Data-adaptive RKHS regularization for learning kernels in operators

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Which norm $\|x\|_*$ to use in $\|Ax - b\|^2 + \lambda \|x\|_*^2$
when solving ill-posed inverse problems ?

$(A) \|x\|$

$(B) \|\phi\|_{L^2}$ for $\phi(s) = \sum_i x_i e_i(s)$

(C) Total variation

(D) RKHS

(E) Try all

Learning kernels in operators

Learn the kernel ϕ: $$R_\phi[u] + \epsilon = f$$

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

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

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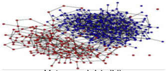
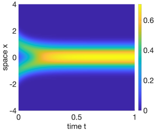
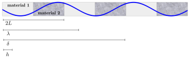


Voter model (wiki)





- Interacting particles/agents $K_\phi(x) = \phi(|x|)\frac{x}{|x|} \in \mathbb{R}^d$

$$R_\phi[\mathbf{X}_t] = \Big[-\frac{1}{n}\sum_{j=1}^{n} K_\phi(X_t^i - X_t^j)\Big]_i = \dot{\mathbf{X}}_t + \dot{\mathbf{W}}_t, \qquad \mathbb{R}^{nd}$$

$$R_\phi[u] = \nabla \cdot [u(K_\phi * u)] = \partial_t u - \sigma \Delta u,$$

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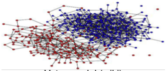

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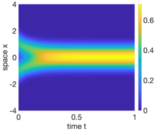

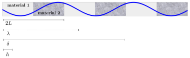

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$$R_\phi[u] = \nabla \cdot [u(K_\phi * u)] = \partial_t u - \sigma \Delta u,$$

- Nonlocal PDEs:

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

Learning kernels in operators

Learn the kernel ϕ: $R_\phi[u] + \epsilon = f$

from data:

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

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

  linear or nonlinear in u, but linear in ϕ

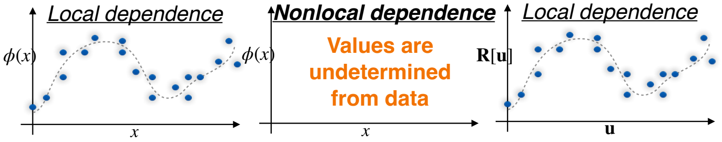
- Statistical learning $\bigcap$ inverse problem
  - random $\{(u_k, f_k)\}$: statistical learning
  - deterministic (e.g., N small): inverse problem

Learning kernels in operators

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

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

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



Inverse problem: well-posed **ill-posed** well-posed

This talk: $\Rightarrow$ introduce a data-adaptive regularization norm

- Convergent estimator as mesh refines

$$\mathcal{D} = \{(u_k(x_j), f_k(x_j))\}_{k=1}^N, \quad \Delta x = |x_{j+1} - x_j| \to 0$$

Part 2: Regression and regularization

Learn the kernel ϕ:

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

from data:

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

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

Nonparametric regression

- Loss functional: $\mathcal{E}(\phi) = \frac{1}{N}\sum_{i=1}^{N} \|R_\phi[u_i] - f_i\|_{\mathbb{Y}}^2$
  - Crucial!
  - Derivative-free Monte Carlo suitable [Lang+Lu22SISC]
- Hypothesis space $\mathcal{H}_n = \mathrm{span}\{\phi_i\}_{i=1}^{n}$: $\phi = \sum_{i=1}^{n} c_i \phi_i$,

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

Goal: $\widehat{\phi}_{\mathcal{H}_n}$ converges as data mesh Δx refines

Challenges

- Choice of $\mathcal{H}_n$: $\{\phi_i\}_{i=1}^{n}$ and $n = n(\Delta x)$
- $\overline{A}_n^{-1}$: ill-conditioned/singular

Regularization

Regularization is necessary:

- $\overline{A}_n$ ill-conditioned
- $\overline{b}_n$: noise or numerical error

Tikhonov/ridge Regularization:

$$\mathcal{E}_\lambda(\phi) = \mathcal{E}(\phi) + \lambda \|\phi\|_*^2 \Rightarrow c^\top \overline{A}_n c - 2\overline{b}_n^\top c + \lambda c^\top B_* c$$

$$\widehat{\phi}_{\mathcal{H}_n}^\lambda = \sum_i \widehat{c}_{\lambda,i}\phi_i, \quad \text{where } \widehat{c}_\lambda = (\overline{A}_n + \lambda B_*)^{-1}\overline{b}_n,$$

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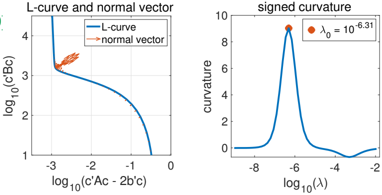
- λ: L-curve[Hansen00], GCV[Golub+Heath+Wahba79]

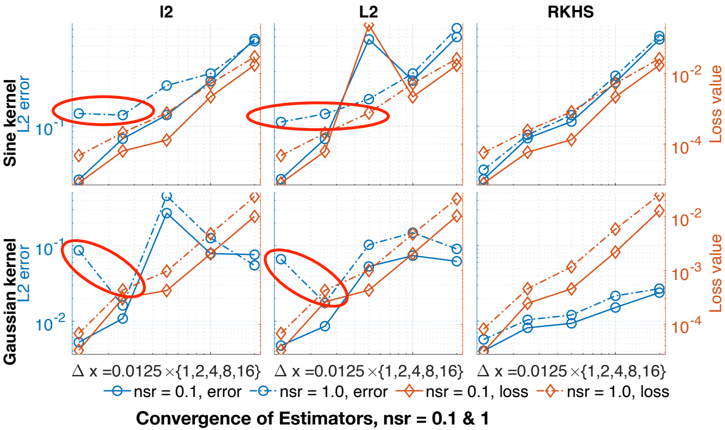
$$(x,y) := (\log(\mathcal{E}(\widehat{c}_\lambda)), \log(\widehat{c}_\lambda^\top B_* \widehat{c}_\lambda)),$$

$$\lambda_* = \text{maximal curvature}$$

- Which norm $\|\cdot\|_*$ to use? $\|c\|$, $\|\phi\|$?



l2: $\|c\|$ L2: $\|\phi\|_{L^2}$



- Risk of blowing up in the small noise limit [Chada-Wang-Lang-Lu22]

Principle: [Stuart2010]
Avoid **discretization** until the last possible moment

$\downarrow$

Avoid basis selection until the last possible moment

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

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

Function space of ϕ? Identifiability?

Part 3: Identifiability & regularization

DARTR: Data adpative RKHS Tikhonov regularization

Identifiability

- An exploration measure: $\rho(dr)$ $\Rightarrow \phi \in L^2_\rho$

  $R_\phi[u](x) = \int_\Omega \phi(|x-y|) g[u](x,y) dy, \quad \rho(dr) \propto \int\int \delta_{|x-y|}(dr) \big| g[u](x,y) \big| dxdy$

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- An integral operator $\Leftarrow$ the Fréchet derivative of loss functional

$$\mathcal{E}(\phi) = \frac{1}{N}\sum_{i=1}^{N} \|R_\phi[u_i] - f_i\|^2_{L^2} = \langle \mathcal{L}_{\overline{G}}\phi, \phi\rangle_{L^2_\rho} - 2\langle \phi^D, \phi\rangle_{L^2_\rho} + C$$

$$\nabla\mathcal{E}(\phi) = 2\mathcal{L}_{\overline{G}}\phi - 2\phi^D = 0 \quad \Rightarrow \widehat{\phi} = \mathcal{L}_{\overline{G}}^{-1}\phi^D$$

  - $\mathcal{L}_{\overline{G}}$: nonnegative compact, $\{(\lambda_i, \psi_i)\}$, $\lambda_i \downarrow 0$
  - $\phi^D = \mathcal{L}_{\overline{G}}\phi_{true} + \phi^{\text{error}}$

Identifiability

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- Function space of identifiability (**FSOI**):

$$\widehat{\phi} = \mathcal{L}_{\overline{G}}^{-1}(\mathcal{L}_{\overline{G}}\phi_{true} + \phi^{\mathrm{error}}) \Rightarrow \quad H = \mathrm{Null}(\mathcal{L}_{\overline{G}})^\perp = \overline{\mathrm{span}\{\psi_i\}_{i:\lambda_i>0}}$$

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

DARTR: Data Adaptive RKHS Tikhonov Regularization

A new task for Regularization:

ensure that the learning takes place in the FSOI

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

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

- $\overline{G} \Rightarrow$RKHS: $H_G = \mathcal{L}_{\overline{G}}^{1/2}(L^2_\rho)$
- $\|\phi\|^2_{H_G} = \langle \mathcal{L}_{\overline{G}}^{-1}\phi, \phi\rangle_{L^2_\rho}$

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$\Rightarrow$ Regularization norm: $\|\phi\|^2_{H_G}$ [Lu+Lang+An22MSML]

$$\mathcal{E}_\lambda(\phi) = \mathcal{E}(\phi) + \lambda\|\phi\|^2_{H_G} = \langle(\mathcal{L}_{\overline{G}} + \lambda\mathcal{L}_{\overline{G}}^{-1})\phi, \phi\rangle_{L^2_\rho} - 2\langle\phi^D, \phi\rangle_{L^2_\rho}$$

$$\widehat{\phi}_\lambda = (\mathcal{L}_{\overline{G}} + \lambda\mathcal{L}_{\overline{G}}^{-1})^{-1}\phi^D = (\mathcal{L}_{\overline{G}}^2 + \lambda I)^{-1}\mathcal{L}_{\overline{G}}\phi^D$$

What DARTR has done:
remove error outside FSOI + regularize in FSOI

- No regularization:

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

- DARTR: $\mathcal{L}_{\overline{G}}\phi_{H^\perp}^{\text{error}} = 0$ or $\|\phi_{H^\perp}^{\text{error}}\|_{H_G}^2 = \infty$

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

- l^2 or L^2 regularizer: with $C = \sum \phi_i \otimes \phi_j$ or $C = I$

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

DARTR: computation

$$\mathcal{E}_\lambda(\phi) = \mathcal{E}(\phi) + \lambda\|\phi\|_{H_G}^2 \Rightarrow c^\top A_n c - 2b_n^\top c + \lambda\|c\|_{B_{rkhs}}^2$$

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

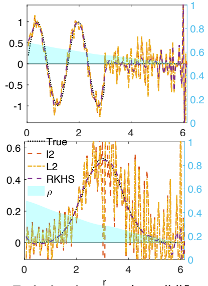
$$\widehat{c}_\lambda = (A_n + \lambda_* B_{rkhs})^{-1} b_n$$

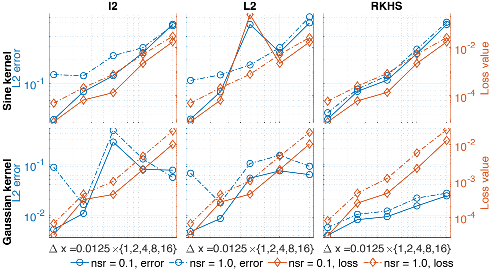
- Generalized eigenvalue problem $(A_n, B_n) \leftrightarrow \mathcal{L}_{\overline{G}}$
  $A_n V = B_n V \Lambda$ and $V^\top B_n V = I_n$
  $B_{rkhs} = (V \Lambda V^\top)^\dagger$; ($B_{rkhs} = A_n^\dagger$ if $B_n = I_n$)
- L-curve to select λ_*

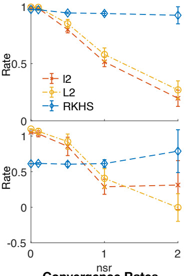
Interaction kernel in a nonlinear operator

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

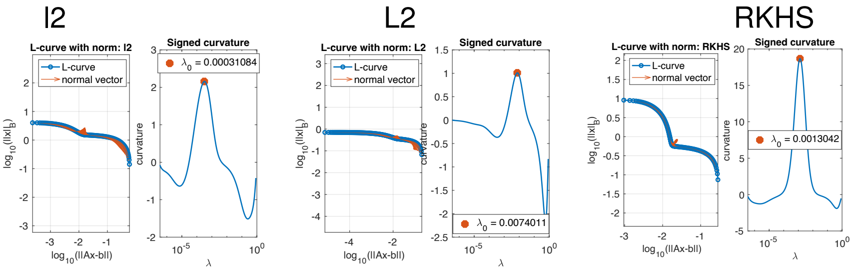
- Recover kernel from discrete noisy data
- Robust in accuracy, consistent rates as mesh refines


Typical estimators, $\Delta x = 0.05$


Convergence of Estimators, nsr = 0.1 & 1

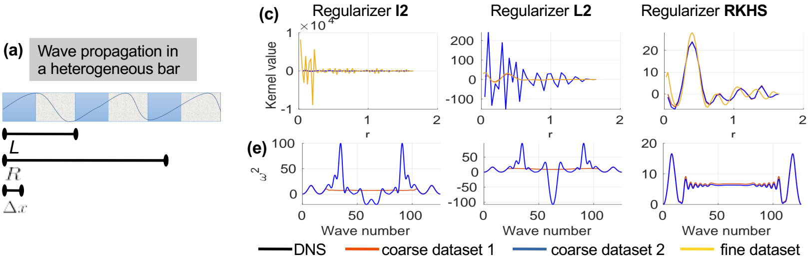

Convergence Rates

More robust L-curve



Homogenization of wave propagation in meta-material

- heterogeneous bar with microstructure + DNS $\Rightarrow$ Data
- Homogenization: [Lu+An+Yu23]
  $R_{\phi}[u] = \int_{\Omega} \phi(|y|)[u(x+y) - u(x)]dy = \partial_{tt}u - v.$



- (c): resolution-invariant
- (e): l^2 and $L2$ leading to non-physical kernel

Part 4: Iterative method

Large scale $Ax = b$, $A \in \mathbb{R}^{m\times n}$ ill-conditioned , $n >> 1$
b: noisy

Direct method: DARTR for $Ax = b$

$$A_n = A^\top A, b_n = A^\top b: \Rightarrow \quad A_n x = b_n$$

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

- $\rho \propto \sum_j |A_{ij}|$: measure of A exploring x
- $B_n = \mathrm{diag}(\rho)$: pre-conditioning
- Generalized eigenvalue problem (A_n, B_n)
  $A_n V = B_n V \Lambda$ and $V^\top B_n V = I_n \Rightarrow B_{rkhs} = (V \Lambda V^\top)^\dagger$
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- L-curve to select λ_*

Direct method: based on **costly** matrix decomposition, $O(n^3)$.

Iterative method: without computing B_{rkhs}?

Iterative Data Adaptive RKHS regularization

Solve: $x_k = \arg\min_{x\in\mathcal{X}_k} \|x\|_{B_{rkhs}}, \ \mathcal{X}_k = \{x : \min_{x\in\mathcal{S}_k} \|Ax - b\|\}$

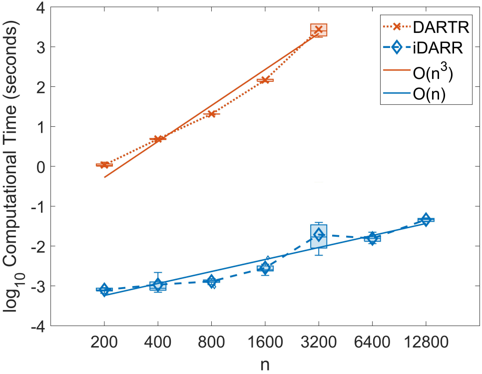
$$\mathcal{S}_k = \mathrm{span}\{(B^{\dagger}_{rkhs}A^\top A)^i B^{\dagger}_{rkhs}A^\top b\}_{i=0}^{k}$$

- Use $B^{\dagger}_{rkhs}$, not B_{rkhs}: $B^{\dagger}_{rkhs} = B^{-1}A^\top A B^{-1}$
- generalized Golub-Kahan bidiagonalization (gGKB)
  $\Rightarrow$ construct $\mathcal{S}_k$ only using matrix-vector product
- $\mathcal{S}_k$ = RKHS-restricted Krylov subspace
- Early stopping: select k

[Li+Feng+Lu, arXiv2401: Scalable iterative data-adaptive RKHS regularization]

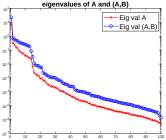
Computational complexity

Direct method: DARTR, $O(n^3)$
Iterative method: iDARR, $O(3mnk)$



Fredholm integral equation: 1st kind

Iterative method ≈ direct method



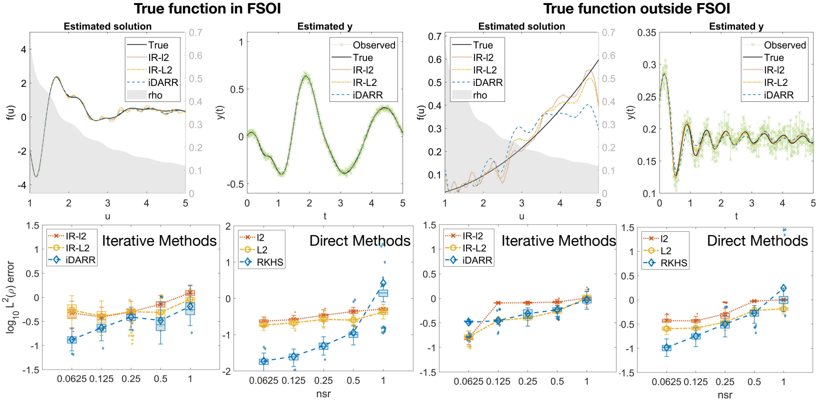
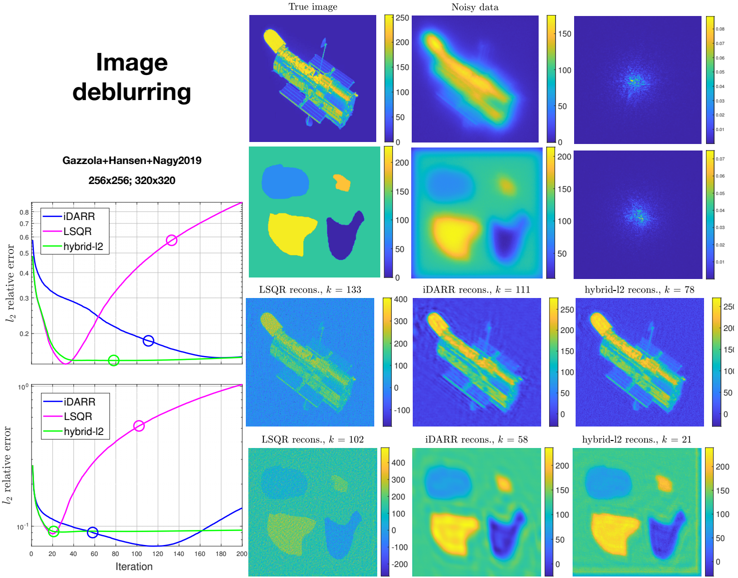


Image deblurring

Image deblurring

Gazzola+Hansen+Nagy2019

256x256; 320x320



Regularization:

Is DA-RKHS better than other norms?

- Small noise analysis [Chada+Lang+Lu+Wang22,Lu+Ou23,LangLu23]
  - Data-Adaptive is important
    fractional space $H_G^s = L_G^{s/2} L_\rho^2$
  - Convergence rate: same as L^2, a smaller factor
- Open: is there a regularizer universally "best"?

Summary

Learning kernels in operators:

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

Nonlocal dependence

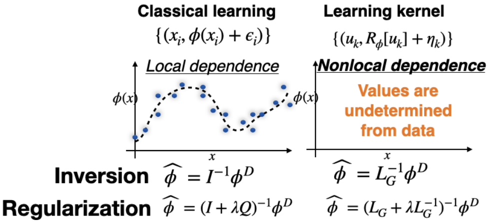
- Identifiability
- DARTR: data adaptive RKHR Tikhonov-Reg
  - Synthetic data: convergent, robust to noise
  - Homogenization: resolution-invariant
- Iterative method: iDARR

Regularization: $A_n x_n = b_n \Rightarrow$ "$x_{\lambda,n} = (A_n + \lambda A_n^{-1}) b_n$ "

Future directions

Learning with nonlocal dependence

- Convergence: $\Delta x, N$
- Automatic kernel for GPR
- Regularization for ML: $\|\phi_\theta\|^2_{rkhs}$, not $\|\theta\|$



Thank you for your attention!