Introduction to Nonparametric Learning of Kernels in Operators

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Plan:

Lecture 1. Overview and a review of classical learning theory Lecture 2. Learning interaction kernels in interacting particle systems Lecture 3. Coercivity condition and minimax rate of convergence Lecture 4. Learning interaction kernels in mean-field equations Lecture 5. Data adaptive RKHS Tikhonov regularization Lecture 6. Small noise analysis of RKHS regularizations Lecture 5. DARTR: data adaptive RKHS Tikhonov regularization

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

$$dX_t^i = \frac{1}{N} \sum_{j=1}^N K_{\phi}(X_t^j - X_t^i) dt + \sqrt{2\nu} dB_t^i \quad \Leftrightarrow R_{\phi}(\mathbf{X}_t) = \dot{\mathbf{X}}_t - \sqrt{2\nu} \dot{\mathbf{B}}_t$$
$$\partial_t u = \nu \Delta u + \nabla \cdot [u(K_{\phi} * u)] \quad \Leftrightarrow R_{\phi}[u(\cdot, t)] = f(\cdot, t)$$

▶ *N* small: M trajectories $\{\mathbf{X}_{t_1:t_L}^{(m)}\}_{m=1}^M \Rightarrow$ statistical learning

► $N = \infty$: $\{u_N(x, t_l) = \frac{1}{N} \sum_i \delta_{X_{t_l}^i}(x)\}$ or $\{u(x_m, t_l)\}_{m,l} \Rightarrow$ inverse problem

Nonparametric regression: $\phi = \sum_{k=1}^{n} c_k \phi_k$

$$A_n c = b_n$$

Ill-conditioned $A_n \Rightarrow$ Regularization

$$||A_n c - b_n||^2 + \lambda ||c||_*^2$$

How to choose $||c||_*^2$?

- 1. Learning kernels
- 2. Regression and regularization
- 3. Identifiability and DARTR
- 4. Adaptive prior for Bayesian inverse
- LLA22: Lu, Lang, and An. MSML22.
- LAY22: Lu, An and Yu. arXiv2205
- CLLW22: Chada, Lang, L.& Wang.arXiv2212

Outline

1. Learning kernels

2. Regression and regularization

3. Identifiability and DARTR

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1 Learning kernels

Learning kernels in operators

Learn the kernel ϕ :

$$R_{\phi}[u] + \epsilon = f$$

from data: $\mathcal{D} = \{(u_k, f_k)\}_{k=1}^n, (u_k, f_k) \in \mathbb{X} \times \mathbb{Y}$

• Operator $R_{\phi}[u](x) = \int \phi(|x-y|)g[u](x,y)dy$

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- interacting particles/agents

$$R_{\phi}[u] = \nabla \cdot [u(K_{\phi} * u)] = \partial_{t}u - \sigma \Delta u, \quad K_{\phi}(x) = \phi(|x|)\frac{x}{|x|} \in \mathbb{R}^{d}$$
$$R_{\phi}[\mathbf{X}_{t}] = \left[-\frac{1}{N}\sum_{j=1}^{N}K_{\phi}(X_{t}^{i} - X_{t}^{j})\right]_{i} = \dot{\mathbf{X}}_{t} + \dot{\mathbf{W}}_{t}, \qquad u = \frac{1}{N}\sum_{i=1}^{N}\delta(X_{t}^{i} - x)$$
$$- \text{ nonlocal PDEs: } R_{\phi}[u] = \partial_{tt}u - v$$

$$R_{\phi}[u](x) = \int_{\Omega} \phi(|x-y|)[u(y) - u(x)]dy = \partial_{tt}u - v.$$

– Integral operators, deconvolution, Toeplitz/Hankel matrix ... Toeplitz matrix: $R_{\phi}u = f$, $R_{\phi}(i,j) = \phi(i-j)$

1 Learning kernels

Learning kernels in operators

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

• Operator $R_{\phi}[u]$: linear in ϕ

Data: discrete/noisy, Nonlocal dependence

- random $(u_k, f_k) \sim \mu \otimes \nu$: statistical learning
- deterministic (e.g., N small): inverse problem

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Nonparametric regression

Loss functional: $\mathcal{E}(\phi) = \frac{1}{N} \sum_{i=1}^{N} \|R_{\phi}[u_i] - f_i\|_{\mathbb{Y}}^2$.

Hypothesis space: $\phi = \sum_{i=1}^{n} c_i \phi_i \in \mathcal{H}_n = \operatorname{span} \{\phi_i\}_{i=1}^{n}$:

$$\mathcal{E}(\phi) = c^{\top} \overline{A}_n c - 2c^{\top} \overline{b}_n + C_N^f, \Rightarrow \widehat{\phi}_{\mathcal{H}_n} = \sum_i \widehat{c}_i \phi_i, \text{ where } \widehat{c} = \overline{A}_n^{-1} \overline{b}_n,$$

Nonparametric regression

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Three issues

- $\blacktriangleright \overline{A}_n^{-1}$: ill-conditioned/singular
- Choice of \mathcal{H}_n : $\{\phi_i\}_{i=1}^n$ and n
- Convergence when data mesh refines $\Delta x \rightarrow 0$

Regularization

Regularization is necessary:

- \blacktriangleright \overline{A}_n ill-conditioned
- \overline{b}_n : noisy or with numerical error

Tikhonov/ridge Regularization: ($||c||_{B_*}^2 = c^\top B_*c$)

$$\mathcal{E}_{\lambda}(\phi) = \mathcal{E}(\phi) + \lambda \|\phi\|_{*}^{2} \Rightarrow c^{\top}\overline{A}_{n}c - 2\overline{b}_{n}^{\top}c + \lambda \|c\|_{B_{*}}^{2}$$
$$\hat{\phi}_{\mathcal{H}_{n}}^{\lambda} = \sum_{i} \widehat{c}_{i}^{\lambda}\phi_{i}, \quad \text{where } \widehat{c} = (\overline{A}_{n} + \lambda B_{*})^{-1}\overline{b}_{n},$$

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,

- hyper-parameter λ: CV, truncated SVD, ...
- The L-curve method [Hansen00]

$$\begin{split} t(\lambda) &= (x(\lambda), y(\lambda)) := (\log(\mathcal{E}(\widehat{c_{\lambda}}), \log(\|\widehat{c_{\lambda}}\|_{*}^{2}) \\ \lambda_{*} &= \operatorname*{arg\,max}_{\lambda_{\min} \leq \lambda \leq \lambda_{\max}} \frac{x' y'' - x' y''}{(x' \,^{2} + y' \,^{2})^{3/2}}, \end{split}$$





2 Regression and regularization

Regularization

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- \overline{b}_n : noisy or with numerical error

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$$l(\lambda) = (x(\lambda), y(\lambda)) := (\log(\mathcal{E}(\widehat{c_{\lambda}}), \log(\|\widehat{c_{\lambda}}\|_{*}^{2}),$$

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Principle: $_{[Stuart2010]}$ Avoid **discretization** until the last possible moment \downarrow Avoid basis selection until the last possible moment

Hypothesis space:
$$\phi = \sum_{i=1}^{n} c_i \phi_i \in \mathcal{H}_n = \operatorname{span} \{\phi_i\}_{i=1}^{n}$$

$$R_{\phi}[u](x) = \int_{\Omega} \phi(|x-y|)g[u](x,y)dy = f$$

Function space of ϕ ? Identifiability?

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Identifiability

• An exploration measure: $\rho(dr) \Rightarrow \phi \in L^2(\rho)$ $R_{\phi}[u](x) = \int_{\Omega} \phi(|x-y|)g[u](x,y)dy, \quad \rho(dr) \propto \int \int \delta_{|x-y|}(dr)|g[u](x,y)|dxdy$

Identifiability

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$$\begin{aligned} \mathcal{E}(\psi) &= \frac{1}{N} \sum_{i=1}^{N} \|R_{\psi}[u_i] - f_i\|_{L^2}^2 = \langle \mathcal{L}_{\overline{G}}\psi, \psi \rangle_{L^2(\rho)} - 2\langle \phi^D, \psi \rangle_{L^2(\rho)} \\ \nabla \mathcal{E}(\psi) &= 2\mathcal{L}_{\overline{G}}\psi - 2\phi^D = 0 \quad \Rightarrow \widehat{\phi} = \mathcal{L}_{\overline{G}}^{-1}\phi^D \\ - \mathcal{L}_{\overline{G}} \text{ is a nonnegative compact operator: } \{(\lambda_i, \psi_i)\}, \lambda_i \downarrow 0 \\ - \phi^D &= \mathcal{L}_{\overline{G}}\phi_{true} + \phi^{\text{error}} \end{aligned}$$

Identifiability

• An exploration measure: $\rho(dr) \Rightarrow \phi \in L^2(\rho)$ $R_{\phi}[u](x) = \int_{\Omega} \phi(|x-y|)g[u](x,y)dy, \quad \rho(dr) \propto \int \int \delta_{|x-y|}(dr) |g[u](x,y)|dxdy$

► An integral operator ⇐ the Fréchet derivative of loss functional

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► Function space of identifiability (**FSOI**): $\widehat{\phi} = \mathcal{L}_{\overline{G}}^{-1}(\mathcal{L}_{\overline{G}}\phi_{true} + \phi^{error}) \Rightarrow \quad H = \operatorname{span}\{\psi_i\}_{i:\lambda_i>0}$

- ill-defined beyond H; ill-posed in H

DARTR: Data Adaptive RKHS Tikhonov Regularization

$$\widehat{\phi} = \mathcal{L}_{\overline{G}}^{-1} \phi^D = \mathcal{L}_{\overline{G}}^{-1} (\mathcal{L}_{\overline{G}} \phi_{true} + \phi^{\text{error}})$$

A new task for Regularization: ensure that the learning takes place in the FSOI

data-dependent $H = \operatorname{span}\{\psi_i\}_{i:\lambda_i>0}$

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A new task for Regularization: ensure that the learning takes place in the FSOI

data-dependent $H = \operatorname{span}\{\psi_i\}_{i:\lambda_i > 0} = \overline{H_G}^{L^2(\rho)}$

►
$$\overline{G} \Rightarrow \mathsf{RKHS}$$
: $H_G = \mathcal{L}_{\overline{G}}^{-1/2}(L^2(\rho))$
► For $\phi = \sum_k c_k \psi_k$, $\|\phi\|_{L^2(\rho)}^2 = \sum_k c_k^2$, $\|\phi\|_{H_G}^2 = \sum_k \lambda_k^{-1} c_k^2$

Why DARTR is good: FSOI is fundamental:

$$\widehat{\phi} = \mathcal{L}_{\overline{G}}^{-1} \phi^{D} = \mathcal{L}_{\overline{G}}^{-1} (\mathcal{L}_{\overline{G}} \phi_{true} + \phi_{H}^{\text{error}} + \phi_{H^{\perp}}^{\text{error}})$$

• DARTR: $\|\phi_{H^{\perp}}^{\text{error}}\|_{H_G}^2 = \infty$

$$(\mathcal{L}_{\overline{G}} + \lambda \mathcal{L}_{\overline{G}}^{-1})^{-1} \phi^{D} = (\mathcal{L}_{\overline{G}} + \lambda \mathcal{L}_{\overline{G}}^{-1})^{-1} (\mathcal{L}_{\overline{G}} \phi_{true} + \phi_{H}^{\text{error}})$$

• l^2 or L^2 regularizer: with $C = \sum_i \phi_i \otimes \phi_i$ or C = I

$$(\mathcal{L}_{\overline{G}} + \lambda C)^{-1} \phi^{D} = (\mathcal{L}_{\overline{G}} + \lambda C)^{-1} (\mathcal{L}_{\overline{G}} \phi_{true} + \phi^{\text{error}}_{H} + \phi^{\text{error}}_{H^{\perp}})$$

DARTR: computation

Input: A_n, b_n and $B_n = (\langle \phi_i, \phi_j \rangle_{L^2(\rho)})_{i,j}$. **Output:** reguarized estimator

$$\widehat{c}_{\lambda} = (A_n + \lambda_* B_{rkhs})^{-1} b_n$$

- Generalized eigenvalue problem (A_n, B_n) : $A_n V = BV\Lambda$
- ► $B_{rkhs} = (V\Lambda V^{\top})^{-1}$: avoid inverse \downarrow Set $D = B_n^{-1}A_n^{1/2}$, then, $\hat{c}_{\lambda} = D(D^{\top}A_nD + \lambda I)^{-1}D^{\top}b_n$
- L-curve to select \u03c6_{*}

Connecting computation with theory

$$\widehat{c}_{\lambda} = (A_n + \lambda_* B_{rkhs})^{-1} b_n \quad \leftrightarrow \qquad \widehat{\phi} = \mathcal{L}_{\overline{G}}^{-1} \phi^D$$

Theorem: If $\mathcal{L}_{\overline{G}}(L^2(\rho)) \subset \mathcal{H}$, then, $\mathcal{L}_{\overline{G}}$ eigenvalues $\leftrightarrow \text{GEP}(A_n, B_n)$.

- If $B_n = I_n$: $B_{rkhs} = A_n^{-1}$, the Zellner's g-prior;
- If $\phi_i = \psi_i$: $A_n = \operatorname{diag}(\lambda_i)$, $B_{rkhs} = A_n^{-1}$: $\widehat{c}_{\lambda} = \sum_{i:\lambda_i > 0} (\lambda_i + \lambda \lambda_i^{-1})^{-1} (v_i^\top \overline{b}) v_i$
- ► L^2 regularizer: $\hat{c}_{\lambda} = [\sum_{i:\lambda_i>0} + \sum_{i:\lambda_i=0}](\lambda_i + \lambda)^{-1}(v_i^\top \overline{b})v_i$

Interaction kernel in a nonlinear operator

$$R_{\phi}[u] = \nabla \cdot [u(K_{\phi} * u)] = f, \quad K_{\phi} = \phi(|x|) \frac{x}{|x|}$$

- Recover kernel from discrete noisy data
- Robust in accuracy, consistent rates as mesh refines



More robust L-curve



Linear integral operator:



Robust in accuracy, consistent rates

Homogenization of wave propagation in meta-material

heterogeneous bar with microstructure + DNS \Rightarrow Data

• Homogenization: $R_{\phi}[u] = \int_{\Omega} \phi(|y|)[u(x+y) - u(x)]dy = \partial_{tt}u - g.$



- (c): resolution-invariant
- ▶ (e): *l*² and *L*2 leading to non-physical kernel

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Bayesian inverse problem

Variational inverse problem: ill-posed

$$\widehat{\phi} = rgmin_{\phi} \mathcal{E}(\phi) = \langle \mathcal{L}_{\overline{G}} \phi, \phi
angle_{L^2(
ho)} - 2 \langle \phi^{
ho}, \phi
angle_{L^2(
ho)} + C.$$

Finite dimensional case:

- Prior $\mathcal{N}(0, \mathcal{Q}_0)$ with $\mathcal{Q}_0 > 0$: $\frac{d\pi_0(\phi)}{d\phi} \propto e^{-\frac{1}{2}\langle \phi, \mathcal{Q}_0^{-1}\phi \rangle_{L^2(\rho)}}$
- Likelihood of data: $\pi_L \sim \mathcal{N}(\mathcal{L}_{\overline{G}}^{-1}\phi^{\scriptscriptstyle D}, \sigma_\eta^2 \mathcal{L}_{\overline{G}}^{-1})$

$$rac{l\pi_L(\phi)}{d\phi} \propto \exp(-rac{1}{2\sigma_\eta^2} \mathcal{E}(\phi))$$

Posterior = Gaussian $\mathcal{N}(\mu_1, \mathcal{Q}_1)$ well-posed

$$\frac{d\pi_1(\phi)}{d\phi} \propto \exp\left(-\frac{1}{2}[\sigma_\eta^{-2}\mathcal{E}(\phi) + \langle \mathcal{Q}_0^{-1}\phi,\phi\rangle_{L^2(\rho)}]\right)$$

$$\mu_1 = (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \mathcal{Q}_0^{-1})^{-1} \phi^{\scriptscriptstyle D}, \text{ and } \mathcal{Q}_1 = \sigma_\eta^2 (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \mathcal{Q}_0^{-1})^{-1}$$

Infinite-dimensional prior and posterior

$\phi \in L^2_{\rho}$, infinite-dimensional:

- **Prior** $\mathcal{N}(0, \mathcal{Q}_0)$, where $\mathcal{Q}_0 > 0$, trace-class operator;
- **Posterior** $\mathcal{N}(\mu_1, \mathcal{Q}_1)$: Radon–Nikodym derivative w.r.t the prior

$$\frac{d\pi_1}{d\pi_0} \propto \exp(-\frac{1}{2}\sigma_\eta^{-2}\mathcal{E}(\phi)) = \exp\left(-\frac{1}{2}\sigma_\eta^{-2}[\langle \mathcal{L}_{\overline{G}}\phi,\phi\rangle_{L^2(\rho)} - 2\langle\phi^D,\phi\rangle_{L^2(\rho)} + C]\right),$$

$$\mu_1 = (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \mathcal{Q}_0^{-1})^{-1} \phi^{\scriptscriptstyle D}, \text{ and } \mathcal{Q}_1 = \sigma_\eta^2 (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \mathcal{Q}_0^{-1})^{-1}.$$

Is it a good idea to choose $Q_0 > 0$?

Risk in a non-degenerate prior

Theorem ([CLLW22])

A non-degenerate prior has the risk of leading to a divergent posterior mean in the small noise limit.

I.e., $\lim_{\sigma_\eta \to 0} (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \mathcal{Q}_0^{-1})^{-1} \phi^{{}_D} " = "\infty$ under Assumption (next page).

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Assumptions: $\mathcal{L}_{\overline{G}} \sim \{(\lambda_k, \psi_k)\}$

- ► Finite rank $\mathcal{L}_{\overline{G}}$: $\lambda_k > 0$ for $1 \le k \le K$, $\lambda_k = 0$ for k > K. $\dim(L^2(\rho)) > K$. As a result, the FSOI $H = \operatorname{span}\{\psi_i\}_{i=1}^K \subseteq L^2_{\rho}$.
- Prior covariance commutes with L_G: The prior N(0, Q₀) satisfies Q₀ψ_i = r_iψ_i with r_i > 0 for all i.
- Error outside of FSOI.

$$\phi^{\scriptscriptstyle D} = \mathcal{L}_{\overline{G}} \phi_{true} + \epsilon^{\xi} + \epsilon^{\eta},$$

The model error $\epsilon^{\xi} = \sum_{i} \epsilon_{i}^{\xi} \psi_{i}$ has $\epsilon_{i_{0}}^{\xi} \neq 0$ with $i_{0} > K$. Note: $\epsilon^{\eta} \sim \mathcal{N}(0, \sigma_{\eta}^{2} \mathcal{L}_{\overline{G}})$ comes from noise.

Proof:

$$\phi^{\scriptscriptstyle D} = \sum_i \phi^{\scriptscriptstyle D}_i \psi_i, \text{ with } \phi^{\scriptscriptstyle D}_i = \lambda_i \phi_{true,i} + \sigma_\eta \lambda_i^{1/2} \epsilon^{\eta}_i + \epsilon_i^{\xi}.$$

The posterior mean $\mu_1 = (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \mathcal{Q}_0^{-1})^{-1} \phi^{\scriptscriptstyle D}$ becomes

$$\mu_{1} = \sum_{i} \left(\lambda_{i} + \sigma_{\eta}^{2} r_{i}^{-1}\right)^{-1} \phi_{i}^{D} \psi_{i} = \sum_{i=1}^{K} \left(\lambda_{i} + \sigma_{\eta}^{2} r_{i}^{-1}\right)^{-1} \phi_{i}^{D} \psi_{i} + \sum_{i>K} \sigma_{\eta}^{-2} r_{i} \epsilon_{i}^{\xi} \psi_{i}.$$

The first term $\rightarrow \sum_{1 \le i \le K} \left(\phi_{true,i} + \lambda_i^{-1} \epsilon_i^{\xi} \right) \psi_i$ But the 2nd term $\sum_{i>K} \sigma_{\eta}^{-2} r_i \epsilon_i^{\xi} \psi_i$ diverges because $\exists \epsilon_{i_0}^{\xi} \neq 0$.

Data-adaptive prior

Fixed prior $\phi \sim \pi_0 = \mathcal{N}(0, \mathcal{Q}_0), \pi_1 = \mathcal{N}(\mu_1, \mathcal{Q}_1)$

$$\mu_1 = (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \mathcal{Q}_0^{-1})^{-1} \phi^{\scriptscriptstyle D}$$

Data-adaptive prior $\phi \sim \pi_0 = \mathcal{N}(0, \lambda_*^{-1} \mathcal{L}_{\overline{G}}), \pi_1 = \mathcal{N}(\mu_1, \mathcal{Q}_1^{\scriptscriptstyle D})$

$$\mu_1^{\scriptscriptstyle D} = (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \lambda_* \mathcal{L}_{\overline{G}}^{-1})^{-1} \phi^{\scriptscriptstyle D}$$
$$\mathcal{Q}_1^{\scriptscriptstyle D} = \sigma_\eta^2 (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \lambda_* \mathcal{L}_{\overline{G}}^{-1})^{-1}$$

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Data-adaptive prior $\phi \sim \pi_0 = \mathcal{N}(0, \lambda_*^{-1} \mathcal{L}_{\overline{G}}), \pi_1 = \mathcal{N}(\mu_1, \mathcal{Q}_1^p)$

$$\mu_1^{\scriptscriptstyle D} = (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \lambda_* \mathcal{L}_{\overline{G}}^{-1})^{-1} \phi^{\scriptscriptstyle D}$$

$$\mathcal{Q}_1^{\scriptscriptstyle D} = \sigma_\eta^2 (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \lambda_* \mathcal{L}_{\overline{G}}^{-1})^{-1}$$

Theorem (Small noise limit of the posterior mean [CLLW22]) Fixed prior with $Q_0 = I_d$: blows up; Data-adaptive prior: stable and convergent **Proof** With $\sigma_{\eta}^2 \lambda_* > 0$:

$$\begin{split} (\mathcal{L}_{\overline{G}} + \sigma_{\eta}^{2} \lambda_{*} \mathcal{L}_{\overline{G}}^{-1})^{-1} \psi_{i} &= (\mathcal{L}_{\overline{G}}^{-2} + \sigma_{\eta}^{2} \lambda_{*} I)^{-1} \mathcal{L}_{\overline{G}} \psi_{i} \\ &= \frac{\lambda_{i}}{\lambda_{i}^{2} + \sigma_{\eta}^{2} \lambda_{*}} \psi_{i} = 0 \,, \text{ if } i \geq K + 1 \,. \end{split}$$

Then, the posterior mean is:

$$\mu_1^{\scriptscriptstyle D} = (\mathcal{L}_{\overline{G}} + \sigma_\eta^2 \lambda_* \mathcal{L}_{\overline{G}}^{-1})^{-1} \phi^{\scriptscriptstyle D} = \sum_{1 \le i \le K} \left(\lambda_i + \sigma_\eta^2 \lambda_* \lambda_i^{-1} \right)^{-1} \phi_i^{\scriptscriptstyle D} \psi_i.$$

The limit exist as $\sigma_{\eta} \to 0$: (recall that $\phi^{\scriptscriptstyle D} = \sum_i \phi^{\scriptscriptstyle D}_i \psi_i$, with $\phi^{\scriptscriptstyle D}_i = \lambda_i \phi_{true,i} + \sigma_{\eta} \lambda_i^{1/2} \epsilon^{\eta}_i + \epsilon^{\xi}_i$)

$$\lim_{\sigma_{\eta}\to 0}\mu_1^{\scriptscriptstyle D} = \sum_{i=1}^K \left(\phi_{true,i} + \lambda_i^{-1}\epsilon_i^{\xi}\right)\psi_i.$$

Small noise limit of posterior mean

Integral operator, ϕ_{true} inside the FSOI:



Fixed prior: blowup Data-adaptive prior: stable and convergent

Small noise limit of posterior mean

Integral operator, ϕ_{true} outside the FSOI:



Fixed prior: blowup Data-adaptive prior: stable and convergent

Summary

Learning kernels in operators:

$$R_{\phi}[u] = f \quad \Leftarrow \quad \mathcal{D} = \{(u_k, f_k)\}_{k=1}^N$$

Nonlocal dependence

- Identifiability: data-dependent FSOI
- DARTR: data adaptive RKHR Tikhonov-Reg
 - Synthetic data: convergent, robust to noise
 - Homogenization: resolution-independent
- Small noise analysis in Bayesian

Next:

How do we theoretically compare different regularizations? Small noise analysis_[L023,LL23] Future directions

Inverse problems \leftrightarrow Learning with nonlocal dependence

- Iterative methods for DARTR
- Convergence: $\Delta x, N$
- Regularization for ML: $\|\phi_{\theta}\|_{rkhs}^2$, not $\|\theta\|$

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References

(@ http://www.math.jhu.edu/~feilu)

- LLA22: Lu, Lang, and An. MSML22. (Matlab code available)
- LAY22: Lu, An and Yu. arXiv2205
- CLLW22: Chada, Lang, Lu, and Wang. arXiv2212