Nonparametric inference of interaction laws in particle/agent systems

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Joint with:

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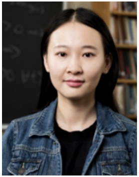

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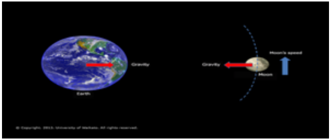
Outline

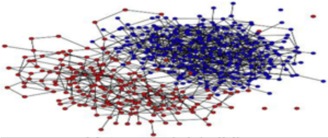
1. Motivation and problem statement
2. Learning via nonparametric regression
3. Numerical examples
4. Ongoing work and open problems

Motivation

Q: What is the law of interaction between particles/agents?



Popkin. Nature(2016)



Voter model (wiki)

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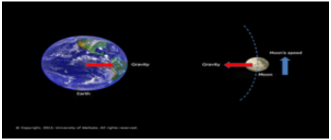


$$m\ddot{x}_i(t) = -\nu \dot{x}_i(t) + \frac{1}{N}\sum_{j=1, j\neq i}^{N} K(x_i, x_j),$$

- Newton's law of gravitation:

$$K(x,y) = G\frac{m_1 m_2}{r^2}, r = |x-y|$$

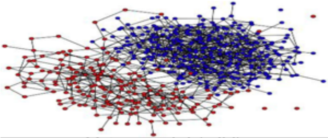
Popkin. Nature(2016)

- Molecular fluid: $K(x,y) = \nabla_x[\Phi(|x-y|)]$
  Lennard-Jones potential: $\Phi(r) = \frac{c_1}{r^{12}} - \frac{c_2}{r^6}$.

- flocking birds/school of fish

$$K(x,y) = \phi(|x-y|)\frac{x-y}{|x-y|}$$

- opinion/voter models, bacteria/cells ...[a]



Voter model (wiki)

[a] (1) Cucker+Smale: On the mathematics of emergence. 2007. (2) Vicsek+Zafeiris: Collective motion. 2012. (3) Mostch+Tadmor: Heterophilious Dynamics Enhances Consensus. 2014 ...

An inference problem:

Infer the rule of interaction in the system

$$m\ddot{x}_i(t) = -\nu\dot{x}_i(t) + \frac{1}{N}\sum_{j=1, j\neq i}^{N} K(x_i - x_j), \quad i = 1, \cdots, N, \; x_i(t) \in \mathbb{R}^d$$

from observations of trajectories.

- x_i is the position of the i-th particle/agent
- **Data**: many independent trajectories $\{\boldsymbol{x}^j(t) : t \in \mathcal{T}\}_{j=1}^{M}$
- **Goal**: infer $\phi : \mathbb{R}+ \to \mathbb{R}$ in

$$K(x) = -\nabla\Phi(|x|) = -\phi(|x|)\frac{x}{|x|}$$

For simplicity, we consider only first-order systems ($m = 0$) $\downarrow$

$$\dot{x}_i(t) = \frac{1}{N}\sum_{j=1, j\neq i}^{N} \phi_{true}(|x_i - x_j|)\frac{x_j - x_i}{|x_j - x_i|} \quad \rightarrow \quad \dot{\boldsymbol{x}} = \mathbf{f}_{\phi_{true}}(\boldsymbol{x}(t))$$

Least squares regression: with $\mathcal{H}_n = \mathrm{span}\{e_i\}_{i=1}^n$,

$$\hat{\phi}_n = \arg\min_{\phi \in \mathcal{H}_n} \mathcal{E}_M(\phi) := \sum_{m=1}^{M} |||\dot{\boldsymbol{x}}^m - \mathbf{f}_{\phi}(\boldsymbol{x}^m)|||^2$$

- Choice of $\mathcal{H}_n$ & function space of learning?
- Inverse problem well-posed/ identifiability?
- Consistency and rate of “convergence”?
  $\rightarrow$ hypothesis testing and model selection

Outline

1. Motivation and problem statement
2. Learning via nonparametric regression:
   - Function space of regression
   - Identifiability: a coercivity condition
   - Consistency and rate of convergence
3. Numerical examples
4. Ongoing work and open problems

Learning via nonparametric regression

The dynamical system:

$$\dot{x} = \mathbf{f}_{\phi_{true}}(\boldsymbol{x}(t))$$

Data: M-trajectories $\{\boldsymbol{x}^m(t) : t \in \mathcal{T}\}_{m=1}^{M}$

- $\boldsymbol{x}^m(0) \overset{i.i.d}{\sim} \mu_0 \in \mathcal{P}(\mathbb{R}^{dN})$
- $\mathcal{T} = [0, T]$ or $\{t_1, \cdots, t_L\}$ with $\dot{\mathbf{x}}(t_i)$

Goal: nonparametric inference[1] of ϕ_{true}

[1] (1) Bongini, Fornasier, Hansen, Maggioni: Inferring Interaction Rules for mean field equations, M3AS, 2017.
(2) Binev, Cohen, Dahmen, Devore and Temlyakov: Universal Algorithms for learning theory, JMLR 2005.
(3) Cucker, Smale: On the mathematical foundation of learning. Bulletin of AMS, 2001.

$$\hat{\phi}_{M,\mathcal{H}} = \underset{\phi \in \mathcal{H}}{\arg\min}\, \mathcal{E}_M(\phi) := \frac{1}{ML} \sum_{l,m=1}^{L,M} \|\mathbf{f}_{\phi}(\boldsymbol{X}^m(t_l)) - \dot{\boldsymbol{X}}^m(t_l)\|^2$$

- $\mathcal{E}_M(\phi)$ is quadratic in ϕ, and $\mathcal{E}_M(\phi) \geq \mathcal{E}_M(\phi_{true}) = 0$
- The minimizer exists for any $\mathcal{H} = \mathcal{H}_n = span\{e_1, \ldots, e_n\}$

Tasks

- Choice of $\mathcal{H}_n$ & function space of learning?
- Inverse problem well-posed/ identifiability?
- Consistency and rate of "convergence"?

$$\begin{tikzcd}
\mathcal{E}_M(\cdot) \arrow[r, "M\to\infty"] \arrow[d] & \mathcal{E}_\infty(\cdot) \arrow[d] \\
\widehat{\phi}_{M,\mathcal{H}} \arrow[r, "?M\to\infty"] \arrow[dr, "??"] & \widehat{\phi}_{\infty,\mathcal{H}} \arrow[d, "?dist(\mathcal{H},\phi_{true})\to 0"] \\
 & \phi_{true}
\end{tikzcd}$$

Review of classical nonparametric regression:

Estimate $y = \phi(z) : \mathbb{R}^D \to \mathbb{R}$ from data $\{z_i, y_i\}_{m=1}^M$.

- $\{z_i, y_j\}$ are iid samples;
- $\hat{\phi}_n := \arg\min_{f \in \mathcal{H}_n} \mathcal{E}_M(f) := \sum_{m=1}^M \|y_i - f(z_i)\|^2 \quad \to \mathbb{E}[Y|Z = z]$
- Optimal rate: if $\mathrm{dist}(\mathcal{H}_n, \phi_{true}) \lesssim n^{-s}$ and $n_* = (M/\log M)^{\frac{1}{2s+1}}$,
$$\|\hat{\phi}_{n_*} - \phi\|_{L^2(\rho_Z)} \lesssim M^{-\frac{s}{2s+D}}$$

[2]

[2] (1) F.Cucker and S.Smale. On the mathematical foundations of learning. Bulletin of the AMS, 2002
(2) L.Györfi, M.Kohler, A.Krzyzak, H.Walk, A Distribution-Free Theoryof Nonparametric Regression (Springer 2002).

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$$\|\hat{\phi}_{n_*} - \phi\|_{L^2(\rho_Z)} \lesssim M^{-\frac{s}{2s+D}}$$

Our case: learning of kernel $\phi : \mathbb{R}^+ \to \mathbb{R}$ from data $\{\boldsymbol{x}^m(t)\}$

$$\dot{x}_i(t) = \frac{1}{N} \sum_{j=1, j\neq i}^{N} \phi(|x_i - x_j|) \frac{x_j - x_i}{|x_j - x_i|}$$

- $\{r_{ij}^m(t) := |x_i^m(t) - x_j^m(t)|\}$ not iid
- The values of $\phi(r_{ij}^m(t))$ unknown

Regression measure

Distribution of pairwise-distances $\rho : \mathbb{R}_+ \to \mathbb{R}$

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

- unknown, estimated by empirical distribution $\rho_T^M \xrightarrow{M\to\infty} \rho_T$ (LLN)
- intrinsic to the dynamics

Regression function space $L^2(\rho_T)$

- the admissible set $\subset L^2(\rho_T)$
- $\mathcal{H} =$ piecewise polynomials $\subset L^2(\rho_T)$
- singular kernels $\subset L^2(\rho_T)$

Identifiability: a coercivity condition

$$\begin{tikzcd}
\mathcal{E}_M(\cdot) \arrow[r, "M\to\infty"] \arrow[d] & \mathcal{E}_\infty(\cdot) \arrow[d] \\
\widehat{\phi}_{M,\mathcal{H}} \arrow[r, "?M\to\infty"] \arrow[dr, "?"] & \widehat{\phi}_{\infty,\mathcal{H}} \arrow[d, "?"] \\
& \phi_{true}
\end{tikzcd}$$

$$\hat{\phi}_{M,\mathcal{H}} = \underset{\phi\in\mathcal{H}}{\arg\min}\ \mathcal{E}_M(\phi)$$

$$\mathcal{E}_\infty(\hat{\phi}) - \mathcal{E}_\infty(\phi_{true}) = \frac{1}{NT}\int_0^T \mathbb{E}_{\mu_0}\|\mathbf{f}_{\hat{\phi}-\phi_{true}}(\boldsymbol{X}(t))\|^2 dt \geq c\|\hat{\phi} - \phi_{true}\|^2_{L^2(\rho_T)}$$

Coercivity condition. $\exists\ c_{T,\mathcal{H}} > 0$ s.t. for all $\varphi \in \mathcal{H} \subset L^2(\rho_T)$

$$\frac{1}{NT}\int_0^T \mathbb{E}_{\mu_0}\|\mathbf{f}_\varphi(\boldsymbol{x}(t))\|^2 dt = \langle\langle \varphi, \varphi \rangle\rangle \geq c_{T,\mathcal{H}}\|\varphi\|^2_{L^2(\rho_T)}$$

- coercivity: bilinear functional $\langle\langle \varphi, \psi \rangle\rangle := \frac{1}{NT}\int_0^T \mathbb{E}_{\mu_0}\langle \mathbf{f}_\varphi, \mathbf{f}_\psi\rangle(\boldsymbol{x}(t))dt$
- controls condition number of regression matrix

Consistency of estimator

Theorem (L., Maggioni, Tang, Zhong)

Assume the coercivity condition. Let $\{\mathcal{H}_n\}$ be a sequence of compact convex subsets of $L^\infty([0,R])$ such that $\inf_{\varphi \in \mathcal{H}_n} \|\varphi - \phi_{true}\|_\infty \to 0$ as $n \to \infty$. Then

$$\lim_{n\to\infty} \lim_{M\to\infty} \|\widehat{\phi}_{M,\mathcal{H}_n} - \phi_{true}\|_{L^2(\rho_T)} = 0, \text{ almost surely.}$$

- For each n, compactness of $\{\widehat{\phi}_{M,\mathcal{H}_n}\}$ and coercivity implies that $\widehat{\phi}_{M,\mathcal{H}_n} \to \widehat{\phi}_{\infty,\mathcal{H}_n}$ in L^2
- Increasing $\mathcal{H}_n$ and coercivity implies consistency.
- In general, truncation to make $\mathcal{H}_n$ compact

Optimal rate of convergence

Theorem (L. Maggioni, Tang, Zhong)

Let $\{\mathcal{H}_n\}$ be a seq. of compact convex subspaces of $L^\infty[0,R]$ s.t.

$$\dim(\mathcal{H}_n) \le c_0 n, \ \textit{and} \ \inf_{\varphi\in\mathcal{H}_n} \|\varphi - \phi_{true}\|_\infty \le c_1 n^{-s}.$$

Assume the coercivity condition. Choose $n_* = (M/\log M)^{\frac{1}{2s+1}}$: then

$$\mathbb{E}_{\mu_0}[\|\widehat{\phi}_{T,M,\mathcal{H}_{n_*}} - \phi_{true}\|_{L^2(\rho_T)}] \le C\left(\frac{\log M}{M}\right)^{\frac{s}{2s+1}}.$$

- The 2nd condition is about regularity: $\phi \in C^s$
- Choice of $\dim(\mathcal{H}_n)$: adaptive to s and M

Prediction of future evolution

Theorem (L., Maggioni, Tang, Zhong)

Denote by $\widehat{\boldsymbol{X}}(t)$ and $\boldsymbol{X}(t)$ the solutions of the systems with kernels $\widehat{\phi}$ and ϕ respectively, starting from the same initial conditions that are drawn i.i.d from μ_0. Then we have

$$\mathbb{E}_{\mu_0}[\sup_{t\in[0,T]} \|\widehat{\boldsymbol{X}}(t) - \boldsymbol{X}(t)\|^2] \lesssim \sqrt{N}\|\widehat{\phi} - \phi_{true}\|^2_{L^2(\rho_T)},$$

- Follows from Grownwall's inequality

Outline

1. Motivation and problem statement
2. Learning via nonparametric regression:
   - A regression measure and function space
   - Learnability: a coercivity condition
   - Consistency and rate of convergence
3. Numerical examples
   - A general algorithm
   - Lennard-Jones model
   - Opinion dynamics and multiple-agent systems
4. Ongoing work and open problems

The regression algorithm

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

$$\mathcal{H}_n := \{\varphi = \sum_{p=1}^{n} a_p \psi_p(r) : \mathbf{a} = (a_1, \ldots, a_n) \in \mathbb{R}^n\},$$

$$\mathcal{E}_{L,M}(\varphi) = \mathcal{E}_{L,M}(\mathbf{a}) = \frac{1}{M} \sum_{m=1}^{M} \|\mathbf{d}^m - \Psi_L^m \mathbf{a}\|_{\mathbb{R}^{LNd}}^2 .$$

$$\frac{1}{M} \sum_{m=1}^{M} A_L^m \mathbf{a} = \frac{1}{M} \sum_{m=1}^{M} b_L^m , \text{ rewrite as } A_M \mathbf{a} = b_M$$

- can be computed parallelly
- Caution: choice of $\{\psi_p\}$ affects condi(A_M)

Assume the coercivity condition: $\langle\!\langle \varphi, \varphi \rangle\!\rangle \geq c_{T,\mathcal{H}} \|\varphi\|^2_{L^2(\rho_T)}$.

Proposition (Lower bound on smallest singular value of A_M)

Let $\{\psi_1, \cdots, \psi_n\}$ be a basis of $\mathcal{H}_n$ s.t.

$$\langle \psi_p, \psi_{p'} \rangle_{L^2(\rho_T^L)} = \delta_{p,p'}, \|\psi_p\|_\infty \leq S_0.$$

Let $A_\infty = \left(\langle\!\langle \psi_p, \psi_{p'} \rangle\!\rangle\right)_{p,p'} \in \mathbb{R}^{n \times n}$. Then $\sigma_{\min}(A_\infty) \geq c_{T,\mathcal{H}}$. Moreover, A_∞ is the a.s. limit of A_M. Therefore, for large M, the smallest singular value of A_M satisfies with a high probability that

$$\sigma_{\min}(A_M) \geq (1 - \epsilon) c_{T,\mathcal{H}}$$

- Choose $\{\psi_p\}$ linearly independent in $L^2(\rho_T)$
- Piecewise polynomials: on a partition of support(ρ_T)
- Finite difference $\approx$ derivatives $\Rightarrow$ an $O(\Delta t)$ error to estimator

Implementation

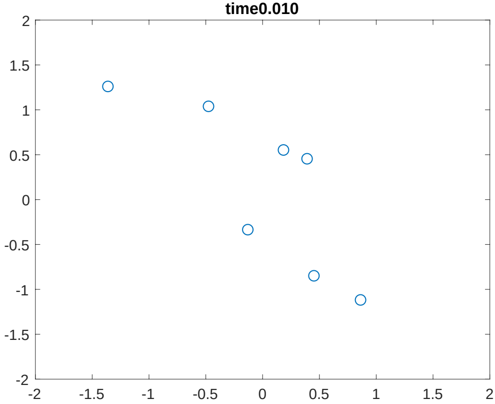
1. Approximate regression measure
   - Estimate the ρ_T with large datasets
   - Partition on support(ρ_T)
2. Construct hypothesis space $\mathcal{H}$:
   - choose the degree of piecewise polynomials
   - set dimension of $\mathcal{H}$ according to sample size
3. Regression:
   - Assemble the arrays (in parallel)
   - Solve the normal equation

Examples: Lennard-Jones Dynamics

The Lennard-Jones potential

$$V_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \Rightarrow \quad \phi(r)r = V'_{LJ}(r)$$

$$\dot{x}_i(t) = \frac{1}{N}\sum_{j=1, j\neq i}^{N} \phi(|x_i - x_j|)(x_j - x_i)$$



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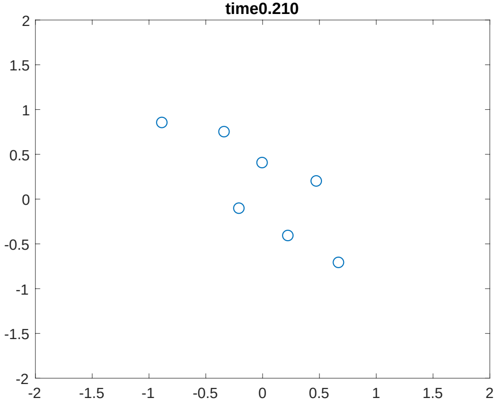

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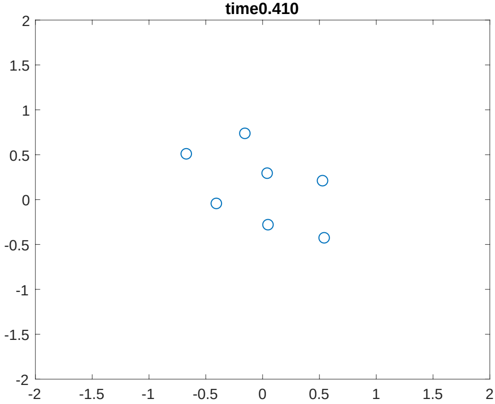

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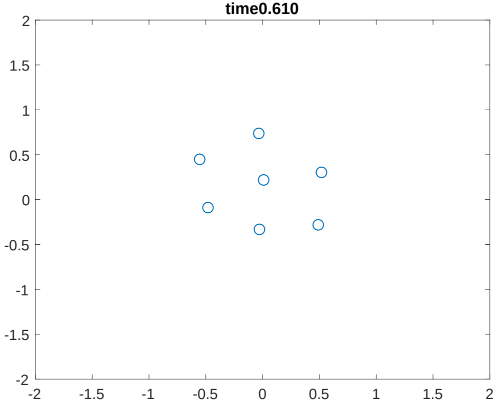
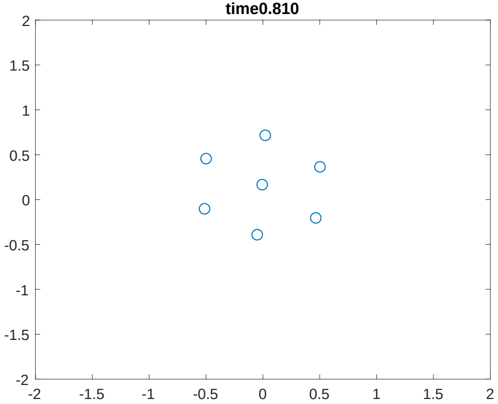


The Lennard-Jones potential

$$V_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \Rightarrow \quad \phi(r)r = V_{LJ}'(r)$$

$$\dot{x}_i(t) = \frac{1}{N}\sum_{j=1, j\neq i}^{N} \phi(|x_i - x_j|)(x_j - x_i)$$



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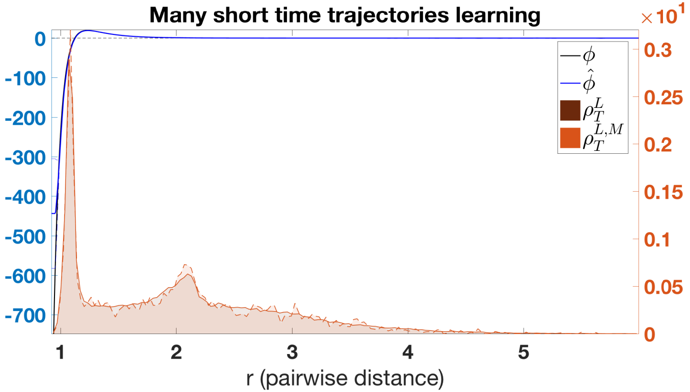
$$V_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \Rightarrow \quad \phi(r)r = V'_{LJ}(r)$$

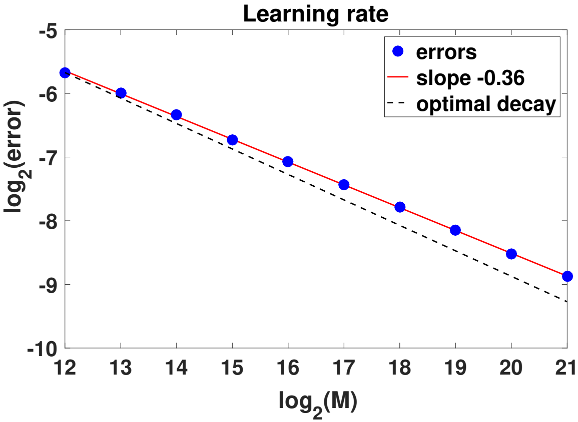
- piecewise linear estimator; Gaussian initial conditions.



Optimal rate

$$V_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \Rightarrow \quad \phi(r)r = V'_{LJ}(r)$$

- V_{LJ} is highly singular, yet we get close to optimal rate (-0.4).



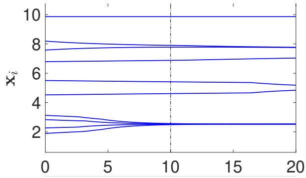
Example: Opinion Dynamics

$N = 10, \boldsymbol{x}_i \in \mathbb{R}$.

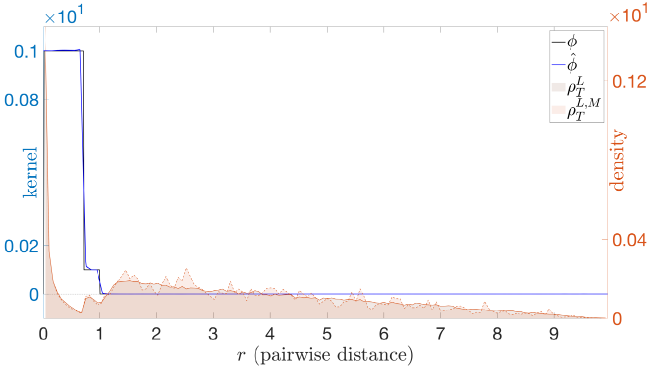
$M = 250, \mu_0 = Unif[0, 10]^{10}$

$\mathcal{T} = [0, 10]$, 200 discrete instances

$\mathcal{H} =$ piecewise constant functions



The estimated kernels:



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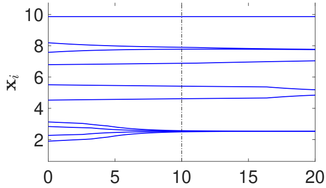
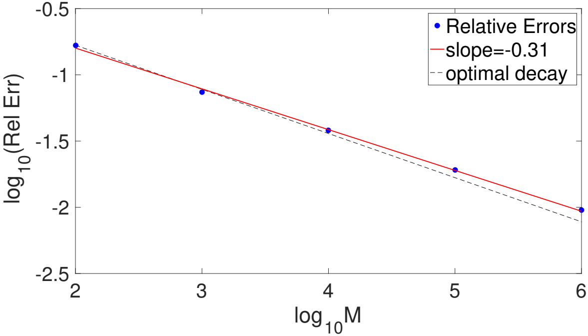
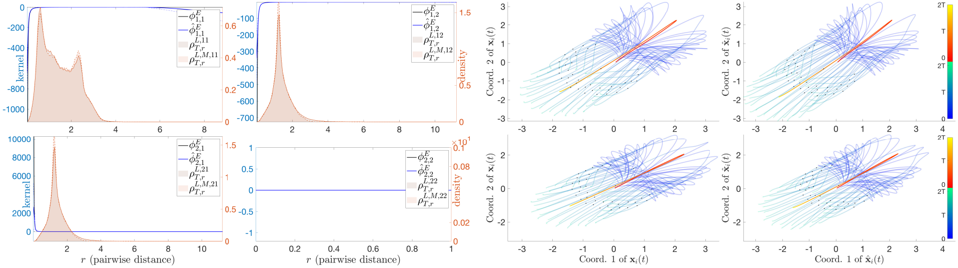


The rate of convergence:



Example: 2nd-order Prey-Predator system

$$\begin{cases} \ddot{\boldsymbol{X}}^m = \mathcal{F}^{\boldsymbol{v}}(\dot{\boldsymbol{X}}^m, \Xi^m) + \mathbf{f}_{\boldsymbol{\phi}^E}(\boldsymbol{X}^m) + \mathbf{f}_{\boldsymbol{\phi}^A}(\boldsymbol{X}^m, \dot{\boldsymbol{X}}^m) \\ \dot{\Xi}^m = \mathcal{F}^{\xi}(\Xi^m) + \mathbf{f}_{\boldsymbol{\phi}^{\xi}}(\boldsymbol{X}^m, \Xi^m), \end{cases}$$

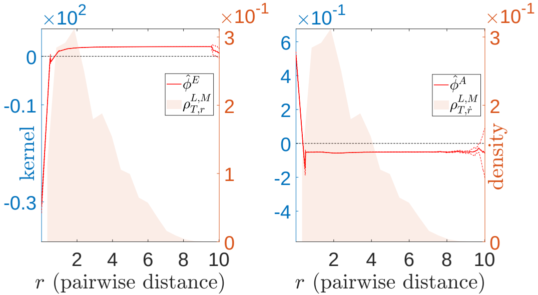


Example: model selection

- **Order selection**

	Learned as 1^{st} order	Learned as 2^{nd} order
1^{st} order system	**0.01** $\pm$ **0.002**	1.6 $\pm$ 1.1
2^{nd} order system	1.7 $\pm$ 0.3	**0.2** $\pm$ **0.06**

- **Interaction type selection**



Summary and open problems

$$\begin{tikzcd}
\mathcal{E}_{T,M}(\cdot) \arrow[r] \arrow[d] & \mathcal{E}_{T,\infty}(\cdot) \arrow[d] \\
\widehat{\phi}_{T,M,\mathcal{H}} \arrow[r, "M\to\infty"] \arrow[dr, "optimal\ \mathcal{H}"] & \widehat{\phi}_{T,\infty,\mathcal{H}} \arrow[d, "dist(\mathcal{H},\phi)\to 0"] \\
 & \phi
\end{tikzcd}$$

Learning theory

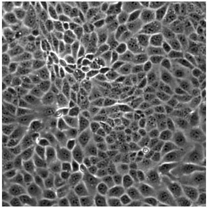
- extended the classical regression theory
- a coercivity condition for identifiability

Theory guided regression algorithms

- Selection of $\mathcal{H}$ (basis functions & dimension)
- Measurement of error of estimators
- Optimal learning rate
- Model selection

Ongoing work

- Different type of systems:
  - 1st- and 2nd-order
  - Multiple type of agents (leader-follower, predator-prey)
  - Stochastic systems
- Coercivity condition
- Adaptive basis functions
- Partial and noisy observations; Mean field equations
- Real data applications:
  learning cell-dynamics



Ongoing work: The coercivity condition

$$\langle\!\langle \varphi, \varphi \rangle\!\rangle \geq c_{\mathcal{H}}^{T} \|\varphi\|_{L^2(\rho_T)}^2, \mathcal{H} \text{ compact}$$

Exchangeability, $g(r) = \phi(r)r \Updownarrow U_t = x_1(t) - x_2(t),\, V_t = x_1(t) - x_3(t)$

$$\int_0^T \underbrace{\mathbb{E}\left[g(|U_t|)g(|V_t|)\frac{\langle U_t, V_t\rangle}{|U_t||V_t|}\right]}_{\int_{\mathbb{R}}^{+}\int_{\mathbb{R}}^{+} g(r)g(s)\mathcal{K}_t(r,s)drds} dt > 0$$

Proposition (Li-Lu19)

Coercivity condition holds for systems with $\Phi(r) = r^{\beta}$, $\beta \in [1,2]$.

- positiveness of integral operator $\leftrightarrow \mathcal{K}(\cdot,\cdot) := \int_0^T \mathcal{K}_t(\cdot,\cdot)dt$
  - Müntz type theorem: $\mathrm{span}\{r^{2n}e^{-r}\}_{n=1}^{\infty}$ dense in $L^2(\mathbb{R}^+)$.
- **Conjecture:** true for general systems

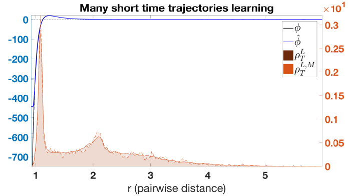
Ongoing work: Adaptive basis functions $\{\psi_p\}$

$$A_M \mathbf{a} = b_M, \text{ with } \mathbb{E}[A_M] = \Big(\underbrace{\langle\langle \psi_p, \psi_{p'} \rangle\rangle}_{\int_{\mathbb{R}}^{+} \int_{\mathbb{R}}^{+} \psi_p(r)\psi_{p'}(s)\mathcal{K}(r,s)drds} \Big)_{p,p' \in 1,\dots,n}$$

Current: piecewise polynomials + uniform partition supp($\bar{\rho}$)

Adaptive strategies:

- Adaptive partition based on $\bar{\rho}$
- Eigenfunctions of integral kernel $\mathcal{K}$
  - $\widehat{\mathcal{K}}$ from data: noisy
  - goal: smooth eigenfunctions



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Thank you!