Data-efficient Kernel Methods for Learning Differential Equations and their Solution Operators

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New talk ...
new typos ...

Matthew Thorpe

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Outline

Overview

Solving PDEs / Learning PDEs / Operator Learning

Generic nonlinear PDE

$$\mathfrak{P}(u) = f$$

- (PDE solvers) Given $\mathfrak{P}, f$ find $\widehat{u}$ such that $\mathfrak{P}(\widehat{u}) \approx f$

$$\widehat{\mathfrak{P}^{-1}} : f \mapsto u$$

- (Learning PDEs) Given training data $\{u_m, f_m\}_{m=1}^M$ find $\widehat{\mathfrak{P}}$ such that $\widehat{\mathfrak{P}}(u) \approx f$

$$\widehat{\mathfrak{P}} : u \mapsto f$$

- (Operator learning) Given training data $\{u_m, f_m\}_{m=1}^M$ find $\widehat{\mathfrak{P}^{-1}}$ such that $\widehat{\mathfrak{P}^{-1}}(f) \approx u$

$$\widehat{\mathfrak{P}^{-1}} : f \mapsto u$$

[1] Brunton, Proctor, and Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems".

[2] Kovachki, Lanthaler, and Stuart, "Operator learning: Algorithms and analysis".

- Sparse observation meshes $X_m := \{x_{m,1}, \ldots, x_{m,N}\} \subset \Omega$

Goal

Given sparse and noisy observations

$$\{u_m(X_m) + \epsilon_m, f_m\}_{m=1}^M$$

learn $\widehat{\mathfrak{P}} \approx \mathfrak{P}$ and $\widehat{\mathfrak{P}^{-1}} \approx \mathfrak{P}^{-1}$.

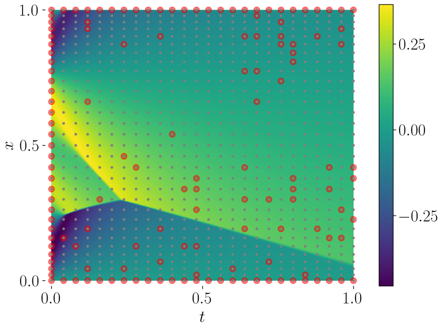
Idea

First learn $\widehat{\mathfrak{P}}$ assuming it is local. Then "invert" $\widehat{\mathfrak{P}}$ to obtain $\widehat{\mathfrak{P}^{-1}}$.

E.g. Burgers' PDE

$$\mathfrak{P}(u) = u_t + uu_x - \nu u_{xx} = 0$$

While $\mathfrak{P}$ is simple, the solution map $\mathfrak{P}^{-1} : u(x,0) \mapsto u(x,t)$ is complex.



Problem Setup

$$\mathfrak{P}(u)(x) = f(x) \qquad x \in \Omega$$

$$\begin{aligned} \mathfrak{P}(u)(x) &= p \circ (x, Du(x), D^2u(x), \dots,) \\ &= p \circ \Phi(u, x) \end{aligned}$$

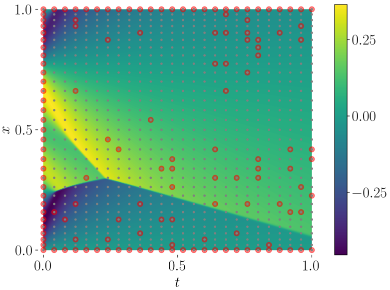
- **(known)** Mapping $\Phi : \mathcal{U} \times \Omega \to \mathbb{R}^Q$, linear in u and nonlinear in x
- **(unknown)** Nonlinear function $p : \mathbb{R}^Q \to \mathbb{R}$

E.g. Nonlinear, Variable Coefficient, Elliptic PDE

$$\begin{aligned} \mathfrak{P}(u) &= -\partial_x \left(a(x)\partial_x u\right) + \alpha u^3 = f \\ \Phi(u, x) &= (x, u(x), u_x(x), u_{xx}(x)) \\ p(s_1, s_2, s_3, s_4) &= -a_x(s_1)s_3 - a(s_1)s_4 + \alpha s_2^3 \end{aligned}$$

Kernel Equation Learning (KEqL): Formulation

- Assumption $\mathfrak{P} = p \circ \Phi(u, x) = f(x)$
- Training data $(u_m(X_m), f_m)_{m=1}^{M}$
- Banach spaces $(\mathcal{U}, \|\cdot\|_{\mathcal{U}})$ and $(\mathcal{P}, \|\cdot\|_{\mathcal{P}})$
- Optimal recovery problem



$$(\widehat{u}_m, \widehat{p}) = \underset{v_m \in \mathcal{U}, q \in \mathcal{P}}{\arg\min} \|q\|_{\mathcal{P}} + \lambda \sum_{m=1}^{M} \|v_m\|_{\mathcal{U}}$$

s.t. $v_m(X_m) = u_m(X_m)$ (Observation/data)

$q \circ \Phi(v_m, x) = f_m(x), \quad \forall x \in \Omega$ (PDE constraint)

Reproducing Kernel Hilbert Spaces (RKHS)

- Set Ω
- Positive definite and symmetric (PDS) kernel $K : \Omega \times \Omega \to \mathbb{R}$:
  - $K(x, x') = K(x', x), \ \forall x, x' \in \Omega$
  - For any set of points $X = \{x_1, \ldots, x_N\} \subset \Omega$ the matrix $K(X, X) = (K(x_i, x_j))$ is PDS.
- Pre-Hilbert space

$$\mathcal{K}_0 := \left\{ f : \Omega \to \mathbb{R} \middle| f = \sum_{j=1}^{N_f} \alpha_{f,j} K(\cdot, x_{f,j}) = K(\cdot, X_f)\boldsymbol{\alpha}_f \right\}$$

- Define inner product

$$\langle f, g \rangle_{\mathcal{K}_0} := \boldsymbol{\alpha}_f^T K(X_f, X_g)\boldsymbol{\alpha}_g$$

- Complete $\mathcal{K}_0$ to get RKHS $\mathcal{K}$
- $\mathcal{K}$ is uniquely defined by K
- Reproducing property: $\forall f \in \mathcal{K}$

$$f(x) = \langle f, K(\cdot, x) \rangle_{\mathcal{K}}$$

- In fact, for any $\phi \in \mathcal{K}^\star$

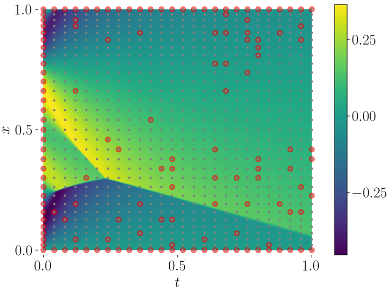
$$\phi(f) = \langle f, K(\cdot, \phi) \rangle_{\mathcal{K}}$$

where

$$K(x, \phi) = \phi(K(x, \cdot))$$

Kernel Equation Learning (KEqL): Formulation

- Assumption $\mathfrak{P} = p \circ \Phi(u, x) = f(x)$
- Training data $(u_m(X_m), f_m)_{m=1}^M$
- RKHS space $\mathcal{U}$ with kernel U
- RKHS space $\mathcal{P}$ with kernel P
- Collocation mesh $X \supseteq \cup_m X_m$



$$(\widehat{u}_m, \widehat{p}) = \underset{v_m \in \mathcal{U}, q \in \mathcal{P}}{\arg\min} \|q\|_{\mathcal{P}}^2 + \lambda \sum_{m=1}^{M} \|v_m\|_{\mathcal{U}}^2$$

s.t. $v_m(X_m) = u_m(X_m)$ (Observation/data)

$q \circ \Phi(v_m, X) = f_m(X)$ (Discrete PDE constraint)

KEqL: All-at-once Inversion

$$
\begin{aligned}
(\widehat{u}_m, \widehat{p}) = \underset{v_m \in \mathcal{U}, q \in \mathcal{P}}{\arg\min} \; & \|q\|_{\mathcal{P}}^2 + \lambda \sum_{m=1}^{M} \|v_m\|_{\mathcal{U}}^2 \\
\text{s.t.} \qquad & v_m(X_m) = u_m(X_m) \qquad && \text{(Observation/data)} \\
& q \circ \Phi(v_m, X) = f_m(X) && \text{(Discrete PDE constraint)}
\end{aligned}
$$

[3] Chen, Liu, and Sun, "Physics-informed learning of governing equations from scarce data".
[4] Sun, Liu, and Sun, "Physics-informed Spline Learning for Nonlinear Dynamics Discovery".
[5] Haber and Oldenburg, "Joint inversion: a structural approach".
[6] Kaltenbacher, "Regularization based on all-at-once formulations for inverse problems".

KEqL: Algorithm Summary

- Relax equality constraints

$$(\widehat{u}_m, \widehat{p}) = \underset{v_m \in \mathcal{U}, q \in \mathcal{P}}{\arg\min} \|q\|_{\mathcal{P}}^2 + \sum_{m=1}^{M} \lambda \|v_m\|_{\mathcal{U}}^2 + \lambda' \|u_m(X^m) - v_m(X^m)\|_2^2 + \lambda'' \|q \circ \Phi(v_m, X) - f_m(X)\|_2^2$$

- Apply kernel trick (representer theorem) or use feature maps
- Solve using a Levenberg–Marquardt-type algorithm

Operator Learning via KEqL

- Given KEqL solution $\widehat{p}$ approximate PDE solution map $\mathfrak{P}^{-1}$ with pseudo inverse of

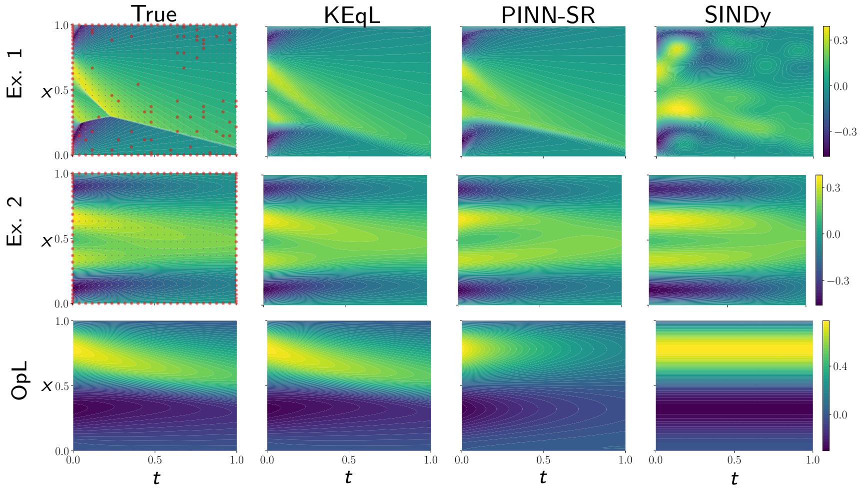
$$\widehat{\mathfrak{P}} := \widehat{p} \circ \Phi.$$

$$\widehat{\mathfrak{P}}^{\dagger}(f) := \operatorname*{arg\,min}_{v \in \mathcal{U}} \|v\|_{\mathcal{U}}^2 + \lambda'' \|\widehat{p} \circ \Phi(v, X) - f(X)\|_2^2.$$

[7] Chen et al., "Solving and learning nonlinear PDEs with Gaussian processes".
[8] Long et al., "A kernel framework for learning differential equations and their solution operators".

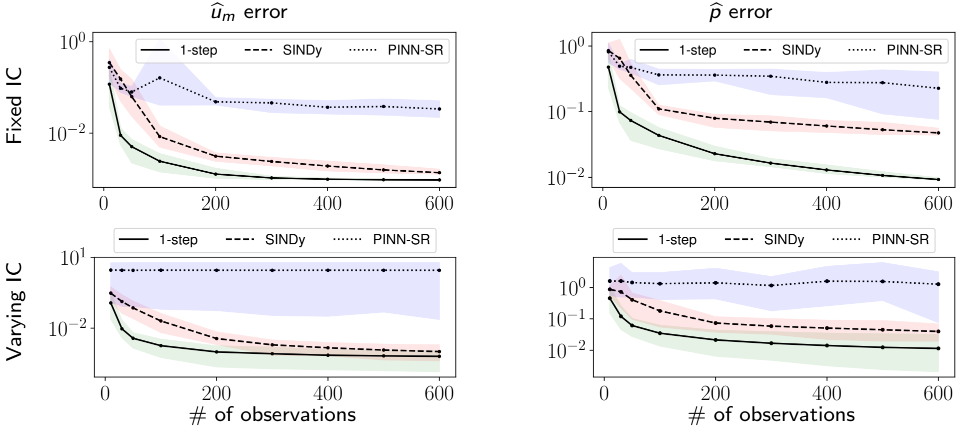
Burgers' Benchmark: Shocks with Sparse Data

$$\mathfrak{P}(u) = u_t + uu_x - 0.1u_x x = 0 \quad \text{plus B.C and I.C}$$



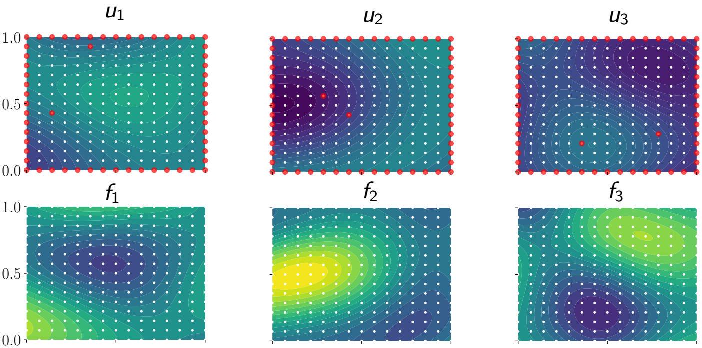
Burgers' Benchmark: Comparison to PINN-SR and SINDy

- Large performance gap with PINN model



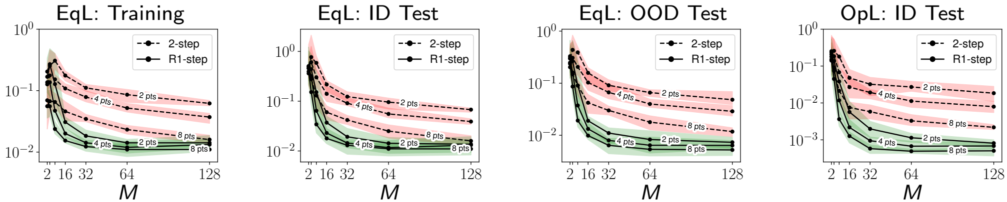
Darcy Flow PDE: Variable Coefficients with Sparse Data

$$\mathfrak{P}(u) = -\text{div } a \nabla u = f \qquad a(x) = \exp(\sin(\cos(x_1) + \cos(x_2))) \qquad + \text{B.C.}$$



Darcy Flow PDE: EqL and OpL Errors

- M – # of solution and source pairs $(u_m(X), f_m)_{m=1}^{M}$
- 2-step – Methods like SINDy that infer u_m first before learning p
- R1-step – KEqL with reduced basis for better performance



Quantitative Error Analysis

Theorem [JOHHO] (Part 1)

Consider $\{u_m(X), f_m\}_{m=1}^M$ defined on a smooth domain $\Omega \subset \mathbb{R}^d$ and observation mesh $X_{\text{obs}} \subset \Omega$ with $|X_{\text{obs}}| = N$. Suppose that $u^m \in H^\gamma(\Omega)$ for $\gamma > d/2 +$ order of $\mathfrak{P}$ and $\mathfrak{P} = p \circ \Phi$ such that $\Phi(u,x) \in \mathbb{R}^Q$. Define the fill distance

$$\rho := \sup_{x' \in \Omega} \inf_{x \in X_{\text{obs}}} |x - x'|,$$

Then under sufficient smoothness assumptions it holds for $0 \leq \gamma' \leq \gamma$

$$\sum_{m=1}^M \|u_m - \widehat{u}_m\|^2_{H^{\gamma'}(\Omega)} \lesssim \rho^{2(\gamma-\gamma')} \left(\|p\|^2_{\mathcal{P}} + \sum_{m=1}^M \|u_m\|^2_{\mathcal{U}} \right).$$

[9] Zhang and Schaeffer, "On the convergence of the SINDy algorithm".
[10] Scholl et al., "The uniqueness problem of physical law learning".
[11] He, Zhao, and Zhong, "How much can one learn a partial differential equation from its solution?"
[12] Boullé, Halikias, and Townsend, "Elliptic PDE learning is provably data-efficient".

Quantitative Error Analysis

Theorem [JOHHO] (Part 2)

Consider $\{u_m(X), f_m\}_{m=1}^M$ defined on a smooth domain $\Omega \subset \mathbb{R}^d$ and observation mesh $X_{\mathrm{obs}} \subset \Omega$ with $|X_{\mathrm{obs}}| = N$. Suppose that $u^m \in H^\gamma(\Omega)$ for $\gamma > d/2 + \text{order of } \mathfrak{P}$ and $\mathfrak{P} = p \circ \Phi$ such that $\Phi(u, x) \in \mathbb{R}^Q$ and $p \in H^\eta(\mathbb{R}^Q)$ for $\eta > Q/2$. Define the set $S := \cup_{m=1}^M \cup_{x \in X_{\mathrm{obs}}} \Phi(u_m, x)$ along with the fill distances

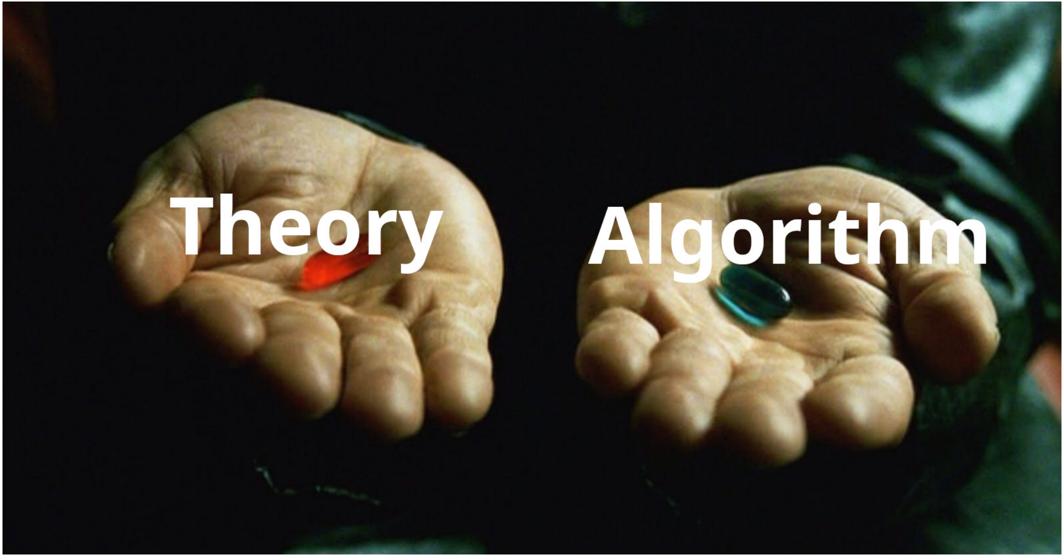
$$\rho := \sup_{x' \in \Omega} \inf_{x \in X_{\mathrm{obs}}} |x - x'|, \qquad \varrho(B) := \sup_{s' \in B} \inf_{s \in S \cap B} |s - s'|,$$

for any smooth and bounded set $B \subset \mathbb{R}^Q$. Then under sufficient smoothness assumptions it holds for $d/2 + \text{order of } \mathfrak{P} \leq \gamma' \leq \gamma$

$$\sum_{m=1}^M \|p - \widehat{p}\|_{L^\infty(B)} \lesssim \left[\rho^{\gamma-\gamma'} + \varrho(B)^{\eta - Q/2}\right] \left(\|p\|_{\mathcal{P}} + \sum_{m=1}^M \|u_m\|_{\mathcal{U}}\right).$$

Summary

- A kernel method for learning PDEs and filtering solutions
- Joint/simultaneous recovery of solutions and PDE form
- Successful recovery of PDEs and their solution maps with very scarce data
- Optimization problem is amenable to quasi-newton algorithms, easier and more efficient training
- Better performance compared to some neural net models or two step learning
- Operator learning through equation learning, going well beyond typical operator learning setups
- Quantitative convergence analysis, reminiscent of Sobolev sampling inequalities for scattered data approximation


Theory
Algorithm

Outline

Algorithms

RKHS Representer Theorems

$$\widehat{f} = \arg\min_{f \in \mathcal{K}} \|f\|_{\mathcal{K}} \quad \text{s.t.} \quad \boldsymbol{\phi}(f) = \mathbf{z}$$

- Shorthand notation $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_N) \in (\mathcal{K}^\star)^N$
- Data $\mathbf{z} \in \mathbb{R}^N$
- Closed form solution

$$\widehat{f} = K(\cdot, \boldsymbol{\phi}) K(\boldsymbol{\phi}, \boldsymbol{\phi})^{-1} \mathbf{z}, \qquad \|\widehat{f}\|_{\mathcal{K}}^2 = \mathbf{z}^T K(\boldsymbol{\phi}, \boldsymbol{\phi})^{-1} \mathbf{z}$$

- Vector field $K(\cdot, \boldsymbol{\phi}) = (K(\cdot, \phi_1), \ldots, K(\cdot, \phi_N)) \in \mathcal{K}^N$
- Matrix $K(\boldsymbol{\phi}, \boldsymbol{\phi}) \in \mathbb{R}^{N \times N}$

$$K(\boldsymbol{\phi}, \boldsymbol{\phi})_{ij} = \phi_i(K(\cdot, \phi_j))$$

Feature Map Perspective

$$\widehat{f} = \arg\min_{f \in \mathcal{K}} \|f\|_{\mathcal{K}} \quad \text{s.t.} \quad \boldsymbol{\phi}(f) = \mathbf{z}$$

- Solution

$$\widehat{f} = K(\cdot, \boldsymbol{\phi}) K(\boldsymbol{\phi}, \boldsymbol{\phi})^{-1} \mathbf{z}, \qquad \|\widehat{f}\|_{\mathcal{K}}^2 = \mathbf{z}^T K(\boldsymbol{\phi}, \boldsymbol{\phi})^{-1} \mathbf{z}$$

- Coefficient vector $\boldsymbol{\alpha} = K(\boldsymbol{\phi}, \boldsymbol{\phi})^{-1} \mathbf{z}$

$$\widehat{f} = K(\cdot, \boldsymbol{\phi}) \boldsymbol{\alpha} = \sum_{j=1}^{N} \alpha_j K(\cdot, \phi_j)$$

- Using reproducing property

$$\|\widehat{f}\|_{\mathcal{K}}^2 = \boldsymbol{\alpha}^T K(\boldsymbol{\phi}, \boldsymbol{\phi}) \boldsymbol{\alpha}$$

Reformulate KEqL

$$(\widehat{u}_m, \widehat{p}) = \underset{v_m \in \mathcal{U}, q \in \mathcal{P}}{\arg\min} \|q\|_{\mathcal{P}}^2 + \sum_{m=1}^{M} \|v_m\|_{\mathcal{U}}^2 + \|u_m(X^m) - v_m(X^m)\|_2^2 + \|q \circ \Phi(v_m, X) - f_m(X)\|_2^2$$

- Take $\lambda = \lambda' = \lambda'' = 1$ for simplicity
- Reduced model $v_m = U(\cdot, X)\boldsymbol{\alpha}_m$ and define $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_M)$
- Recall X is the collocation mesh
- Define $S(\boldsymbol{\alpha}) = \cup_{m=1}^{M} \cup_{x \in X} \Phi(K(\cdot, X)\boldsymbol{\alpha}, x)$ and $S(\boldsymbol{\alpha}_m) = \cup_{x \in X} \Phi(K(\cdot, X)\boldsymbol{\alpha}_m, x)$
- Take $q = P(\cdot, S(\boldsymbol{\alpha}))\beta$

$$(\widehat{\boldsymbol{\alpha}}, \widehat{\beta}) = \underset{\boldsymbol{\alpha}, \beta}{\arg\min} \, \beta^T P(S(\boldsymbol{\alpha}), S(\boldsymbol{\alpha}))\beta + \sum_{m=1}^{M} \boldsymbol{\alpha}_m^T U(X, X)\boldsymbol{\alpha}_m + \|u_m(X^m) - U(X^m, X)\boldsymbol{\alpha}_m\|_2^2 + \|P(S(\boldsymbol{\alpha}_m), S(\boldsymbol{\alpha}))\beta - f_m(X)\|_2^2$$

Reformulate KEqL

$$
\begin{aligned}
(\widehat{\boldsymbol{\alpha}}, \widehat{\boldsymbol{\beta}}) = \underset{\boldsymbol{\alpha},\boldsymbol{\beta}}{\arg\min}\, & \boldsymbol{\beta}^T P(S(\boldsymbol{\alpha}), S(\boldsymbol{\alpha}))\boldsymbol{\beta} + \sum_{m=1}^{M} \boldsymbol{\alpha}_m^T U(X, X)\boldsymbol{\alpha}_m \\
& + \|u_m(X^m) - U(X^m, X)\boldsymbol{\alpha}_m\|_2^2 + \|P(S(\boldsymbol{\alpha}_m), S(\boldsymbol{\alpha}))\boldsymbol{\beta} - f_m(X)\|_2^2
\end{aligned}
$$

- Compositional structure
- Quadratic in $\boldsymbol{\alpha}$ for fixed $\boldsymbol{\beta}$
- Quadratic in $\boldsymbol{\beta}$ for fixed $\boldsymbol{\alpha}$
- Propose sequential quadratic approximations
- Additional regularization to control deviation in each step, similar to Levenberg–Marquardt (LM)

LM for KEqL

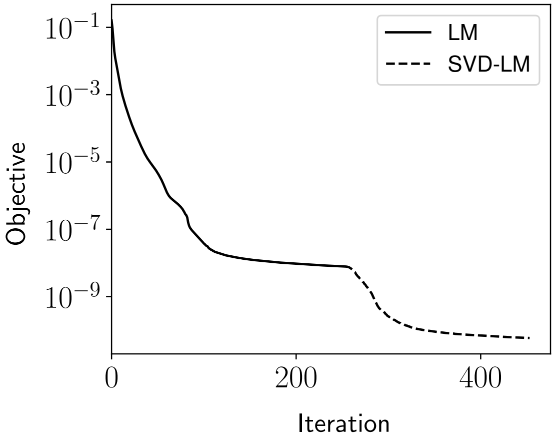
$$(\widehat{\boldsymbol{\alpha}}, \widehat{\boldsymbol{\beta}}) = \operatorname*{arg\,min}_{\boldsymbol{\alpha},\boldsymbol{\beta}} \boldsymbol{\beta}^T P(S(\boldsymbol{\alpha}), S(\boldsymbol{\alpha}))\boldsymbol{\beta} + \sum_{m=1}^{M} \boldsymbol{\alpha}_m^T U(X,X)\boldsymbol{\alpha}_m$$
$$+ \|u_m(X^m) - U(X^m, X)\boldsymbol{\alpha}_m\|_2^2 + \|P(S(\boldsymbol{\alpha}_m), S(\boldsymbol{\alpha}))\boldsymbol{\beta} - f_m(X)\|_2^2$$

Minimizing sequence $(\boldsymbol{\alpha}^{(k)}, \boldsymbol{\beta}^{(k)})$ given by

$$(\widehat{\boldsymbol{\alpha}}^{(k+1)}, \widehat{\boldsymbol{\beta}}^{(k+1)}) := \operatorname*{arg\,min}_{\boldsymbol{\alpha},\boldsymbol{\beta}} \boldsymbol{\beta}^T P(S(\boldsymbol{\alpha}^{(k)}), S(\boldsymbol{\alpha}^{(k)}))\boldsymbol{\beta} + \sum_{m=1}^{M} \boldsymbol{\alpha}_m^T U(X,X)\boldsymbol{\alpha}_m$$
$$+ \|u_m(X^m) - U(X^m, X)\boldsymbol{\alpha}_m\|_2^2$$
$$+ \left\| \left[P(S(\boldsymbol{\alpha}_m^{(k)}), S(\boldsymbol{\alpha}^{(k)})) + \nabla_{\boldsymbol{\alpha}} P(S(\boldsymbol{\alpha}_m^{(k)}), S(\boldsymbol{\alpha}^{(k)}))(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{(k)}) \right] \boldsymbol{\beta} - f_m(X) \right\|_2^2$$
$$+ \sigma_k(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{(k)})^T U(X,X)(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{(k)}) + \sigma_k'(\boldsymbol{\beta} - \boldsymbol{\beta}^{(k)})^T P(S(\boldsymbol{\alpha}_m^{(k)}), S(\boldsymbol{\alpha}^{(k)}))(\boldsymbol{\beta} - \boldsymbol{\beta}^{(k)})$$

Choose σ_k, σ_k' based on decrease of objective, established heuristics for LM

LM for KEqL



Theory

Sobolev Sampling Inequalities

Sobolev Sampling Inequality

Suppose $\Omega \subset \mathbb{R}^d$ is a bounded set with Lipschitz boundary and consider a set of points $X = \{x_1, \ldots, x_N\} \subset \overline{\Omega}$ with fill distance $h_X := sup_{x\in\Omega} \inf_{x'\in X} \|x - x'\|_2$. Let $u|_X$ denote the restriction of u to the set X. Further consider $\gamma > d/2$ and $0 \le \gamma' \le \gamma$ and let $u \in H^\gamma(\Omega)$.

1. (Noiseless) Suppose $u|_X = 0$. Then there exists $h_0 > 0$ so that whenever $h_X \le h_0$ we have $\|u\|_{H^{\gamma'}(\Omega)} \le C_\Omega h_X^{\gamma-\gamma'} \|u\|_{H^\gamma(\Omega)}$, where $C_\Omega > 0$ is a constant that depends only on Ω.
2. (Noisy) Suppose $u|_X \neq 0$. Then there exists $h_0 > 0$ so that whenever $h_X \le h_0$ we have $\|u\|_{L^\infty(\Omega)} \le C_\Omega h_X^{\gamma-d/2} \|u\|_{H^\gamma(\Omega)} + 2\|u|_X\|_\infty,$ where $C_\Omega > 0$ is a constant that depends only on Ω.

Controlling the Filtering Error

$$(\widehat{u}_m, \widehat{p}) = \underset{v_m \in \mathcal{U}, q \in \mathcal{P}}{\arg\min} \|q\|_{\mathcal{P}}^2 + \sum_{m=1}^{M} \|v_m\|_{\mathcal{U}}^2$$

$$\text{s.t.} \qquad v_m(X_{\text{obs}}) = u_m(X_{\text{obs}}) \qquad \text{(Observation/data)}$$

$$q \circ \Phi(v_m, X_{\text{obs}}) = f_m(X_{\text{obs}}) \quad \text{(Discrete PDE constraint)}$$

- Apply Sobolev sampling inequality, recalling $\rho = \sup_{x' \in \Omega} \inf_{x \in X_{\text{obs}}} |x - x'|$

$$\|\widehat{u}_m - u_m\|_{H^{\gamma'}(\Omega)} \lesssim \rho^{(\gamma - \gamma')} \|\widehat{u}_m - u_m\|_{H^{\gamma}(\Omega)}$$

- Sum up, use assumed embedding $\mathcal{U} \subset H^{\gamma}(\Omega)$, and optimality

$$\sum_m \|\widehat{u}_m - u_m\|_{H^{\gamma'}(\Omega)}^2 \lesssim \rho^{2(\gamma - \gamma')} \left(\sum_m \|\widehat{u}_m\|_{H^{\gamma}(\Omega)}^2 + \|\widehat{u}_m\|_{H^{\gamma}(\Omega)}^2 \right)$$

$$\lesssim \rho^{2(\gamma - \gamma')} \left(\sum_m \|\widehat{u}_m\|_{\mathcal{U}}^2 + \|u_m\|_{\mathcal{U}}^2 \right) \lesssim \rho^{2(\gamma - \gamma')} \left(\|p\|_{\mathcal{P}}^2 + \sum_m \|u_m\|_{\mathcal{U}}^2 \right)$$

Controlling the Equation Error

$$(\widehat{u}_m, \widehat{p}) = \underset{v_m \in \mathcal{U}, q \in \mathcal{P}}{\arg\min} \ \|q\|_{\mathcal{P}}^2 + \sum_{m=1}^{M} \|v_m\|_{\mathcal{U}}^2$$

$$\text{s.t.} \qquad v_m(X_{\text{obs}}) = u_m(X_{\text{obs}})$$

$$q \circ \Phi(v_m, X_{\text{obs}}) = f_m(X_{\text{obs}}) = p \circ \Phi(u_m, X_{\text{obs}})$$

- Observe this is "almost" an interpolation problem for p
- $S = \cup_m \cup_{x \in X_{\text{obs}}} \Phi(u_m, x)$ then constraint is

$$q(S + \text{noise}) = p(S)$$

- Akin to total least squares!
- We need to do more work

Controlling the Equation Error

- Basic idea

$$\begin{aligned} \widehat{p}(S+\delta S) &= p(S) \\ \widehat{p}(S) + \nabla \widehat{p}(S)\delta S &\approx p(S) \\ \Rightarrow |\widehat{p}(S) - p(S)| &\approx |\nabla \widehat{p}(S)\delta S| \end{aligned}$$

- Use Sobolev sampling inequality again but with noisy RHS
- Local Lipschitz assumption for $q \in \mathcal{P}$:

$$|q(s) - q(s')| \leq C(B)\|q\|_{\mathcal{P}}|s - s'|, \quad \forall s, s' \in B,$$

for any bounded set $B \subset \mathbb{R}^Q$

Controlling the Equation Error

$$\widehat{p} \circ \Phi(\widehat{u}_m, x_k) = p \circ \Phi(u_m, x_k) = f(x_k)$$

$$\Rightarrow |(\widehat{p} - p) \circ \Phi(u_m, x_k)| = |\widehat{p} \circ \Phi(\widehat{u}_m, x_k) - \widehat{p} \circ \Phi(u_m, x_k)|$$

$$\text{(Lipschitz assumption)} \qquad \leq C(B)\|\widehat{p}\|_{\mathcal{P}} |\Phi(\widehat{u}_m, x_k) - \Phi(u_m, x_k)|$$

Suppose $\Phi(u, x) = (x, u(x), \partial^{\boldsymbol{a}} u(x))$ for some multi-index $\boldsymbol{a}$ s.t. $|\boldsymbol{a}| \leq k \in \mathbb{N}$

$$|(\widehat{p} - p) \circ \Phi(u_m, x_k)| \lesssim C(B)\|\widehat{p}\|_{\mathcal{P}} \|\widehat{u}_m - u_m\|_{C^k(\Omega)}$$

$$\text{(Sobolev embedding)} \qquad \lesssim C(B)\|\widehat{p}\|_{\mathcal{P}} \|\widehat{u}_m - u_m\|_{H^{\gamma'}(\Omega)}$$

$$\text{(From filtering bound)} \qquad \lesssim C(B)\|\widehat{p}\|_{\mathcal{P}} \rho^{\gamma - \gamma'} (\|p\|_{\mathcal{P}} + \textstyle\sum_m \|u_m\|_{\mathcal{U}})$$

Controlling the Equation Error

$$|(\widehat{p} - p) \circ \Phi(u_m, x_k)| \lesssim C(B) \|\widehat{p}\|_{\mathcal{P}} \, \rho^{\gamma - \gamma'} \left(\|p\|_{\mathcal{P}} + \sum_m \|u_m\|_{\mathcal{U}} \right)$$

- Extra lemma: $\|\widehat{p}\|_{\mathcal{P}} \leq \|p\|_{\mathcal{P}} + \rho^\gamma \sum_m \|u_m\|_{\mathcal{U}^2}^2$ where $\|\cdot\|_{\mathcal{U}^2}$ is stronger norm on $\mathcal{U}$.
- Up to leading order

$$|(\widehat{p} - p) \circ \Phi(u_m, x_k)| \lesssim C(B) \|p\|_{\mathcal{P}} \, \rho^{\gamma - \gamma'} \left(\|p\|_{\mathcal{P}} + \sum_m \|u_m\|_{\mathcal{U}} \right)$$

- Apply sampling inequality for p and $\widehat{p}$ with fill distance

$$\varrho(B) := \sup_{s' \in B} \inf_{m,k} |s' - \Phi(u_m, x_k)|$$

$$\|\widehat{p} - p\|_{L^\infty(\Omega)} \leq C(B) \left(\varrho(B)^{\eta - Q/2} + \rho^{(\gamma - \gamma')} \right) \left(\|p\|_{\mathcal{P}} + \sum_m \|u_m\|_{\mathcal{U}} \right)$$

Thank you

Yasamin Jalalian, Juan Felipe Osorio Ramirez, Alex Hsu,, Bamdad Hosseini, and Houman Owhadi, **Data-Efficient Kernel Methods for Learning Differential Equations and Their Solution Operators: Algorithms and Error Analysis**, arXiv:2503.01036, 2025

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