Learning interacting kernels of mean-field equations of particle systems

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Joint work with Quanjun Lang

Related work with: Mauro Maggioni, Sui Tang, Ming Zhong, Zhongyang Li and Cheng Zhang

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Outline

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

An inverse problem

Consider the mean-field equation

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)], \quad x \in \mathbb{R}^d, t > 0,$$

where $K_\phi(x) = \nabla(\Phi(|x|)) = \phi(|x|)\frac{x}{|x|}$.

Question: identify ϕ from data $\{u(x_m, t_l)\}_{m,l=1}^{M,L}$?

Goal:

- An algorithm $\to \widehat{\phi}$
- identifiability: function space of learning
- convergence rate when $\Delta x = M^{-1/d} \to 0$

Motivation

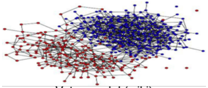
$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)]$$

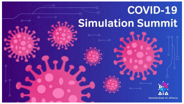
Interacting particles/agents:

$$\frac{d}{dt} X_t^i = \frac{1}{N} \sum_{i'=1}^{N} \phi(|X_t^j - X_t^i|) \frac{X_t^j - X_t^i}{|X_t^j - X_t^i|} + \sqrt{2\nu} dB_t^i, \quad i = 1, \ldots, N$$

- X_t^i: the i-th particle's position; B_t^i: Brownian motion
- $u(x,t) = \lim_{N\to\infty} \sum_{i=1}^N \delta(X_t^i - x)$ Propagation of chaos
- 1st- and 2nd-order models
- Application in many disciplines:
  - Statistical physics, quantum mechanics
  - Biology [Keller-Segal1970, Cucker-Smale2000]
  - Social science [Motsch-Tadmor2014]
  - Monte Carlo sampling [Del Moral13]
  - Epidemiology (Agent-based model for COVID19 at Imperial)


Popkin. Nature(2016)


Voter model (wiki)



Previous work: finite N

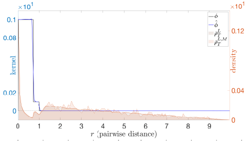
$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)]$$

Interacting particles/agents:

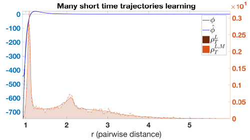
$$\frac{d}{dt} X_t^i = \frac{1}{N} \sum_{i'=1}^{N} \phi(|X_t^j - X_t^i|) \frac{X_t^j - X_t^i}{|X_t^j - X_t^i|} + \sqrt{2\nu} dB_t^i, \quad i = 1, \ldots, N$$

Maggioni JHU team: [M., L., Tang, Zhong, Miller, Li, Zhang: PNAS19, SPA20, etc]

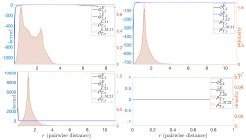
- Data: many trajectories $\{X_{[0,T]}^{(m)}\}_{m=1}^{M}$, $\nu = 0; \nu > 0$, **finite N**
- Function space of learning: $\phi \in L^2(\rho_T)$ with $\rho_T \leftarrow |X_t^j - X_t^i|$
- Nonparametric estimation ($Ac = b$)



Opinion Dynamics



Lennard-Jones



Prey-Predator

Previous work: finite N

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)]$$

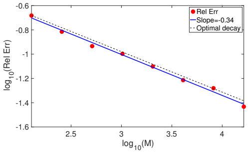
Interacting particles/agents:

$$\frac{d}{dt} X_t^i = \frac{1}{N} \sum_{i'=1}^{N} \phi(|X_t^j - X_t^i|) \frac{X_t^j - X_t^i}{|X_t^j - X_t^i|} + \sqrt{2\nu} dB_t^i, \quad i = 1, \ldots, N$$

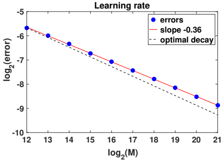
Maggioni JHU team: [M., L., Tang, Zhong, Miller, Li, Zhang: PNAS19, SPA20, etc]

- Identifiability: a coercivity condition for $L^2(\rho_T)$
- Optimal convergence rate:

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



Opinion Dynamics



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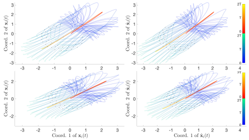

Prey-Predator

What if $N \to \infty$?

~~Data: many trajectories $\{X^{(m)}_{[0,T]}\}_{m=1}^{M}$;~~

Data: density $u(x,t) = \lim_{N\to\infty} \sum_{i=1}^{N} \delta(X_t^i - x)$

$$\{u(x_m, t_l)\}_{m,l=1}^{M,L}$$

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)]$$

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$$\{u(x_m, t_l)\}_{m,l=1}^{M,L}$$

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)]$$

How to estimate ϕ from data?

$$\text{Minimize } \mathcal{E}_0(\psi) = \int_0^T \int_{\mathbb{R}^d} \left|\nabla.(u(K_\psi * u)) - g\right|^2 dx\, dt?$$

(with $g = \partial_t u - \nu \Delta u$)

Derivatives not available from data.

Outline

1. Motivation and problem statement
2. Nonparametric learning
   - A probabilistic error functional
   - Identifiability: function spaces of learning
   - Rate of convergence
3. Numerical examples
4. Ongoing work and open problems

A probabilistic error functional

$$\mathcal{E}(\psi) := \frac{1}{T}\int_0^T \int_{\mathbb{R}^d} \left[\left| K_\psi * u \right|^2 u - 2\nu u(\nabla \cdot K_\psi * u) + 2\partial_t u(\Psi * u) \right] dx\, dt$$
$$= \langle\!\langle \psi, \psi \rangle\!\rangle_{\overline{G}_T} - 2 \langle\!\langle \psi, \phi \rangle\!\rangle_{\overline{G}_T}$$

- Expectation of the negative log-likelihood of the process

$$\begin{cases} d\overline{X}_t = -K_\phi * u(\overline{X}_t, t)dt + \sqrt{2\nu} dB_t, \\ \mathcal{L}(\overline{X}_t) = u(\cdot, t), \end{cases}$$

- Derivative-in-space free!
- $\overline{G}_T$ is a reproducing kernel for a RKHS

$$\langle \phi, \psi \rangle_{\overline{G}_T} := \frac{1}{T}\int_0^T \int_{\mathbb{R}^d} \langle (K_\phi * u), (K_\psi * u) \rangle u(x,t) dx\, dt = \int_{\mathbb{R}+} \int_{\mathbb{R}+} \phi(r)\psi(s)\, \overline{G}_T(r,s)\, dr\, ds$$

- $\psi = \sum_{i=1}^n c_i \phi_i \Rightarrow \mathcal{E}(\psi) = c^\top A c - 2b^\top c$ with $A_{ij} = \langle\!\langle \phi_i, \phi_j \rangle\!\rangle_{\overline{G}_T}$

$$\Rightarrow \quad \textbf{Estimator:} \quad \widehat{\phi}_n = \sum_{i=1}^n \widehat{c}_i \phi_i, \qquad \widehat{c} = A^{-1} b$$

Discrete data

From data $\{u(x_m, t_l)\}_{m,l=1}^{M,L}$: $\mathcal{H}_n = \mathrm{span}\{\phi_i\}_{i=1}^n$,

$$\widehat{\phi}_{n,M,L} = \sum_{i=1}^{n} \widehat{c}^i_{n,M,L}\phi_i, \quad \text{with } \widehat{c}_{n,M,L} = A^{-1}_{n,M,L} b_{n,M,L}.$$

- Inverse problem: well-posed/ identifiable, A^{-1}?
- Choice of $\mathcal{H}_n$: $\{\phi_i\}$ and n ?
- Convergence rate when $\Delta x = M^{-1/d} \to 0$?
  $\to$ hypothesis testing and model selection

Invertibility of A and function space

Recall that $\mathcal{H} = \mathrm{span}\{\phi_i\}_{i=1}^n$,

$$A_{ij} = \langle\langle \phi_i, \phi_j \rangle\rangle_{\overline{G}_T},$$

with integral kernel $\overline{G}_T \to$ RKHS $H_{\overline{G}_T}$.

- if $\{\phi_i\}$ orthonormal in $H_{\overline{G}_T}$: $A = I_n$
- if $\{\phi_i\}$ orthonormal in $L^2(\rho_T)$: minimal eigenvalue of A =

$$c_{\mathcal{H},T} = \inf_{\psi \in \mathcal{H}, \|\psi\|_{L^2(\rho_T)}=1} \langle\langle \psi, \psi \rangle\rangle_{\overline{G}_T} > 0 \quad \text{(Coercivity condition)}$$

  - measure $\rho_T \leftarrow |\overline{X}_t - \overline{X}'_t|$ (“pairwise distance”)

Error bounds

$\mathbb{H} = L^2(\rho_T)$ or RKHS $H_{\overline{G}_T}$.

Theorem (Lang-Lu20)

Let $\mathcal{H} = \mathrm{span}\{\phi_i\}_{i=1}^n$ and $\widehat{\phi}_n$ the projection of ϕ on $\mathcal{H} \subset \mathbb{H}$. Assume regularity conditions. Then

$$\|\widehat{\phi}_{n,M,L} - \widehat{\phi}_n\|_{\mathbb{H}} \leq 2c_{\mathcal{H},T}{}^{-1} \left(C^b\sqrt{n} + C^A n \|\phi\|_{\mathbb{H}}\right) (\Delta x + \Delta t),$$

- If if $\mathbb{H} = L^2(\rho_T)$: assume coercivity condition on $\mathcal{H}$ with $c_{\mathcal{H},T} > 0$, if $\mathbb{H}$ = RKHS, set $c_{\mathcal{H},T} = 1$
- $\Delta x + \Delta t$ comes from numerical integrator (Riemann sum)
- Dominating order: $n\Delta x$ (if $\Delta t = 0$)

Optimal dimension and rate of convergence

Total error: trade-off

$$\|\widehat{\phi}_{n,M,\infty} - \phi\|_{\mathbb{H}} \leq \underbrace{\|\widehat{\phi}_{n,M,\infty} - \widehat{\phi}_n\|_{\mathbb{H}}}_{\text{inference error}} + \underbrace{\|\widehat{\phi}_n - \phi\|_{\mathbb{H}}}_{\text{approximation error}}$$

Theorem (Lang-Lu20)

Assume $\|\widehat{\phi}_{n,M,\infty} - \widehat{\phi}_n\|_{\mathbb{H}} \lesssim n(\Delta x)^{\alpha}$ *and* $\|\widehat{\phi}_n - \phi\|_{\mathbb{H}} \lesssim n^{-s}$. *Then, with optimal dimension* $n \approx (\Delta x)^{-\alpha/(s+1)}$:

$$\|\widehat{\phi}_{n,M,\infty} - \phi\|_{\mathbb{H}} \lesssim (\Delta x)^{\alpha s/(s+1)}$$

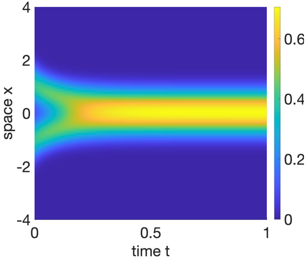
Outline

1. Motivation and problem statement
2. Nonparametric learning
3. Numerical examples
   - Granular media: smooth kernel $\phi(r) = 3r^2$
   - Opinion dynamics: piecewise linear ϕ
   - Repulsion-attraction: singular ϕ
4. Ongoing work and open problems

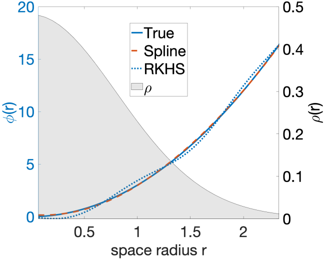
Numerical example 1: granular media

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)], \quad x \in \mathbb{R}^d, t > 0,$$

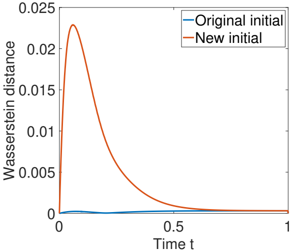
where $K_\phi(x) = \nabla(\Phi(|x|)) = \phi(|x|)\frac{x}{|x|}$. $\phi(r) = 3r^2$



The solution $u(x, t)$

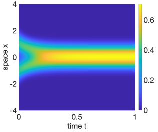


Estimators of ϕ



Wasserstein $W_2(u, \widehat{u})$

Numerical example 1: granular media



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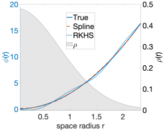
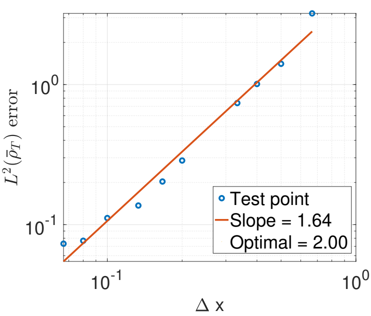
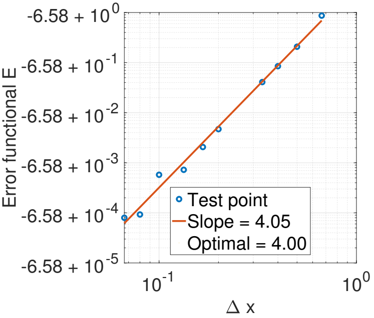


Estimators of ϕ



Convergence rate of $L^2(\rho_T)$ error

almost optimal



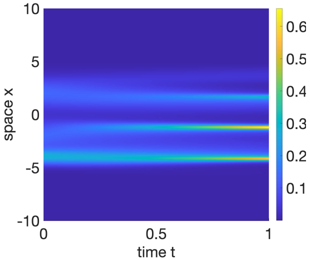
Convergence rate of $\mathcal{E}_{M,L}$

almost optimal

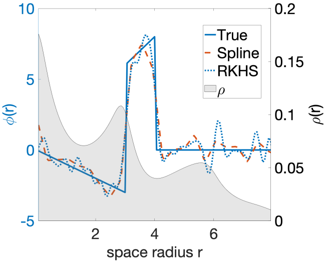
Numerical Example 2: opinion dynamics

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)], \quad x \in \mathbb{R}^d, t > 0,$$

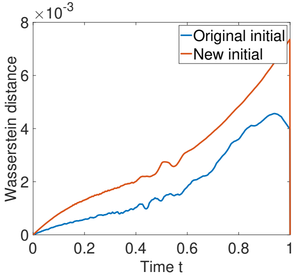
where $K_\phi(x) = \nabla(\Phi(|x|)) = \phi(|x|)\frac{x}{|x|}$. $\phi(r)$ piecewise linear



The solution $u(x,t)$

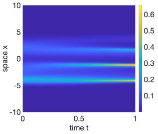


Estimators of ϕ

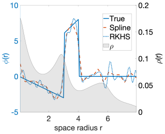


Wasserstein $W_2(u, \widehat{u})$

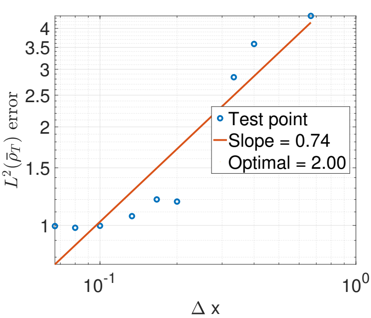
Numerical Example 2: opinion dynamics



The solution $u(x, t)$

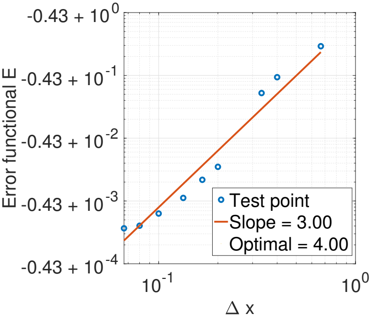


Estimators of ϕ



Convergence rate of $L^2(\rho_T)$ error

sub-optimal ($\phi \notin W^{1,\infty}$)



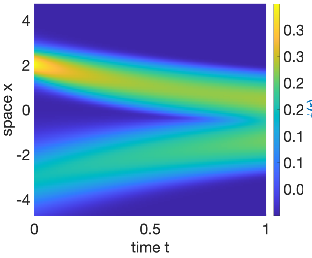
Convergence rate of $\mathcal{E}_{M,L}$

sub-optimal

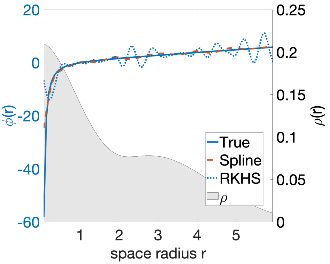
Numerical example 3: repulsion-attraction

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)], \quad x \in \mathbb{R}^d, t > 0,$$

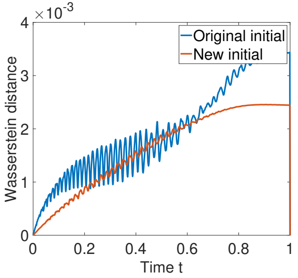
where $K_\phi(x) = \nabla(\Phi(|x|)) = \phi(|x|)\frac{x}{|x|}$. $\phi(r) = r - r^{-1.5}$ singular



The solution $u(x,t)$

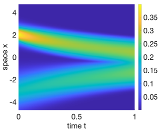


Estimators of ϕ

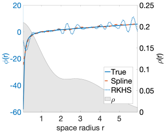


Wasserstein $W_2(u, \widehat{u})$

Numerical example 3: repulsion-attraction



The solution $u(x, t)$



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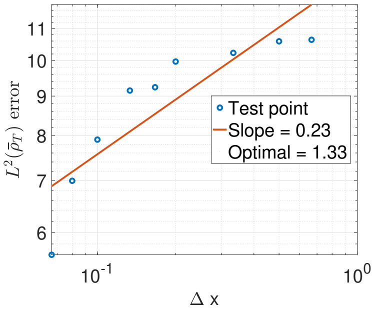
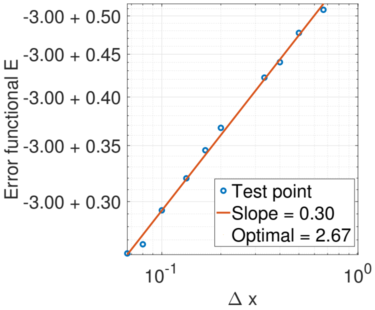


Convergence rate of $L^2(\rho_T)$ error

low rate: theory does not apply



Convergence rate of $\mathcal{E}_{M,L}$

low rate: theory does not apply

Summary and open problems

Problem: Estimate ϕ of Mean-field equation

$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)]$$

from discrete data $\{u(x_m, t_l)\}_{m,l=1}^{M,L}$.

Solution: Algorithm

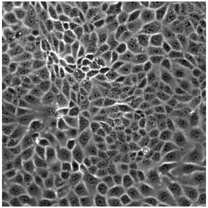
- A probabilistic error functional
- Estimator by least squares

Theory guidance

- Choice of hypothesis space basis functions & dimension
- Function space of learning: RKHS v.s. $L^2(\rho_T)$
- Optimal learning rate

Open problem and future directions

- Learning/computation:
  - 2nd-order systems
  - High-dimensional state space (Monte Carlo)
  - non-radial interaction kernel
  - partial observation of large systems
- Coercivity condition on $L^2(\rho_T)$
  - $\overline{G}_T \to$ strictly positive integral operator?
- Singular kernels?
- Real data applications: learning cell-dynamics



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Thank you!