Neural Information Processing Systems 2024

Neural Persistence Dynamics



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• Neural Persistence Dynamics

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in Sebastian Zeng



• Observation of a coherently moving flock of birds, understood as an evolving 3D point cloud $\mathcal{P} = \{\mathbf{x}^k\}_{k=1}^K$:



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

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

Attraction & Repulsion





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Attraction & Repulsion

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

 $C_r, l_r)$.

• Observation of a coherently moving flock of birds, understood as an evolving 3D point cloud $\mathcal{P} = \{\mathbf{x}^k\}_{k=1}^K$:



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- To predict the models parameters β, understanding the evolving behavioral patterns of a collective is key.
- Solving the Hence, we learn the **dynamics in the topology** of time evolving **point clouds**.
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 - the difficulty of identifying individual motion trajectories $\mathbf{x}^{k}(t)$.



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



Problem setting



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- We assume...
 - (1) individual trajectories of points \mathbf{x}^k are governed by a coupled equation of motion

$$\ddot{\mathbf{x}}^{k} = f_{\boldsymbol{\beta}}\left(\{\mathbf{x}^{k}\}_{l=1}^{K}, \dot{\mathbf{x}}^{k}\right)$$

- (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 \mathbf{Z} .

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We seek to learn **Z** and thus predict β !

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For each sequence \mathcal{P} , we pre-compute topological features **per time point**, by... \bullet



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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 $\{z_{\tau_i}\}_i$ can (i) reproduce the vectorizations, and (ii) serve as input for predicting β .

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- In this setting one chooses... \bullet



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- (1) an encoder network (Enc_{θ}) ,
- (2) an ODE solver,
- (3) a suitable decoder network (Dec_{γ}), <u>and</u>
- (4) a suitable regression network (Reg_{κ}) .

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

$$\boldsymbol{\theta}, \boldsymbol{\gamma}, \boldsymbol{\alpha} = \underset{\boldsymbol{\theta}, \boldsymbol{\gamma}, \boldsymbol{\alpha}}{\operatorname{arg\,max}} \mathbb{E}_{\mathbf{z}_{t_0} \sim q_{\boldsymbol{\theta}}} \left[\sum_{j} \log p_{\boldsymbol{\gamma}} \left(\mathbf{v}_{\tau_j} | \mathbf{z}_{\tau_j} \right) \right] - \mathcal{D}_{\mathsf{KL}} \left(q_{\boldsymbol{\theta}} \left(\mathbf{z}_{t_0} | \{ \mathbf{v}_{\tau_j} \}_j \right) \| p\left(\mathbf{z}_{t_0} \right) \right) - \underbrace{\mathsf{ELBO}}_{\mathsf{ELBO}} \right]$$

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

 $\operatorname{loss}_{\operatorname{aux}}\left(\operatorname{Reg}_{\alpha}(\{\mathbf{z}_{\tau_i}\}_j),\boldsymbol{\beta}\right)$.

auxiliary loss

		⊘ VE ↑	⊘ SMAPE↓
dorsogna-10k	Ours	0.851 <u>+</u> 0.008	0.097 ±0.005
	PSK	0.828 <u>+</u> 0.016	0.096 <u>+</u> 0.006
	Crocker Stacks	0.746 <u>+</u> 0.023	0.150 <u>+</u> 0.005
vicsek-10k	Ours	0.579 <u>+</u> 0.034	0.146 ±0.006
	PSK	0.466 <u>+</u> 0.009	0.173 <u>+</u> 0.003
	Crocker Stacks	0.345 <u>+</u> 0.005	0.190 <u>+</u> 0.001

Listed are parameter regression results from two models [D'Orsogna et al. '06 & Vicsek et al. '95] for collective behavior with $|\beta| = 4$, resp.

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- Each dataset contains 10,000 point cloud sequences simulated using SiSyPHE [Diez '21].

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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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- 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).
- 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 numerous regression tasks.

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Thanks for your attention!

Come see us at our **poster**. Fr. 13 Dec 11 a.m. PST – 2 p.m. PST @ Poster Session 5

C Full source code is available!





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