Statistical learning and inverse problems from interacting particle systems

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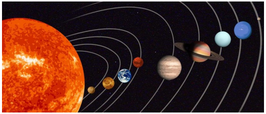
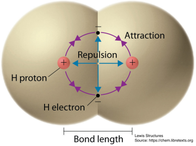
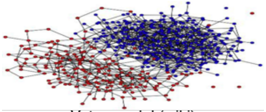
What is the law of interaction ?





Popkin. Nature(2016)



Voter model (wiki)

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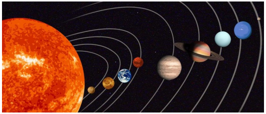

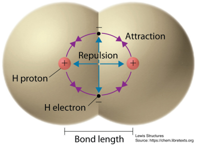

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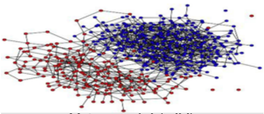

Voter model (wiki)

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

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

- 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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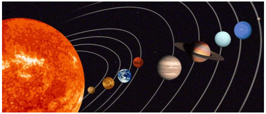

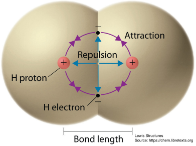

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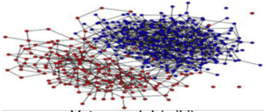

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- flocking birds, bacteria/cells ?
- opinion/voter/multi-agent models, ...? [a]

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 ...

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

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

Finite N: [a]

- Data: M trajectories of particles : $\{\boldsymbol{X}_{t_1:t_L}^{(m)}\}_{m=1}^{M}$
- Statistical learning
- ODEs/SDEs: Opinion Dynamics, Lennard-Jones, Prey-Predator; 1st/2nd order

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Large N ($>>1$)[b]

- 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

[a] [Maggioni, Lu, Tang, Zhong, Miller, Li, Zhang: PNAS19, SPA20,FOC22,JMLR21] [b] [Lang-Lu 20,21]

Learning kernels in operators: $R_\phi : \mathbb{X} \to \mathbb{Y}$

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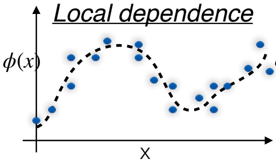
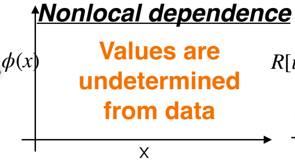
Classical learning

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



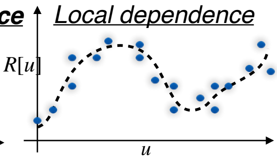
Learning kernel

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



Operator learning

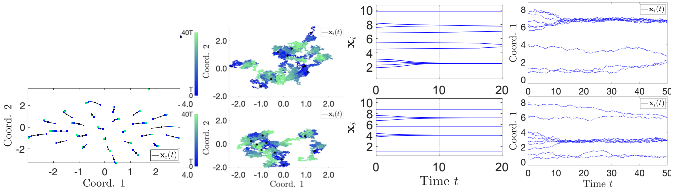
$\{(u_k, R[u_k] + \eta_k)\}$



Nonparametric learning:
Loss function? Identifiability? Convergence?

Finite many particles

$$R_\phi(\boldsymbol{X}_t) = \dot{\boldsymbol{X}}_t - \sqrt{2\nu}\dot{\boldsymbol{B}}_t \quad \& \text{ Data} \qquad \Rightarrow \hat{\phi}_{n,M} = \underset{\psi \in \mathcal{H}_n}{\arg\min}\, \mathcal{E}_M(\psi)$$



- Loss function (log-likelihood, or MSE for ODEs): quadratic
- Regression: with $\psi = \sum_i c_i \phi_i \in \mathcal{H}_n = \mathrm{span}\{\phi_i\}_{i=1}^n$:

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

Finite many particles

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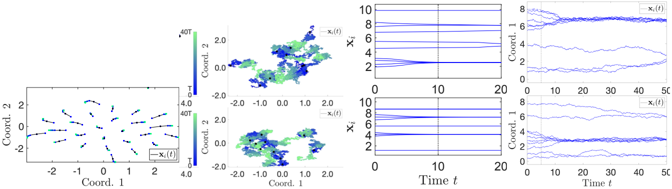

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  - Choice of $\mathcal{H}_n$ & function space of learning?
  - Well-posed/ identifiability?
  - Convergence and rate?

Classical learning theory

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

Goal: find f s.t. $Y = \phi(X)$

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

Learning kernel

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

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

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

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- 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 $L^2(\rho_X)$.

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

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

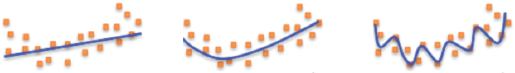
$$\mathcal{E}(\widehat{\phi}_{n_M}) - \mathcal{E}(\phi_{\mathcal{H}}) \geq c_{\mathcal{H}} \|\widehat{\phi}_{n_M} - \phi_{\mathcal{H}}\|^2$$

Theorem (LZTM19,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*

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

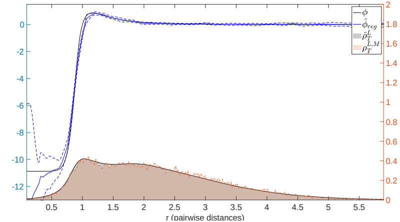
- $\dim(\mathcal{H}_n)$ adaptive to s ($\phi_{true} \in C^s$) and M:

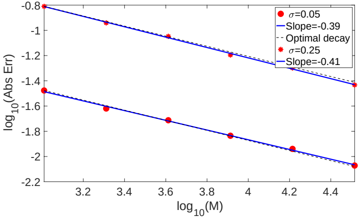


Underfitting | **Balanced** | **Overfitting**

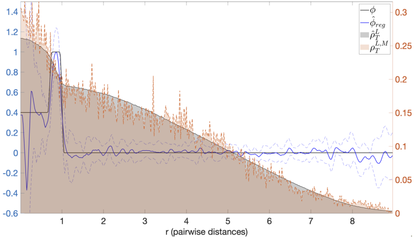
- Concentration inequalities for r.v. or martingale

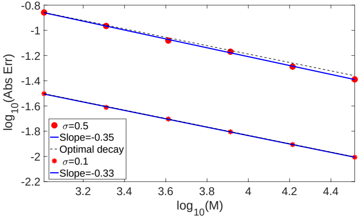
Lennard-Jones kernel estimators:





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 $c_{\mathcal{H}} \to 0$

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: $\mathcal{E}(\psi) = \|\partial_t u - \nu \Delta u - \nabla.(u(K_\psi * u))\|^2$
- Free energy: $\mathcal{E}(\psi) = C + |\int_{\mathbb{R}^d} u[(\Psi - \Phi) * u]dx|^2$
- Wasserstein-2: $\mathcal{E}(\psi) = W_2(u^\psi, u)$
  costly: requires many PDE simulations in optimization
- A probabilistic loss functional

A probabilistic loss functional

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

- $= -\mathbb{E}[$ 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: $Z_t = \overline{X}_t - \overline{X}_t'$

$$\mathcal{E}(\psi) = \frac{1}{T}\int_0^T \left(\mathbb{E}|\mathbb{E}[K_\psi(Z_t)|\overline{X}_t]|^2 - 2\nu\mathbb{E}[\nabla \cdot K_\psi(Z_t)] + \partial_t \mathbb{E}\Psi(Z_t) \right) dt$$

Nonparametric regression

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

LS-regression $\psi = \sum_{i=1}^n c_i \phi_i \in \mathcal{H}_n$:

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

- Choice of $\mathcal{H}_n$ & function space of learning?
  - Exploration measure $\rho_T \leftarrow |\overline{X}_t - \overline{X}'_t|$
- Inverse problem well-posed/ identifiability?
- Convergence and rate? $\Delta x = M^{-1/d} \to 0$

Identifiability

$$A_{ij} = \langle\!\langle \phi_i, \phi_j \rangle\!\rangle = \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \phi_i(r) \psi_j(s) \overline{G}_T(r,s) \rho_T(dr) \rho_T(ds)$$
$$= \langle L_{\overline{G}_T} \phi_i, \phi_j \rangle_{L^2(\rho_T)}$$

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$$= \langle L_{\overline{G}_T} \phi_i, \phi_j \rangle_{L^2(\rho_T)}$$

- Positive compact operator $L_{\overline{G}_T}$
  - normal matrix $A \sim L_{\overline{G}_T}|_{\mathcal{H}}$ in $L^2(\rho_T)$

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

- Identifiability: $A^{-1}b \leftrightarrow L_{\overline{G}_T}^{-1}\phi^D$
  - Function space of identifiability (FSOI): $\overline{\mathrm{span}\{\psi_i\}_{\lambda_i>0}}$
  - Closure of RKHS $H_{\overline{G}} = L_{\overline{G}_T}^{1/2}(L^2(\rho_T))$ [LangLu21]

Convergence rate

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

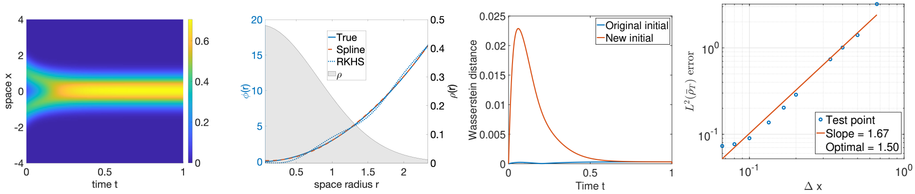
Theorem (Numerical error bound [Lang-Lu20])

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

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

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

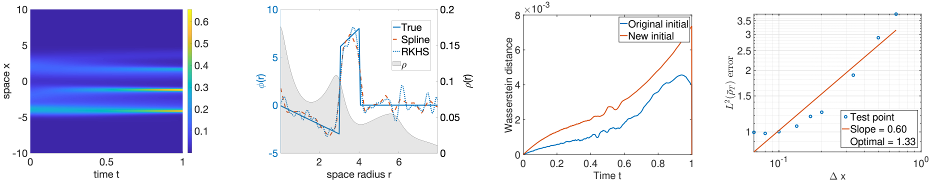
Example 1: granular media $\phi(r) = 3r^2$



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

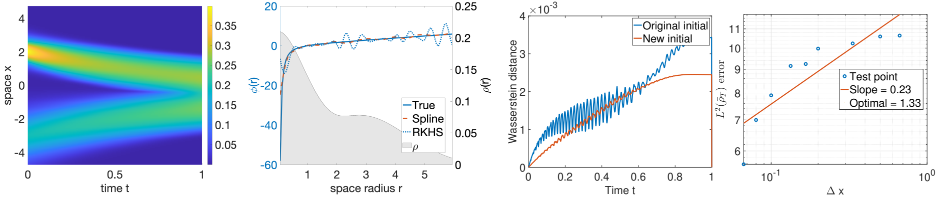
- near optimal rate ($\phi \in W^{1,\infty}$)

Example 2: Opinion dynamics $\phi(r)$ piecewise linear



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

Example 3: repulsion-attraction $\phi(r) = r - r^{-1.5}$ (singular)



- low rate: theory does not apply

Ongoing projects and open problems:

- Coercivity condition
- General systems:
  - Aggression equations (inviscid MFE)
  - non-radial kernels
  - Systems on graph
- Other types of data:
  - Partial data: observability and randomization
  - Multiple MFE solutions

Learning kernels in operators: regularization

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

$$\mathcal{E}(\psi) = \|R_\psi[u] - f\|_{\mathbb{Y}}^2 = \langle L_G\psi, \psi\rangle_{L^2(\rho)} - 2\langle \phi^D, \psi\rangle_{L^2(\rho)} + C$$

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

$$\phi^D = L_G\phi_{true} + \phi^D_{noise} + \phi^D_{model\ error} + \phi^D_{numerical\ error}$$

Ill-posed inverse problem

$$\mathcal{E}(\psi) = \|R_\psi[u] - f\|_{\mathbb{Y}}^2 = \langle L_G \psi, \psi \rangle_{L^2(\rho)} - 2\langle \phi^D, \psi \rangle_{L^2(\rho)} + C$$

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

$$\phi^D = L_G \phi_{true} + \phi^D_{noise} + \phi^D_{model\ error} + \phi^D_{numerical\ error}$$

Regularization

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

- λ by the L-curve method [Hansen00]
- Regularization norm $\|\cdot\|_Q$?

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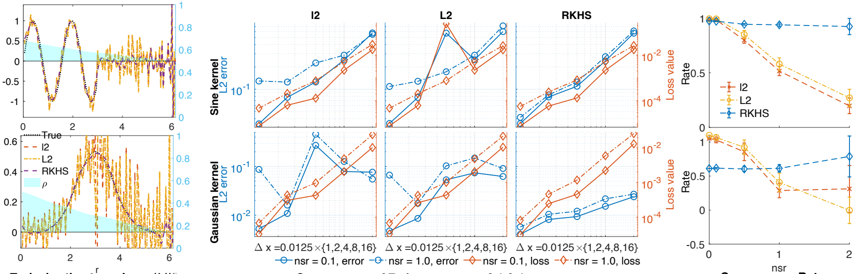
ANSWER: norm of RKHS $H_G = L_G^{1/2}L^2(\rho) \leftrightarrow Q = L_G^{-1}$ [Lu+Lang+An22]

- DARTR: Data Adaptive RKHS Tikhonov Regularization

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

Open questions and ongoing projects:

- Regularized estimator: convergence and rate?
- Regularization for NN in function space
- Data-adaptive priors for Bayesian inverse problems
- Applications: deconvolution, homogenization,...

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:

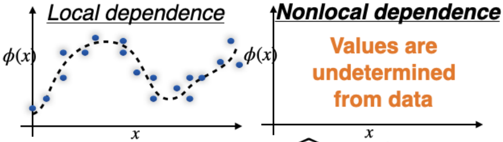
- Probabilistic loss functionals
- Identifiability
- Coercivity condition
  - yes: convergence
  - no: DARTR

Learning with nonlocal dependence: a new direction?

- Coercivity condition
- Regularization
- Convergence (minimax rate)

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

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



Inversion $\widehat{\phi} = I^{-1}\phi^D$ $\qquad$ $\widehat{\phi} = L_G^{-1}\phi^D$

Regularization $\widehat{\phi} = (I + \lambda Q)^{-1}\phi^D$ $\qquad$ $\widehat{\phi} = (L_G + \lambda L_G^{-1})^{-1}\phi^D$

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