Statistical learning and inverse problems from interacting particle systems

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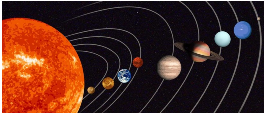
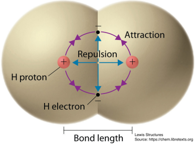
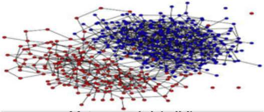
What is the law of interaction ?





Popkin. Nature(2016)



Voter model (wiki)

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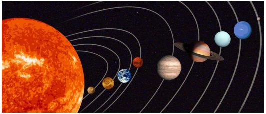

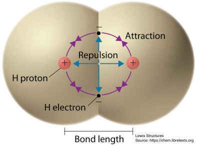

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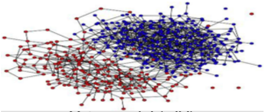

Voter model (wiki)

$$m_i \ddot{X}_t^i = -\gamma \dot{X}_t^i + \frac{1}{N} \sum_{j=1, j\neq i}^{N} K_\phi(X_t^i, X_t^j),$$

$$K_\phi(x,y) = \nabla_x[\Phi(|x-y|)] = \phi(|x-y|)\frac{x-y}{|x-y|}.$$

- Newton's law of gravity $\phi(r) = G\frac{m_1 m_2}{r^2}$
- Lennard-Jones potential: $\Phi(r) = \frac{c_1}{r^{12}} - \frac{c_2}{r^6}$.

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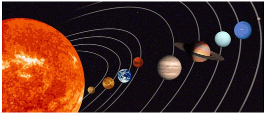

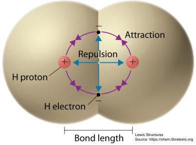


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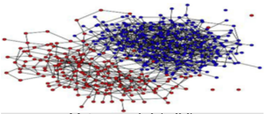
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- flocking birds, bacteria/cells ?
- opinion/voter/multi-agent models, ...? [a]

Infer the interaction kernel from data?

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

Part 0: statistical learning & inverse problem

- Part 1: statistical learning — Finitely many particles
- Part 2: inverse problem — infinitely many particles
- Part 3: Regularization for learning kernels in operators

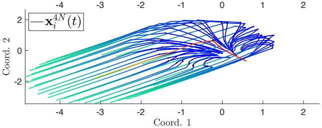
Learning the interaction kernel

$$dX_t^i = \frac{1}{N}\sum_{j=1}^{N} K_\phi(X_t^j, X_t^i)dt + \sqrt{2\nu}dB_t^i \quad \Leftrightarrow \dot{\boldsymbol{X}}_t = R_\phi(\boldsymbol{X}_t) + \sqrt{2\nu}\dot{\boldsymbol{B}}_t$$

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

Finite N:

- Data: M trajectories of particles $\{\boldsymbol{X}_{t_1:t_L}^{(m)}\}_{m=1}^{M}$
- Statistical learning



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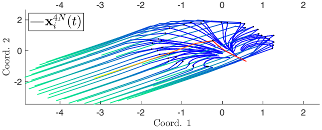
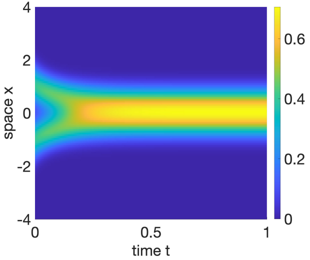


Large N ($>> 1$)

- Data: density of particles $\{u(x_m, t_l) \approx N^{-1}\sum_i \delta(X_{t_l}^i - x_m)\}_{m,l}$

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

- Inverse problem for PDEs



Statistical learning & inverse problem

- What's in common and what's different?
- What is new from
  - classical learning $\{(x_i, y_i)\}_{i=1}^M \Rightarrow y = \phi(x)$?
  - operator learning $\{u_k, f_k\}_{k=1}^M \Rightarrow f = R[u]$?

Learning kernels in operators:

$$dX_t^i = \frac{1}{N}\sum_{j=1}^{N} K_\phi(X_t^j, X_t^i)dt + \sqrt{2\nu}dB_t^i \quad \Leftrightarrow R_\phi(\boldsymbol{X}_t) = \dot{\boldsymbol{X}}_t - \sqrt{2\nu}\dot{\boldsymbol{B}}_t$$

$$\partial_t u = \nu\Delta u + \nabla\cdot[u(K_\phi * u)] \quad \Leftrightarrow R_\phi[u(\cdot,t)] = f(\cdot,t)$$

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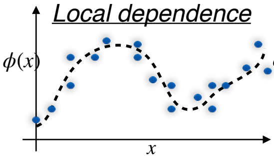
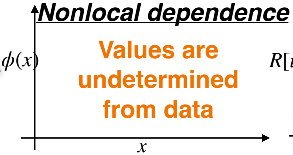
Classical learning

$\{(x_i, \phi(x_i) + \epsilon_i)\}$



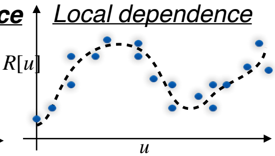
Learning kernel

$\{(u_k, R_\phi[u_k] + \eta_k)\}$



Operator learning

$\{(u_k, R[u_k] + \eta_k)\}$



Part 1: Finitely many particles

Statistical learning from sample trajectories

Finitely many particles

$$R_{\phi}(\boldsymbol{X}_t) = \dot{\boldsymbol{X}}_t - \sqrt{2\nu}\dot{\boldsymbol{B}}_t \quad \text{\& Data } \{\boldsymbol{X}_{t_1:t_L}^{(m)}\}_{m=1}^{M}$$

- Loss function (or log-likelihood for SDEs):

$$\hat{\phi}_{n,M} = \underset{\phi\in\mathcal{H}_n}{\arg\min}\, \mathcal{E}_M(\phi) = \frac{1}{M}\sum_{m=1}^{M}\int_0^T |\dot{\boldsymbol{X}}_t^m - R_\phi(\boldsymbol{X}_t^m)|^2 dt$$

- Nonparametric Regression: $\mathcal{H}_n = \mathrm{span}\{\phi_i\}_{i=1}^n$, $\phi = \sum_i c_i\phi_i$

$$\mathcal{E}_M(\phi) = c^\top A c - 2b^\top c \quad \Rightarrow \quad \widehat{\phi}_{n,M} = \sum_{i=1}^{n} \widehat{c}_i\phi_i, \quad \widehat{c} = A^{-1}b$$

Finitely many particles

$$R_{\phi}(\boldsymbol{X}_t) = \dot{\boldsymbol{X}}_t - \sqrt{2\nu}\dot{\boldsymbol{B}}_t \quad \text{\& Data } \{\boldsymbol{X}^{(m)}_{t_1:t_L}\}_{m=1}^{M}$$

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  - Choice of $\mathcal{H}_n$ & function space of learning?
  - Well-posedness/ identifiability?
  - Convergence and rate?

Classical learning in a nutshell

$$\text{Data}\{(x_m, y_m)\}_{m=1}^M \sim (X, Y) \Rightarrow \text{find } \phi \text{ s.t. } Y = \phi(X)$$

- Loss function: $\hat{\phi}_{n,M} = \underset{\phi \in \mathcal{H}_n}{\arg\min}\, \mathcal{E}_M(\phi) = \frac{1}{M}\sum_{m=1}^M |Y_m - \phi(X_m)|^2$.
- Regression: with $\psi = \sum_i c_i \phi_i \in \mathcal{H}_n = \text{span}\{\phi_i\}_{i=1}^n$:

$$\mathcal{E}_M(\psi) = c^\top A c - 2b^\top c \quad \Rightarrow \quad \widehat{\phi}_{n,M} = \sum_{i=1}^n \widehat{c}_i \phi_i, \quad \widehat{c} = A^{-1} b$$

-
  - Choice of $\mathcal{H}_n \subset C^s$ in $L^2(\rho_X)$: $n_* = (M/\log M)^{\frac{1}{2s+d}}$

Underfitting **Balanced** **Overfitting**

  - Well-posedness/ identifiability: $\phi_{optimal} = \mathbb{E}[Y|X = x]$
  - minimax rate $\mathbb{E}[\|\widehat{\phi}_{n_*,M} - \phi_{optimal}\|^2_{L^2(\rho_X)}] \approx \left(\frac{\log M}{M}\right)^{\frac{s}{2s+d}}$

Classical learning theory

Given: Data$\{(x_m, y_m)\}_{m=1}^M \sim (X, Y)$

Goal: find ϕ s.t. $Y = \phi(X)$

Learning kernel

Given: Data$\{\boldsymbol{X}_{[0,T]}^{(m)}\}_{m=1}^M$

Goal: find ϕ s.t. $\dot{\boldsymbol{X}}_t = R_\phi(\boldsymbol{X}_t)$

$$\mathcal{E}(\phi) = \mathbb{E}|Y - \phi(X)|^2 = \|\phi - \phi_{true}\|^2_{L^2(\rho_X)} \quad \mathcal{E}(\phi) = \mathbb{E}|\dot{\boldsymbol{X}} - R_\phi(\boldsymbol{X})|^2 \neq \|\phi - \phi_{true}\|^2_{L^2(\rho)}$$

Classical learning theory

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Goal: find ϕ s.t. $Y = \phi(X)$

$$\mathcal{E}(\phi) = \mathbb{E}|Y - \phi(X)|^2 = \|\phi - \phi_{true}\|^2_{L^2(\rho_X)}$$

- Function space: $L^2(\rho_X)$.
- Identifiability: $\mathbb{E}[Y|X = x] = \arg\min_{\phi \in L^2(\rho_X)} \mathcal{E}(\phi)$.
- $A \approx \mathbb{E}[\phi_i(X)\phi_j(X)] = I_n$ by setting $\{\phi_i\}$ ONB in $L^2(\rho_X)$.

Learning kernel

Given: Data$\{\boldsymbol{X}^{(m)}_{[0,T]}\}_{m=1}^{M}$

Goal: find ϕ s.t. $\dot{\boldsymbol{X}}_t = R_\phi(\boldsymbol{X}_t)$

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- Function space: $L^2(\rho)$. measure $\rho \sim |X^i - X^j|$
- Identifiability: $\arg\min_{\phi \in L^2(\rho)} \mathcal{E}(\phi)$??
- $A \approx \mathbb{E}[R_{\phi_i}(\boldsymbol{X})R_{\phi_j}(\boldsymbol{X})]$? $\geq$?$c_{\mathcal{H}} I_n$ Coercivity condition

Classical learning theory

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- $A \approx \mathbb{E}[R_{\phi_i}(\boldsymbol{X})R_{\phi_j}(\boldsymbol{X})]? \geq ? c_{\mathcal{H}} I_n$ Coercivity condition

Error bounds for $\widehat{\phi}_{n_M}$: asymptotic/non-asymptotic (CLT/concentration)

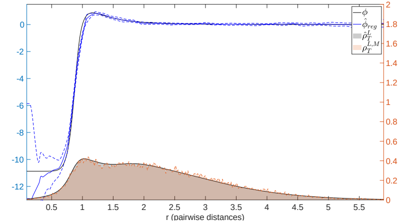
$$\mathcal{E}(\widehat{\phi}_{n_M}) - \mathcal{E}(\phi_{\mathcal{H}}) \geq c_{\mathcal{H}} \|\widehat{\phi}_{n_M} - \phi_{\mathcal{H}}\|^2$$

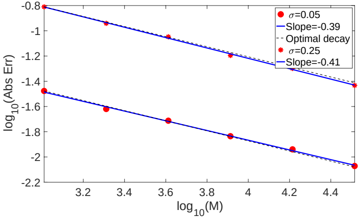
Theorem (Convergence with minimax rate [LZTM19,LMT21,LMT22])

Let $\{\mathcal{H}_n\}$ compact convex in L^∞ with $\mathrm{dist}(\phi_{true}, \mathcal{H}_n) \sim n^{-s}$. Assume the coercivity condition on $\cup_n \mathcal{H}_n$. Set $n_* = (M/\log M)^{\frac{1}{2s+1}}$. Then

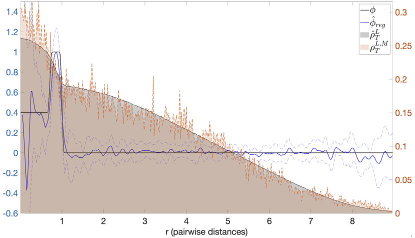
$$\mathbb{E}_{\mu_0}[\|\widehat{\phi}_{n_*,M} - \phi_{true}\|_{L^2(\rho)}] \leq C \left(\frac{\log M}{M}\right)^{\frac{s}{2s+1}} .$$

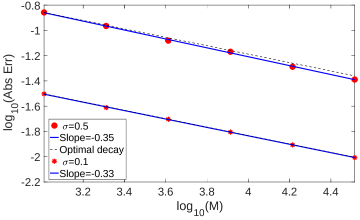
Lennard-Jones kernel estimators:





Opinion dynamics kernel estimators:





Coercivity condition on $\mathcal{H}$

$$\langle\langle \phi, \phi \rangle\rangle = \frac{1}{T}\int_0^T \mathbb{E}[R_\phi(\boldsymbol{X}_t)R_\phi(\boldsymbol{X}_t)]dt \geq c_{\mathcal{H}} \|\phi\|^2_{L^2(\rho)}, \quad \forall \phi \in \mathcal{H}$$

- Partial results: $c_{\mathcal{H}} = \frac{1}{N-2}$ for $\mathcal{H} = L^2(\rho)$
  - Gaussian or $\Phi(r) = r^{2\beta}$ stationary [LLMTZ21spa,LL20]
  - Harmonic analysis: strictly positive definite integral kernel

$$\mathbb{E}[\phi(|X-Y|)\phi(|X-Z|)\frac{\langle X-Y, X-Z\rangle}{|X-Y||X-Z|}] \geq 0, \forall \phi \in L^2(\rho)$$

- Open: non-stationary? A compact $\mathcal{H} \subset C(\mathrm{supp}(\rho))$?
- No coercivity on $L^2(\rho)$ when $N \to \infty$ since $c_{\mathcal{H}} \to 0$

Part 2: Infinitely many particles

Inverse problem for mean-field PDEs

Inverse problem for Mean-field PDE

Goal: Identify ϕ from discrete data $\{u(x_m, t_l)\}_{m,l=1}^{M,L}$ of

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

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

Loss functional

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

Candidates:

- Discrepancy: $\mathcal{E}(\phi) = \|\partial_t u - \nu \Delta u - \nabla.(u(K_\phi * u))\|^2$
  - derivatives approx. from discrete data
  - Weak SINDY [Bortz etc21,22], denoising+smoothing [Kang+Liao etc22]
- Wasserstein-2: $\mathcal{E}(\phi) = W_2(u^\phi, u)$

  costly: requires many PDE simulations in optimization
- A probabilistic loss functional

A probabilistic loss functional

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

- $= -\mathbb{E}[$ log-likelihood $]$: McKean–Vlasov process

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

- Derivative free
- Suitable for high dimension: $Z_t = \overline{X}_t - \overline{X}'_t$

$$\mathcal{E}(\phi) = \frac{1}{T}\int_0^T \Big(\mathbb{E}|\mathbb{E}[K_\phi(Z_t)|\overline{X}_t]|^2 - 2\nu\mathbb{E}[\nabla \cdot K_\phi(Z_t)] + \partial_t \mathbb{E}\Phi(Z_t) \Big) \, dt$$

Nonparametric regression $\phi = \sum_{i=1}^{n} c_i \phi_i \in \mathcal{H}_n$:

$$\mathcal{E}_M(\phi) = c^\top A c - 2b^\top c \quad \Rightarrow \quad \widehat{\phi}_{n,M} = \sum_{i=1}^{n} \widehat{c}_i \phi_i, \quad \widehat{c} = A^{-1} b$$

- Choice of $\mathcal{H}_n$ & function space of learning?
  - Exploration measure $\rho_T \leftarrow |\overline{X}_t - \overline{X}_t'|$
- Inverse problem well-posedness/ identifiability?
  - $\arg\min_{\phi \in L^2(\rho)} \mathcal{E}(\phi)$
- Convergence and rate? $\Delta x = M^{-1/d} \to 0$

Identifiability

$$\mathcal{E}(\phi) = \langle L_{\overline{G}}\phi, \phi\rangle - 2\langle \phi^D, \phi\rangle + const.$$
$$\nabla\mathcal{E}(\phi) = L_G\phi - \phi^D = 0 \quad \Rightarrow \widehat{\phi} = L_G^{-1}\phi^D$$

- Identifiability: $A^{-1}b \leftrightarrow L_{\overline{G}}^{-1}\phi^D$
  - $L_{\overline{G}}$: positive compact operator
  - Function space of identifiability (FSOI): $\overline{\mathrm{span}\{\psi_i\}_{\lambda_i>0}}$
- Coercivity condition on $\mathcal{H}$ (not $L^2(\rho)$)

$$c_{\mathcal{H}} = \inf_{\phi\in\mathcal{H}, \|\phi\|_{L^2(\rho_T)}=1} \langle L_{\overline{G}}\phi, \phi\rangle > 0$$

Convergence rate

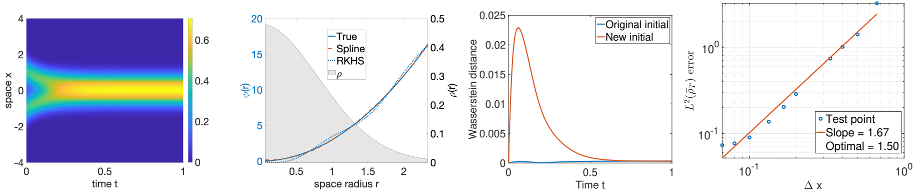
Theorem (Numerical error bound [Lang-Lu20])

Let $\mathcal{H}_n = \mathrm{span}\{\phi_i\}_{i=1}^n$ s.t. $\|\phi_{\mathcal{H}_n} - \phi\|_{L^2(\rho_T)} \lessapprox n^{-s}$. Assume the coercivity condition on $\cup\mathcal{H}_n$. Then, with $n \approx (\Delta x)^{-\alpha/(s+1)}$, we have:

$$\|\widehat{\phi}_{n,M} - \phi\|_{L^2(\rho_T)} \lessapprox (\Delta x)^{\alpha s/(s+1)}$$

- Δx^{α} comes from numerical integrator (e.g.,Riemann sum)
  - In statistical learning: $\alpha = 1/2$ (Monte Carlo, CLT)
- Trade-off: numerical error v.s. approximation error

Example: granular media $\phi(r) = 3r^2$



Data $u(x,t)$ Estimator Wasserstein-2 Rate

- Near optimal rate ($\phi \in W^{1,\infty}$)
- Other examples:
  suboptimal when ϕ discontinuous,
  low rate for singular ϕ

Part 3: Learning kernels in operators

Regularization

Learning kernels in operators

Learn the kernel ϕ:

$$R_\phi[u] = f$$

from data:

$$\mathcal{D} = \{(u_k, f_k)\}_{k=1}^N, \quad (u_k, f_k) \in \mathbb{X} \times \mathbb{Y}$$

- R_ϕ linear/nonlinear in u, but linear in ϕ
- Examples:
  - interaction kernel: $R_\phi[u] = \nabla \cdot [u(K_\phi * u)] = \partial_t u - \nu \Delta u$
  - Toeplitz/Hankel matrix
  - integral/nonlocal operators,...

Ill-posed inverse problem

$$\mathcal{E}(\phi) = \|R_\phi[u] - f\|_{\mathbb{Y}}^2$$

$$\nabla\mathcal{E}(\phi) = L_G\phi - \phi^D = 0 \quad \Rightarrow \widehat{\phi} = L_G^{-1}\phi^D$$

Regularization

$$\mathcal{E}_\lambda(\phi) = \mathcal{E}(\phi) + \lambda\|\psi\|_Q^2 \to \widehat{\phi} = (L_G + \lambda Q)^{-1}\phi^D$$

- λ by the L-curve method [Hansen00]
- Regularization norm $\|\cdot\|_Q$? $Q = Id$, $Q = RKHS$?

Ill-posed inverse problem

$$\mathcal{E}(\phi) = \|R_\phi[u] - f\|_{\mathbb{Y}}^2$$
$$\nabla\mathcal{E}(\phi) = L_G\phi - \phi^D = 0 \quad \Rightarrow \widehat{\phi} = L_G^{-1}\phi^D$$

Regularization

$$\mathcal{E}_\lambda(\phi) = \mathcal{E}(\phi) + \lambda\|\psi\|_Q^2 \to \widehat{\phi} = (L_G + \lambda Q)^{-1}\phi^D$$

- λ by the L-curve method [Hansen00]
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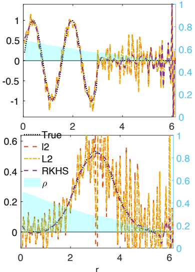
Data Adaptive RKHS Tikhonov Regularization [Lu+Lang+An22]

- norm of RKHS $H_G = L_G^{1/2}L^2(\rho) \leftrightarrow Q = L_G^{-1}$
- L_G is data dependent
- Computation: $\widehat{\phi} = (L_G + \lambda L_G^{-1})^{-1}\phi^D = (L_G^2 + \lambda I)^{-1}L_G\phi^D$

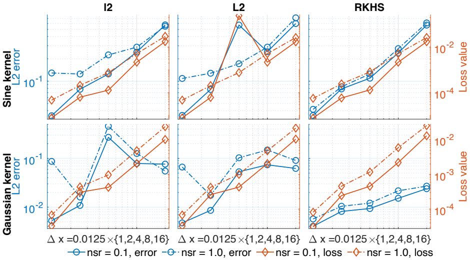
DARTR: Data Adaptive RKHS Tikhonov Regularization

$$R_\phi[u] = \nabla \cdot [u(K_\phi * u)] = f$$

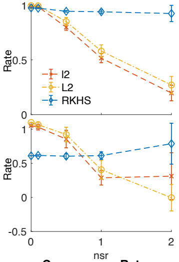
- Recover kernel from discrete noisy data
- Consistent convergence as mesh refines



Typical estimators, $\Delta x = 0.05$



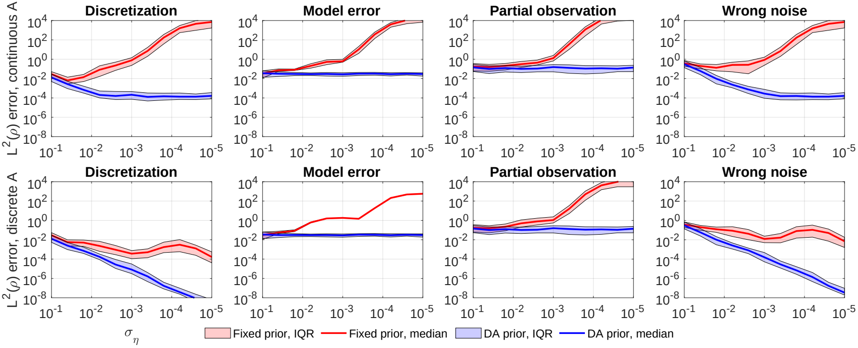
Convergence of Estimators, nsr = 0.1 & 1



Convergence Rates

Small noise limit:

- $Q = I$: divergent estimator
- $Q = L_G^{-1}$: stable/convergent



Summary and future directions

Nonparametric regression for interaction kernels

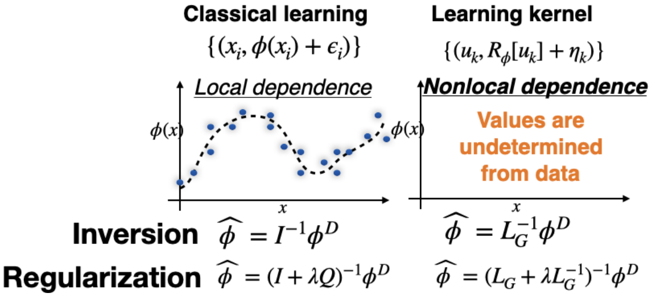
- Finite N (ODEs/SDEs): statistical learning
- $N = \infty$ (Mean-field PDEs): inverse problem

Learning kernels in operators:

- Probabilistic loss functionals
- Identifiability: $\widehat{\phi} = L_G^{-1}\phi^D$
- Coercivity condition
  - yes: convergence
  - no: regularization — DARTR (ill-posed inverse problem)

Learning with nonlocal dependence: a new direction?

- Coercivity condition, spectrum decay
- Regularization for NN in function space?
- Convergence (minimax rate)



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