Solving and Learning Nonlinear PDEs with Gaussian Processes

Yifan Chen, Caltech

Joint work with

Bamdad Hosseini, Houman Owhadi and Andrew Stuart

SIAM Uncertainty Quantification, 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
  - Physics informed ML (Deep Ritz methods, PINNs, SDEs...)
  - Operator learning techniques (Neural Operators, DeepONets...)
  - Bayes probabilistic numerics, Gaussian processes and kernel methods
  - ...

This talk*

Our Goal

A general GP framework for solving and learning nonlinear PDEs

- Intepretable, convergent and amenable to numerical analysis*
- Near-linear time and space complexity implementation*
- Hierarchical parameter learning in the GP, or kernel learning

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

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

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

Roadmap

A Nonlinear Elliptic PDE Example

- Consider the stationary elliptic PDE

$$\begin{cases} -\Delta u(\mathbf{x}) + u(\mathbf{x})^3 = f(\mathbf{x}), & \forall \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = g(\mathbf{x}), & \forall \mathbf{x} \in \partial\Omega. \end{cases}$$

  - 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

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

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")

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

[4] 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

Representation of the Minimizer

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

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

$$\begin{cases} \underset{\mathbf{z}=(\mathbf{z}^{\mathsf{bd}},\mathbf{z}^{\mathsf{int}},\mathbf{z}_{\Delta}^{\mathsf{int}})\in\mathbb{R}^N}{\text{minimize}} \begin{cases} \underset{u\in\mathcal{U}}{\text{minimize}} \ \|u\| \\ \text{s.t.} \quad u(X^{\mathsf{bd}}) = \mathbf{z}^{\mathsf{bd}} \\ \qquad u(X^{\mathsf{int}}) = \mathbf{z}^{\mathsf{int}} \\ \qquad \Delta u(X^{\mathsf{int}}) = \mathbf{z}_{\Delta}^{\mathsf{int}} \end{cases} \\ \text{s.t.} \quad -\mathbf{z}^{\mathsf{int}} + (\mathbf{z}_{\Delta}^{\mathsf{int}})^3 = f(X^{\mathsf{int}}) \\ \qquad \mathbf{z}^{\mathsf{bd}} = g(X^{\mathsf{bd}}) \end{cases}$$

Inner optimization

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

- 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

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

$$K(\boldsymbol{\phi}, \boldsymbol{\phi}) =$$

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

- **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 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"

Roadmap

- Nonlinear Elliptic Equation

$$\begin{cases} -\Delta u(\mathbf{x}) + u(\mathbf{x})^3 = f(\mathbf{x}), & \forall \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = g(\mathbf{x}), & \forall \mathbf{x} \in \partial\Omega. \end{cases}$$

- 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: $K(\mathbf{x}, \mathbf{y}; \sigma) = \exp(-\frac{|\mathbf{x}-\mathbf{y}|^2}{2\sigma^2})$

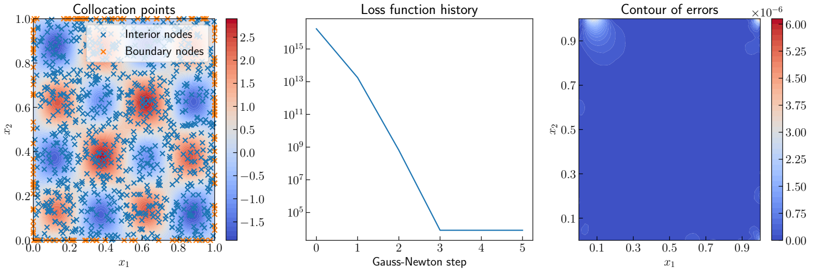


Figure: $N_{\text{domain}} = 900, N_{\text{boundary}} = 124$

Scalability: Taming the Dense Kernel Matrice

Dense kernel matrix $K(\phi, \phi)$

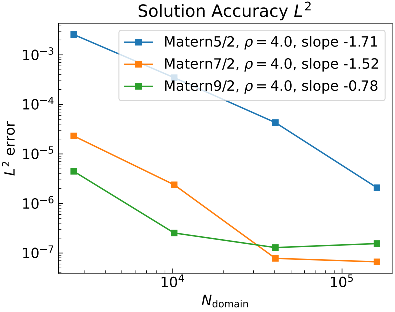
- Poor conditioning, and scale imbalance between blocks
  Adding scale-aware nugget term $K(\phi, \phi) + \lambda \mathrm{diag}(K(\phi, \phi))$
- Sparse Cholesky factorization under "coarse to fine" ordering
  Thanks to screening effects hold for PDE-type measurements

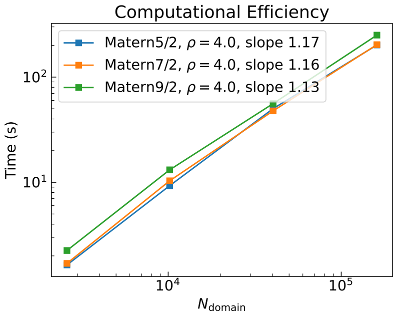
[5] Michael L Stein. "The screening effect in kriging". In: *Annals of statistics* 30.1 (2002), pp. 298–323.

[6] 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.

Near Linear Complexity by Sparse Cholesky

- Sparse Cholesky parameter $\rho = 4.0$
- Matérn kernel regularity parameter $\nu = 5/2, 7/2, 9/2$





- Accuracy floor due to finite ρ and nugget terms

[7] Michael L Stein. *Interpolation of spatial data: some theory for kriging*. Springer Science & Business Media, 1999.

Roadmap

Numerical Experiments: Time Dependent Problems

Viscous Burgers' Equation

- Viscosity $\nu = 0.02$

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

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

Numerical Experiments: Viscous Burgers' Equation

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

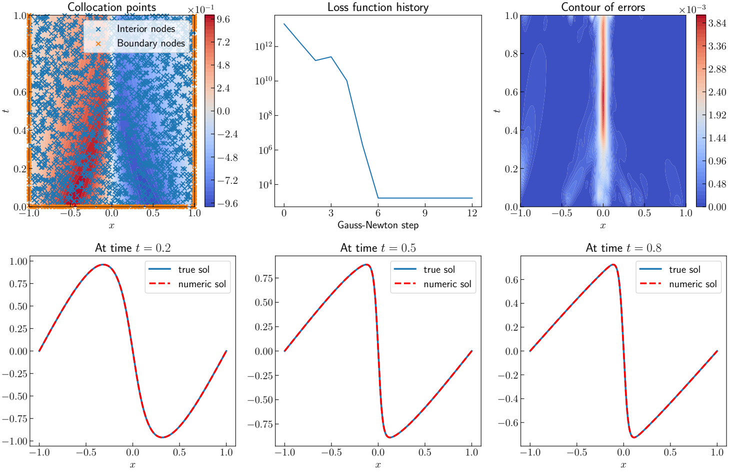


Figure: $N_{\text{domain}} = 2000, N_{\text{boundary}} = 400$

Roadmap

Numerical Experiments: Inverse Problems

Darcy Flow inverse problems

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

- 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

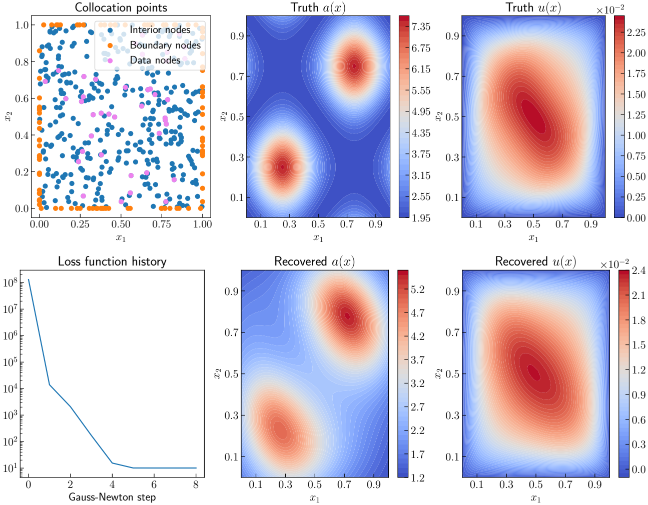


Figure: $N_{\text{domain}} = 400, N_{\text{boundary}} = 100, N_{\text{observation}} = 50$

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 Ω and in $H^t(\Omega)$ for $t \in (s^*, s)$.

Roadmap

Take-aways

Solving and Learning Nonlinear PDEs with Gaussian Processes

Algorithm

- A simple framework for solving and learning PDEs, via GPs
- Near-linear complexity treatment of the dense kernel matrices
- Experiments: stationary PDEs, time dependent, inverse problems

Theory

- Consistency as fill-in distance goes to 0
- Consistency of kernel learning: Kernel Flow and Empirical Bayes

Thank you!