L}_{con} = \frac{1}{2}\sum_{t=2}^{T}\left(\log|\boldsymbol{\Sigma}| + (\tilde{\boldsymbol{z}}_t - \boldsymbol{z}_{1:K,t})^\top \boldsymbol{\Sigma}^{-1}(\tilde{\boldsymbol{z}}_t - \boldsymbol{z}_{1:K,t})\right)$$

Data likelihoods from PLRNN

$$\mathcal{L}_{\mathrm{PLRNN}} = -\sum_{t=1}^{T}\left(\log p_{\boldsymbol{\theta}}(\boldsymbol{x_t}|\boldsymbol{z}_{1:K,t}) + \log p_{\boldsymbol{\theta}}(\boldsymbol{o}_t|\boldsymbol{z}_{1:K,t}) + \log p_{\boldsymbol{\theta}}(\boldsymbol{c}_t|\boldsymbol{z}_{1:K,t})\right)$$



Multimodal Reconstructions

Randomly initialized obs. models

Underlying DS

$\boldsymbol{z}_t$

Noisy Gaussian Obs.

$$\boldsymbol{x}_t |\, \boldsymbol{z}_t \sim \mathcal{N}(\boldsymbol{z}_t, \boldsymbol{\Gamma})$$

Ordinal Obs.

$$\boldsymbol{o}_t |\, \boldsymbol{z}_t \sim \text{Ordinal}(\beta \boldsymbol{z}_t, \epsilon)$$

Poisson Obs.

$$\boldsymbol{p}_t |\, \boldsymbol{z}_t \sim \text{Poisson}(\lambda(\boldsymbol{z}_t))$$

Multimodal Reconstructions

Randomly initialized obs. models

Underlying DS

z_t

Noisy Gaussian Obs.

$x_t | z_t \sim \mathcal{N}(z_t, \Gamma)$

Ordinal Obs.

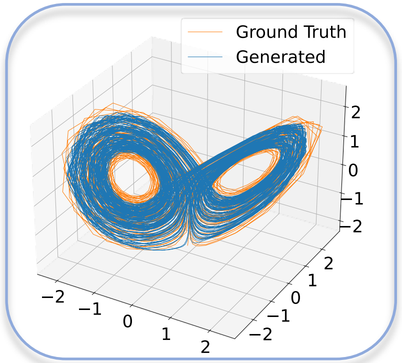
$o_t | z_t \sim \text{Ordinal}(\beta z_t, \epsilon)$

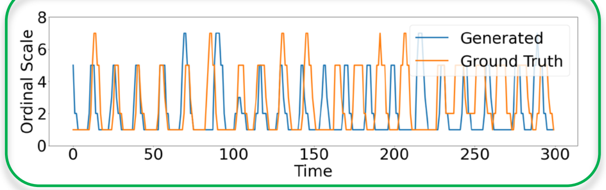
Poisson Obs.

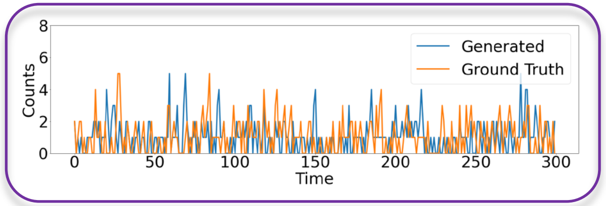
$p_t | z_t \sim \text{Poisson}(\lambda(z_t))$

Geometric Agreement

$$p_{\text{gen}}(\mathbf{x} \mid \mathbf{z})) \approx \sum_{k=1}^{K} \hat{p}_{\text{true}}^{(k)}(\mathbf{x}) \log \left(\frac{\hat{p}_{\text{true}}^{(k)}(\mathbf{x})}{\hat{p}_{\text{gen}}^{(k)}(\mathbf{x} \mid \mathbf{z})} \right)$$

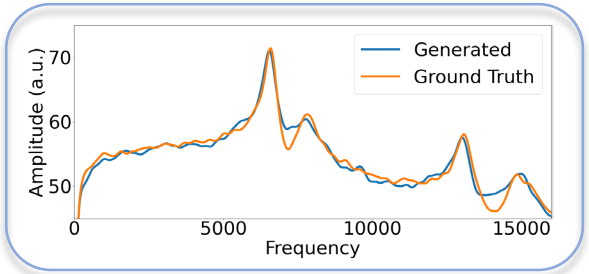


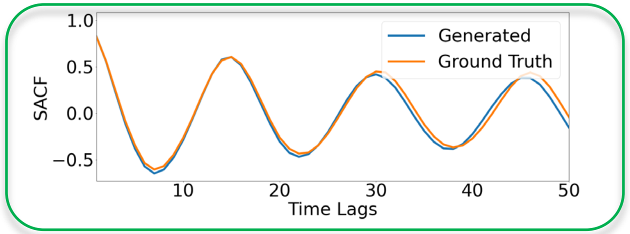


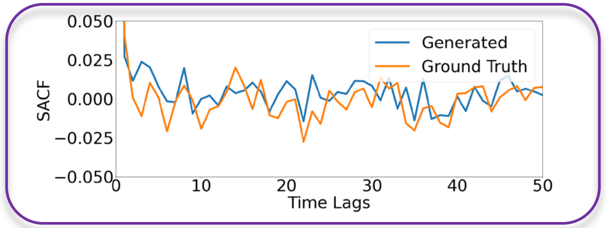


Temporal Agreement

$$H(F(\omega), G(\omega)) = \sqrt{1 - \int_{-\infty}^{\infty} \sqrt{F(\omega)G(\omega)} d\omega} \in [0,1]$$

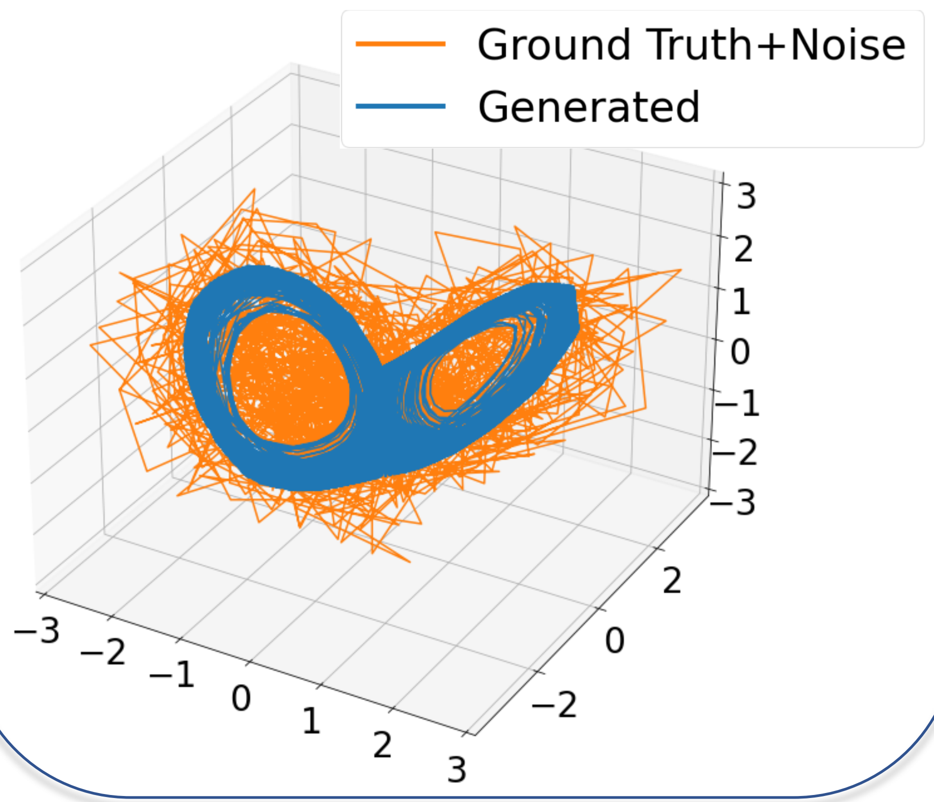




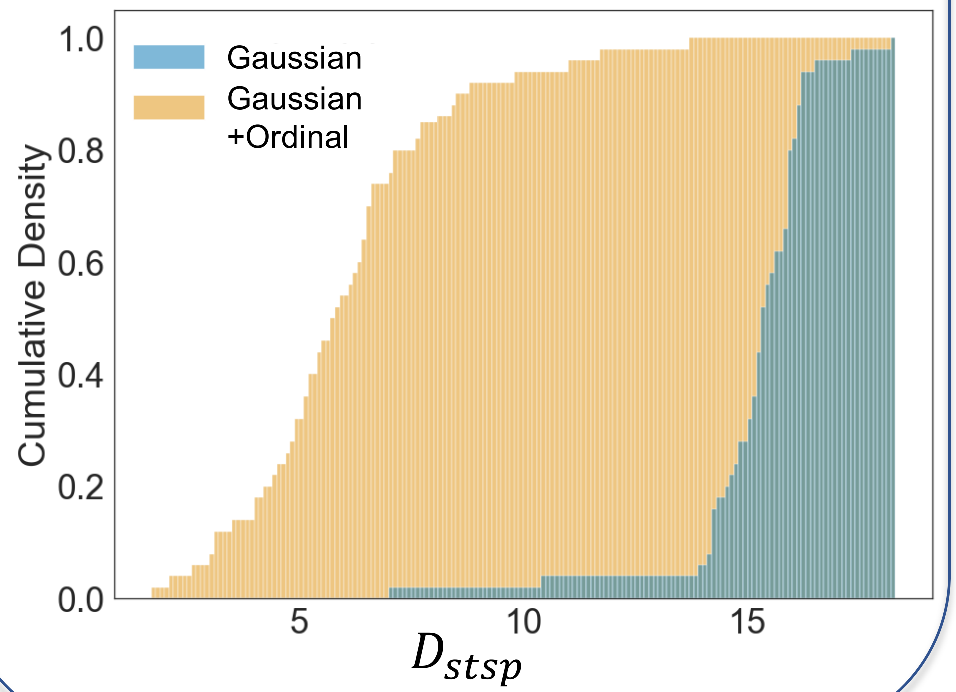


Challenging Data Settings

Reconstructed State Space

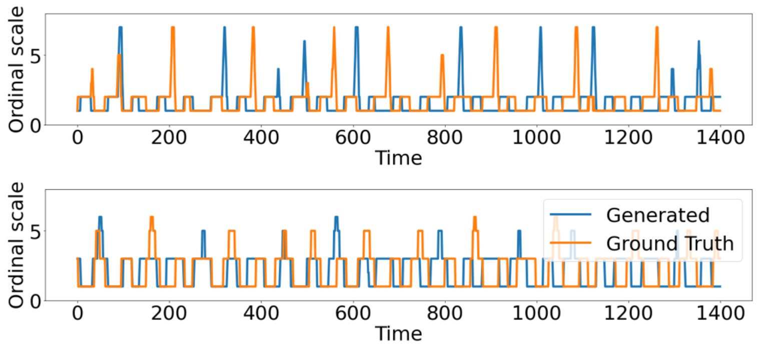


Multimodal Data Improve DSR

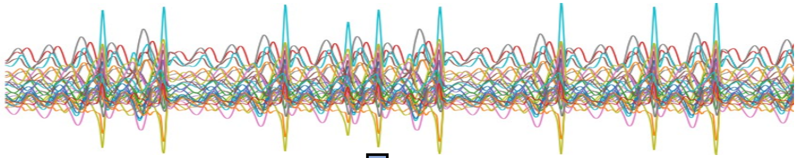


Discrete Observations&Experimental Data

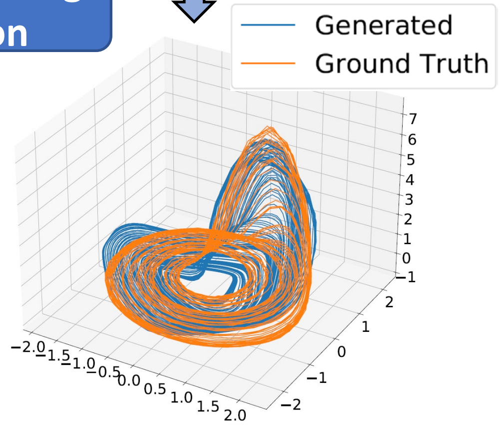
Chaotic Rössler attractor from discrete ordinal observations



Train RNN model



Geometry preserving transformation



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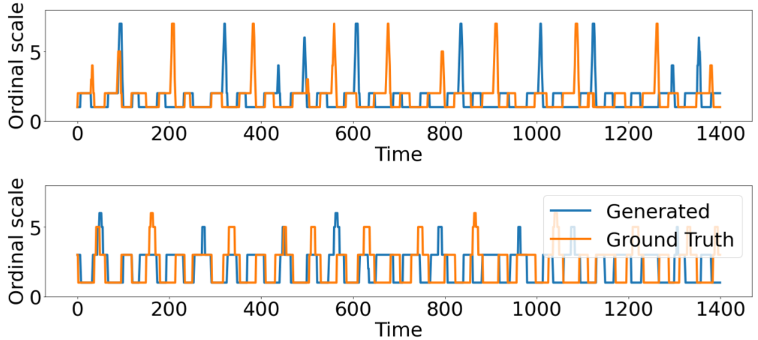
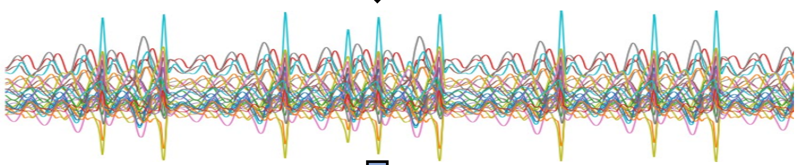
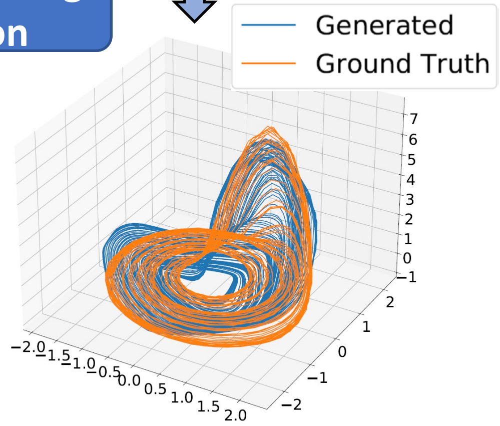


Train RNN model



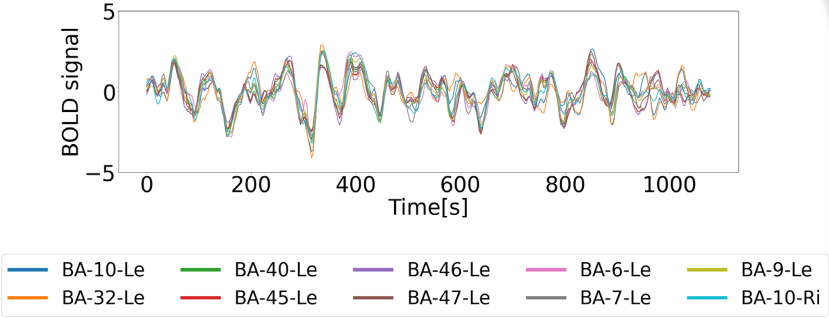
Geometry preserving transformation



Neurophysiological Data+Behavioral Data

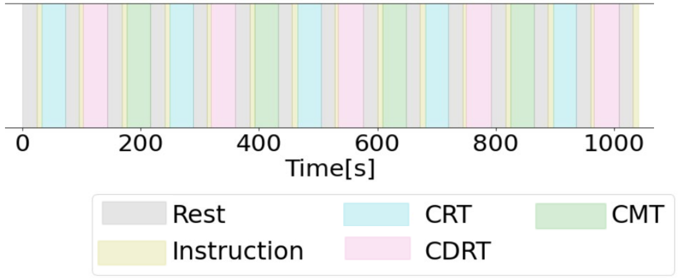
Gaussian Data

$$\boldsymbol{x}_t | \boldsymbol{z}_t \sim \mathcal{N}(\mathbf{B}\boldsymbol{z}_t, \boldsymbol{\Gamma})$$

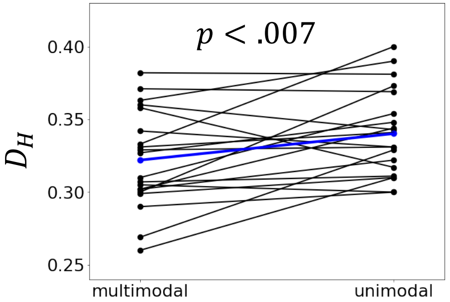


Categorical Data

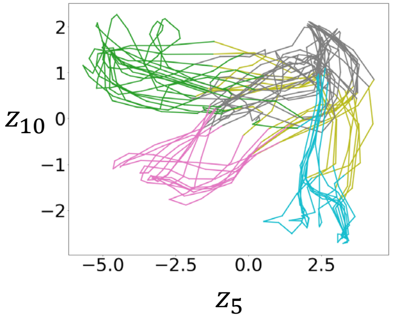
$$\boldsymbol{c}_t | \boldsymbol{z}_t \sim Cat(\boldsymbol{z}_t, \boldsymbol{\beta})$$



Improved DSR



Structured latent activity



Competitive Performance

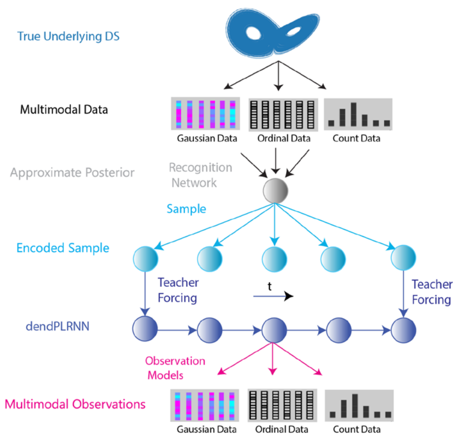
Dataset	Method	$D_{stsp}\downarrow$	$D_H\downarrow$	PE$\downarrow$	OPE$\downarrow$	SCC$\downarrow$	OACF$\downarrow$	CACF$\downarrow$
Lorenz	MVAE-TF	$\mathbf{3.4\pm0.35}$	$\mathbf{0.30\pm0.06}$	$\mathbf{1.3e{-}2\pm2e{-}4}$	$\mathbf{0.12\pm0.03}$	$\mathbf{0.07\pm0.01}$	$\mathbf{0.07\pm0.01}$	$\mathbf{6.6e{-}5\pm8.1e{-}6}$
	SVAE	11.1 ± 0.6	0.82 ± 0.05	$6.3e{-}1\pm5.1e{-}2$	0.68 ± 0.03	0.14 ± 0.01	0.18 ± 0.02	$8.5e{-}5\pm1.6e{-}5$
	GVAE-TF	4.3 ± 0.3	0.47 ± 0.07	$3.6e{-}1\pm1.5e{-}3$	X	X	X	X
	BPTT-TF	8.8 ± 1.9	0.86 ± 0.05	$4.4e{-}1\pm2.2e{-}2$	X	X	X	X
	MS	4.5 ± 1.5	0.61 ± 0.08	X	X	0.14 ± 0.04	0.11 ± 0.02	$\mathbf{6.5e{-}5\pm3.8e{-}6}$
Rössler	MVAE-TF	$\mathbf{1.45\pm0.71}$	$\mathbf{0.32\pm0.03}$	$\mathbf{1.9e{-}3\pm7.1e{-}5}$	$\mathbf{0.08\pm0.02}$	$\mathbf{0.04\pm0.004}$	$\mathbf{0.017\pm0.003}$	$\mathbf{6.5e{-}5\pm1.2e{-}5}$
	SVAE	10.7 ± 1.5	0.66 ± 0.05	$1.5e{-}1\pm3.1e{-}2$	0.24 ± 0.02	0.17 ± 0.03	0.13 ± 0.02	$1.1e{-}4\pm1.4e{-}5$
	GVAE-TF	12.1 ± 0.5	0.55 ± 0.04	$4.9e{-}2\pm3.4e{-}3$	X	X	X	X
	BPTT-TF	8.9 ± 1.4	0.64 ± 0.07	$2.8e{-}1\pm1.8e{-}3$	X	X	X	X
	MS	3.99 ± 1.1	0.59 ± 0.04	X	X	0.08 ± 0.04	0.09 ± 0.02	$1.6e{-}4\pm5.9e{-}5$
Lewis-Glass	MVAE-TF	$\mathbf{0.27\pm0.07}$	$\mathbf{0.33\pm0.02}$	$\mathbf{2.1e{-}3\pm7e{-}5}$	$\mathbf{0.11\pm0.01}$	0.12 ± 0.03	$\mathbf{0.05\pm0.02}$	$2.3e{-}4\pm2.0e{-}5$
	SVAE	2.6 ± 0.5	0.52 ± 0.03	$8.0e{-}2\pm4e{-}3$	0.26 ± 0.01	0.4 ± 0.05	0.18 ± 0.03	$7.5e{-}3\pm4.7e{-}3$
	GVAE-TF	$\mathbf{0.28\pm0.08}$	0.44 ± 0.02	$4.6e{-}3\pm4e{-}4$	X	X	X	X
	BPTT-TF	2.51 ± 0.71	0.43 ± 0.03	$2.6e{-}2\pm3e{-}3$	X	X	X	X
	MS	$\mathbf{0.33\pm0.06}$	$\mathbf{0.35\pm0.01}$	X	X	$\mathbf{0.08\pm0.01}$	$\mathbf{0.04\pm0.002}$	$\mathbf{1.9e{-}4\pm7.5e{-}6}$

Neurophysiological Data

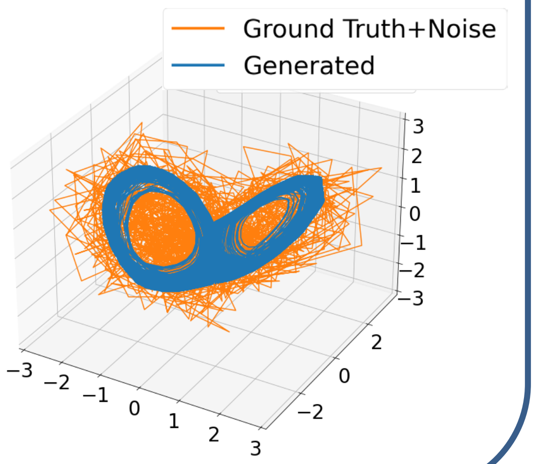
Dataset	Method	$D_{stsp}\downarrow$	$D_H\downarrow$	PE$\downarrow$
fMRI	MVAE-TF	$\mathbf{0.55\pm0.04}$	$\mathbf{0.301\pm0.007}$	$\mathbf{1.21\pm0.08}$
	SVAE	1.9 ± 0.22	0.441 ± 0.019	2.34 ± 0.12
	GVAE-TF	0.67 ± 0.06	0.335 ± 0.011	1.64 ± 0.07
	BPTT-TF	0.63 ± 0.03	0.312 ± 0.006	1.39 ± 0.05
	MS	1.06 ± 0.14	0.373 ± 0.012	X

Conclusions

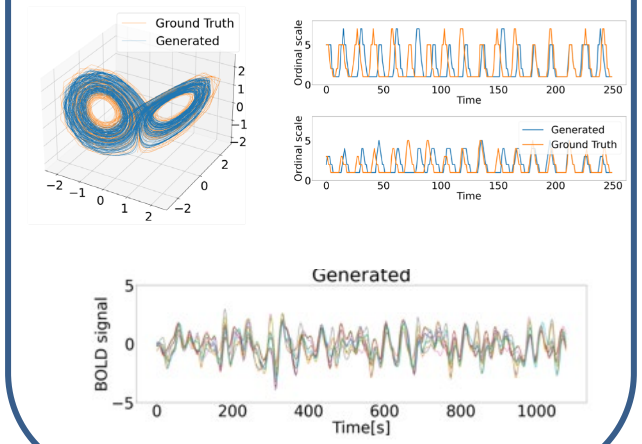
Flexible training framework for DSR from multimodal time series combining sparse TF with MVAEs



DSR from highly noisy and and non-Gaussian obs. from chaotic systems



State of the art performance on benchmark & experimental datasets



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