Machine Learning of Self Organization from Observation

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Emergent Collective Behaviors: Integrating Simulation and Experiment 2022

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Motivation: Interesting Patterns

Self Organization

Figure: Stripes on Zebra, Source: Wiki

Motivation: Interesting Patterns

Self Organization

Figure: Flocking of Birds, Source: Wiki

Motivation: Interesting Patterns

Self Organization

Figure: Milling of Fish, Source: Wiki

Learning Self Organization

Interaction Laws[1]

Inferring ϕ from observation

Can the interaction be learned?

[1] Lu, **Zhong**, Tang, Maggioni, PNAS, 2019.

Learning Self Organization

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Consider a system of N agents, each of which is assigned $\mathbf{x}_i \in R^d$,

$$\frac{d\mathbf{x}_i(t)}{dt} = -\partial_{\mathbf{x}_i} E(\mathbf{x}_1(t), \ldots, \mathbf{x}_N(t)), \quad i = 1, \ldots, N.$$

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$$\frac{d\mathbf{x}_i(t)}{dt} = -\partial_{\mathbf{x}_i}\Big(\underbrace{\frac{1}{N}\sum_{1\le i<i'\le N} U(\big|\mathbf{x}_{i'}(t) - \mathbf{x}_i(t)\big|)}_{=E(\mathbf{x}_1(t),\ldots,\mathbf{x}_N(t))}\Big), \quad i = 1,\ldots,N.$$

Here $U(0) = 0$ and $\lim_{\mathbf{r}\to\mathbf{0}} U'(\big|\mathbf{r}\big|)\mathbf{r} = \mathbf{0}$.

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Consider a system of N agents, each of which is assigned $\mathbf{x}_i \in R^d$,

$$\dot{\mathbf{x}}_i = \frac{1}{N}\sum_{i'=1}^{N} \phi(\left|\mathbf{x}_{i'} - \mathbf{x}_i\right|)(\mathbf{x}_{i'} - \mathbf{x}_i), \quad i = 1, \dots, N. \tag{1}$$

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- $\phi : \mathbb{R}^+ \to \mathbb{R}$ with $\phi(r) = \frac{U'(r)}{r}$ is the **interaction law**; $\left|\cdot\right|$: Euclidean norm.

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- Known ϕ

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- $\phi : \mathbb{R}^+ \to \mathbb{R}$ with $\phi(r) = \frac{U'(r)}{r}$ is the **interaction law**; $\left| \cdot \right|$: Euclidean norm.
- Known $\phi \Rightarrow$ emergent behaviors (clustering, flocking, milling, etc.).

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- Known $\phi \Rightarrow$ emergent behaviors (clustering, flocking, milling, etc.).

For Example:

$$\phi(r) = \mathbf{1}_{[0,\frac{1}{2})} + 0.1 * \mathbf{1}_{[\frac{1}{\sqrt{2}},1]}.$$

It induces clusters.

[1] Lu, **Zhong**, Tang, Maggioni, PNAS, 2019.

Learning Self Organization

Interaction Laws, cont.

Moreover

$$\phi(r) = r^{q-1} - r^{p-1}, \quad 0 \leq p < q.$$

It induces ring-like patterns.

Learning Self Organization

Interaction Laws, cont.

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$$\phi(r) = r^{q-1} - r^{p-1}, \quad 0 \leq p < q.$$

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$$\phi(r) = -\frac{\tanh((1-r)a) + b}{r}, \quad a > 0, -1 < b < 1.$$

It induces soccer ball like patterns.

Learning Self Organization

Interaction Laws, cont.

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It induces soccer ball like patterns.

Inverse Problem

Given $\{\mathbf{x}_i(t), \dot{\mathbf{x}}_i(t)\}_{i=1}^N$ for $t \in [0, T]$, can ϕ be learned?
Input: $\{\mathbf{x}_i(t), \dot{\mathbf{x}}_i(t)\}_{i=1}^N$ for $t \in [0, T]$, including agent information.
Output: ϕ: **interaction law**.

Learning Self Organization

The Variational Approach

Given $\{\mathbf{X}_{t_l}^{(m)}, \dot{\mathbf{X}}_{t_l}^{(m)}\}_{l,m=1}^{L,M}$ with $0 = t_1 < \cdots < t_L = T$ and $\mathbf{X}_0^{(m)} \sim \mu^N(\mathbb{R}^D)$

Learning Self Organization

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$$\mathcal{E}_{L,M,\mathcal{H}}(\varphi) = \frac{1}{LM}\sum_{l,m=1}^{L,M} \left|\dot{\mathbf{X}}_{t_l}^{(m)} - \mathbf{f}_\varphi(\mathbf{X}_{t_l}^{(m)})\right|_{\mathcal{S}}^2,$$

Here $\left|\mathbf{X}_t\right|_{\mathcal{S}}^2 = \frac{1}{N}\sum_{i=1}^N \left|\mathbf{x}_i(t)\right|^2$ and $\varphi \in \mathcal{H}$ (compact and convex).

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Theorem (Lu, Maggioni, Tang, **Zhong**, 2019)

When $\hat{\phi}_{L,M,\mathcal{H}_M}$*'s constructed from* $\mathcal{H}_M$ *with* $\dim(\mathcal{H}_M) = \mathcal{O}(M^{\frac{1}{3}})$,

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- Independent of the dimension of the observation data, i.e. $D = Nd \gg 1$.

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- Learning Rate in M is optimal ($1D$ regression rate).
- Independent of the dimension of the observation data, i.e. $D = Nd \gg 1$.
- Package: `https://github.com/MingZhongCodes/LearningDynamics`.

Learning Self Organization

Opinion Dynamics

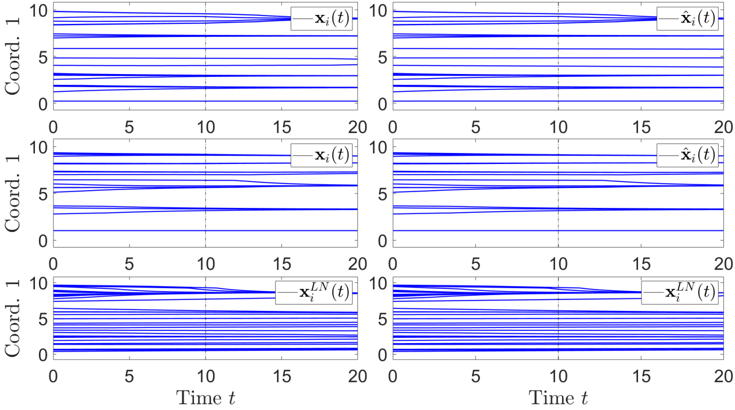

Figure: $\mathbf{X}$ vs. $\hat{\mathbf{X}}$[2].

[2] Lu, Z., Tang, Maggioni, PNSA, 2019.

Learning Self Organization

Opinion Dynamics

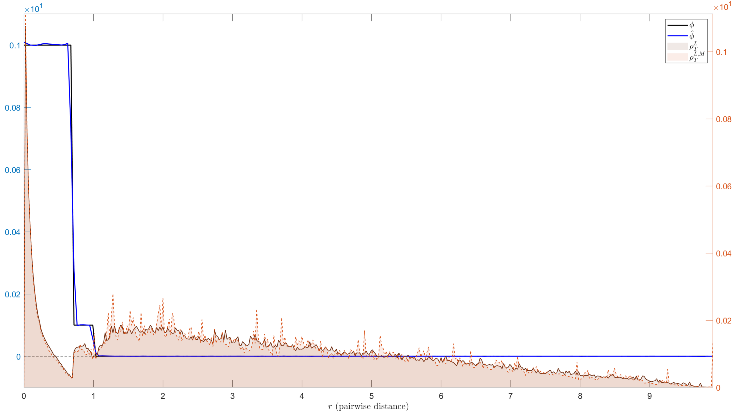

Figure: ϕ vs. $\hat{\phi}$, ρ_T^L vs. $\rho_T^{L,M2}$.

[2] Lu, Z., Tang, Maggioni, PNSA, 2019.

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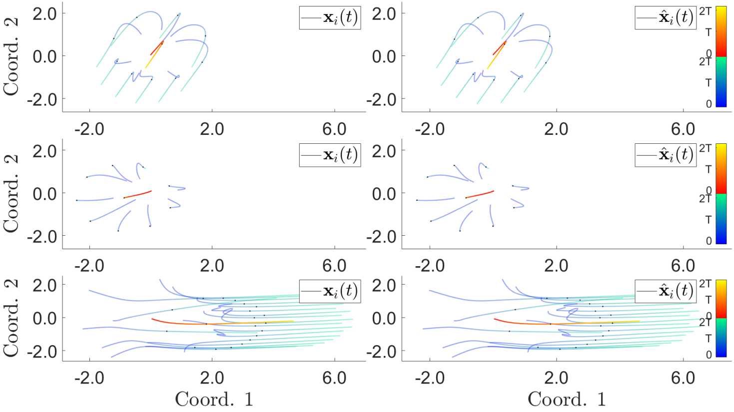
Applications

Heterogeneous Agents[3]

Predator-Preys Dynamics



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Heterogeneous Agents[3]

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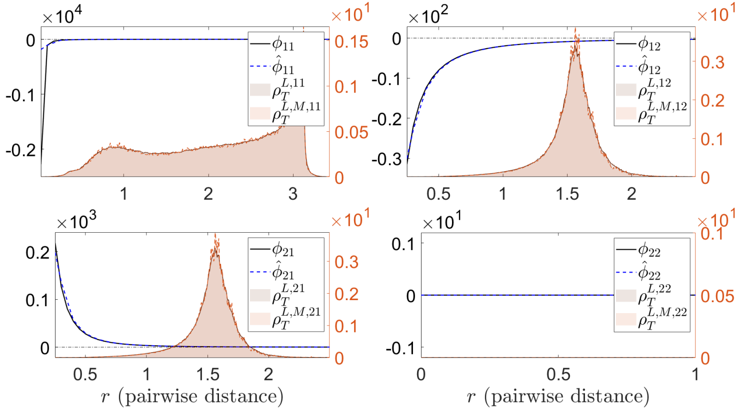

Figure: $\phi_{k,k'}$ vs. $\hat{\phi}_{k,k'}$.

[3]Lu, **Zhong**, Tang, Maggioni, PNSA, 2019.

Applications

Second Order Systems

Fill-Mill $2D$

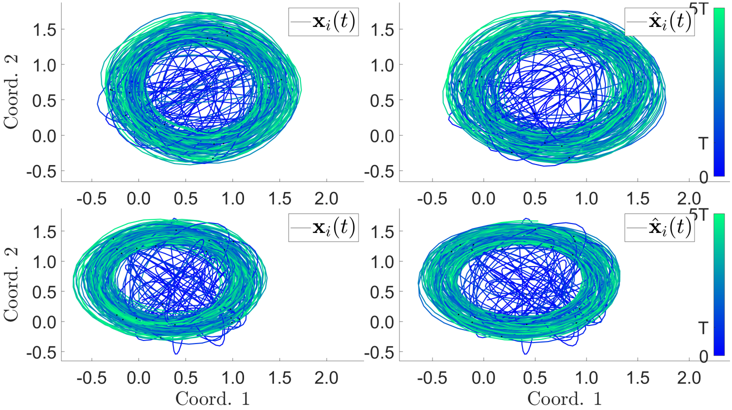

Figure: **X** vs. $\hat{\mathbf{X}}$[4].

[4] **Zhong**, Miller, Maggioni, Physica D, 2020.

Applications

Second Order Systems

Anticipation Dynamics

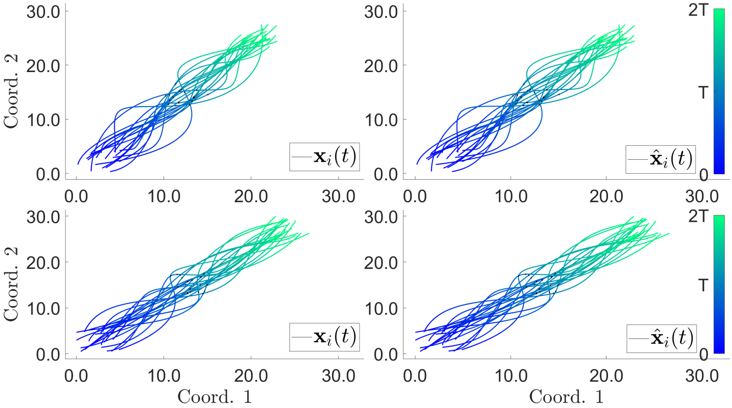

Figure: ϕ vs. $\hat{\phi}$[4].

[4] Miller, Tang, **Zhong**, Maggioni, submitted, 2020

Applications

Dynamics on Manifold[5]

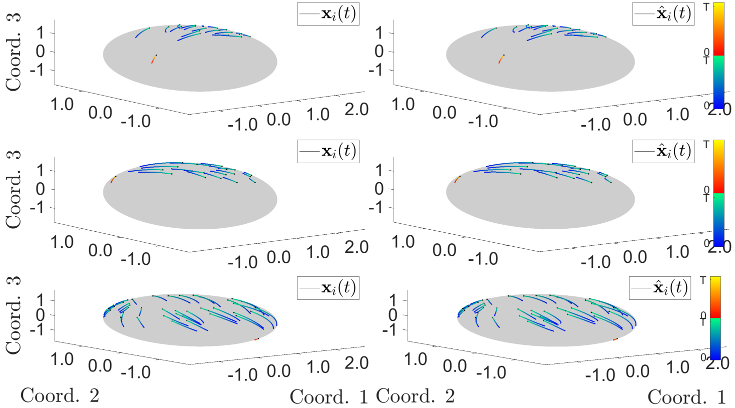

Figure: **X** vs. $\hat{\mathbf{X}}$.

[5]Maggioni, Miller, Qiu, **Zhong**, PMLR for 38^{th} ICML, 2021.

Applications

Dynamics on Manifold[5]

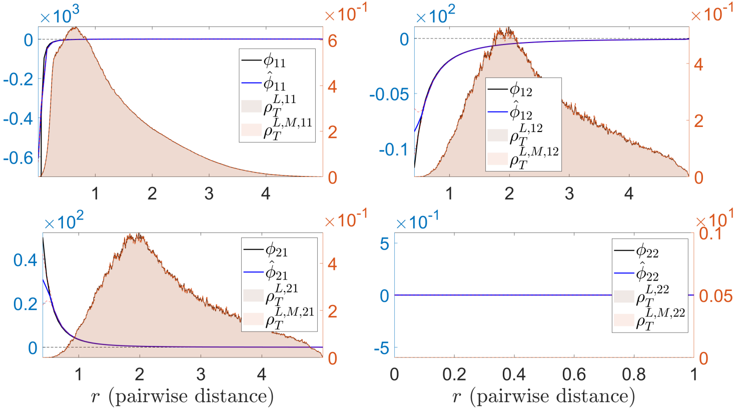

Figure: $\phi_{k,k'}$ vs. $\hat{\phi}_{k,k'}$.

[5] Maggioni, Miller, Qiu, **Zhong**, PMLR for 38^{th} ICML, 2021.

Applications

Celestial Dynamics (Traj)[6]

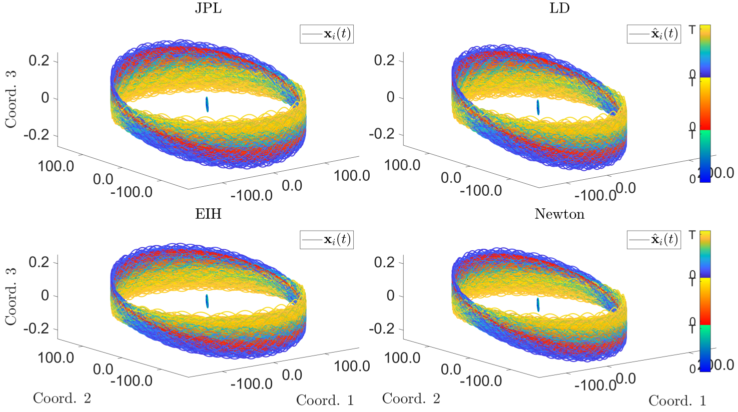

Figure: Earth-Moon-Sun System

[6] **Zhong**, Miller, Maggioni, submitted, 2021.

Applications

Celestial Dynamics (Traj)[6]

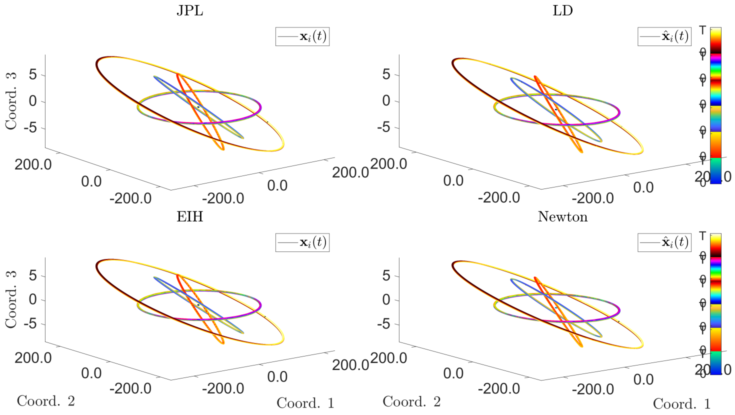

Figure: Inner Solar System

[6] **Zhong**, Miller, Maggioni, submitted, 2021.

Applications

Celestial Dynamics (Traj)[6]

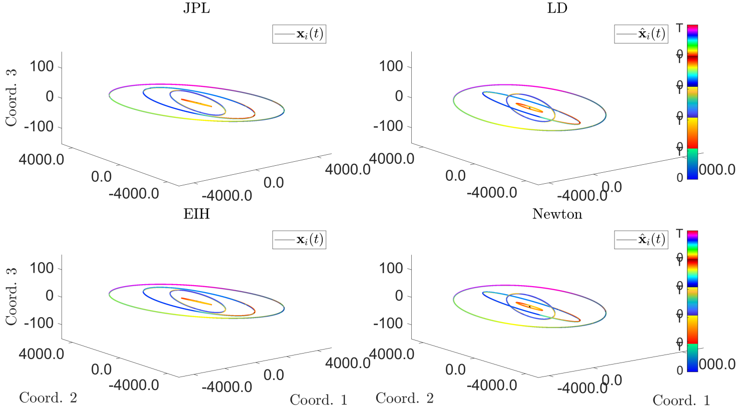

Figure: Outer Solar System

[6] **Zhong**, Miller, Maggioni, submitted, 2021.

Applications

Celestial Mechanics: Estimating Masses

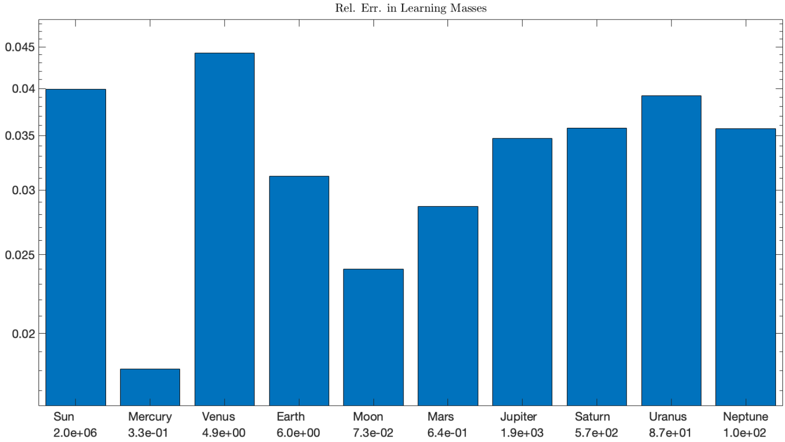

Figure: Mass Estimation from Learned Interaction Kernels.

Applications

Celestial Mechanics: Estimating Masses

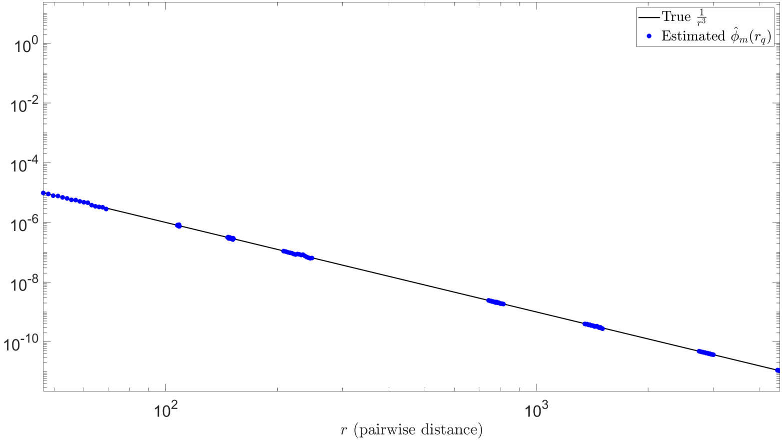

Figure: Shared Kernel Function.

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Ongoing Projects

Feature Map Learning[7]

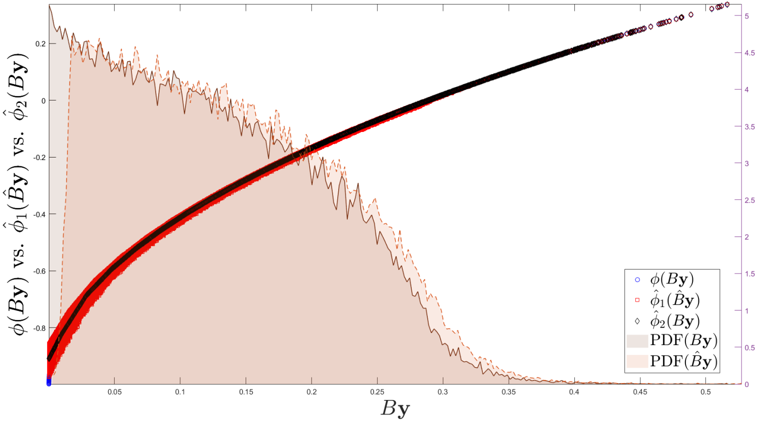

Figure: $\Phi(\mathbf{x}_i, \mathbf{x}_{i'})$ vs other estimated pairs (Power Law).

[7] Feng, Maggioni, Martin, **Zhong**, submitted 2022.

Ongoing Projects

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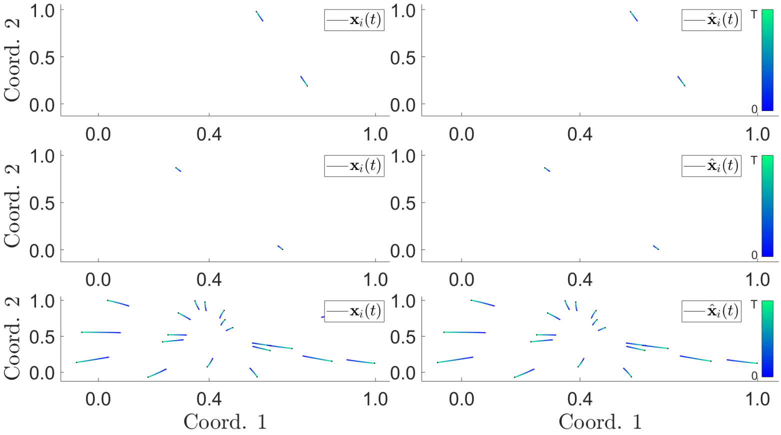

Figure: **X** vs. $\hat{\mathbf{X}}$.

[7] Feng, Maggioni, Martin, **Zhong**, submitted 2022.

Ongoing Projects

Learning from Steady State Patterns[8]

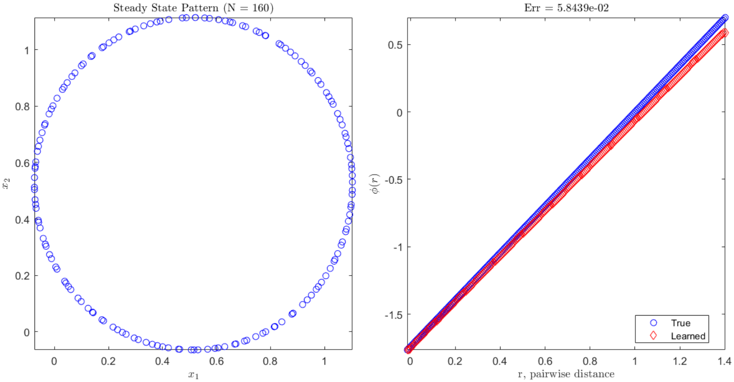

Figure: Learn from Steady State Patterns.

[8] Maggioni, **Zhong**, in preparation, 2022.

Future Projects

Physics-informed Machine Learning

Ongoing:

Future Projects

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- Semi-supervised learning: no type information; changing types, changing N, etc.

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Forward Approach

For different kinds of Self Organization

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Inverse Problem Approach

SINDy, ROM, PINN, Neural ODEs, Bayesian Inference, etc.

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Q and A

Questions?

Thank You!!