Learning interaction laws in particle-based systems

IPAM - Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry

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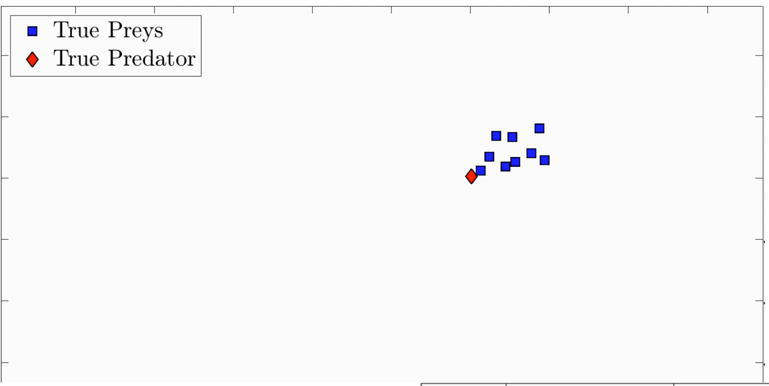
Learning in Interacting Particle Systems

- Inference problem for interaction kernels
  - Problem setup
  - Proposed estimator
  - Regularized Least Squares
  - Performance guarantees
- Examples and Extensions:
  - Second order systems
  - Emergent behaviors
  - Stochastic systems
- Learning the interaction network
- Conclusions

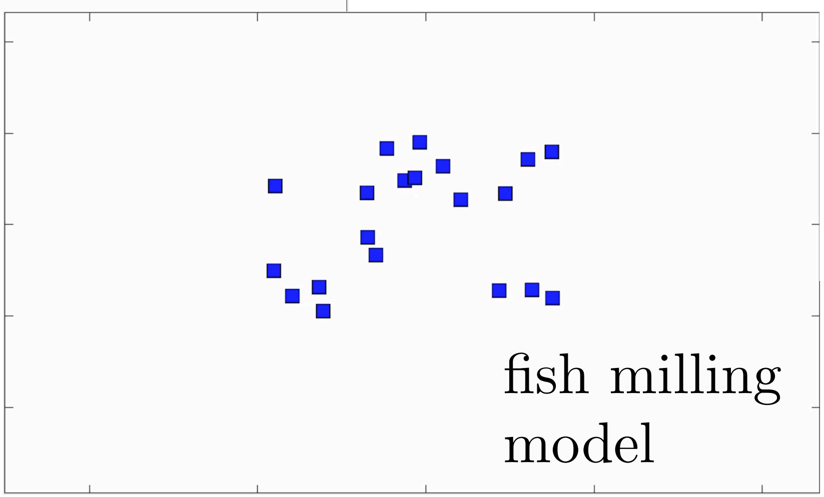
Felix Munoz, https://www.youtube.com/watch?v=OxYn3e_imhA

Introduction and motivation

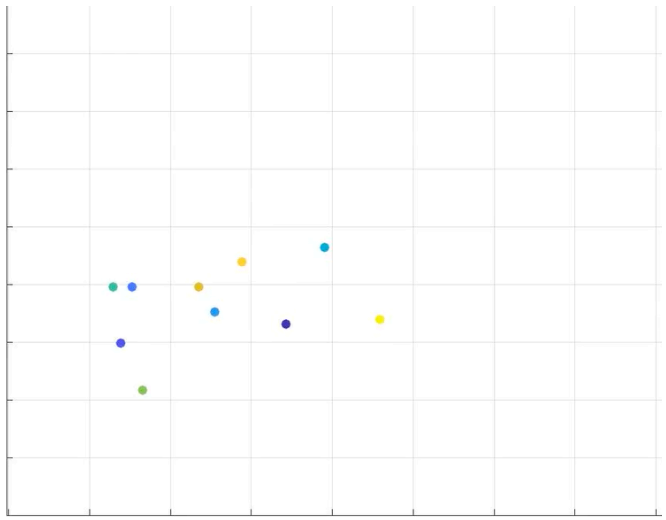
Problem: Given observations of trajectories of a dynamical system of interacting agents, learn the interaction rules.
Motivation: particle-/agent-based systems ubiquitous in Physics, Biology, social sciences, Economics, ... Beyond model-based interaction rules.
Further goals: hypothesis testing for agent-based systems; transfer learning; agents on networks; collaborative and competitive games.



prey/predator model



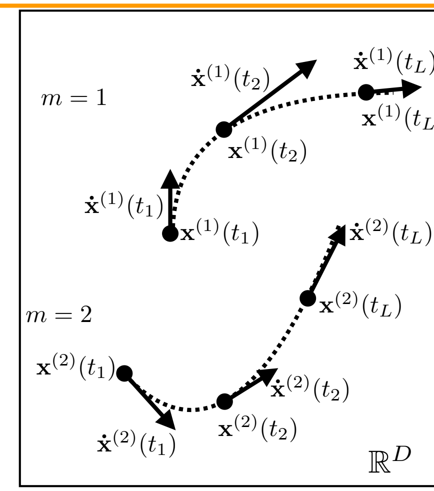
fish milling model



stochastic Lennard-Jones

Problem formulation

Suppose we have a system driven by of ODEs in the form



$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t)) \qquad , \mathbf{x} \in \mathbb{R}^D, \mathbf{f} : \mathbb{R}^D \to \mathbb{R}^D$$

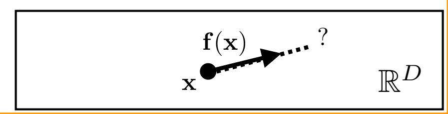
and we are given observations of positions and velocities

$$(\mathbf{x}^{(m)}(t_l), \dot{\mathbf{x}}^{(m)}(t_l))_{l=1,\dots,L; m=1,\dots,M} \ ,$$

where:

- $0 = t_1 < \cdots < t_L = T$;
- m indexes trajectories corresponding to different initial conditions at $t_1 = 0$

Problem: construct an estimator $\hat{\mathbf{f}}_n$ that is close to $\mathbf{f}$.



Statistical learning version:
given $(\mathbf{x}^{(m)}(t_l), \dot{\mathbf{x}}^{(m)}(t_l))_{l=1,\dots,L; m=1,\dots,M}$, with $\mathbf{x}^{(m)}(t_1) \sim_{\text{i.i.d.}} \mu_0$, we want to construct an estimator $\hat{\mathbf{f}}_n$ for the unknown $\mathbf{f}$ in $\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t))$.

We are interested in the *nonparametric* setting, i.e. no assumptions on $\mathbf{f}$ except some regularity.

Nonparametric regression

Statistical learning version:
given $(\mathbf{x}^{(m)}(t_l), \dot{\mathbf{x}}^{(m)}(t_l))_{l=1,\ldots,L; m=1,\ldots,M}$, with $\mathbf{x}^{(m)}(t_1) \sim_{\text{i.i.d.}} \mu_0$, we want to construct an estimator $\hat{\mathbf{f}}_n$ for the unknown $\mathbf{f}$ in $\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t))$.

Possible approach: regression. In regression one is given pairs

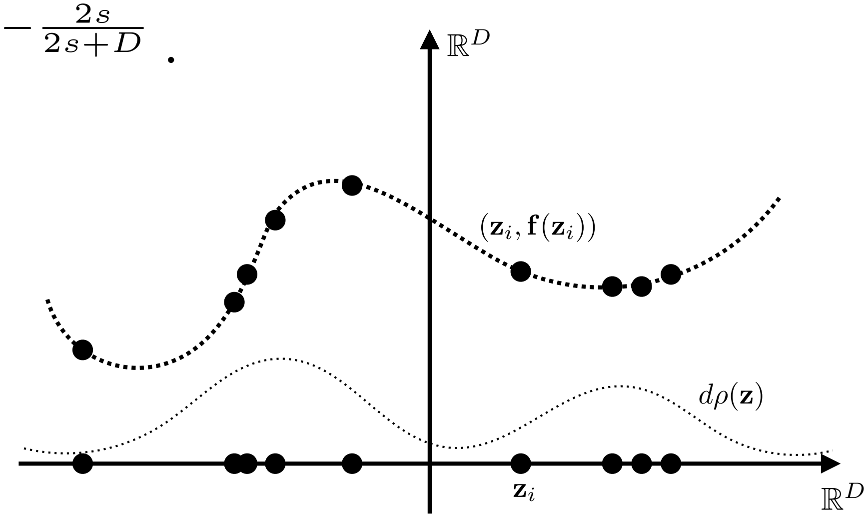
$$\{(\mathbf{z}_i, \mathbf{f}(\mathbf{z}_i) + \eta_i)\}_{i=1}^n \,, \text{with } \mathbf{z}_i \in \mathbb{R}^D, \mathbf{z}_i \sim_{\text{i.i.d.}} \rho\,, \text{ a prob. measure on } \mathbb{R}^D\,,$$

with η independent noise, and outputs an estimator $\hat{\mathbf{f}}_n$.

Well-understood problem: estimators that, for $\mathbf{f}$ s-Hölder regular, satisfy

$$\mathbb{E}[||\hat{\mathbf{f}}_n - \mathbf{f}||^2_{L^2(\rho)}] \lesssim n^{-\frac{2s}{2s+D}}\,.$$

Moreover, this *learning rate* is optimal (in the so-called min-max sense: for any estimator one can find $\mathbf{f}$ for which the estimator does not converge to $\mathbf{f}$ any faster than this).



Nonparametric estimation

Suppose we have a system driven by of ODEs in the form

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t)) \qquad , \mathbf{x} \in \mathbb{R}^D, \mathbf{f} : \mathbb{R}^D \to \mathbb{R}^D$$

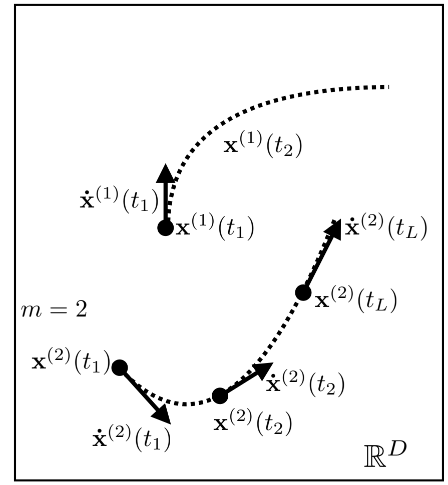
and we are given observations of positions and velocities

$$(\mathbf{x}^{(m)}(t_l), \dot{\mathbf{x}}^{(m)}(t_l))_{l=1,\dots,L;m=1,\dots,M} \, ,$$

where:

- $0 = t_1 < \cdots < t_L = T$;
- m indexes trajectories corresponding to different initial conditions at $t_1 = 0$

Problem: construct an estimator $\hat{\mathbf{f}}_n$ that is close to $\mathbf{f}$.



$(\mathbf{x}^{(m)}(t_l), \dot{\mathbf{x}}^{(m)}(t_l))_{l=1,\dots,L;m=1,\dots,M}$, with $\mathbf{x}^{(m)}(t_1) \sim_{\text{i.i.d.}} \mu_0$, construct $\hat{\mathbf{f}}_n$.

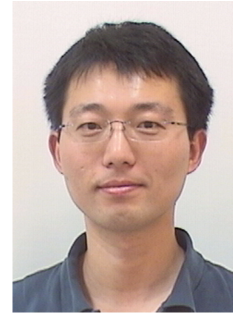
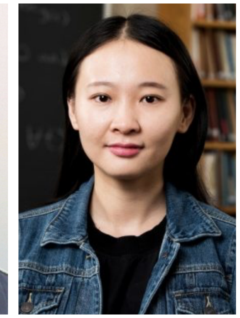
$\mathbf{z}_i$ ↗ $\mathbf{f}(\mathbf{z}_i)$ ↗

The observations are independent in m, but not in l.

Pretending we had independence, under the only assumption that $\mathbf{f}$ is s-Hölder, the best attainable learning rate is $\mathbb{E}[||\hat{\mathbf{f}}_n - \mathbf{f}||_{L^2}] \lesssim n^{-\frac{s}{2s+D}}$, where $n = LM$ (L obs. in each of M traj.) and $D = Nd$ (N agents in $\mathbb{R}^d$).

For a system of N agents in $\mathbb{R}^d$, $D = Nd$ is typically very large, and the rate $n^{-\frac{s}{2s+D}}$ unsatisfactory. Further assumptions are needed for better rates.

Particle-based systems

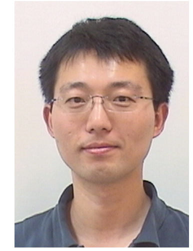
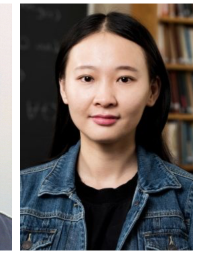

Particle- and agent-based systems are driven by ODEs with special structure. A simple prototypical model:

$$\dot{\mathbf{x}}_i^{(m)}(t) = \frac{1}{N}\sum_{i'} \phi(||\mathbf{x}_{i'}^{(m)}(t) - \mathbf{x}_i^{(m)}(t)||)(\mathbf{x}_{i'}^{(m)}(t) - \mathbf{x}_i^{(m)}(t))\,.$$

Given observations $\{(\mathbf{x}_i, \dot{\mathbf{x}}_i)\}_{i=1}^N$ at different times $\{t_l\}_{l=1}^L$ and/or for different initial conditions $\{\mathbf{x}^{(m)}(0)\}_{m=1}^M$, we want to learn the interaction kernel ϕ. Different limits: $N \to +\infty$ (mean-field limit, joint work with M. Fornasier and M. Bongini), $M \to +\infty$ (joint work with F. Lu, S. Tang and M. Zhong).

- Strong model assumption on the form of the ODE system. Now the unknown is the function ϕ of 1 variable, r.
- We may be able avoid the curse of dimensionality.
- No value $\phi(r)$ is observed, so this is not regression, but an inverse problem.

Particle-based systems


Particle- and agent-based systems are driven by ODEs with special structure. A simple prototypical model:

$$\dot{\mathbf{x}}_i^{(m)} = \frac{1}{N}\sum_{i'=1}^{N} \phi(||\mathbf{x}_i^{(m)} - \mathbf{x}_{i'}^{(m)}||)(\mathbf{x}_{i'}^{(m)} - \mathbf{x}_i^{(m)})$$

Given observations $\{(\mathbf{x}_i, \dot{\mathbf{x}}_i)\}_{i=1}^N$ at different times $\{t_l\}_{l=1}^L$ and/or for different initial conditions $\{\mathbf{x}^{(m)}(0)\}_{m=1}^M$, we want to learn the interaction kernel ϕ.

Different limits: $N \to +\infty$ (mean-field limit, joint work with M. Fornasier and M. Bongini), $M \to +\infty$ (joint work with F. Lu, S. Tang and M. Zhong).

For fixed $t = t_l$ and m, we cannot solve for $\phi(r_{ii'})$: $N(N-1)/2$ unknowns, only dN known quantities (typically $d \ll N$). Need to leverage observations in time.

At time scale $[0, T]$, we define the probability measure on $\mathbb{R}_+$:

$$\rho_T^L(r) := \mathbb{E}_{x(0)\sim\mu_0} \frac{1}{L}\sum_{l=1}^{L} \frac{1}{\binom{N}{2}} \sum_{i,i'=1, i<i'}^{N} \delta_{r_{ii'}^{(m)}(t_l)}(r)\,.$$

- ↑ average over initial conditions
- ↑ average over observations in time
- ↑ average over pairs of agents
- ↑ δ function on $\mathbb{R}_+$ at every observed pairwise distance

The Mean-field limit

Rewriting

$$\dot{\mathbf{x}}_i = \frac{1}{N}\sum_{i'}\phi(||\mathbf{x}_i - \mathbf{x}_{i'}||)(\mathbf{x}_{i'} - \mathbf{x}_i) = \frac{1}{N}\sum_{i'}\frac{\Phi'(||\mathbf{x}_i - \mathbf{x}_{i'}||)}{||\mathbf{x}_i - \mathbf{x}_{i'}||}(\mathbf{x}_i - \mathbf{x}_{i'})$$

we see this is the gradient flow of the energy $\mathcal{J}_N(\mathbf{X}) = \frac{1}{2N}\sum_{i,i'=1}^{N}\Phi(||\mathbf{x}_i - \mathbf{x}_{i'}||)$.

Considering the measure $\mu^N(t) = \frac{1}{N}\sum_{i=1}^{N}\delta_{\mathbf{x}_i(t)}$, we may let $N \to +\infty$ to obtain (under suitable regularity assumptions on Φ) the mean field equations

$$\partial_t\mu(t) = -\nabla\cdot\left(\left(-\frac{\Phi'(||\cdot||)}{||\cdot||} * \mu(t)\right)\mu(t)\right)\,, \quad \mu(0) = \mu_0\,.$$

This is also a gradient flow for the energy $\mathcal{J}(\mu) = \int_{\mathbb{R}^{d\times d}}\Phi(||\mathbf{x} - \mathbf{y}||)d\mu(\mathbf{x})d\mu(\mathbf{y})$ on the space of probability measures with Wasserstein distance.

Estimation in the limit as $N \to \infty$: studied in *Inferring Interaction Rules from Observations of Evolutive Systems I: The Variational Approach*, M. Bongini, M. Fornasier, M. Hansen, MM, published in M3S, 2017

Measures on pairwise distances

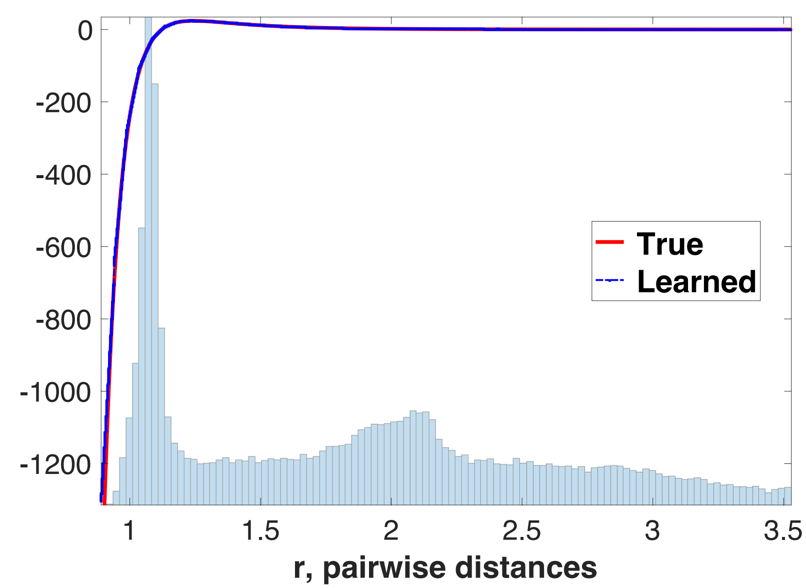
Observations: $\{(\mathbf{x}_i, \dot{\mathbf{x}}_i)^{(m)}(t_l)\}_{i=1,l=1,m=1}^{N,L,M}$, where $\mathbf{x}^{(m)}(0) \sim \mu_0$ for some μ_0 on $\mathbb{R}^d$. Note that each state of the system is in $\mathbb{R}^{dN}$.

$$\dot{\mathbf{x}}_{i'}^{(m)}(t) = \frac{1}{N}\sum_{i'=1}^{N} \phi(\underbrace{||\mathbf{x}_{i'}^{(m)}(t) - \mathbf{x}_i^{(m)}(t)||}_{r_{ii'}^{(m)}(t)})(\mathbf{x}_{i'}^{(m)}(t) - \mathbf{x}_i^{(m)}(t)) \,.$$

At time scale $[0, T]$, we define the probability measure on $\mathbb{R}_+$:

$$\rho_T^L(r) := \mathbb{E}_{x(0)\sim\mu_0} \frac{1}{\binom{N}{2} L} \sum_{l=1}^{L} \sum_{i,i'=1, i<i'}^{N} \delta_{r_{ii'}^{(m)}(t_l)}(r) \,.$$

Example. The Lennard Jones force is the derivative of the potential $V_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$.
Right figure: In blue the LJ ϕ, superimposed to an empirical estimate of ρ_T^L, for a system of $N = 7$ agents, and L, T small.



The estimator for the interaction kernel

Observations: $\{(\mathbf{x}_i^{(m)}, \dot{\mathbf{x}}_i^{(m)})(t_l)\}_{I=1,l=1,m=1}^{N,L,M}$, for M different initial conditions i.i.d. $\sim \mu_0$, from

$$\dot{\mathbf{x}}_i^{(m)}(t) = \frac{1}{N}\sum_{i'} \phi(||\mathbf{x}_{i'}^{(m)}(t) - \mathbf{x}_i^{(m)}(t)||)(\mathbf{x}_{i'}^{(m)}(t) - \mathbf{x}_i^{(m)}(t)) =: \mathbf{f}_\phi((\mathbf{x}_i^{(m)}(t))_i)\,.$$

linear map (in ϕ) applied to unknown ϕ

Consider the empirical error functional, for "any" ψ,

$$\mathcal{E}_{L,M}(\psi) := \frac{1}{LMN}\sum_{l,m,i=1}^{L,M,N} \left\|\dot{\mathbf{x}}_i^{(m)}(t_l) - \mathbf{f}_\psi((\mathbf{x}_i^{(m)}(t_l))_i)\right\|^2 .$$

Our estimator is defined as a minimizer of $\mathcal{E}_{L,M}$ over $\psi \in \mathcal{H}$, a suitable hypothesis space of functions on $\mathbb{R}_+$, with $\dim(\mathcal{H}) = n$ (with $n = n(M)$):

$$\hat{\phi}_{L,M,\mathcal{H}} := \arg\min_{\psi\in\mathcal{H}} \mathcal{E}_{L,M}(\psi)\,.$$

For $\mathcal{H}$ linear subspace, this is a least squares problem (Gauss, Legendre). We want a large $\mathcal{H}$ to reduce bias, but not too large as that increases the number of parameters to be estimated for a given amount of data, and therefore the variance of the estimator.

Coercivity condition

$$\mathcal{E}_{L,M}(\psi) := \frac{1}{LMN} \sum_{l,m,i=1}^{L,M,N} \left\| \dot{\mathbf{x}}_i^{(m)}(t_l) - \mathbf{f}_\psi(\mathbf{x}_i^{(m)}(t_l)) \right\|^2,$$

$$\hat{\phi}_{L,M,\mathcal{H}} := \arg\min_{\psi \in \mathcal{H}} \mathcal{E}_{L,M}(\psi)\,.$$

We shall assume that the unknown interaction kernel ϕ is in the admissible class $\mathcal{K}_{R,S} := \{\psi \in C^1(\mathbb{R}_+) :\ \text{supp}.\psi \subset [0,R], \sup_{r\in[0,R]} |\psi(r)| + |\psi'(r)| \leq S\}$.

Coercivity condition: $\exists c_{L,N,\mathcal{H}} > 0$ s.t. $\forall \psi : \psi(\cdot)\cdot \in \mathcal{H}$, $\mathbf{r}_{ii'} := \mathbf{x}_i - \mathbf{x}_{i'}$

$$c_{L,N,\mathcal{H}} \|\psi(\cdot)\cdot\|^2_{L^2(\rho_T^L)} \leq \frac{1}{NL} \sum_{l,i=1}^{L,N} \mathbb{E} \left\| \frac{1}{N} \sum_{i'=1}^{N} \psi(\|\mathbf{r}_{ii'}(t_l)\|)\mathbf{r}_{ii'}(t_l) \right\|^2.$$

Lemma. Coercivity $\implies$ unique minimizer of $\lim_{M\to+\infty} \mathcal{E}_{L,M}(\psi)$ over $\psi \in \mathcal{H}$

$$\psi - \phi \in \mathcal{H} \implies c_{L,N,\mathcal{H}} \|\psi(\cdot)\cdot - \phi(\cdot)\cdot\|^2_{L^2(\rho_T^L)} \leq \mathcal{E}_{L,\infty}(\psi)$$

$c_{L,N,\mathcal{H}}$ also controls the condition number of the LS problem for $\hat{\phi}_{L,M,\mathcal{H}}$.

Bias/variance trade-off

$$\mathcal{E}_{L,M}(\varphi) := \frac{1}{LMN}\sum_{l,m,i=1}^{L,M,N} \left\|\dot{\mathbf{x}}_i^{(m)}(t_l) - \mathbf{f}_\varphi(\mathbf{x}_i^{(m)}(t_l))\right\|^2,$$

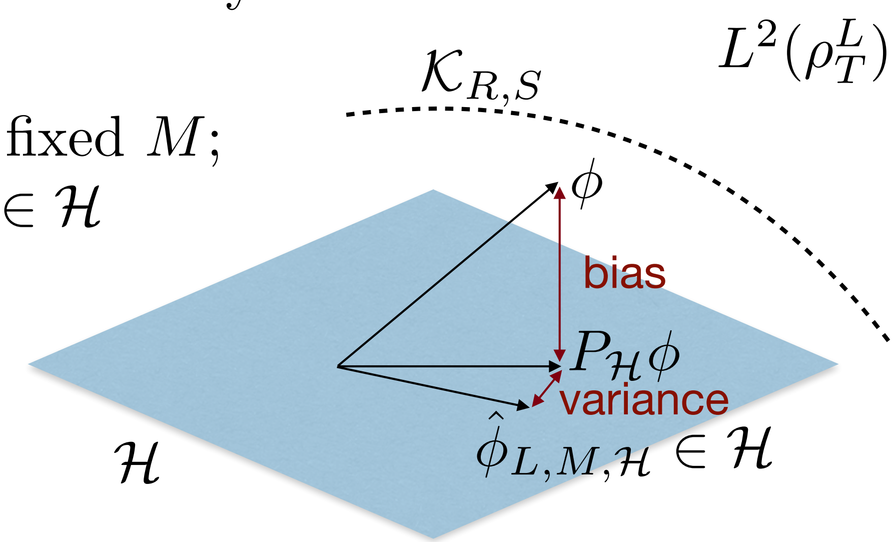
$$\hat{\phi}_{L,M,\mathcal{H}} := \arg\min_{\varphi\in\mathcal{H}} \mathcal{E}_{L,M}(\varphi)\,.$$

$$+\text{ coercivity}$$

bias decreases as $\dim\mathcal{H}$ increases; depends only on approximation properties of $\mathcal{H}$

variance increases as $\dim\mathcal{H}$ increases, for fixed M; measures randomness of $\hat{\phi}_{L,M,\mathcal{H}} \in \mathcal{H}$

Pick $\dim\mathcal{H}$ an increasing function of M, to attain the minimum of the sum of bias (squared) and variance.



Unlike regression, we do not have access to values of ϕ, but only observations that are linear functions (via f_ϕ) of ϕ; coercivity implies stable invertibility.

Main Theorem (first order systems)

Theorem. Let $\{\mathcal{H}_n\}_n \subseteq \mathcal{H}$ be a sequence of subspaces of $L^\infty[0,R]$, with $\dim(\mathcal{H}_n) \leq c_0 n$ and $\inf_{\varphi \in \mathcal{H}_n} \|\varphi(\cdot) - \phi(\cdot)\|_{L^\infty([0,R])} \leq c_1 n^{-s}$, for some constants $c_0, c_1, s > 0$. It exists, for example, if ϕ is s-Hölder regular.
Choose $n_* = (M/\log M)^{\frac{1}{2s+1}}$: then for some $C = C(c_0, c_1, R, S)$

$$\mathbb{E}[\|\widehat{\phi}_{L,M,\mathcal{H}_{n_*}}(\cdot)\cdot - \phi(\cdot)\cdot\|_{L^2(\rho_L^T)}] \leq \frac{C}{c_{L,N,\mathcal{H}}} \left(\frac{\log M}{M}\right)^{\frac{s}{2s+1}} .$$

this is just the function that, evaluated at r, gives $\phi(r)r$

this is an occupancy measure for pairwise distances, over trajectories

coercivity constant: it is a crucial parameter controlling how well-conditioned the inverse problem is. Depends on the system.

- The good: Rate in M is optimal, in fact even optimal in the case of regression, where we would be given $(r_m, \phi(r_m))_{m=1}^M$.
- The bad: no dependency on L. Numerical examples suggest that the effective sample size can be LM = #obs; but that cannot be always true.

In the examples we choose $\mathcal{H}_n$ to be the space of piecewise linear functions on a uniform partition of cardinality n of $[0, R_{\max}]$ (estimated supp.ρ_L^T), for $n = n_*$. Fourier, wavelets, etc...would be other natural choices.

In the end solving the minimization problem is a least-squares problem in $n = n_*$ dimensions. Algorithms for constructing the LS matrix and computing the estimator run in time $O(N^2 Ld \cdot M + Mn_*^2)$ (online versions also possible).

Errors on trajectories

Standard arguments yield bounds on the distance between trajectories of the true system and those of the system driven by the estimated interaction kernel.

Proposition. Assume $\widehat{\phi}(\|\cdot\|)\cdot \in \mathrm{Lip}(\mathbb{R}^d)$, with Lipschitz constant C_{Lip}. Let $\widehat{\mathbf{X}}(t)$ and $\mathbf{X}(t)$ be the solutions of systems with kernels $\widehat{\phi}$ and ϕ respectively, started from the same initial condition. Then for each trajectory

$$\sup_{t\in[0,T]} \|\widehat{\mathbf{X}}(t) - \mathbf{X}(t)\|^2 \le 2Te^{8T^2C_{\mathrm{Lip}}^2}\int_0^T \left\|\dot{\mathbf{X}}(t) - \mathbf{f}_{\hat{\phi}}(\mathbf{X}(t))\right\|^2 dt\,,$$

and on average w.r.t. the distribution μ_0 of initial conditions:

$$\mathbb{E}_{\mu_0}[\sup_{t\in[0,T]} \|\widehat{\mathbf{X}}(t) - \mathbf{X}(t)\|] \le C(T, C_{\mathrm{Lip}})\sqrt{N}\|\hat{\phi}(\cdot)\cdot - \phi(\cdot)\cdot\|_{L^2(\rho_T)},$$

distances between trajectories

quantity controlled by theorem on learning rate

where $C(T, C_{\mathrm{Lip}})$ is a constant depending on T and C_{Lip}.

Overview

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Example: 2nd order systems

$$
\begin{cases}
m_i \ddot{\boldsymbol{x}}_i = F_i^{\boldsymbol{v}}(\dot{\boldsymbol{x}}_i, \xi_i) + \sum_{i'=1}^{N} \frac{\kappa^{\boldsymbol{v}}_{\mathcal{k}_{i'}}}{N_{\mathcal{k}_{i'}}} \left(\phi^E_{\mathcal{k}_i \mathcal{k}_{i'}}(r_{ii'}) \boldsymbol{r}_{ii'} + \phi^A_{\mathcal{k}_i \mathcal{k}_{i'}}(r_{ii'}) \dot{\boldsymbol{r}}_{ii'} \right) \\
\dot{\xi}_i = F_i^{\xi}(\xi_i) + \sum_{i'=1}^{N} \frac{\kappa^{\xi}_{\mathcal{k}_{i'}}}{N_{\mathcal{k}_{i'}}} \phi^{\xi}_{\mathcal{k}_i \mathcal{k}_{i'}}(r_{ii'}) \xi_{ii'}
\end{cases}
$$

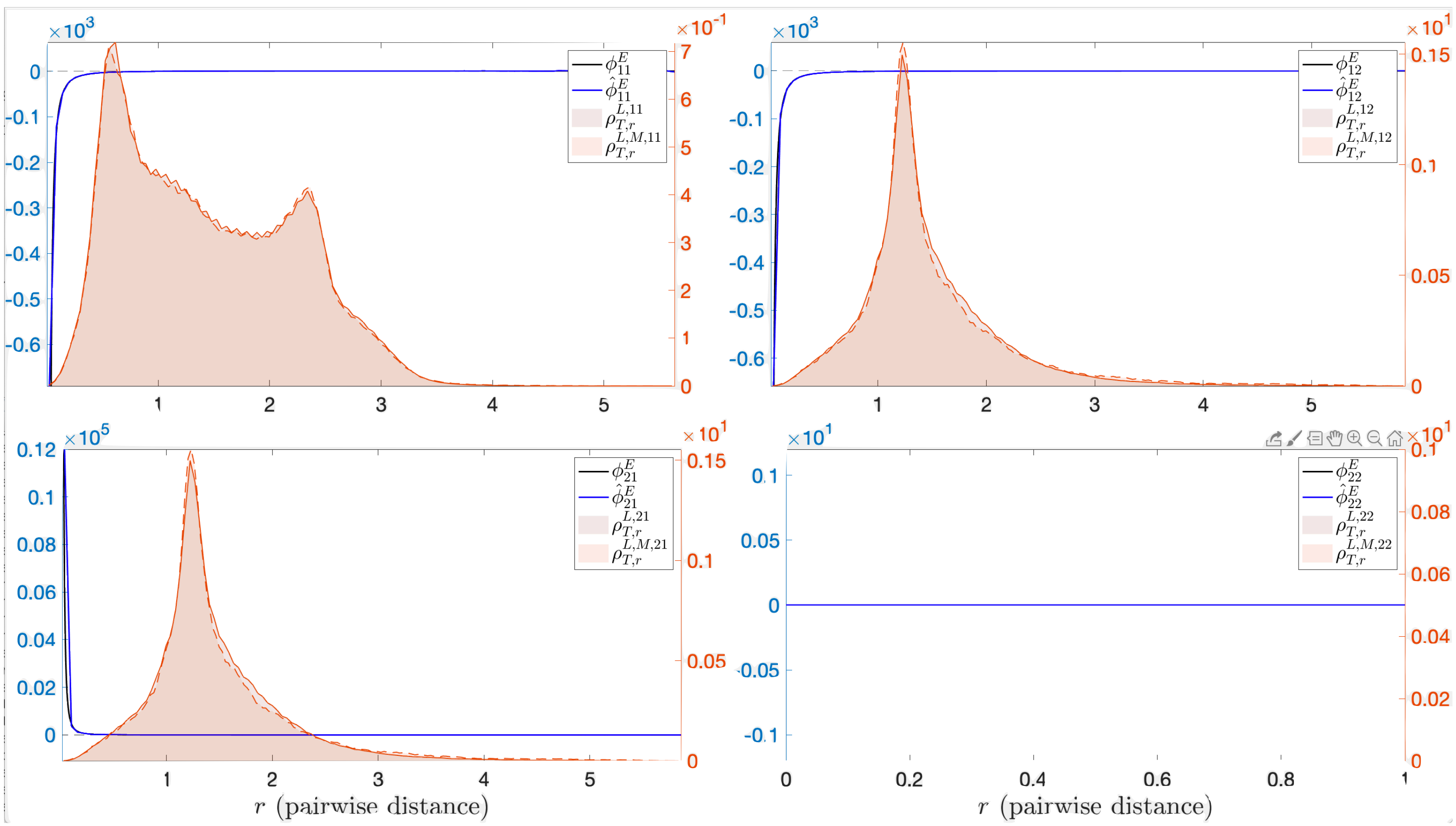
simple environment (food, light, ...)

energy and alignment interactions

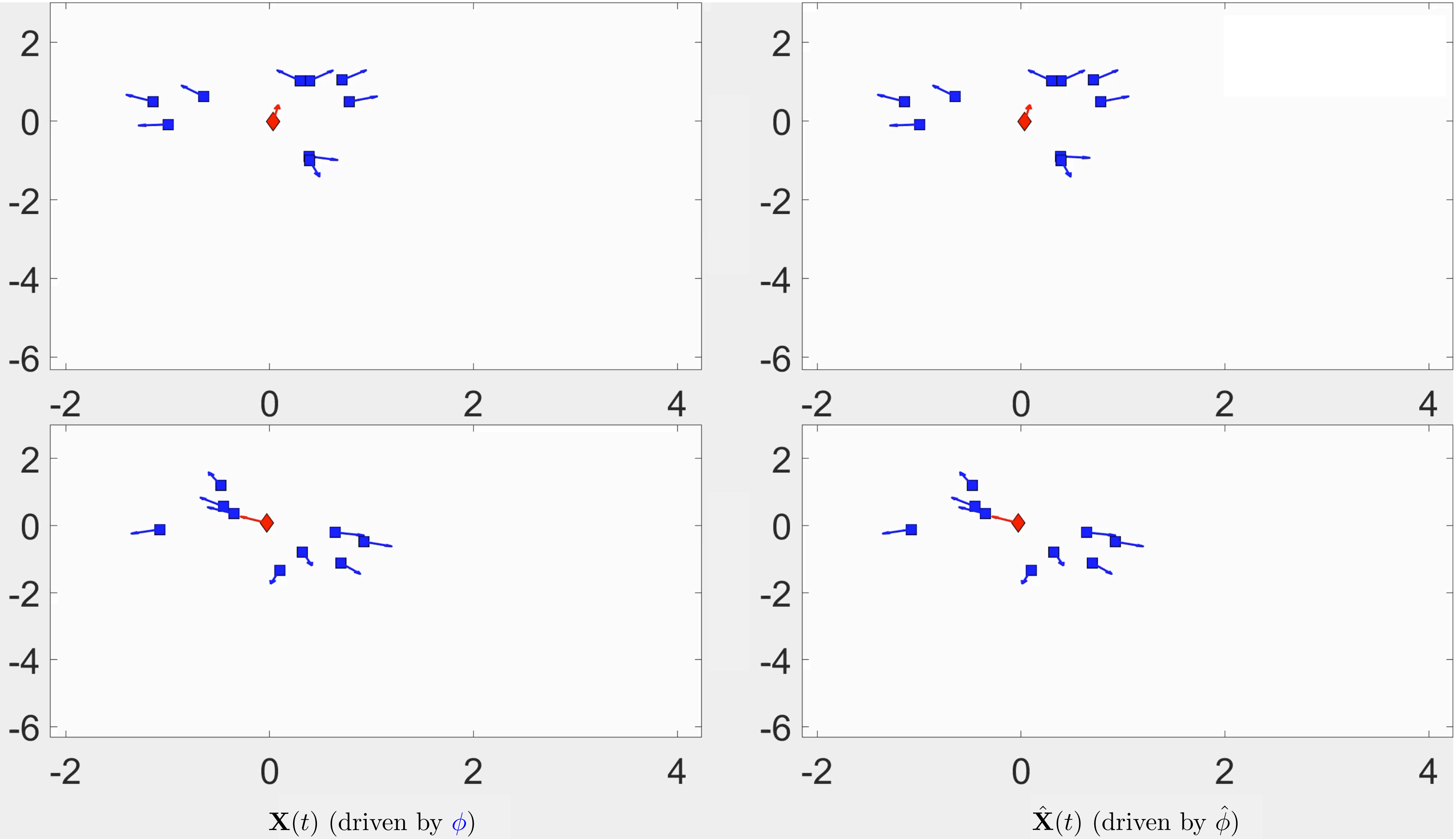
one kernel for each pair of interacting agent **types**

2nd order Prey-Predator system: the interaction kernels and ρ_L^T's.

$\phi^E_{\mathcal{k}_i \mathcal{k}_{i'}}$ vs. $\hat{\phi}^E_{\mathcal{k}_i \mathcal{k}_{i'}}$

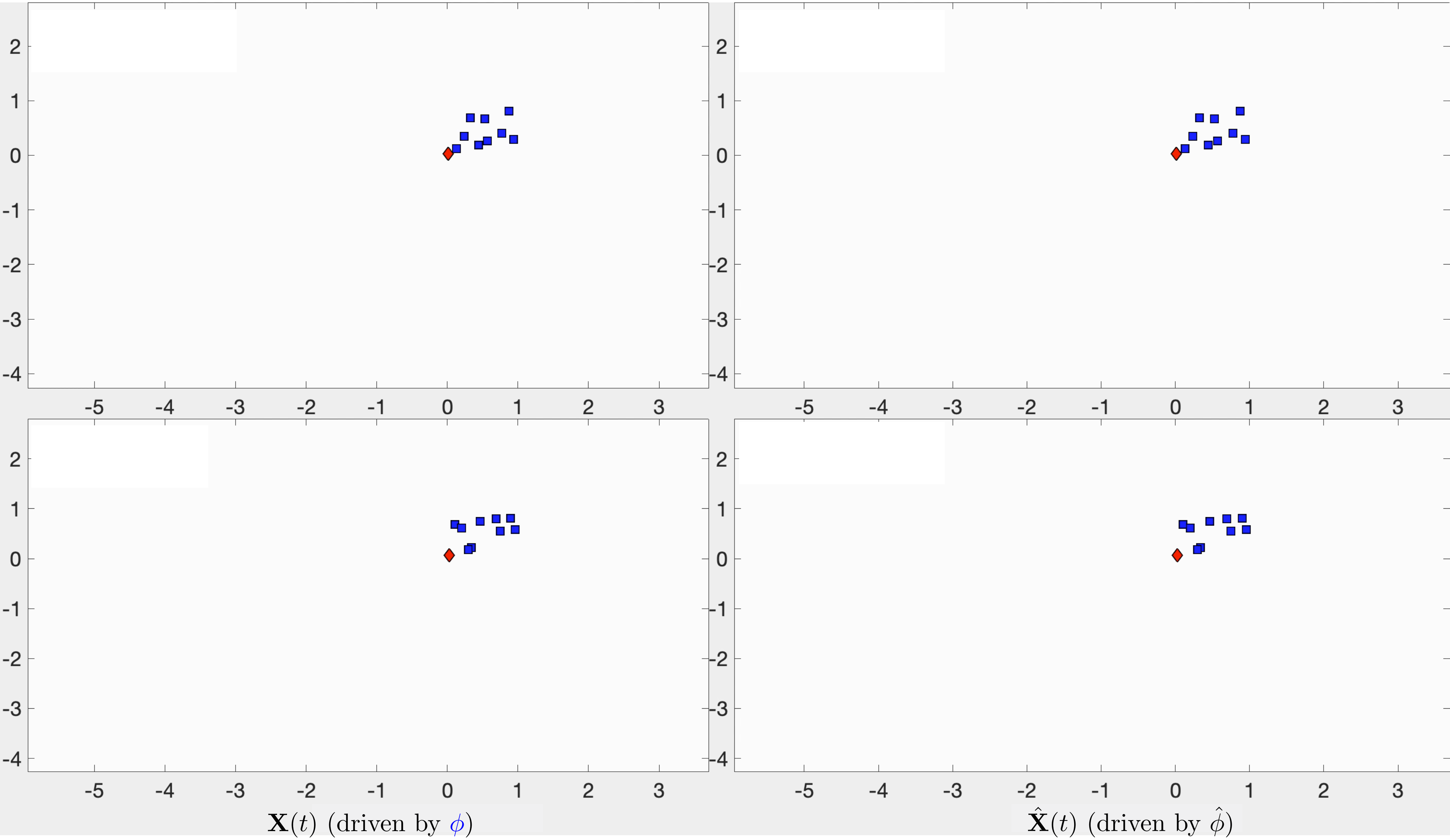


Examples: prey-predator systems



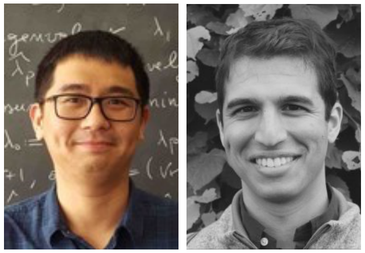
Trajectories of the true system (left col.) and learned system (right col.) with an initial condition from training data (top) and a new one (bottom).

Examples: prey-predator systems



Trajectories of the true system (left col.) and learned system (right col.) with an initial condition from training data (top) and a new one (bottom).

Emerging behaviors



Ming Zhong,
Jason Miller

Organized collecting stable patterns at large spatial/temporal scale.
Simple, local interaction kernels can learn to complex, organized behavior.
Most of the above is ill-defined, and quotes needed a.e.
Examples include flocking of bird, milling of fish, synchronization in systems of oscillators (neurons, frogs, ...), etc...

In general difficult to characterize and predict; however if robust, we may hope to recover them with systems driven by estimated interaction kernels.

Not only we are often able to recover them in general, but even predict them correctly for each initial condition, with good probability of success.

Felix Munoz, https://www.youtube.com/watch?v=OxYn3e_imhA

BBC Blue Planet

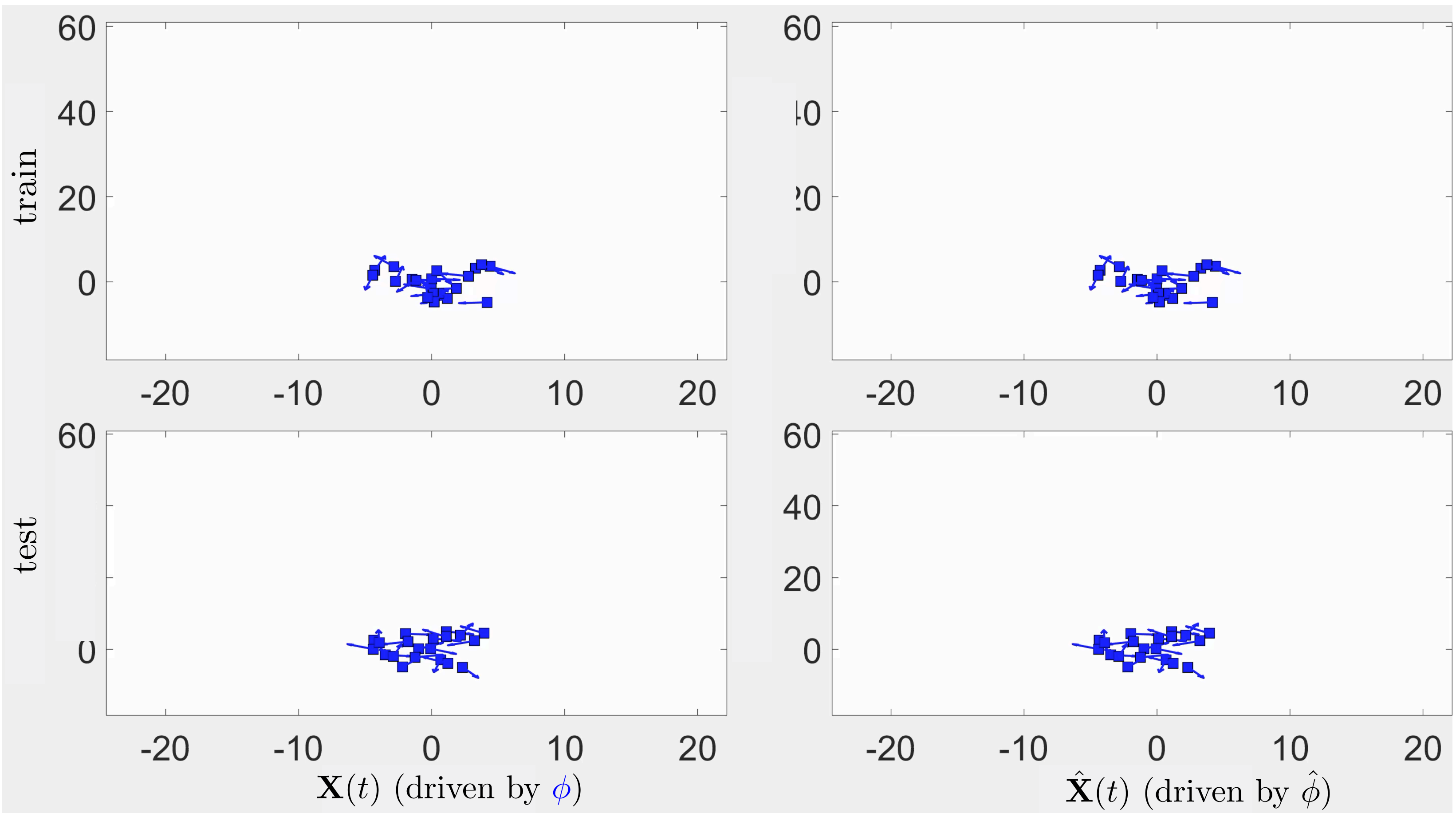
Emerging behaviors: flocking

(*) F. Cucker, J. G. Dong, Avoiding collisions in flocks, IEEE Transactions on Automatic Control, 2010.

The governing equations of Cucker-Smale-Dong (*) dynamics,

$$\ddot{\mathbf{x}}_i = -b_i(t)\dot{\mathbf{x}}_i + \sum_{i'=1}^{N} \left[a_{i,i'}(\mathbf{x})(\dot{\mathbf{x}}_{i'} - \dot{\mathbf{x}}_i) + f(||\mathbf{x}_i - \mathbf{x}_{i'}||^2)(\mathbf{x}_{i'} - \mathbf{x}_i)\right].$$

Here $a_{i,i'}(\mathbf{x}) = H(1 + ||\mathbf{x}_{i'} - \mathbf{x}_i||^2)^{-\beta}$; $b_i : [0,\infty) \to [0,\infty)$ is a bounded and uniformly continuous damping function, and $f : (\delta,\infty) \to [0,\infty)$ is a non-increasing $\mathcal{C}^1$ repulsion function integrable at $+\infty$.

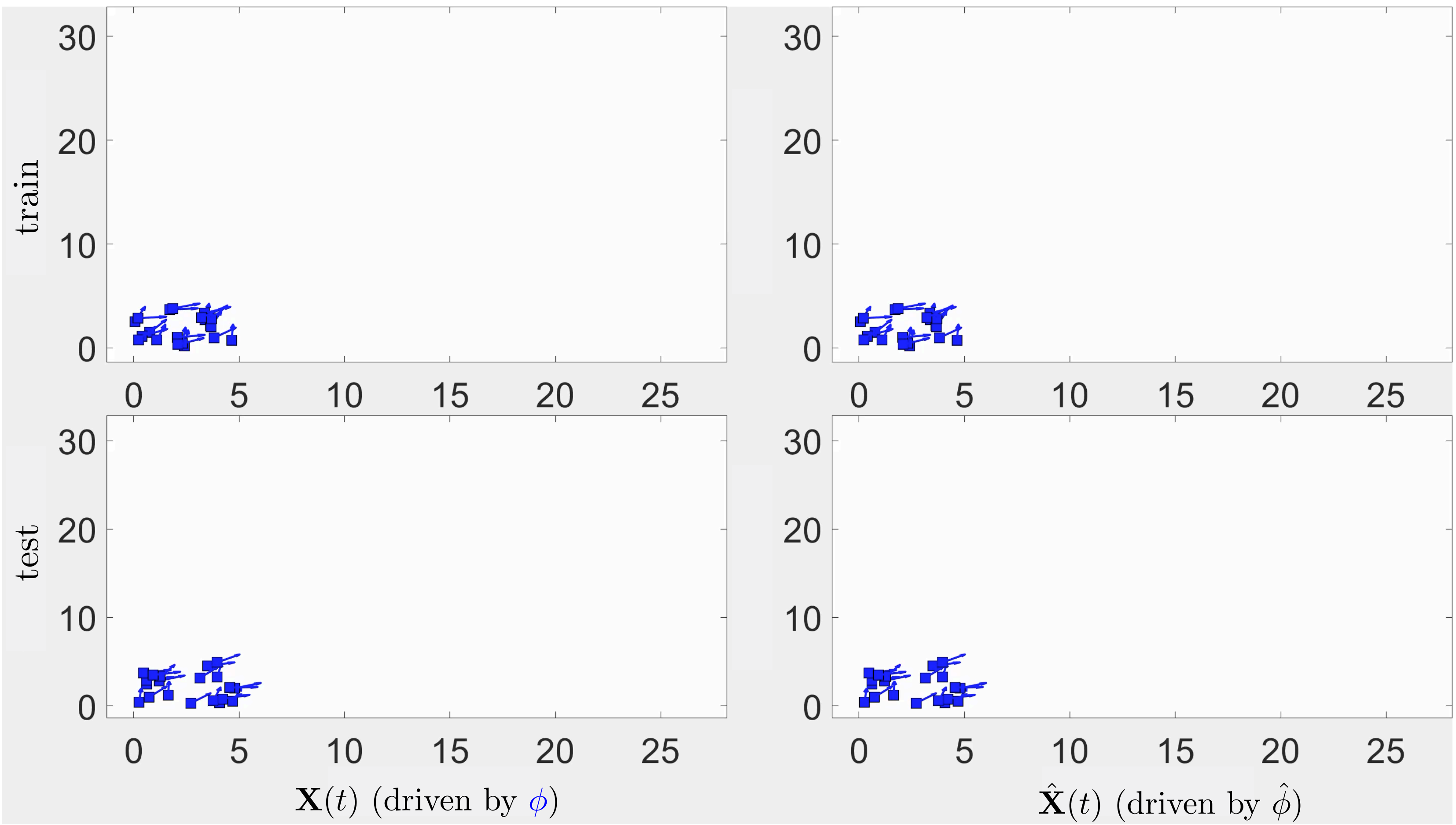


Emerging behaviors: anticipation & flocking

(*) R. Shu and E. Tadmor, Anticipation breeds alignment. arXiv:1905.00633

$$\ddot{\mathbf{x}}_i = \frac{1}{N}\sum_{i'=1,i'\neq i}^{N} \frac{\tau U'(||\mathbf{x}_{i'}-\mathbf{x}_i||)}{||\mathbf{x}_{i'}-\mathbf{x}_i||}(\dot{\mathbf{x}}_{i'}-\dot{\mathbf{x}}_i)$$
$$+\frac{1}{N}\sum_{i'=1,i'\neq i}^{N}\left\{\frac{-\tau U'(||\mathbf{x}_{i'}-\mathbf{x}_i||)(\mathbf{x}_{i'}-\mathbf{x}_i)\cdot(\dot{\mathbf{x}}_{i'}-\dot{\mathbf{x}}_i)}{||\mathbf{x}_{i'}-\mathbf{x}_i||^3}\right.$$
$$\left.+\frac{\tau U''(||\mathbf{x}_{i'}-\mathbf{x}_i||)(\mathbf{x}_{i'}-\mathbf{x}_i)\cdot(\dot{\mathbf{x}}_{i'}-\dot{\mathbf{x}}_i)}{||\mathbf{x}_{i'}-\mathbf{x}_i||^2}+\frac{U'(||\mathbf{x}_{i'}-\mathbf{x}_i||)}{||\mathbf{x}_{i'}-\mathbf{x}_i||}\right\}(\mathbf{x}_{i'}-\mathbf{x}_i).$$

$U(r) = r^{1.5}/1.5$



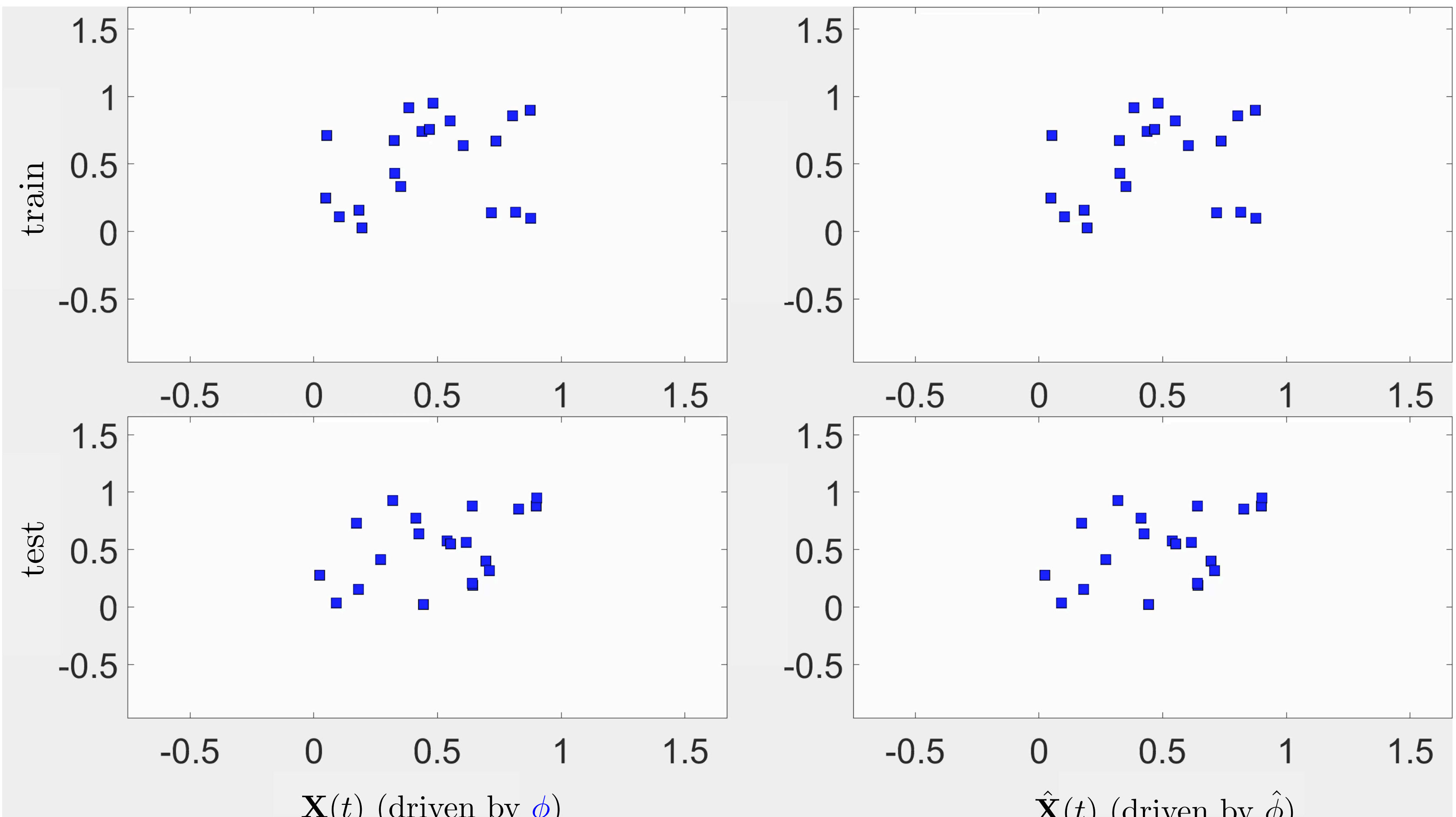
Emerging behaviors: Fish mill patterns

The governing equations of fish milling dynamics in $\mathbb{R}^2$ of (*) are

(*) Y. Li Chuang, M. R. D'Orsogna, D. Marthaler, A. L. Bertozzi, L. S. Chayes, Physica D: Nonlinear Phenomena 232 (2007)

$$m_i \ddot{\mathbf{x}}_i = \alpha \dot{\mathbf{x}}_i - \beta ||\dot{\mathbf{x}}_i||^2 \dot{\mathbf{x}}_i - \sum_{i'} \nabla_2 U(\mathbf{x}_i, \mathbf{x}_{i'}) \,,$$

with $U(\mathbf{x}_i, \cdot)$ is a potential for the interaction of the i^{th} agent with the other agents: $U(\mathbf{x}_i, \mathbf{x}_{i'}) = (-C_a \mathrm{e}^{-||\mathbf{x}_i - \mathbf{x}_{i'}||/\ell_a} + C_r \mathrm{e}^{-||\mathbf{x}_i - \mathbf{x}_{i'}||/\ell_r})$.



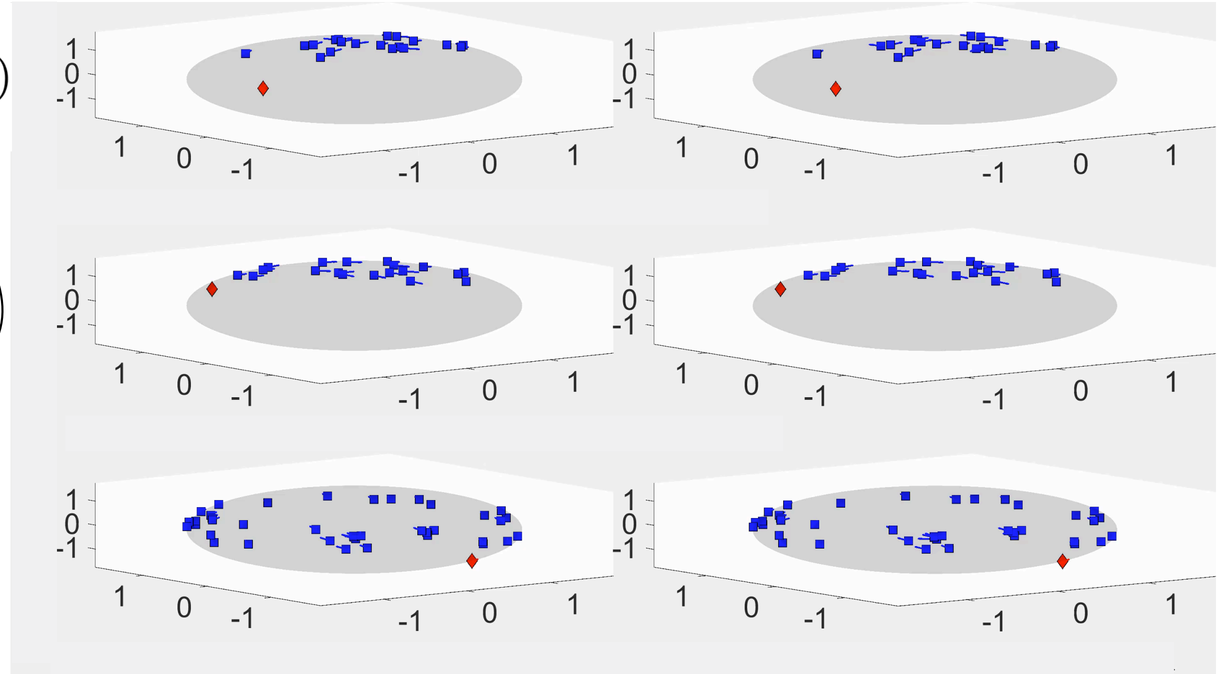
Interacting particles on manifolds

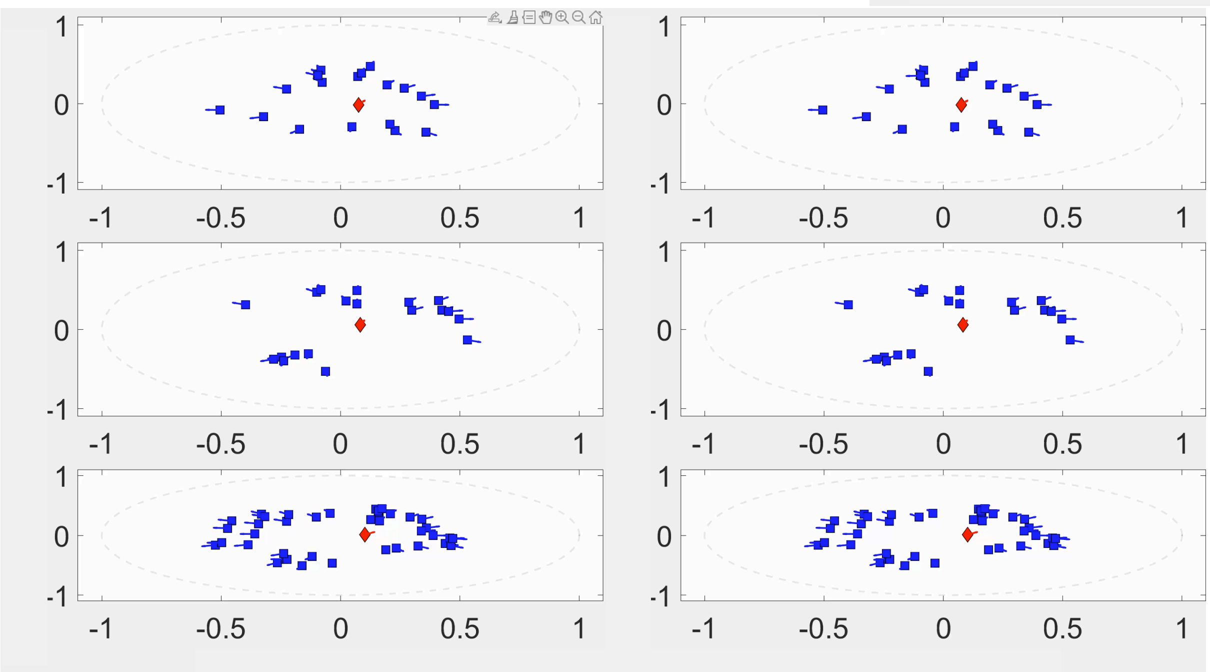
$$\dot{\mathbf{x}}_i^{(m)} = \frac{1}{N}\sum_{i'=1}^{N} \phi(||\mathbf{x}_i^{(m)} - \mathbf{x}_{i'}^{(m)}||)(\mathbf{x}_{i'}^{(m)} - \mathbf{x}_i^{(m)})$$

Generalization to manifolds:

· distances → geodesic distances

· $(\mathbf{x_{i'}} - \mathbf{x_i})/||\mathbf{x_{i'}} - \mathbf{x_i}||$ → direction of tangent to geodesic from $\mathbf{x_i}$ to $\mathbf{x_{i'}}$ at $\mathbf{x_i}$.





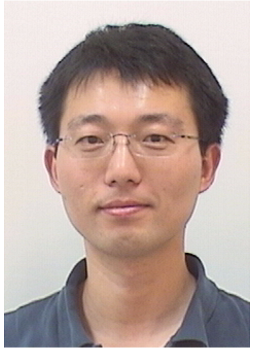
Poincaré disk

$\mathbb{S}^2$

Prey-predator system on...

MM, J. Miller, H. Qiu, M. Zhong, *Learning Interaction Kernels for Agent Systems on Riemannian Manifolds*, ICML 2021

The Stochastic case



We have also generalized these results to the **stochastic** case

$$d\mathbf{x}_{i,t} = \frac{1}{N}\sum_{i'=1}^{N}\phi(\|\mathbf{x}_{i',t}-\mathbf{x}_{i,t}\|)(\mathbf{x}_{i',t}-\mathbf{x}_{i,t})dt + \sigma d\mathbf{B}_{i,t}\,.$$

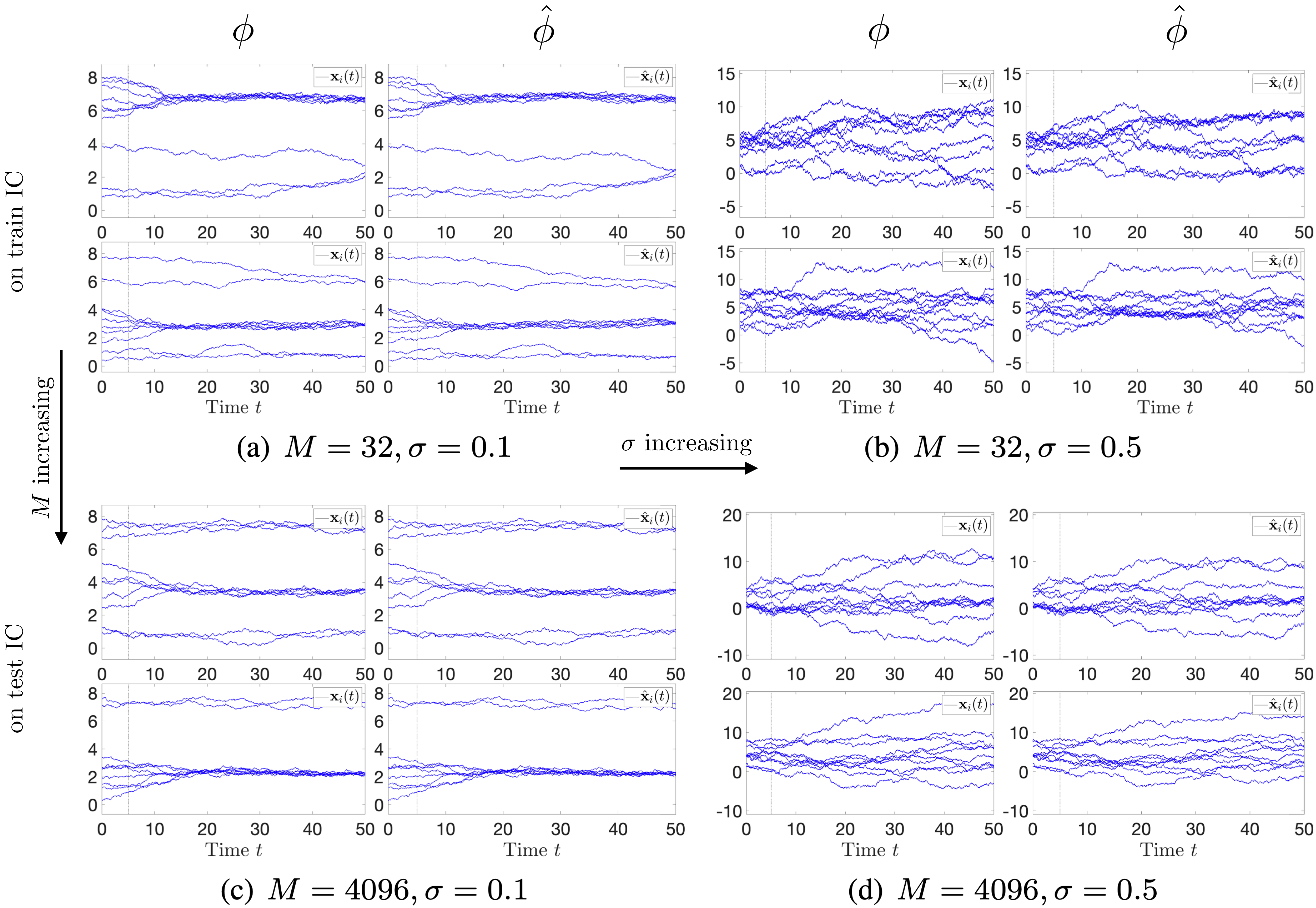
Joint work with F. Lu and S. Tang, *Learning interaction kernels in stochastic systems of interacting particles from multiple trajectories*, FOCM, 2021.

Note that in the stochastic case we do not (cannot!) observe velocities, but only positions. We have studied carefully the dependence on the observation time gap $\Delta t := t_{l+1} - t_l = T/L$:

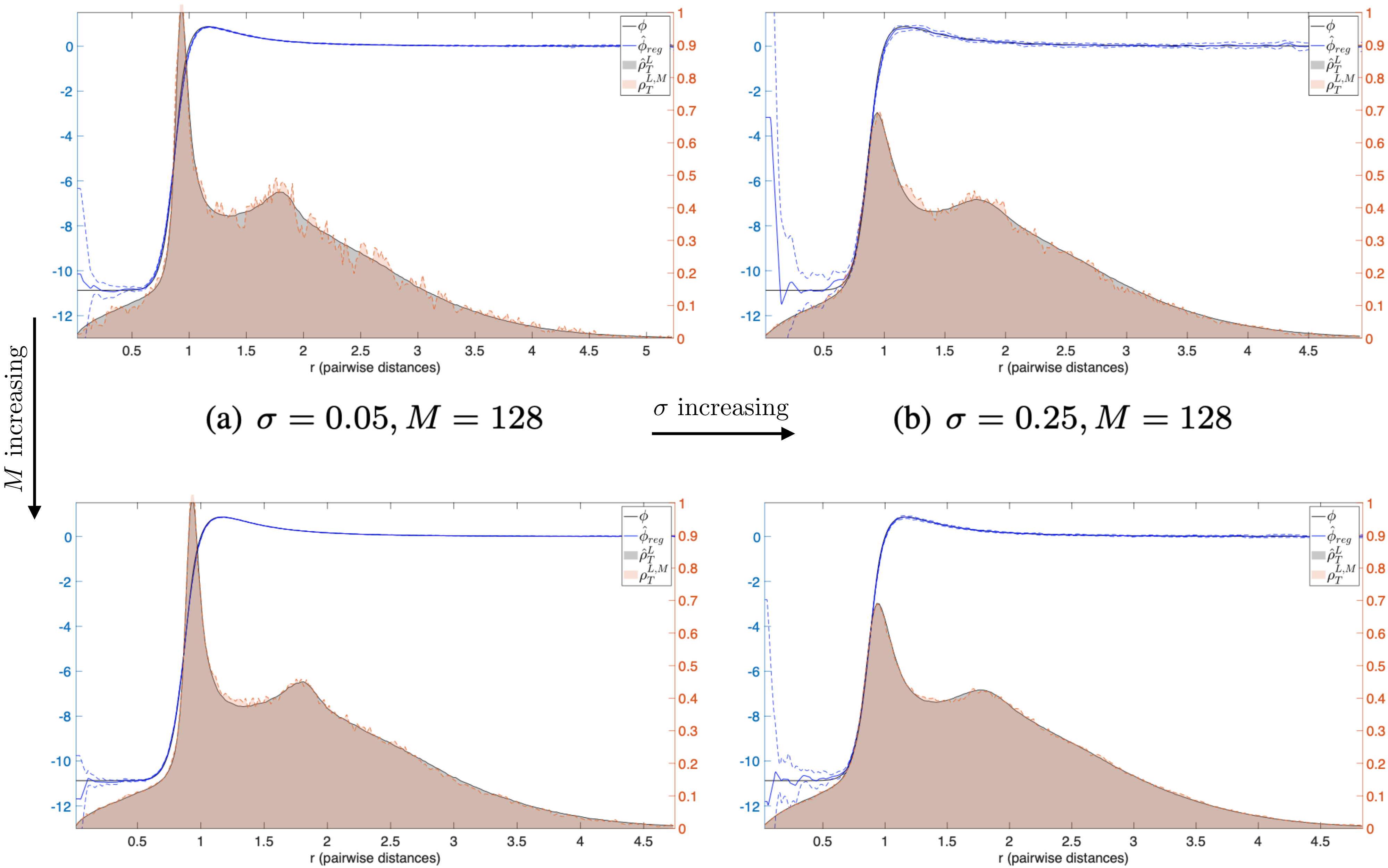
$$||\hat{\phi}_{L,T,M,\mathcal{H}} - \phi||_{L^2(\rho_T)} \leq \underbrace{||\hat{\phi}_{T,\infty,\mathcal{H}} - \phi||_{L^2(\rho_T)}}_{\text{approximation error}} + C\left(\underbrace{\sqrt{\frac{n}{M}}}_{\text{statistical error}} + \underbrace{\sqrt{\frac{T}{L}}}_{\text{discretization error}}\right),$$

where $\hat{\phi}_{T,\infty,\mathcal{H}}$ is the projection of the true kernel ϕ onto $\mathcal{H}$.

Stochastic opinion dynamics



Stochastic Lennard-Jones



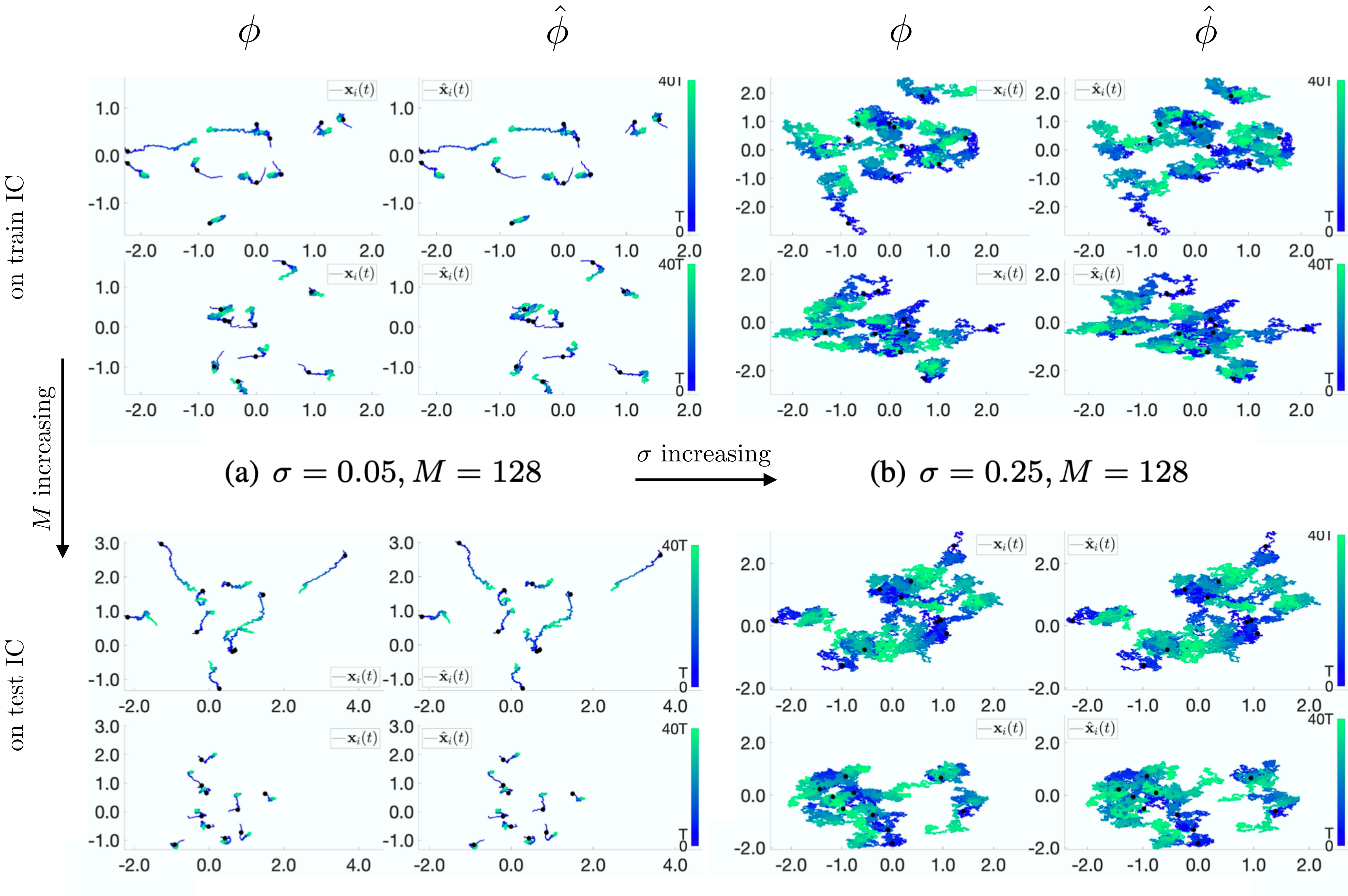
(a) $\sigma = 0.05, M = 128$

(b) $\sigma = 0.25, M = 128$

(c) $\sigma = 0.05, M = 1024$

(d) $\sigma = 0.25, M = 1024$

Stochastic Lennard-Jones



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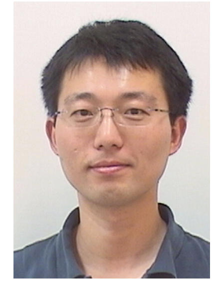
Overview

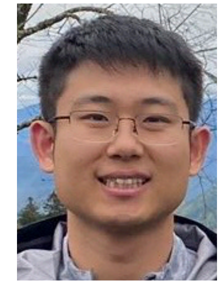
- Inference problem for interaction kernels
  - Problem setup
  - Proposed estimator
  - Regularized Least Squares
  - Performance guarantees
- Examples and Extensions:
  - Second order systems
  - Emergent behaviors
  - Stochastic systems
- Learning the interaction network
- Conclusions

Interacting Particle Systems on Networks



F. Lu

X. Wang



Q. Lang

We consider a heterogeneous dynamical system with N interacting particles on a graph: $G = (V, E, \mathbf{a})$ a graph, $\mathbf{a} = (\mathbf{a}_{ij}) \in [0,1]^{N\times N}$, $\mathbf{a}_{ij} > 0$ iff $(i,j) \in E$. At each vertex $i \in \{1, \ldots, N\}$ there is a particle $X_t^i \in \mathbb{R}^d$, with dynamics

$$\mathcal{S}_{\mathbf{a},\Phi} \ : \qquad dX_t^i = \sum_{j\neq i} \mathbf{a}_{ij}\Phi(X_t^j - X_t^i)dt + \sigma dW_t^i, \qquad i = 1, \ldots, N$$

Observations: $\{\mathbf{X}_{t_l}^{(m)}\}_{l\in[L],m\in[M]}$ + noise, where $\mathbf{X} = (X_i)_{i\in[N]} \in \mathbb{R}^{N\times d}$.

Want to estimate both $\mathbf{a} \in [0,1]^{N\times N}$ and $\Phi : \mathbb{R}^d \to \mathbb{R}^d$.

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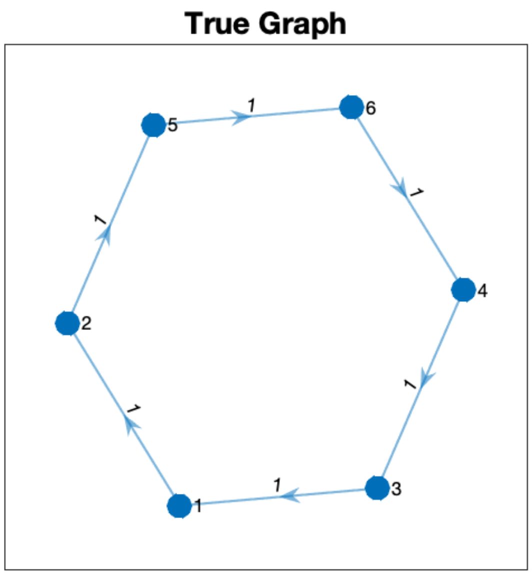

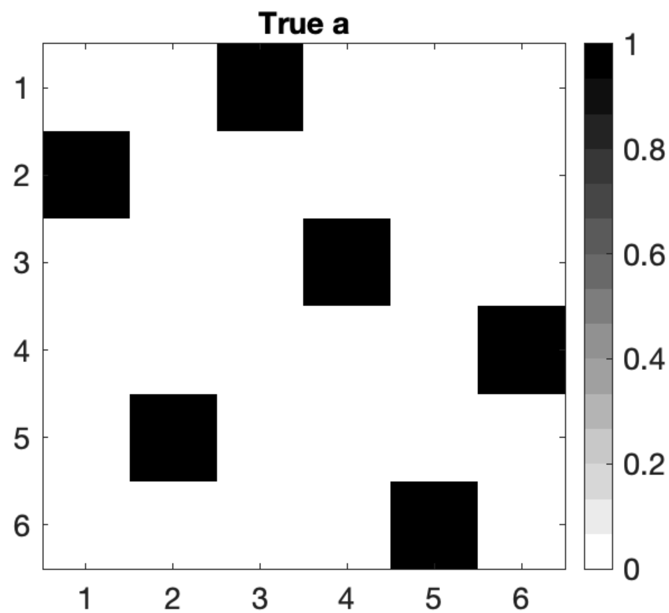

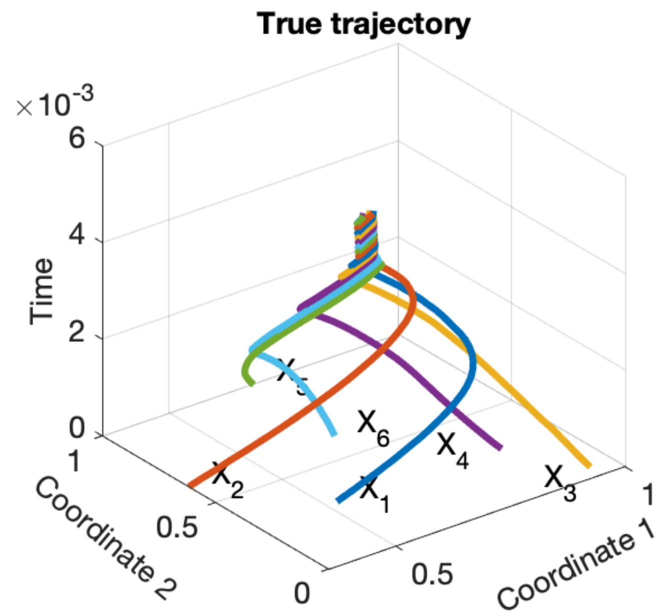

M	N	p	L	T	σ	σ_{obs}
10^3	6	10	50	$5 \cdot 10^{-3}$	10^{-3}	10^{-3}

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Parametric setting for simplicity: $\Phi \in \mathcal{H}$, for some given finite-dimensional hypothesis space $\mathcal{H} = \text{span}\{\psi_k\}_{k\in[p]}$; then $\Phi = \sum_{k\in[p]} c_k\psi_k$.

$$(\widehat{\mathbf{a}}, \widehat{c}) = \text{argmin}_{(\mathbf{a},c)}\mathcal{E}_{L,M}(\mathbf{a}, c)$$

$$\mathcal{E}_{L,M}(\mathbf{a}, c) := \frac{1}{MT}\sum_{l=0,m=1}^{L-1,M} \left\|\Delta\mathbf{X}_{t_l}^m - \mathbf{a}\mathbf{B}(\mathbf{X}_{t_l}^m)c\Delta t\right\|_F^2$$

where $\mathbf{B}(\mathbf{X}_t)_i := \left(\psi_k(X_t^j - X_t^i)\right)_{j,k} \in \mathbb{R}^{N\times 1\times d\times p}$ for each $i \in [N]$.

Interacting Particle Systems on Networks

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Normalization: $||\mathbf{a}_{i,\cdot}||_2 = 1$, defining the set $\mathcal{M}$ of admissible weights.

$\mathcal{E}$ nonlinear, non-convex, but separately convex in each of the two arguments.

Alternating Least Squares

$$(\widehat{\mathbf{a}}, \widehat{c}) = \mathrm{argmin}_{(\mathbf{a},c)} \mathcal{E}_{L,M}(\mathbf{a}, c)$$

$$\mathcal{E}_{L,M}(\mathbf{a}, c) := \frac{1}{MT} \sum_{l=0,m=1}^{L-1,M} \left\| \Delta \mathbf{X}_{t_l}^m - \mathbf{a}\mathbf{B}(\mathbf{X}_{t_l}^m) c \Delta t \right\|_F^2$$

1. Given c, estimate $\mathbf{a}$ by directly solving the minimizer of the quadratic loss function with c fixed, which solves

$$\widehat{\mathbf{a}}_{i\cdot} \mathcal{A}_{c,M,i}^{\mathrm{ALS}} := \widehat{\mathbf{a}}_{i\cdot}([\mathbf{B}(\mathbf{X}_{t_l}^m)_i]_{l,m} c) = [(\Delta \mathbf{X}_{t_l}^m)_i]_{l,m} / \Delta t$$

with $[\mathbf{B}(\mathbf{X}_{t_l}^m)_i]_{l,m} \in \mathbb{R}^{N \times (dLM) \times p}$, $\mathcal{A}_{c,M,i}^{\mathrm{ALS}} := [\mathbf{B}(\mathbf{X}_{t_l}^m)_i]_{l,m} c \in \mathbb{R}^{N \times (dLM)}$ and $[\Delta \mathbf{X}_{t_l}^m]_{l,m} \in \mathbb{R}^{N \times dLMN}$ obtained by multiplying appropriate tensor slices by c.

2. Given $\mathbf{a}$, estimate c by minimizing the loss function with fixed $\mathbf{a}$ by solving

$$\mathcal{A}_{\mathbf{a},M}^{\mathrm{ALS}} \widehat{c} := [\mathbf{a}\mathbf{B}(\mathbf{X}_{t_l}^m)]_{l,m} \widehat{c} = [\Delta \mathbf{X}_{t_l}^m]_{l,m} / \Delta t \,,$$

where $\mathcal{A}_{\mathbf{a},M}^{\mathrm{ALS}} := [\mathbf{a}\mathbf{B}(\mathbf{X}_{t_l}^m)]_{l,m} \in \mathbb{R}^{dLMN \times p}$ is again obtained by stacking in a block-row fashion and $\mathcal{A}_{\mathbf{a},M,i}^{\mathrm{ALS}} := [\mathbf{a}\mathbf{B}(\mathbf{X}_{t_l}^m)_i]_{l,m}$.

Operation Regression + ALS

$$(\widehat{\mathbf{a}}, \widehat{c}) = \mathrm{argmin}_{(\mathbf{a},c)} \mathcal{E}_{L,M}(\mathbf{a}, c)$$

$$\mathcal{E}_{L,M}(\mathbf{a}, c) := \frac{1}{MT} \sum_{l=0,m=1}^{L-1,M} \left\| \Delta \mathbf{X}_{t_l}^m - \mathbf{a}\mathbf{B}(\mathbf{X}_{t_l}^m) c \Delta t \right\|_F^2$$

Operator Regression. Consider $\{\mathbf{Z}_i = \mathbf{a}_{i,\cdot}^\top c^\top \in \mathbb{R}^{(N-1)\times p}\}_{i=1}^N$ treated as vectors $z_i \in \mathbb{R}^{(N-1)p\times 1}$; they solve

$$\mathcal{A}_{i,M} z_i = [\mathcal{A}_i]_{l,m} z_i := [(\mathbf{a}\mathbf{B}(\mathbf{X}_{t_l}^m) c \Delta t)_i]_{l,m} = [(\Delta \mathbf{X}_{t_l}^m)_i]_{l,m}\,, \quad i \in [N],$$

where $\mathcal{A}_{i,M} = [\mathcal{A}_i]_{l,m} \in \mathbb{R}^{dML\times(N-1)p}$, since the loss function can be written as $\frac{1}{ML} \sum_{l,m,i=1}^{L,M,N} \left| [(\Delta \mathbf{X}^m)_i]_{l,m} - [\mathcal{A}_i]_{l,m} z_i \right|^2$.

Deterministic ALS stage. The rows of $\mathbf{a}$ and the vector c are estimated via a joint factorization of the matrices of the estimated vectors $\{\widehat{z}_{i,M}\}$, denoted by $\widehat{\mathbf{Z}}_{i,M}$, with a shared vector c:

$$(\widehat{\mathbf{a}}^M, \widehat{c}^M) = \mathrm{argmin}_{\mathbf{a}\in\mathcal{M},\, c\in\mathbf{R}^p} \mathcal{E}(\mathbf{a}, c) := \sum_{i=1}^N \left\| \widehat{\mathbf{Z}}_{i,M} - \mathbf{a}_{i,\cdot}^\top c^\top \right\|_F^2$$

Theoretical results

The system satisfies a **rank-2 joint coercivity condition** on $\mathcal{H}$ if $\exists\, c_{\mathcal{H}} > 0$ s.t. $\forall\, \Phi_1, \Phi_2 \in \mathcal{H}$ with $\langle \Phi_1, \Phi_2 \rangle_{L^2(\rho_L)} = 0$, $\forall\, \mathbf{a}^{(1)}, \mathbf{a}^{(2)} \in \mathcal{M}$ and $\forall\, i \in [N]$

$$\frac{1}{L}\sum_{l=0}^{L-1} \mathbb{E}\Big[\Big|\sum_{j\neq i}[\mathbf{a}_{ij}^{(1)}\Phi_1(\mathbf{r}_{ij}(t_l)) + \mathbf{a}_{ij}^{(2)}\Phi_2(\mathbf{r}_{ij}(t_l))]\Big|^2\Big] \geq c_{\mathcal{H}}\left[|\mathbf{a}_{i\cdot}^{(1)}|^2\|\Phi_1\|_{\rho_L}^2 + |\mathbf{a}_{i\cdot}^{(2)}|^2\|\Phi_2\|_{\rho_L}^2\right]$$

uniqueness of the minimizer for $M = \infty$, solution of $\mathcal{E}_{L,\infty}(\mathbf{a}, \Phi) = 0$.

matrices in the least squares steps of ALS are well-conditioned.

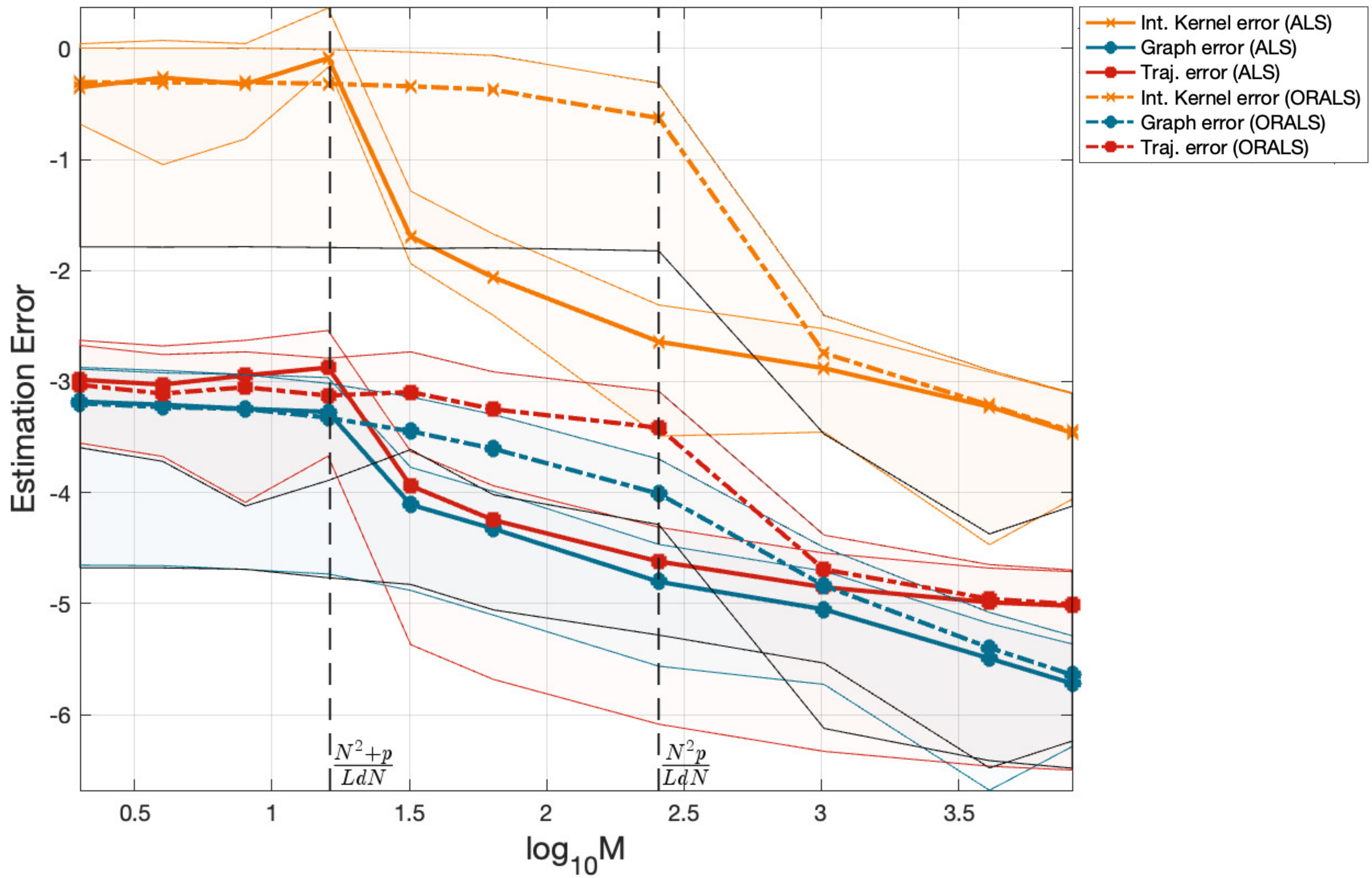
The system satisfies an **interaction kernel coercivity condition** in $\mathcal{H}$ if $\exists c_{0,\mathcal{H}} \in (0,1)$ s.t. $\forall \Phi \in \mathcal{H}$ and $i \in [N]$ $\frac{1}{L(N-1)}\sum_{l=0}^{L-1}\sum_{j\neq i}\mathbb{E}[\operatorname{tr}\operatorname{Cov}(\Phi(\mathbf{r}_{ij}(t_l)) \mid \mathcal{F}_l^i)] \geq c_{0,\mathcal{H}}\|\Phi\|_{\rho_L}^2$ where $\mathcal{F}_l^i$ is the σ-algebra generated by $(\mathbf{X}_{t_{l-1}}, X_{t_l}^i)$.

rank-2 joint coercivity

ORALS yields consistent and asymptotically normal estimator

matrices in ORALS are well-conditioned

Convergence & sampling



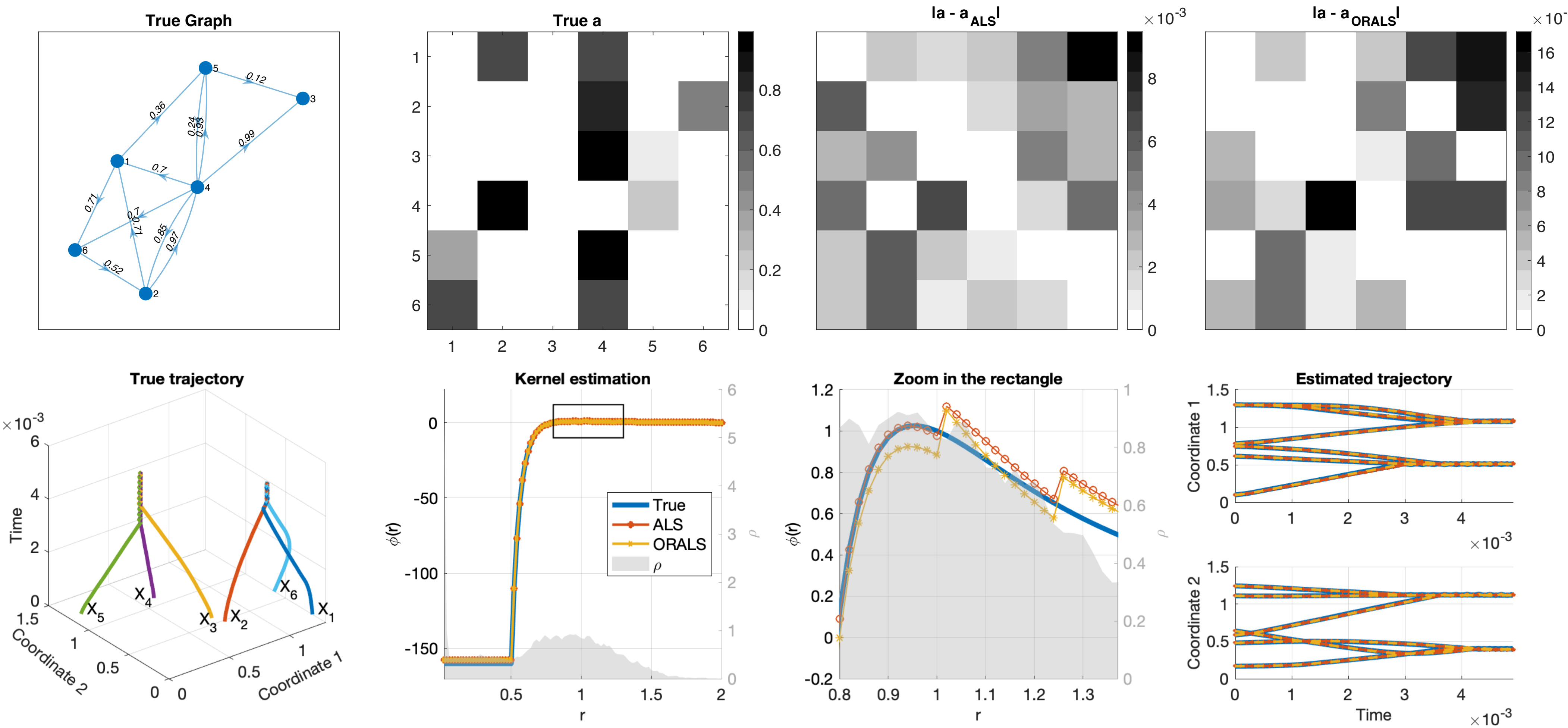
Top: Estimation errors as a function of M (all other parameters fixed), for ALS and ORALS, for a random Fourier interaction kernel with $p = 16$, $N = 32$, $L = 2$. In the small and medium sample regime, between the two vertical bars, ALS significantly and consistently outperforms ORALS; for large sample sizes, the two estimators have similar performance.

Lennard-Jones interactions on a network

$$\phi(x) = (-\tfrac{1}{3}x^{-9} + \tfrac{4}{3}x^{-3})\mathbf{1}_{x\geq 0.5} - 160\,\mathbf{1}_{0\leq x<0.5}$$

M	N	p	L	T	σ	σ_{obs}
10^3	6	10	50	$5\cdot 10^{-3}$	10^{-3}	10^{-3}

$$\{\psi_{1+k} = x^{-9}\mathbf{1}_{[0.25k+0.5,+\infty]}\}_{k=0}^{2} \cup \{\psi_{4+k} = x^{-3}\mathbf{1}_{[0.25k+0.5,+\infty]}\}_{k=0}^{2} \cup \{\psi_{7+k} = \mathbf{1}_{[0,0.25k+0.5]}\}_{k=0}^{3}$$



	Graph error $\varepsilon_{\mathbf{a}}$	Kernel error ε_K	Traj. error $\varepsilon_{\mathbf{X}}$	Exp. traj. error $\varepsilon_{\mathbf{X}}$
ALS	8.47×10^{-3}	1.45×10^{-2}	6.1×10^{-3}	$6.19\times 10^{-3} \pm 8.12\times 10^{-4}$
ORALS	1.67×10^{-2}	1.47×10^{-2}	6.6×10^{-3}	$7.41\times 10^{-3} \pm 1.07\times 10^{-3}$

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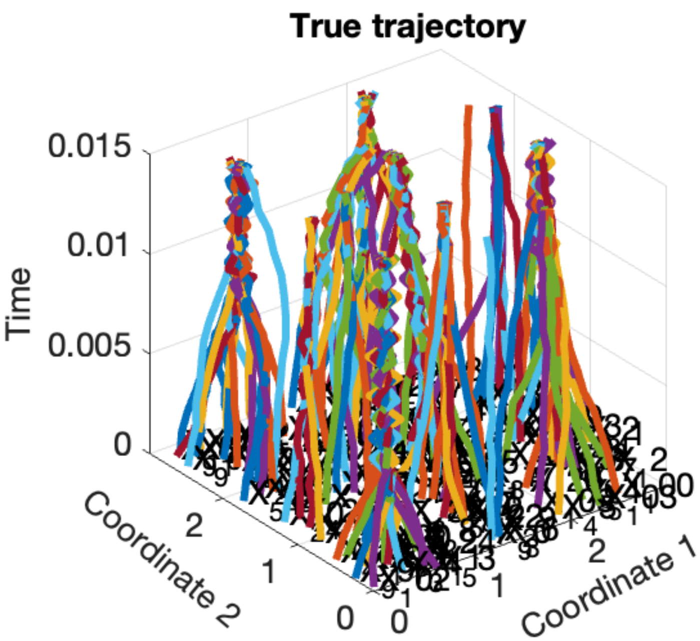
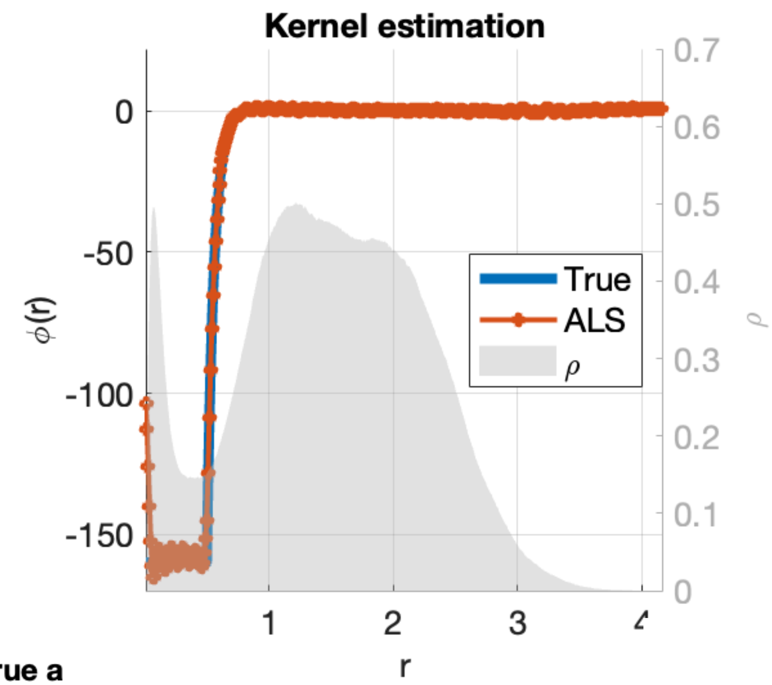
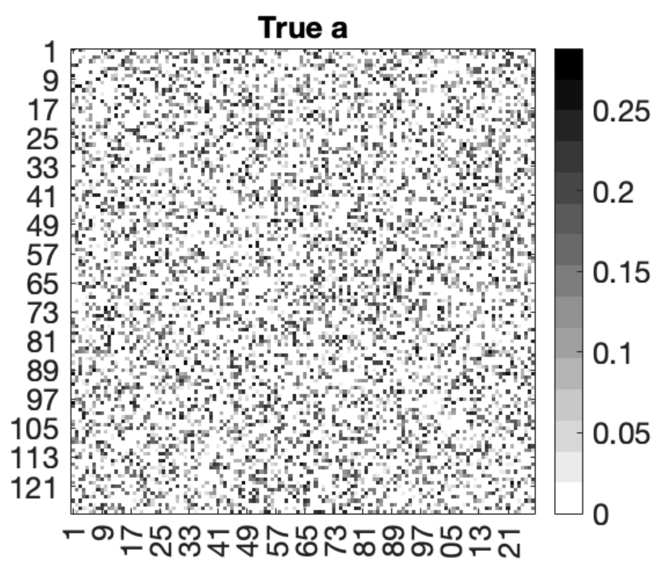
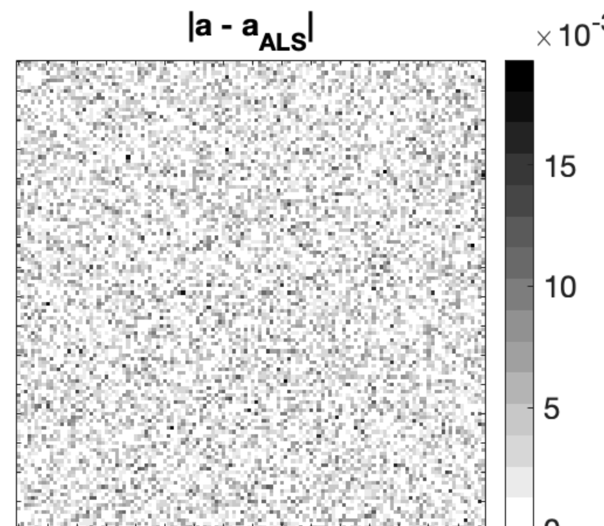
M	N	p	L	T	σ	σ_{obs}
10^3	128	67	50	$5\cdot 10^{-3}$	10^{-3}	10^{-3}







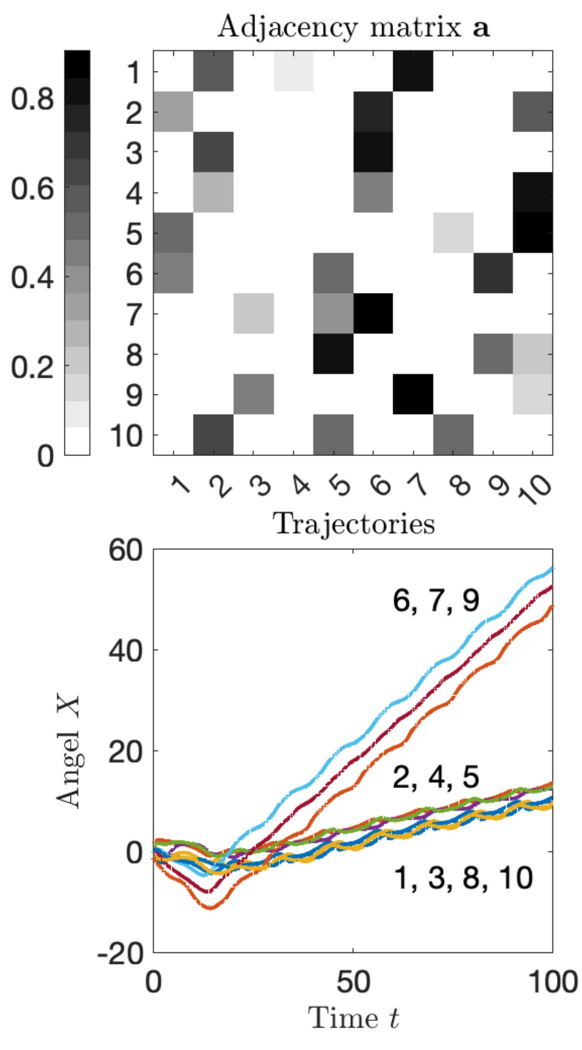


Kuramoto interactions on a network

$$dX_t^i = \kappa \sum_{j \in \mathcal{N}_i} \mathbf{a}_{ij} \sin(X_t^j - X_t^i)dt + \sigma dW_t^i$$

M	N	L	T	σ	σ_{obs}
$8, 64, 512$	10	100	$1 \cdot 10^{-1}$	10^{-4}	10^{-3}

$\mathcal{H} = \text{span}\{\cos(x), \sin(2x), \cos(2x), \dots, \cos(7x), \sin(7x)\}$, which does not contain Φ, and $\mathcal{H}_\phi := \text{span}\{\mathcal{H}, \Phi\}$.



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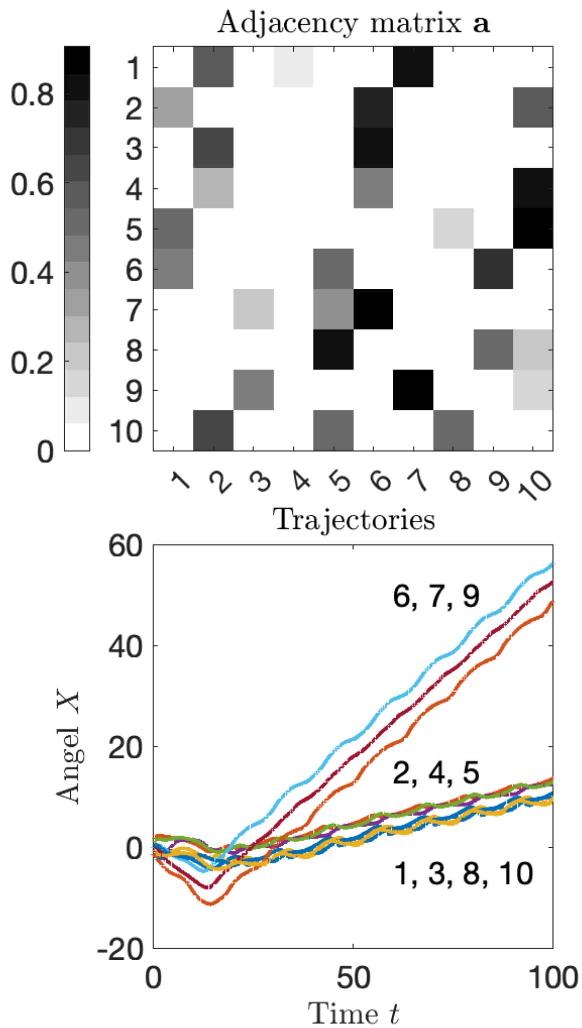

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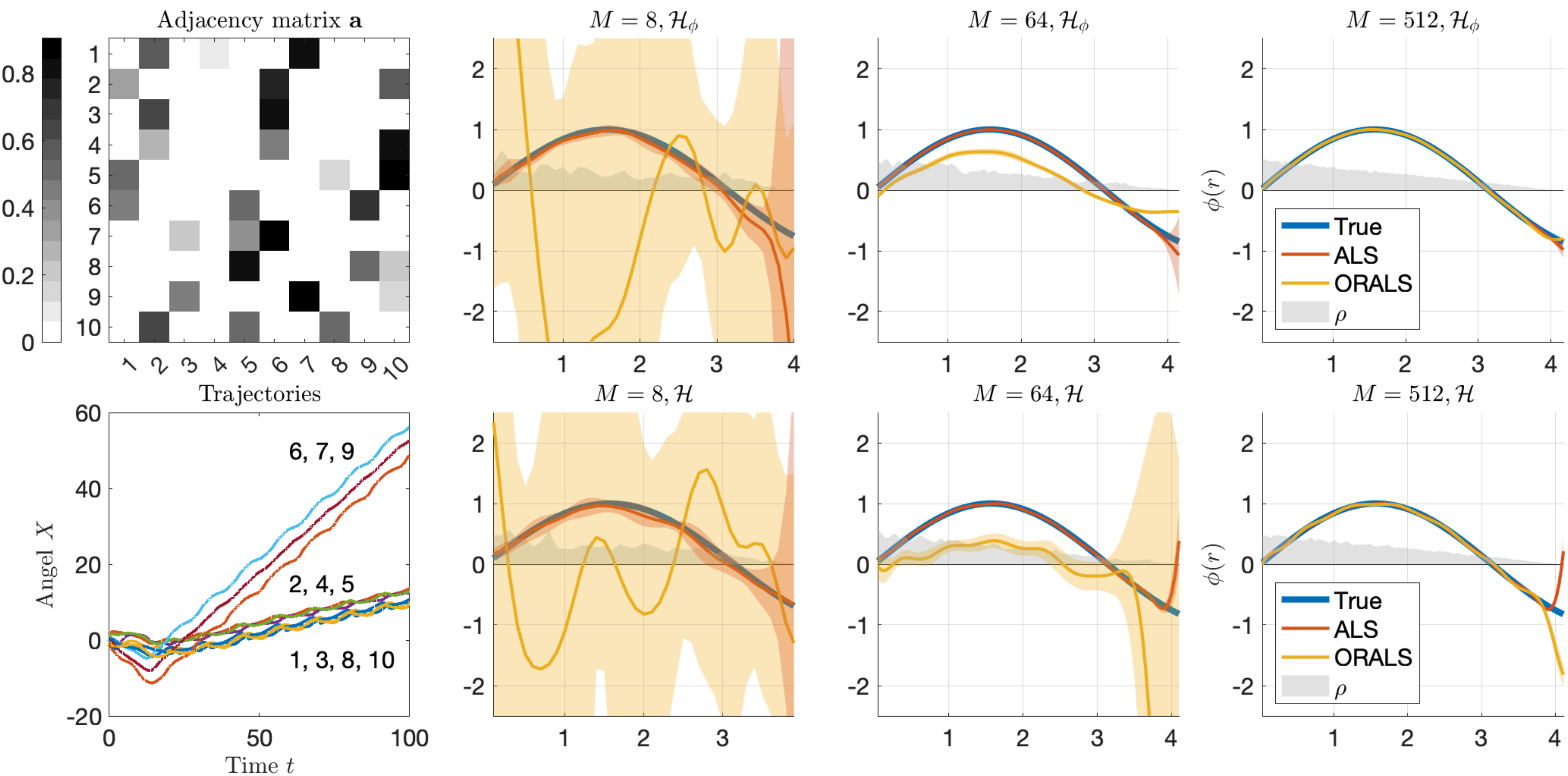


Leader-follower opinion dynamics

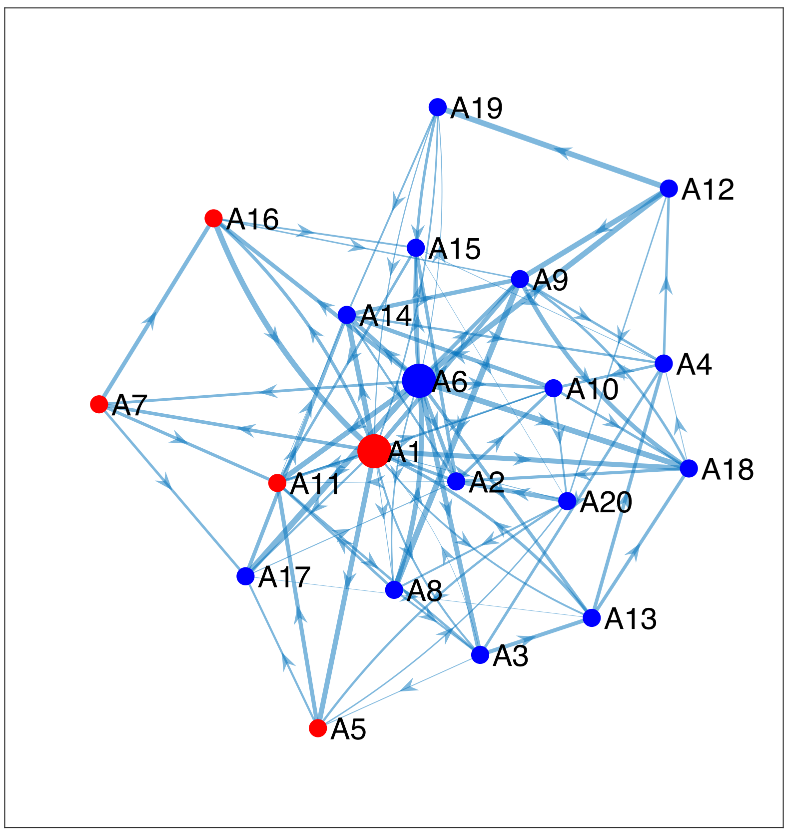
$dX_t^i = \sum_{j \neq i} \mathbf{a}_{ij} \Phi(X_t^j - X_t^i)dt + \sigma dW_t^i$

M	N	L	T	σ	σ_{obs}
$15, 30, 100$	20	100	1	0	0

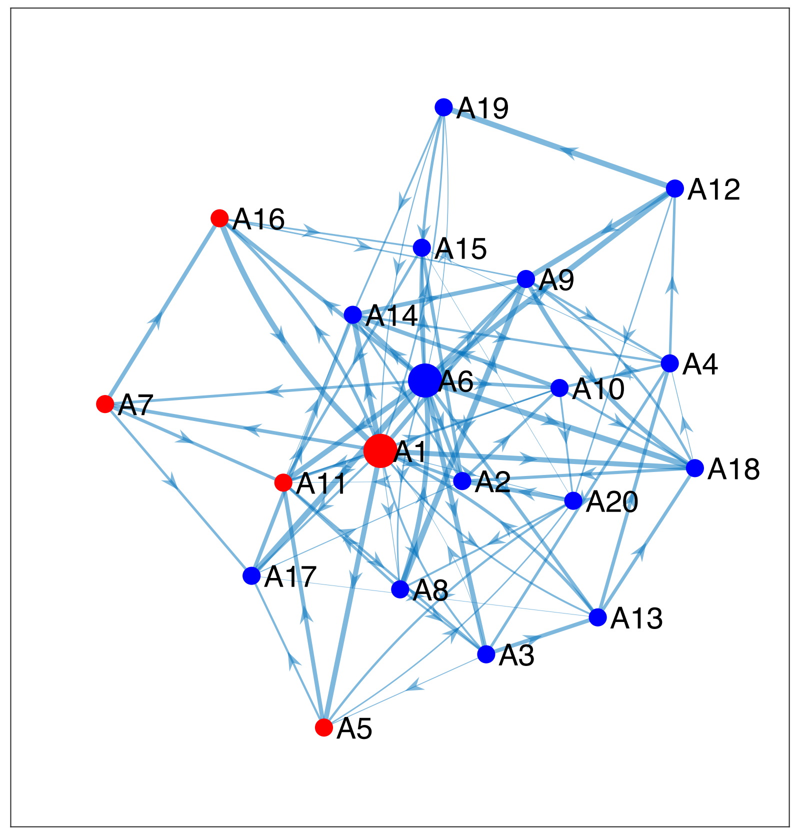
with $\Phi(x) = -\psi_1(x) - 0.1\psi_2(x)$, where $\psi_1(x) = \mathbf{1}_{\{x \leq 1\}}$, $\psi_2(x) = \mathbf{1}_{\{1 < x \leq 1.5\}}$.

"Leaders": consider the feature $L_i = \alpha \|\mathbf{a}_{i\cdot}\|_{\ell_1} + \beta \|\mathbf{a}_{\cdot i}\|_{\ell_1}$, with $\alpha + \beta = 1$. With $\alpha \gg \beta$, clustering yields the set of "leaders".
"Followers": we group them by assigning them to leaders based on a score $\widetilde{L}_j^k = \alpha \sum_{i \in G^k} |\mathbf{a}_{ij}| + \beta \sum_{i \in G^k} |\mathbf{a}_{ji}|$ from groups G^k of "followers" to "leaders".

Leader-follower network M=100



Leader-follower network True

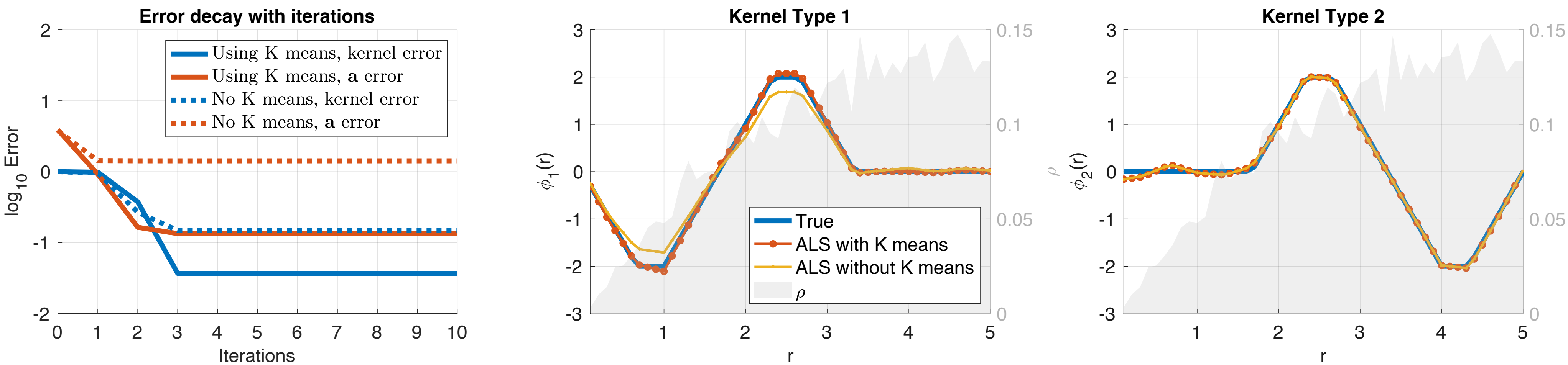


Particles of different types: example

$$dX_t^i = \sum_{j \neq i} \mathbf{a}_{ij} \Phi_{\kappa(i)}(X_t^j - X_t^i)dt + \sigma dW_t^i$$

M	N	L	T	σ	σ_{obs}
400	50	50	$5 \cdot 10^{-2}$	10^{-3}	10^{-3}

$\kappa : [N] \to [Q]$, with $Q = 2$, with Φ_1 short-range, and Φ_2 long-range.



Estimation of two types of kernels: short range and long range. The first panel shows the error decay with respect to iteration numbers. The algorithm using K-means decays faster and reaches lower errors than the algorithm without K-means. The right two columns show the estimation result of the two kernels. The classification is correct for both of the algorithms, and the one with K-means yields more accurate estimators, particularly for the kernel Type 1.

Conclusions and further work

- Learning interaction kernels in particle systems may be performed efficiently, nonparametrically, without curse of dimensionality of the state space...

- ...also on networks, with particles of different types, with interaction kernels, networks and types all unknown.

- Generalizations: 1st- and 2nd-order, multi-type, stochastic; learning variables; more general interaction kernels.

- many open problems and many connected techniques: singular kernels, learning variables inside interaction kernels; estimators that use weak formulations; robustness w.r.t. observational noise and mis-specified models; better connections to mean field equations; uncertainty quantification; learning controls; ternary kernels and beyond; anomaly detection.

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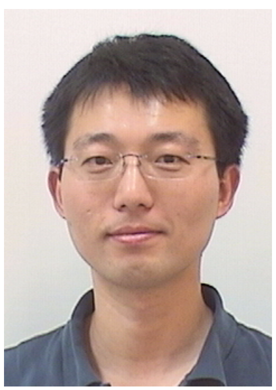
Links to code, papers: https://mauromaggioni.duckdns.org


Fei Lu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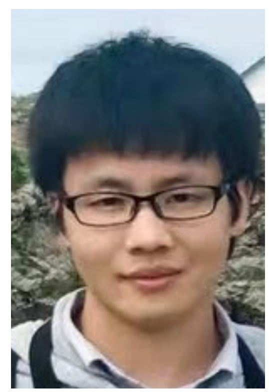
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