Physics-informed Machine Learning of Collective Behaviors

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Abstract

We developed a learning framework in [1] to discover the dynamical structure, namely interaction kernels between agents, for explaining collective behaviors (clustering, flocking, milling, etc.) from observation data. We study the steady state behaviors of the estimated dynamics evolved from the estimated interaction kernels in [2], and completed the learning theory for extended second order systems in [3]. We then extend the learning theory to dynamics constrained on Riemannian manifolds in [4], and apply to study celestial motion in the Solar system from NASA JPL's develop ephemerides in [5]. Our physics-informed machine learning method can be used to validate and improve the modeling of **collective dynamics**.

Model Equations

The governing equations for first-order dynamics is derived from a gradient flow approach,

$$\dot{\boldsymbol{x}}_i(t) = \frac{1}{N}\sum_{i'=1}^{N}\phi(r_{i,i'}(t))\boldsymbol{r}_{i,i'}(t), \quad i = 1, \cdots, N. \tag{1}$$

The second-order dynamics is derived from conservation of a Lagrangian:

$$\begin{aligned} \dot{\boldsymbol{x}}_i(t) &= \boldsymbol{v}_i(t) \\ \dot{\boldsymbol{v}}_i(t) &= \frac{1}{N}\left[\phi^E(r_{i,i'}(t))\boldsymbol{r}_{i,i'}(t) + \phi^A(r_{i,i'}(t))\boldsymbol{s}_{i,i'}(t)\right] \end{aligned}, \quad i = 1, \cdots, N. \tag{2}$$

The variables are:

$\boldsymbol{x}_i \in \mathbb{R}^d$:	state/position vector	$\boldsymbol{v}_i \in \mathbb{R}^d$:	velocity
d:	length of state	N:	Number of agents
ϕ, ϕ^E, ϕ^A:	interaction kernels	$r_{i,i'}$:	$\\|\boldsymbol{x}_{i'} - \boldsymbol{x}_i\\|$, pairwise distance
$\boldsymbol{r}_{i,i'}$:	$\boldsymbol{x}_{i'} - \boldsymbol{x}_i$	$\boldsymbol{s}_{i,i'}$:	$\boldsymbol{v}_{i'} - \boldsymbol{v}_i$

The Empirical Error Functional

Given a set of continuous trajectories, $\{\boldsymbol{x}_i^{(m)}(t), \boldsymbol{v}_i^{(m)}(t)\}_{i,m=1}^{N,M}$ for $t \in [0, T]$, we infer the interaction kernel, ϕ, from minimizing the following **Empirical Error Functional**,

$$\mathcal{E}(\varphi) = \frac{1}{MTN}\sum_{i,m=1}^{N,M}\int_{t=0}^{T}\left\|\dot{\boldsymbol{x}}_i^{(m)}(t) - \frac{1}{N}\sum_{i'=1}^{N}\varphi(r_{i,i'}^{(m)}(t)\boldsymbol{r}_{i,i'}^{(m)}(t)\right\|^2 dt, \tag{3}$$

for $\varphi \in \mathcal{H}$, a compact/convex subspace of $L^2([0, R])$. See [1, 2, 3] for details on second-order learning.

The Algorithm

Given $\{\boldsymbol{x}_i^{(m)}(t_l), \boldsymbol{v}_i^{(m)}(t_l)\}_{i,m,l=1}^{N,M,L}$,

1. Construct a finite dimensional $\mathcal{H}_M$;
2. Discretize (3);
3. Assemble the learning matrix/RHS;
4. Solve the linear system.

Details for the actual algorithms, see [1, 2, 3]

Numerical Results

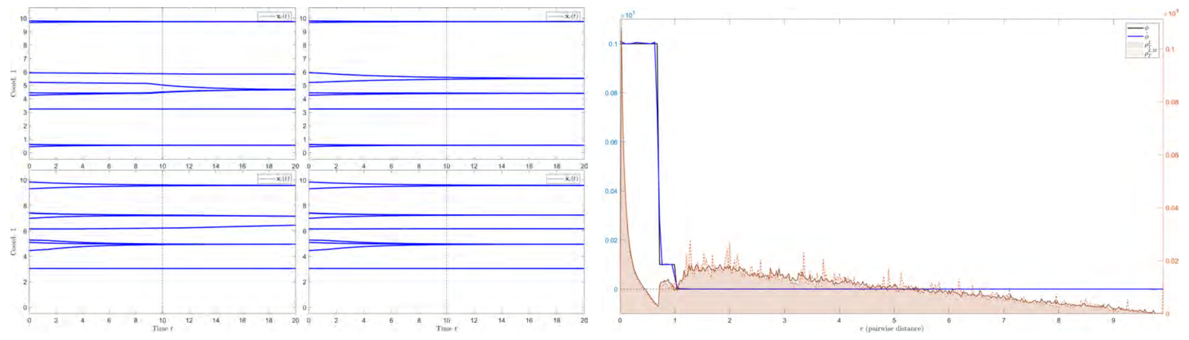

Figure 1: Opinion Dynamics

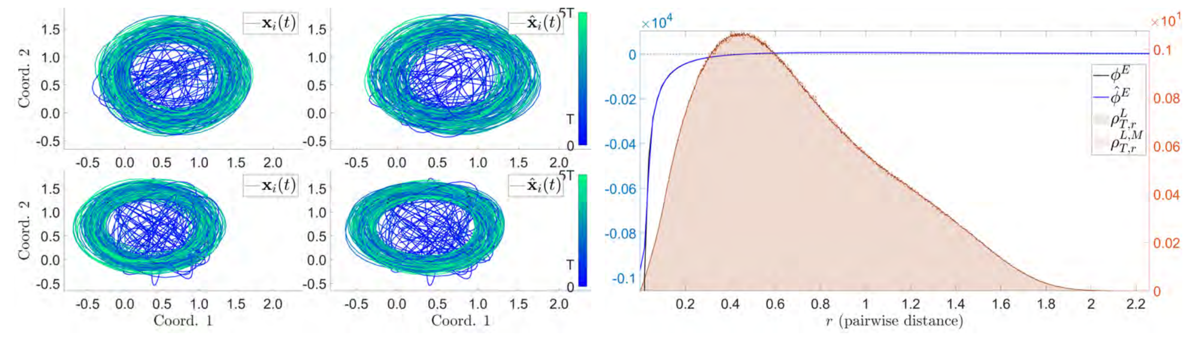

Figure 2: Fish Mill $2D$

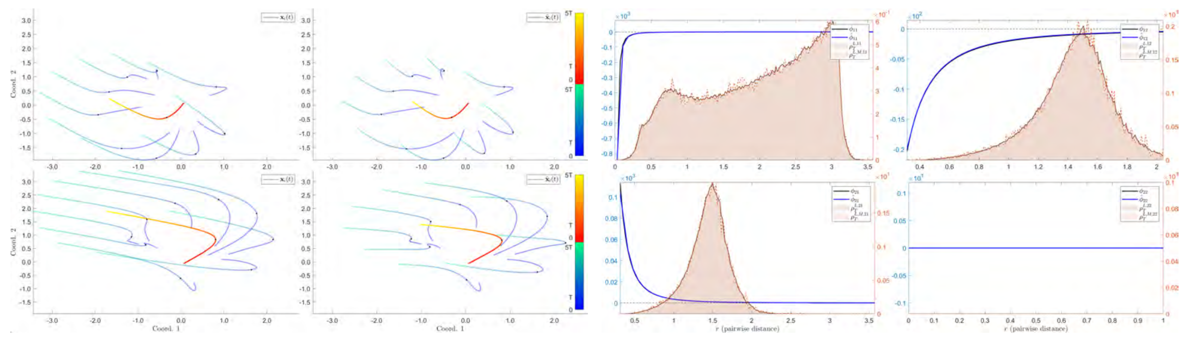

Figure 3: Predator-Preys Dynamics

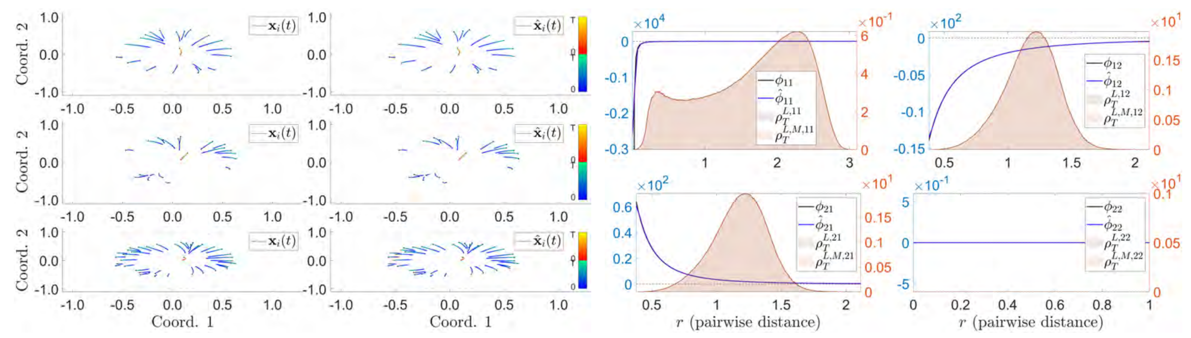

Figure 4: Predator-Preys Dynamics on Manifolds

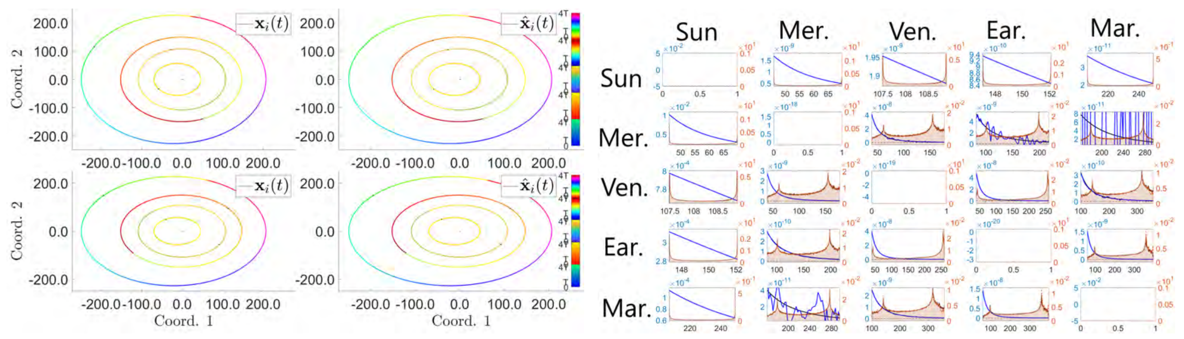

Figure 5: Simulated Newton's

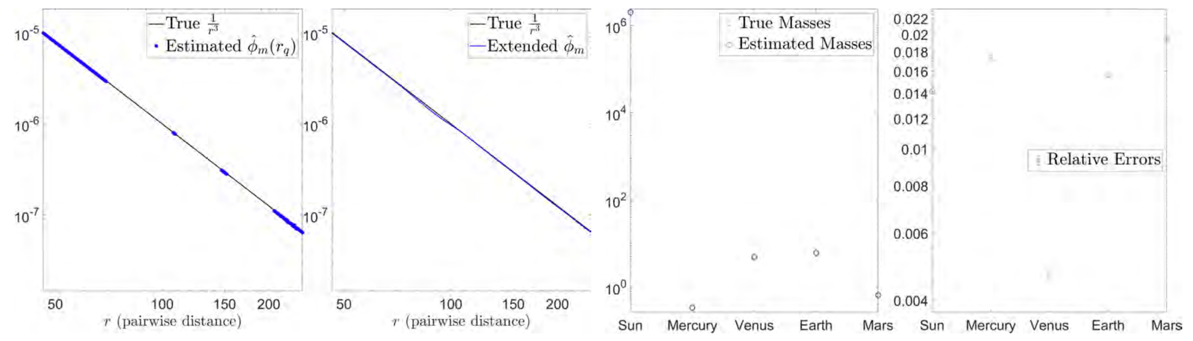

Figure 6: Simulated Newton's

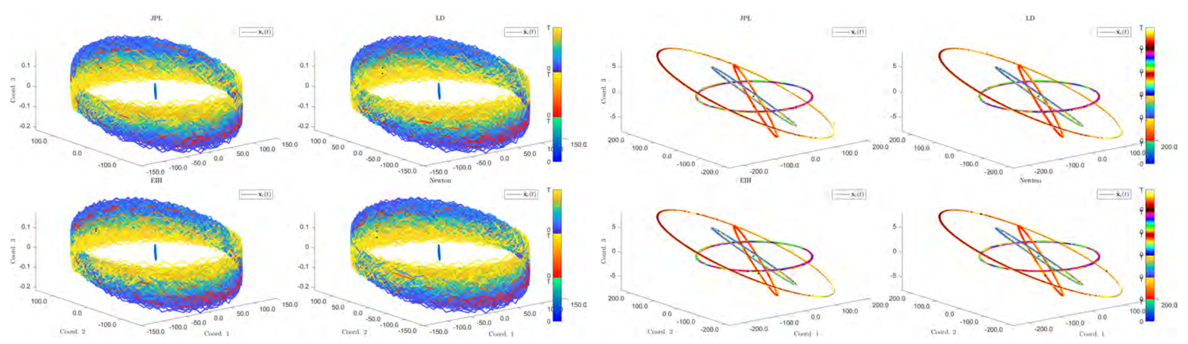

Figure 7: NASA JPL's Ephemeris

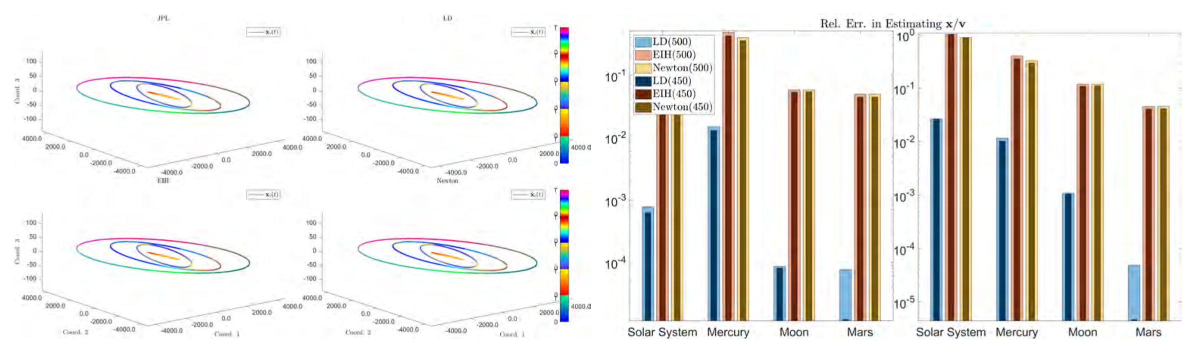

Figure 8: NASA JPL's Ephemeris

References

[1] F. Lu, M. Zhong, S. Tang, and M. Maggioni. Nonparametric inference of interaction laws in systems of agents from trajectory data. *PNAS*, 116(3):14424 – 14433, 2019.

[2] M. Zhong, J. Miller, and M. Maggioni. Data-driven discovery of emergent behaviors in collective dynamics. *Phiysca D: Nonlinear Phenomenon*, 411:132542, 2020.

[3] J. Miller, S. Tang, M. Zhong, and M. Maggioni. Learning theory for inferring interaction kernels in second-order interacting agent systems. Submitted, 2020.

[4] M. Maggioni, J. Miller, H. Qiu, and M. Zhong. Learning interaction kernels for agent systems on riemannian manifolds. Accepted, 2021.

[5] M. Zhong, J. Miller, and M. Maggioni. Machine learning for discovering effective interaction laws between celestial bodies from ephemerides. In Preparation, 2021.