Learning interacting kernels of mean-field equations of particle systems

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Outline

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

An inverse problem

Mean-field equation of interacting particles

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

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

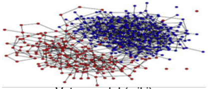
Question: identify ϕ from discrete data $\{u(x_m, t_l)\}_{m,l=1}^{M,L}$?

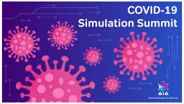
Systems of interacting particles/agents

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

- X_t^i: the i-th particle's position; B_t^i: Brownian motion
- From Newton's law (2nd-order) + 0-mass $\rightarrow$ 1st-order
- Applications in many disciplines:
  Statistical physics, quantum mechanics
  Biology [Keller-Segal1970, Cucker-Smale2000]
  Social science [Motsch-Tadmor2014]
  Monte Carlo sampling [Del Moral13]
  Epidemiology (Agent-based models for COVID19 at Imperial)


Popkin. Nature(2016)

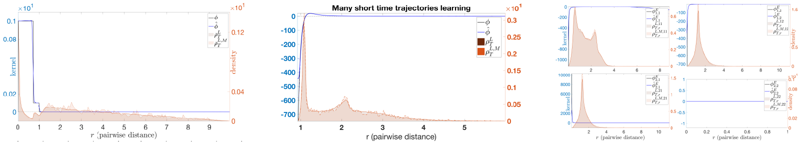

Voter model (wiki)



Previous work: finite N

Maggioni et al: [Maggioni, L., Tang, Zhong, Miller, Li, Zhang: PNAS19, SPA20, etc]

- Data: many trajectories $\{X^{(m)}_{[0,T]}\}_{m=1}^{M}$.
- Nonparametric regression
  - Function space of learning: $\mathcal{H} \subset L^2(\rho_T)$ with $\rho_T \leftarrow |X_t^j - X_t^i|$
  - minimax convergence rate
  - various systems



Opinion Dynamics Lennard-Jones Prey-Predator

Large system challenge: $N \to \infty$

Data at macroscopic scale:

- lack of trajectories $\{X_{[0,T]}^{(m)}\}_{m=1}^{M}$ (recall $X_t \in \mathbb{R}^{Nd}$)
- only population density $u(x,t) = \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \delta(X_t^i - x)$

Discrete in space-time: $\{u(x_m, t_l)\}_{m,l=1}^{M,L}$

$\Rightarrow$ Infer kernel in Mean-field equation:

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

Outline

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

Variational approach: minimize a loss functional $\mathcal{E}(\psi)$

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

Loss functions that do not work (efficiently)

- discrepancy: $\mathcal{E}(\psi) = \|\partial_t u - \nu \Delta u - \nabla.(u(K_\psi * u))\|^2$
  derivatives approx. from discrete data
- Free energy: $\mathcal{E}(\psi) = C + |\int_{\mathbb{R}^d} u[(\Psi - \Phi) * u] dx|^2$
  limitted information from the 1st moment
- Wasserstein-2: $\mathcal{E}(\psi) = W_2(u^\psi, u)$
  costly: require many PDE simulations in optimization

A probabilistic loss functional

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

- $=$ Expectation of the negative log-likelihood of the process

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

A probabilistic loss functional

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

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- Derivative-in-space free!
- Suitable for high-dimension: $K_\psi * u(\overline{X}_t) = \mathbb{E}[K_\psi(\overline{X}_t - \overline{X}_t') | \overline{X}_t]$

$$\mathcal{E}(\psi) = \frac{1}{T}\int_0^T \left(\mathbb{E}|K_\psi * u(\overline{X}_t)|^2 + \partial_t \mathbb{E}\Psi(\overline{X}_t - \overline{X}_t') + 2\nu \mathbb{E}[\Delta\Psi(\overline{X}_t - \overline{X}_t')] \right) dt$$

Least squares estimator

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

- bilinear form $\langle\!\langle \phi, \psi \rangle\!\rangle = \frac{1}{T}\int_0^T \int_{\mathbb{R}^d} \langle (K_\phi * u), (K_\psi * u) \rangle u(x,t) dxdt$
- Hypothesis space $\mathcal{H}_n = \mathrm{span}\{\phi_i\}_{i=1}^n$: $\psi = \sum_{i=1}^n c_i \phi_i$

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

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

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

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

Three fundamental issues

- Identifiability: uniqueness of minimizer, A^{-1}
- Choice of $\mathcal{H}_n$: B-splines $\{\phi_i\}_{i=1}^n$ and n ?
- Convergence rate when $\Delta x = M^{-1/d} \to 0$?
  $\to$ hypothesis testing and model selection

Identifiability and function space of learning

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

$$A_{ij} = \langle\langle \phi_i, \phi_j \rangle\rangle , \quad \langle\langle \phi, \psi \rangle\rangle = \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \phi(r)\psi(s)\overline{G}_T(r,s)drds$$

- function spaces of identifiability: RKHSs [LangLu21]
  - $\overline{G}_T$ is Mercer kernel $\to$ RKHS $H_{\overline{G}_T} \subset L^2(\mathcal{X})$.
  - $\overline{R}_T = \frac{\overline{G}_T}{\rho_T \otimes \rho_T} \to$ RKHS $H_R \subset L^2(\rho_T)$.
- Positive compact operators $L_{\overline{G}_T}$ and $L_{\overline{R}_T}$
  - normal matrix $A = L_{\overline{G}_T} \mid_{\mathcal{H}}$ in $L^2(\mathcal{X})$; $A = L_{\overline{R}_T} \mid_{\mathcal{H}}$ in $L^2(\rho_T)$

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

  - Regularization needed as $Dim(\mathcal{H}) \uparrow \infty$

Error bounds

$$\mathbb{H} = L^2(\rho_T)$$

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

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

- $\Delta x^\alpha + \Delta t$ comes from numerical integrator (Riemann sum)
- Dominating order: $n\Delta x^\alpha$ (neglecting Δt error)

Optimal dimension and rate of convergence

Total error: trade-off

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

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* $n \approx (\Delta x)^{-\alpha/(s+1)}$*:*

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

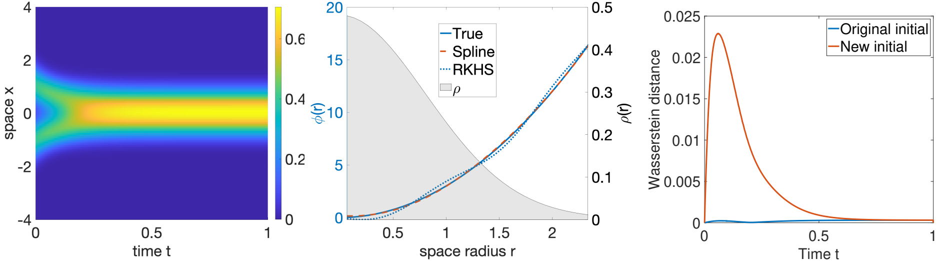
Outline

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 $\phi = r - r^{-1.5}$
4. Ongoing work and open problems

Example 1: granular media

$\phi(r) = 3r^2$

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



The solution $u(x,t)$ Estimators of ϕ Wasserstein $W_2(u, \widehat{u})$

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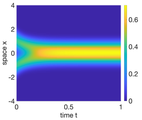
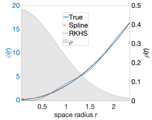
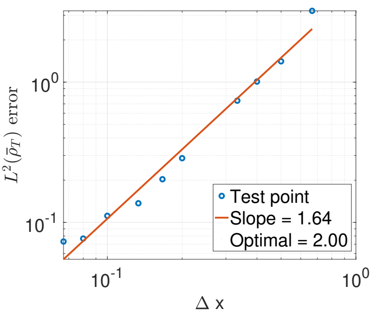
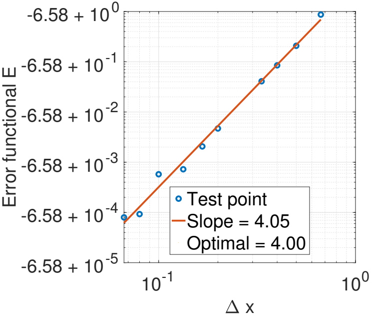








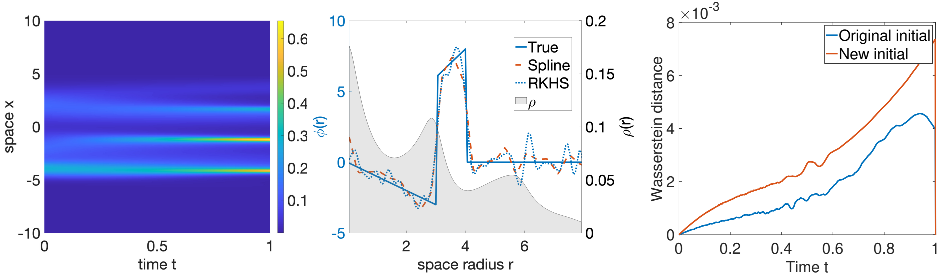
Convergence rate of $L^2(\rho_T)$ error Convergence rate of $\mathcal{E}_{M,L}$

close to optimal

Example 2: opinion dynamics

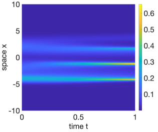
$\phi(r)$ piecewise linear

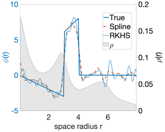
$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)], \quad x \in \mathbb{R}^d, t > 0, \quad K_\phi(x) = \phi(|x|)\frac{x}{|x|}$$

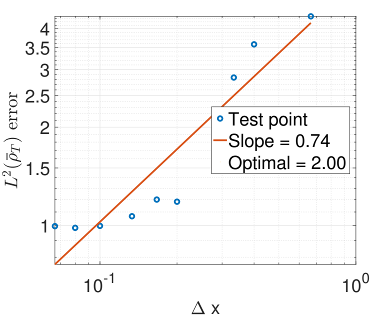


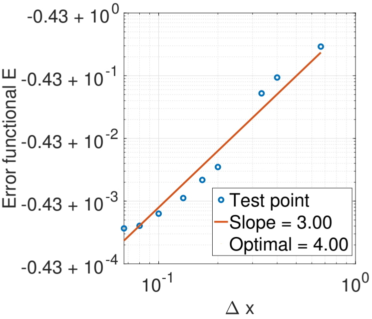
The solution $u(x,t)$ Estimators of ϕ Wasserstein $W_2(u, \widehat{u})$

Example 2: opinion dynamics









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

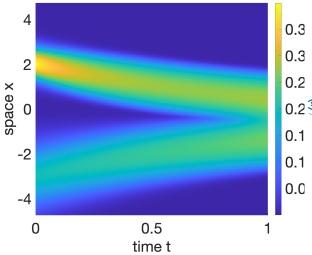
sub-optimal ($\phi \notin W^{1,\infty}$)

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

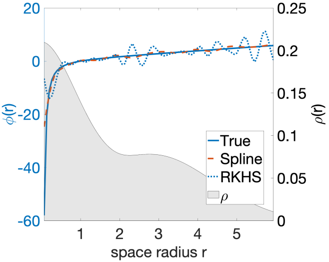
Example 3: repulsion-attraction

$\phi(r) = r - r^{-1.5}$ (singular)

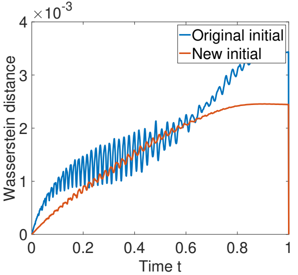
$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_\phi * u)], \quad x \in \mathbb{R}^d, t > 0, \quad K_\phi(x) = \phi(|x|)\frac{x}{|x|}$$



The solution $u(x,t)$

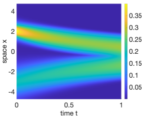


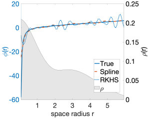
Estimators of ϕ

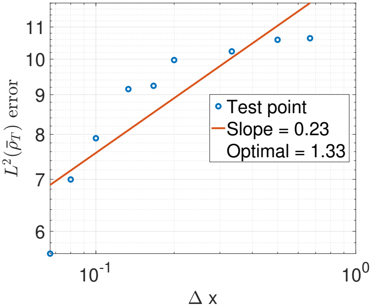


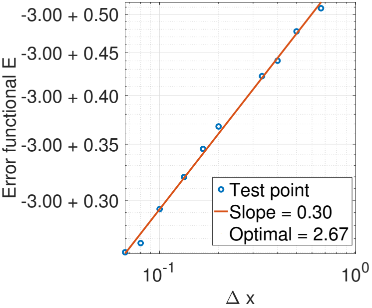
Wasserstein $W_2(u, \widehat{u})$

Example 3: repulsion-attraction









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

low rate: theory does not apply

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

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: Least-squares-based algorithm

- A probabilistic loss functional

Theory:

- Function space of identifiability: intrinsic RKHSs
- Choice of hypothesis space basis functions & dimension
- Optimal convergence rate

Open problem and future directions

- General systems/settings:
  - 2nd-order systems / zero diffusion
  - non-radial interaction kernel, multi-potentials
  - High-dimensional state space (Monte Carlo)
  - partial observation of large systems
- Data-adaptive RKHSs:
  - optimal regularization
  - feature selection
- Applications: graph and networks