Neural Information Processing Systems 2024
 Neural Persistence Dynamics

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◆ [Neural Persistence Dynamics](https://github.com/plus-rkwitt/neural_persistence_dynamics) **◆ Orkwitt1982 in [Sebastian Zeng](https://linkedin.com/in/sebastianzeng)**

[∗]�proprietary data (2024).

$$
m\ddot{\mathbf{x}}^k = \left(\alpha - \beta \|\dot{\mathbf{x}}^k\|^2\right) \dot{\mathbf{x}}^k - \frac{1}{K} \nabla_{\mathbf{x}^k} \sum_{l \neq k} U\left(\|\mathbf{x}^k - \mathbf{x}^l\|, C\right)
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$$

, \boldsymbol{r}

- Solving the **inverse problem**, i.e., predicting $\beta = (m, \alpha, C_r, l_r)$, is inherently difficult due to:
	- o the large number of observed entities, and
	- the difficulty of identifying individual motion trajectories $\mathbf{x}^k(t)$.

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The D **'** <code>Orsogna</code> model [D'Orsogna et al. '06] describes the dynamics of individual entities \mathbf{x}^k

- To predict the **models parameters** $\boldsymbol{\beta}$, understanding the evolving τ_0 τ_{150} τ_{160} τ_{150}
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- Solving th**e oge** Hence, we learn the **dynamics in the topology** of time evolving **point clouds**.
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	- the difficulty of identifying individual motion trajectories $\mathbf{x}^k(t)$.

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Problem setting We seek to learn from spatiotemporal data, i.e., from sequences of 3D point clouds P

For learning, we consider datasets of N time-evolving 3D point clouds \mathcal{P}^1 , \dots , \mathcal{P}^N ; e.g., \bullet

Problem setting

- (2) β control such motions and specify (local) interactions among neighboring points, and
- (3) the dynamics in the topology of the point clouds are determined by a simpler latent process **Z**.

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\ddot{\mathbf{x}}^k = f_{\beta} \left(\{ \mathbf{x}^k \}_{l=1}^K, \dot{\mathbf{x}}^k \right)
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We seek to learn **Z** and thus predict $\boldsymbol{\beta}$!
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- (1) applying Vietoris-Rips persistent homology computation, Rips, and
- (2) vectorizing the persistence diagrams, dgm(Rips), using Hofer et al. '19.
	- **Prior works** predominantly extracted **one** topological summary over time.
	- **We** learn a latent process **Z** whose paths $\{\mathbf{z}_{\tau_j}\}_j$ can **(i)** reproduce the vectorizations, and (ii) serve as input for predicting β .

• Z is modeled via a neural ODE by Rubanova et al. '19 and learned in a variational Bayes regime.

A model incarnation

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- In this setting one chooses... \bullet

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(3) a suitable decoder network (Dec_{γ})

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- (3) a suitable decoder network (Dec_{γ}), and
- (4) a suitable regression network (Reg_{α}).

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- (4) a suitable regression network (Reg $_{\alpha}$).

 $\big) \big) - \mathsf{loss}_\mathsf{aux} \left(\mathsf{Reg}_\pmb{\alpha}(\{ \mathbf{z}_{\tau_j} \}_j) , \pmb{\beta} \right) \, .$

model is trained upon choosing a prior
$$
p(\mathbf{z}_{t_0})
$$
 and maximizing (ELBO – loss_{aux}), i.e.,
\n
$$
\theta, \gamma, \alpha = \underset{\theta, \gamma, \alpha}{\arg \max} \underbrace{\mathbb{E}_{\mathbf{z}_{t_0} \sim q_{\theta}} \Big[\sum_j \log p_{\gamma} (\mathbf{v}_{\tau_j} | \mathbf{z}_{\tau_j}) \Big] - \mathcal{D}_{KL} \big(q_{\theta} \big(\mathbf{z}_{t_0} | \{ \mathbf{v}_{\tau_j} \}_j \big) || p \big(\mathbf{z}_{t_0} \big) \Big) - \underset{\text{aux} \text{aux}}{\text{loss}_{aux}} \big(\text{Reg}_{\alpha}(\{ \mathbf{z}_{\tau_j} \}_j), \beta \big)}.
$$
\n
$$
\text{ELBO} \qquad \text{auxiliary loss}
$$

The model is trained upon choosing a prior $p(\mathbf{z}_{t_0})$ and maximizing (ELBO $-$ loss $_{\mathtt{aux}}$), i.e.,

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- We compare against *path signature kernel (PSK)* [Giusti & Lee '23] & *crocker stacks* [Xian et al. '22] and report *Variance Explained (VE)* and *Symmetric Mean Absolute Percentage Error (SMAPE)*.

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- and report *Variance Explained (VE) and Symmetric Mean Absolute Percentage Error (SMAPE).*
Overall, **Neural Persistence Dynamics (Ours)** largely outperforms the state-of-the-art in all tasks.

In summary, **Neural Persistence Dynamics**...

(1) scales to a **large number** of observation sequences,

(2) is trained with **fixed hyperparameters** across all datasets, <u>and</u>

(3) **outperforms** the state-of-the-art across

Thanks for your attention!

Come see us at our **poster**. Fr. 13 Dec 11 a.m. PST – 2 p.m. PST @ Poster Session 5 In summary, Neural Persistence Dynamics...

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