# Solving and Learning Nonlinear PDEs with Gaussian Processes

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Joint work with

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Rough Path Interest Group, 2022

# Contents

# Roadmap

# Numerical Approximation and Inference

- **Partial Differential Equations**: infinite degrees of freedom (DOF)

$$\mathcal{F}(x, t, u, \partial_t u, \nabla_x u, \nabla_x^2 u, a, \xi, ...) = 0$$

  - Stationary PDEs, time dependent, inverse problems, UQ, ...

- **Numerical Approximation** (finite DOF) designed by experts
  - Finite difference/element/volume
  - Spectral methods
  - Boundary integral methods
  - Meshless methods, collocation methods
  - Multiscale methods, numerical homogenization, ...

- **Inference and ML** to automate the finite $\leftrightarrow$ infinite DOF process
  - Gaussian process (GP) and kernel methods for numerical integration
  - GPs and kernel methods for ODEs, linear PDEs
  - Bayes probabilistic numerics, Bayes numerical analysis, UQ
  - Physics informed ML (Deep Ritz methods, PINNs, SDEs...)
  - Operator learning (Kernels, Neural Operators, DeepONets), ...

# This talk

**Our Goal**

A general GP framework for solving and learning nonlinear PDEs

- Intepretable, convergent and amenable to numerical analysis[1]
  - generalize RBF collocation methods and meshless kernel methods
- Near-linear time and space complexity implementation[2]
  - quantitative screening effects for GPs with PDE measurements
- Hierarchical parameter learning in the GP, or kernel learning[3]
  - consistency analysis of Kernel Flow and Emperical Bayes

[1] Yifan Chen, Bamdad Hosseini, Houman Owhadi, and Andrew M Stuart. "Solving and learning nonlinear pdes with gaussian processes". In: *Journal of Computational Physics* (2021).

[2] Yifan Chen, Florian Schaefer, and Houman Owhadi. "Sparse Cholesky Factorization for Solving Nonlinear PDEs via Gaussian Processes". In preparation.

[3] Yifan Chen, Houman Owhadi, and Andrew Stuart. "Consistency of empirical Bayes and kernel flow for hierarchical parameter estimation". In: *Mathematics of Computation* (2021).

# Roadmap

# A Nonlinear Elliptic PDE Example

- Consider the stationary elliptic PDE

$$\begin{cases} -\Delta u(\mathbf{x}) + \tau(u(\mathbf{x})) = f(\mathbf{x}), & \forall \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = g(\mathbf{x}), & \forall \mathbf{x} \in \partial\Omega. \end{cases}$$

  - Domain $\Omega \subset \mathbb{R}^d$.
  - PDE data $f, g : \Omega \to \mathbb{R}$.

- PDE has a unique strong/classical solution $u^\star$.

# A Nonlinear Elliptic PDE: The Methodology

1. Choose a kernel $K : \overline{\Omega} \times \overline{\Omega} \to \mathbb{R}$
   - Corresponding RKHS $\mathcal{U}$ with norm $\|\cdot\|$

2. Choose some collocation points
   - $X^{\mathsf{int}} = \{\mathbf{x}_1^{\mathsf{int}}, \ldots, \mathbf{x}_{M^{\mathsf{int}}}^{\mathsf{int}}\} \subset \Omega$
   - $X^{\mathsf{bd}} = \{\mathbf{x}_1^{\mathsf{bd}}, \ldots, \mathbf{x}_{M^{\mathsf{bd}}}^{\mathsf{bd}}\} \subset \partial\Omega$

3. Solve the optimization problem

$$\begin{cases} \underset{u \in \mathcal{U}}{\text{minimize}} \ \|u\| \\ \text{s.t.} \quad -\Delta u(\mathbf{x}_m) + \tau(u(\mathbf{x}_m)) = f(\mathbf{x}_m), \quad \text{for } \mathbf{x}_m \subset X^{\mathsf{int}} \\ \qquad\qquad\qquad\qquad\qquad\quad u(\mathbf{x}_n) = g(\mathbf{x}_n), \qquad \text{for } \mathbf{x}_n \subset X^{\mathsf{bd}} \end{cases}$$

# Bayes Inference Interpratation of the Methodology

1. Choose a kernel $K : \overline{\Omega} \times \overline{\Omega} \to \mathbb{R}$ (Choose the prior $\mathcal{GP}(0, K)$)
   - Corresponding RKHS $\mathcal{U}$ with norm $\|\cdot\|$
2. Choose some collocation points (Choose the data/likelihood)
   - $X^{\mathsf{int}} = \{\mathbf{x}_1^{\mathsf{int}}, \ldots, \mathbf{x}_{M^{\mathsf{int}}}^{\mathsf{int}}\} \subset \Omega$
   - $X^{\mathsf{bd}} = \{\mathbf{x}_1^{\mathsf{bd}}, \ldots, \mathbf{x}_{M^{\mathsf{bd}}}^{\mathsf{bd}}\} \subset \partial\Omega$
3. Solve the optimization problem (Find the "MAP")

$$\begin{cases} \underset{u \in \mathcal{U}}{\text{minimize}} \ \|u\| \\ \text{s.t.} \quad -\Delta u(\mathbf{x}_m) + \tau(u(\mathbf{x}_m)) = f(\mathbf{x}_m), \quad \text{for } \mathbf{x}_m \subset X^{\mathsf{int}} \\ \qquad\qquad\qquad\qquad u(\mathbf{x}_n) = g(\mathbf{x}_n), \qquad \text{for } \mathbf{x}_n \subset X^{\mathsf{bd}} \end{cases}$$

Generalize linear PDEs in Bayes probabilistic numerical methods[4][5]

- Solving PDEs as a Bayes inverse problem

[4] Houman Owhadi. "Bayesian numerical homogenization". In: *Multiscale Modeling & Simulation* 13.3 (2015), pp. 812–828.

[5] Jon Cockayne, Chris J Oates, Timothy John Sullivan, and Mark Girolami. "Bayesian probabilistic numerical methods". In: *SIAM Review* 61.4 (2019), pp. 756–789.

# Roadmap

# Introducing Slack Variables

$$
\begin{cases}
\underset{u \in \mathcal{U}}{\text{minimize}} \ \|u\| \\
\text{s.t.} \quad -\Delta u(\mathbf{x}_m) + u(\mathbf{x}_m)^3 = f(\mathbf{x}_m), \quad \text{for } \mathbf{x}_m \subset X^{\mathsf{int}} \\
\qquad\qquad\qquad\qquad u(\mathbf{x}_n) = g(\mathbf{x}_n), \quad \text{for } \mathbf{x}_n \subset X^{\mathsf{bd}}
\end{cases}
$$

$$
\Updownarrow \ (N = M^{\mathsf{bd}} + 2M^{\mathsf{int}})
$$

$$
\begin{cases}
\underset{\mathbf{z}=(\mathbf{z}^{\mathsf{bd}},\mathbf{z}^{\mathsf{int}},\mathbf{z}_{\Delta}^{\mathsf{int}})\in\mathbb{R}^N}{\text{minimize}} \begin{cases}
\underset{u \in \mathcal{U}}{\text{minimize}} \ \|u\| \\
\text{s.t.} \quad u(X^{\mathsf{bd}}) = \mathbf{z}^{\mathsf{bd}} \\
\qquad u(X^{\mathsf{int}}) = \mathbf{z}^{\mathsf{int}} \\
\qquad \Delta u(X^{\mathsf{int}}) = \mathbf{z}_{\Delta}^{\mathsf{int}}
\end{cases} \\
\text{s.t.} \quad -\mathbf{z}^{\mathsf{int}} + \tau(\mathbf{z}_{\Delta}^{\mathsf{int}}) = f(X^{\mathsf{int}}) \\
\qquad \mathbf{z}^{\mathsf{bd}} = g(X^{\mathsf{bd}})
\end{cases}
$$

# Inner optimization

- The inner problem is linear

$$\begin{aligned} &\underset{u\in\mathcal{U}}{\text{minimize}} \ \ \|u\| \\ &\text{s.t.} \quad u(X^{\mathsf{bd}}) = \mathbf{z}^{\mathsf{bd}}, u(X^{\mathsf{int}}) = \mathbf{z}^{\mathsf{int}}, \Delta u(X^{\mathsf{int}}) = \mathbf{z}^{\mathsf{int}}_{\Delta} \end{aligned}$$

- Measurement vector $\boldsymbol{\phi} := (\delta_{X^{\mathsf{bd}}}, \delta_{X^{\mathsf{int}}}, \delta_{X^{\mathsf{int}}} \circ \Delta) \in (\mathcal{U}^*)^{\otimes N}$
- Kernel vector and matrix

$$K(\mathbf{x},\boldsymbol{\phi}) = \left(K(\mathbf{x}, X^{\mathsf{bd}}), K(\mathbf{x}, X^{\mathsf{int}}), \Delta_{\mathbf{y}} K(\mathbf{x}, X^{\mathsf{int}})\right) \in \mathbb{R}^N$$

$$K(\boldsymbol{\phi},\boldsymbol{\phi}) = \begin{pmatrix} K(X^{\mathsf{bd}}, X^{\mathsf{bd}}) & K(X^{\mathsf{bd}}, X^{\mathsf{int}}) & \Delta_{\mathbf{y}} K(X^{\mathsf{bd}}, X^{\mathsf{int}}) \\ K(X^{\mathsf{int}}, X^{\mathsf{bd}}) & K(X^{\mathsf{int}}, X^{\mathsf{int}}) & \Delta_{\mathbf{y}} K(X^{\mathsf{int}}, X^{\mathsf{int}}) \\ \Delta_{\mathbf{x}} K(X^{\mathsf{int}}, X^{\mathsf{bd}}) & \Delta_{\mathbf{x}} K(X^{\mathsf{int}}, X^{\mathsf{int}}) & \Delta_{\mathbf{x}}\Delta_{\mathbf{y}} K(X^{\mathsf{int}}, X^{\mathsf{int}}) \end{pmatrix} \in \mathbb{R}^{N\times N}$$

Minimizer $u(\mathbf{x}) = K(\mathbf{x},\boldsymbol{\phi})K(\boldsymbol{\phi},\boldsymbol{\phi})^{-1}\mathbf{z}$

# Representation of the Minimizer

Combine the two level optimization:

**Representer theorem**

Every minimizer $u^\dagger$ can be represented as

$$u^\dagger(\mathbf{x}) = K(\mathbf{x}, \phi)K(\boldsymbol{\phi}, \boldsymbol{\phi})^{-1}\mathbf{z}^\dagger,$$

where the vector $\mathbf{z}^\dagger \in \mathbb{R}^N$ is a minimizer of

$$\begin{cases} \min\limits_{\mathbf{z}\in\mathbb{R}^N} & \mathbf{z}^T K(\boldsymbol{\phi}, \boldsymbol{\phi})^{-1}\mathbf{z} \\ \text{s.t.} & F(\mathbf{z}) = \mathbf{y} \end{cases}$$

- Function $F : \mathbb{R}^N \to \mathbb{R}^M$ depends on PDE collocation constraints
- $\mathbf{y}$ contains PDE boundary and RHS data

# Roadmap

# Towards A Practical Algorithm

Quadratic optimization with nonlinear constraints

- A simple linearization algorithm $\mathbf{z}^k \to \mathbf{z}^{k+1}$

$$\begin{cases} \min\limits_{\mathbf{z}\in\mathbb{R}^N} & \mathbf{z}^T K(\boldsymbol{\phi},\boldsymbol{\phi})^{-1}\mathbf{z} \\ \text{s.t.} & F(\mathbf{z}^k) + F'(\mathbf{z}^k)(\mathbf{z}-\mathbf{z}^k) = \mathbf{y}. \end{cases}$$

"Newton's iteration for the nonlinear PDE"

- Poor conditioning of $K(\boldsymbol{\phi},\boldsymbol{\phi})$, and scale imbalance between blocks
  Adding scale-aware regularization $K(\boldsymbol{\phi},\boldsymbol{\phi}) + \lambda\text{diag}(K(\boldsymbol{\phi},\boldsymbol{\phi}))$

# Roadmap

# Numerical Experiments: Stationary Problems

- Nonlinear Elliptic Equation, $\tau(u) = u^3$

$$\begin{cases} -\Delta u(\mathbf{x}) + \tau(u(\mathbf{x})) = f(\mathbf{x}), & \forall \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = g(\mathbf{x}), & \forall \mathbf{x} \in \partial\Omega. \end{cases}$$

- Truth: $d = 2$, $u^\star(\mathbf{x}) = \sin(\pi x_1)\sin(\pi x_2) + 4\sin(4\pi x_1)\sin(4\pi x_2)$
- Kernel: $K(\mathbf{x}, \mathbf{y}; \sigma) = \exp(-\frac{|\mathbf{x}-\mathbf{y}|^2}{2\sigma^2})$

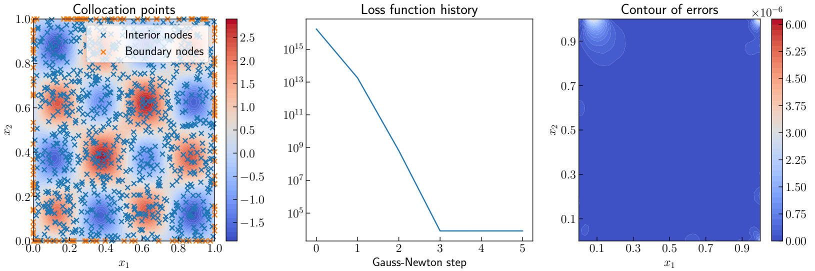



Figure: $N_{\text{domain}} = 900, N_{\text{boundary}} = 124$

# Convergence Study

- For $\tau(u) = 0, u^3$, use Gaussian kernel with lengthscale $\sigma$
- $L^2, L^\infty$ accuracy, compared with Finite Difference (FD)

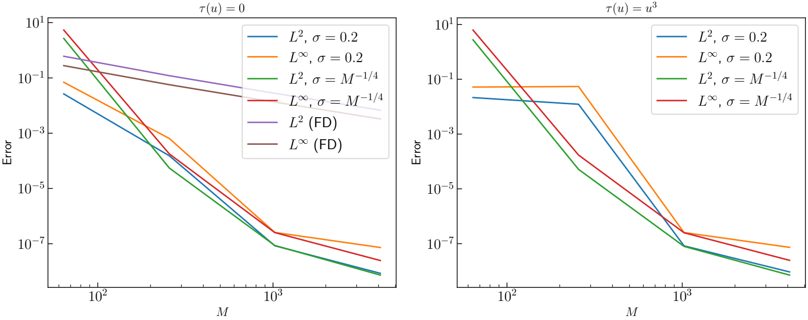
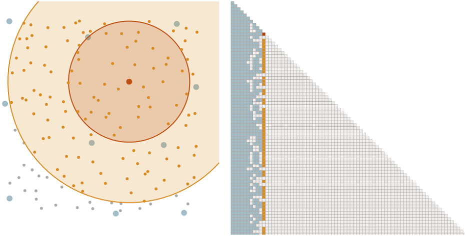



Figure: Convergence of the kernel method is fast, since the solution is smooth

# Roadmap

# Scalability: Taming the Dense Kernel Matrice

Sparse Cholesky factor for kernel matrices under coarse to fine ordering[6]



Coarse to fine: max-min ordering

$$x_k = \mathrm{argmax}_{x_i} d(x_i, \{x_j, 1 \le j < k\})$$

with lengthscale $l_k = d(x_k, \{x_j, 1 \le j < k\})$

[6] F Schäfer, TJ Sullivan, and H Owhadi. "Compression, inversion, and approximate PCA of dense kernel matrices at near-linear computational complexity". In: *Multiscale Modeling & Simulation* 19.2 (2021), pp. 688–730.

# Why Sparse? Cholesky Factors and Screening Effects

Let $\Theta \in \mathbb{R}^{d\times d}$, $\Theta_{ij} = k(x_i, x_j)$, and $X \sim \mathcal{N}(0, \Theta)$

- Cholesky factor of the covariance matrix $\Theta = LL^T$

$$\frac{L_{ij}}{L_{jj}} = \frac{\mathrm{Cov}[X_i, X_j | X_{1:j-1}]}{\mathrm{Var}[X_j | X_{1:j-1}]} \qquad (i \geq j)$$

- Cholesky factor of the precision matrix $\Theta^{-1} = UU^T$

$$\frac{U_{ij}}{U_{jj}} = (-1)^{i\neq j} \frac{\mathrm{Cov}[X_i, X_j | X_{1:j-1\setminus\{i\}}]}{\mathrm{Var}[X_j | X_{1:j-1\setminus\{i\}}]} \qquad (i \leq j)$$

Screening effects: $x_{1:j}$ ordered from coarse to fine; scale of $x_j$ is $l_j$, then for certain kernel arsing from PDEs [8]

$$\mathrm{Cov}[X_i, X_j | X_{1:j-1}] \lesssim \exp\left(-\frac{d(x_i, x_j)}{l_j}\right)$$

[7] Michael L Stein. "The screening effect in kriging". In: *Annals of statistics* 30.1 (2002), pp. 298–323.

[8] Schäfer, Sullivan, and Owhadi, "Compression, inversion, and approximate PCA of dense kernel matrices at near-linear computational complexity".

# Screening Effects with PDE measurements

Recall the kernel matrices

$$\begin{pmatrix} K(X^{\text{bd}}, X^{\text{bd}}) & K(X^{\text{bd}}, X^{\text{int}}) & \Delta_{\mathbf{y}} K(X^{\text{bd}}, X^{\text{int}}) \\ K(X^{\text{int}}, X^{\text{bd}}) & K(X^{\text{int}}, X^{\text{int}}) & \Delta_{\mathbf{y}} K(X^{\text{int}}, X^{\text{int}}) \\ \Delta_{\mathbf{x}} K(X^{\text{int}}, X^{\text{bd}}) & \Delta_{\mathbf{x}} K(X^{\text{int}}, X^{\text{int}}) & \Delta_{\mathbf{x}} \Delta_{\mathbf{y}} K(X^{\text{int}}, X^{\text{int}}) \end{pmatrix}$$

How to order when there are derivative measurements?

- Order pointwise measurements from coarse to fine
- PDE measurements follow behind (with the same ordering)

**Theorem: screening effects hold for such ordering**

Theory: need technical assumptions

- The kernel is the Green function of some differential operator $\mathcal{L} : H_0^s(\Omega) \to H^{-s}(\Omega)$

Practice: works more generally

# Near Linear Complexity by Sparse Cholesky

- Ignore correlation beyond $d(x, x_j) \geq \rho l_j$ (which is $O(\exp(-\rho))$)
- Once ordering and sparsity pattern determined, use KL minimization algorithm[9]: $O(N\rho^d)$ memory and $O(N\rho^{2d})$ time

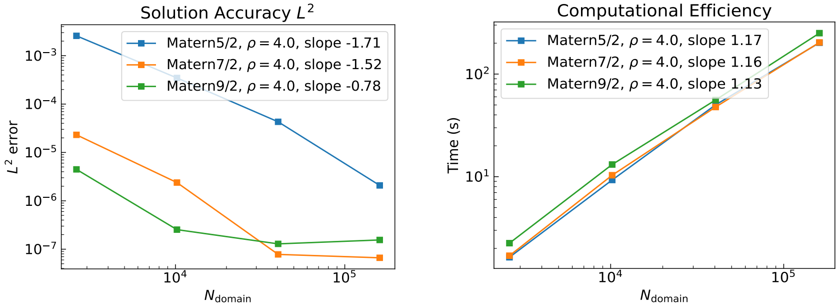



Figure: Run 3 GN iterations. Accuracy floor due to finite $\rho$ and regularization

[9] Florian Schäfer, Matthias Katzfuss, and Houman Owhadi. "Sparse Cholesky Factorization by Kullback–Leibler Minimization". In: *SIAM Journal on Scientific Computing* 43.3 (2021), A2019–A2046.

# Roadmap

# Numerical Experiments: Time Dependent Problems

Viscous Burgers' Equation

- Viscosity $\nu = 0.02$

$$\begin{cases} \partial_t u + u\partial_s u - \nu\partial_s^2 u = 0, \qquad \forall (s,t) \in (-1,1) \times (0,1]. \\ u(s,0) = -\sin(\pi s), \\ u(-1,t) = u(1,t) = 0. \end{cases}$$

- Shock when $\nu = 0$. Problem harder for smaller $\nu$
- Choose an anisotropic spatio-temperal GP

# Numerical Experiments: Viscous Burgers' Equation

- Kernel: $K((s,t),(s',t')) = \exp\left(-20^2|s-s'|^2 - 3^2|t-t'|^2\right)$

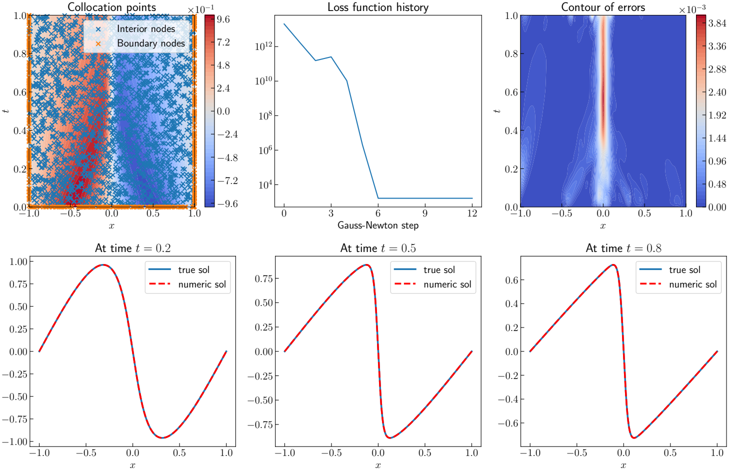



Figure: $N_{\text{domain}} = 2000, N_{\text{boundary}} = 400$

# Push to Small Viscosity

Discretize in time first, then apply the methodology to the resulting spatial PDE: dimension of kernel matrices is reduced

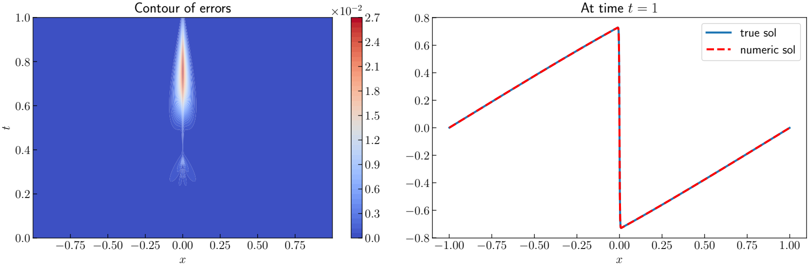



Figure: $\nu = 10^{-3}$; number of spatial points $2000$; time step size $0.01$; Matern7/2 kernel with lengthscale 0.02; use $2$ GN iterations

At time $t = 1$, $L^2$ accuracy: $10^{-4}$

- Observation: accuracy not monotone regarding time $t$
- Implication: further improvement through time-adaptive kernels

# Roadmap

# Numerical Experiments: Inverse Problems

Darcy Flow inverse problems

$$\begin{cases} \min_{u,a} \|u\|_K^2 + \|a\|_\Gamma^2 + \frac{1}{\gamma^2}\sum_{j=1}^{I}|u(\mathbf{x}_j)-o_j|^2, \\ \text{s.t.} \quad -\mathsf{div}(\exp(a)\nabla u)(\mathbf{x}_m) = 1, \quad \forall \mathbf{x}_m \in (0,1)^2 \\ \qquad\qquad u(\mathbf{x}_m) = 0, \quad \forall \mathbf{x}_m \in \partial(0,1)^2. \end{cases}$$

- Recover $a$ from pointwise measurements of $u$
- Model $(u,a)$ as independent GPs
- Impose PDE constraints and formulate Bayesian inverse problem

# Numerical Experiments: Darcy Flow

- Kernel $K(\mathbf{x}, \mathbf{x}'; \sigma) = \exp\left(-\frac{|\mathbf{x}-\mathbf{x}'|^2}{2\sigma^2}\right)$ for both $u$ and $a$

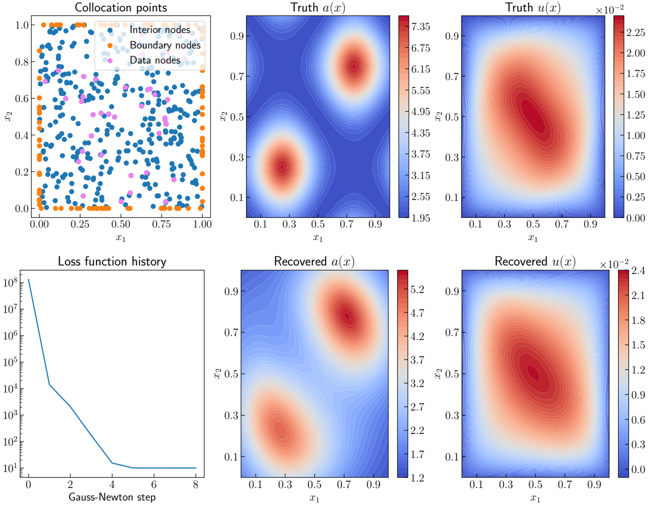



Figure: $N_{\text{domain}} = 400, N_{\text{boundary}} = 100, N_{\text{observation}} = 50$

# Roadmap

# Theoretical Foundation: Consistency

Consistency of the minimizer

$$\begin{cases} \min\limits_{u \in \mathcal{U}} & \|u\| \\ \text{s.t.} & \text{PDE constraints at } \{\mathbf{x}_1, \ldots, \mathbf{x}_M\} \in \overline{\Omega}. \end{cases}$$

### Convergence theory

- $K$ is chosen so that
  - $\mathcal{U} \subseteq H^s(\Omega)$ for some $s > s^*$ where $s^* = d/2 +$ order of PDE.
  - $u^\star \in \mathcal{U}$.
- Fill distance of $\{\mathbf{x}_1, \ldots, \mathbf{x}_M\} \to 0$ as $M \to \infty$.

Then as $M \to \infty$, $u^\dagger \to u^\star$ pointwise in $\Omega$ and in $H^t(\Omega)$ for $t \in (s^*, s)$.

# Roadmap

# Theoretical Foundation: Kernel Learning

Hierarchical parameters in the kernel $K_\theta$

- Good $\theta$ improves the performance

Algorithms for learning $\theta$: another level of optimization

- Bayes approach built in GPs: e.g. Empirical Bayes (EB)
- Kernel Flow (KF)[10]: a variant of cross-validation

$$\min_\theta \ \mathbb{E}_\pi \frac{\|u^\dagger(\cdot, X, \theta) - u^\dagger(\cdot, \pi X, \theta)\|_{K_\theta}^2}{\|u^\dagger(\cdot, X, \theta)\|_{K_\theta}^2}$$

- $u^\dagger(\cdot, X, \theta)$ is the solution using collocation points $X$ and kernel $K_\theta$
- $\pi X$ is a subsampling of $X$
- $\|\cdot\|_{K_\theta}$ is the RKHS norm for the kernel $K_\theta$; attain explicit formula due to representer theorem

Our result: Consistency of learning regularity of Matérn-like kernels

- EB and KF learn different parameters for linear problems

[10] Houman Owhadi and Gene Ryan Yoo. "Kernel flows: From learning kernels from data into the abyss". In: *Journal of Computational Physics* 389 (2019), pp. 22–47.

# Roadmap

# Take-aways

Solving and Learning Nonlinear PDEs with Gaussian Processes

Algorithm

- A simple framework for solving and learning nonlinear PDEs
- Near-linear complexity treatment of the dense kernel matrices
- Experiments: stationary PDEs, time dependent, inverse problems
- Future work: parametric PDEs, high dimensional PDEs, UQ, ...

Convergence theory

- Consistency as fill-in distance goes to 0 (asymptotic only)
- Future work: convergence rates?

Kernel learning (The hard part)

- Consistency of Kernel Flow and Empirical Bayes for linear problem :)

# Thank you!

# References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Owhadi, Houman and Gene Ryan Yoo. "Kernel flows: From learning kernels from data into the abyss". In: *Journal of Computational Physics* 389 (2019), pp. 22–47.