Solving and Learning Nonlinear PDEs with Gaussian Processes

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Joint work with

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SIAM Uncertainty Quantification, 2022

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, dynamical systems, 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 process
  - Physics informed ML (Deep Ritz methods, PINNs, SDEs...)
  - Operator learning techniques (Neural Operators, DeepONets...)
  - Bayes 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 <u>strong/classical</u> 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

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

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)
   - $X^{\text{int}} = \{\mathbf{x}_1^{\text{int}}, \ldots, \mathbf{x}_{M^{\text{int}}}^{\text{int}}\} \subset \Omega$
   - $X^{\text{bd}} = \{\mathbf{x}_1^{\text{bd}}, \ldots, \mathbf{x}_{M^{\text{bd}}}^{\text{bd}}\} \subset \partial\Omega$
3. Solve the optimization problem (Find the "MAP")

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

Roadmap

Representation of the Minimizer

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

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

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

Inner optimization

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

- Bounded linear functionals: $\delta_{\mathbf{x}_m} \circ \Delta$, $\delta_{\mathbf{x}_m}$, $\delta_{\mathbf{x}_n}$ $\in \mathcal{U}^*$
- 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:

$$\begin{aligned} K(\mathbf{x}, \boldsymbol{\phi})_j &:= \boldsymbol{\phi}_j^{\mathbf{x}'} K(\mathbf{x}, \cdot) \\ K(\boldsymbol{\phi}, \boldsymbol{\phi})_{i,j} &:= \boldsymbol{\phi}_i^{\mathbf{x}} (\boldsymbol{\phi}_j^{\mathbf{x}'} K(\cdot, \cdot)) \end{aligned}$$

  Entry examples: $K(\mathbf{x}_i, \mathbf{x}_j), \Delta^{\mathbf{x}} K(\mathbf{x}_i, \mathbf{x}_j), \Delta^{\mathbf{x}} \Delta^{\mathbf{x}'} K(\mathbf{x}_i, \mathbf{x}_j)$

- 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

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

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 $\mathbf{z}^k \rightarrow \mathbf{z}^{k+1}$

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

"Newton's iteration for the nonlinear PDE"

Roadmap

Numerical Experiments: Stationary Problems

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

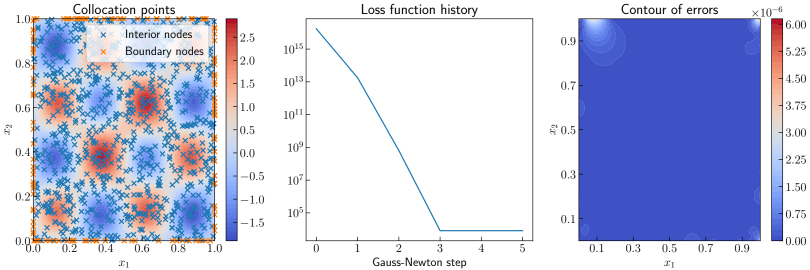


Figure: $N_{\text{domain}} = 900, N_{\text{boundary}} = 124$

Taming the Dense Kernel Matrice Numerically

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

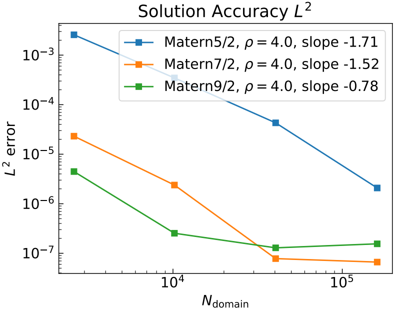
- Poor conditioning, and scale imbalance between blocks
  Adding scale-aware nugget term $K(\phi, \phi) + \lambda \text{diag}(K(\phi, \phi))$
- Sparse Cholesky factorization under "coarse to fine" ordering
  Thanks to screening effects hold for PDE-type measurements

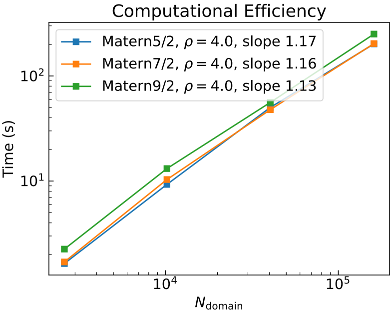
[4] Michael L Stein. "The screening effect in kriging". In: *Annals of statistics* 30.1 (2002), pp. 298–323.

[5] 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

[6] 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 $\nu = 0.02$

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

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

Numerical Experiments: Viscous Burgers' Equation

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

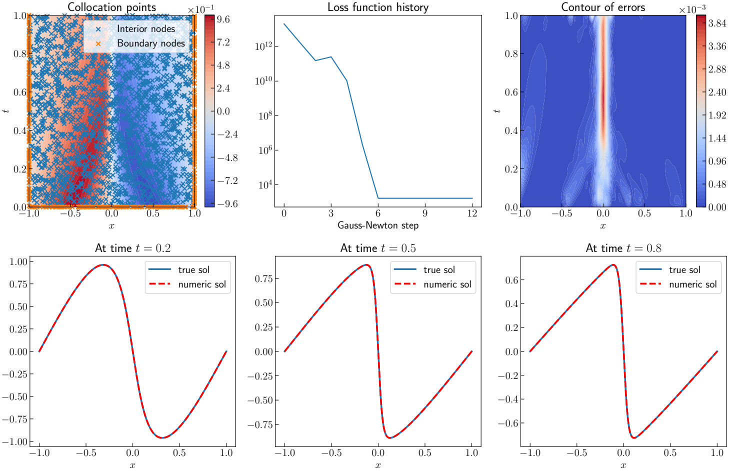


Figure: $N_{\text{domain}} = 2000, N_{\text{boundary}} = 400$

Roadmap

Numerical Experiments: Inverse Problems

Darcy Flow inverse problems

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

- 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

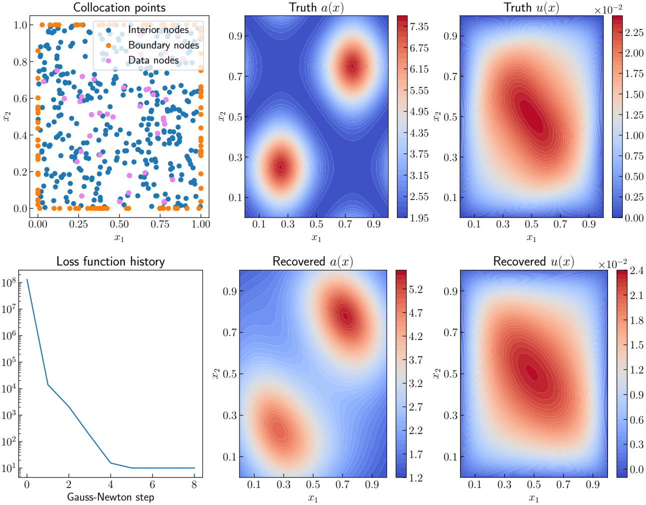


Figure: $N_{\text{domain}} = 400, N_{\text{boundary}} = 100, N_{\text{observation}} = 50$

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!