

Gaussian Processes and Kernel Methods

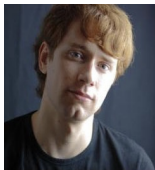
for Solving PDEs and Inverse Problems

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Collaborators



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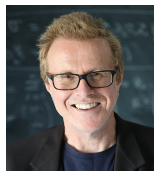
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Solving PDEs/Inverse Problems

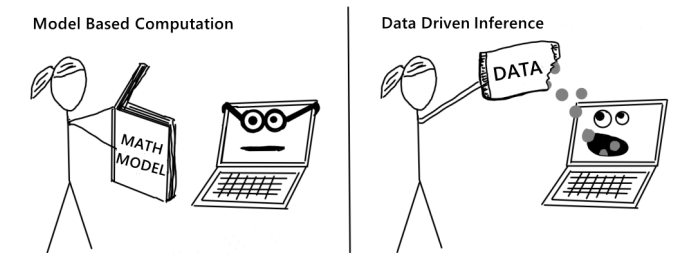
Traditional numerical methods designed by experts

- Finite difference/element/volume, spectral methods, ...
- Adjoint methods, ...

Solving PDEs/Inverse Problems

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Machine learning methods aiming for automation

- Physics informed neural networks, ...
- Operator learning, ...

This Talk: Gaussian Processes and Kernel Methods

Advantages

- Interpretable, amenable to analysis, and built-in UQ
- Connect to traditional meshless methods
- Connect to neural network methods in the infinite-width limit

Many related works in the literature

- [Poincaré 1896], [Palasti, Renyi 1956], [Sul'din 1959], [Sard 1963], [Kimeldorf, Wahba 1970], [Larkin 1972], [Traub, Wasilkowski, Woźniakowski 1988], [Diaconis 1988], [Schaback, Wendland 2006], [Stuart 2010], [Owhadi 2015], [Hennig, Osborne, Girolami 2015], [Cockayne, Oates, Sullivan, Girolami 2017], [Raissi, Perdikaris, Karniadakis 2017], ...

What's new?

- A **rigorous, scalable** computational framework for solving **nonlinear** PDEs and inverse problems

Outline

- 1 The Methodology
- 2 Numerical Examples
 - Nonlinear Elliptic PDEs
 - Darcy Flow Inverse Problem
- 3 Conclusions

A nonlinear elliptic PDE example for demonstration

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

- Domain $\Omega \subset \mathbb{R}^d$.
- PDE data $f, g : \Omega \rightarrow \mathbb{R}$.
- Assume PDE has a unique **strong/classical** solution u^\star .

The Methodology for A Nonlinear Elliptic PDE

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

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

- Convergence guarantee when solution is in \mathcal{U}
- Uncertainty quantification can also be done

How to Solve: Introducing Slack Variables

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

\Updownarrow

$$\left\{ \begin{array}{l} \underset{\mathbf{z}=(\mathbf{z}^{\text{bd}}, \mathbf{z}^{\text{int}}, \mathbf{z}_{\Delta}^{\text{int}}) \in \mathbb{R}^N}{\text{minimize}} \\ \text{s.t.} \end{array} \left\{ \begin{array}{ll} \underset{u \in \mathcal{U}}{\text{minimize}} & \|u\| \\ \text{s.t.} & u(X^{\text{bd}}) = \mathbf{z}^{\text{bd}} \in \mathbb{R}^{M^{\text{bd}}} \\ & u(X^{\text{int}}) = \mathbf{z}^{\text{int}} \in \mathbb{R}^{M^{\text{int}}} \\ & \Delta u(X^{\text{int}}) = \mathbf{z}_{\Delta}^{\text{int}} \in \mathbb{R}^{M^{\text{int}}} \end{array} \right. \right.$$

$$\left\{ \begin{array}{ll} \text{s.t.} & -\mathbf{z}_{\Delta}^{\text{int}} + \tau(\mathbf{z}^{\text{int}}) = f(X^{\text{int}}) \\ & \mathbf{z}^{\text{bd}} = g(X^{\text{bd}}) \end{array} \right.$$

How to Solve: Inner optimization

A linear inner problem

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

- Notations for kernel vectors and matrices

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

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

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

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

How to Solve: Finite Dimensional Representation

Representer Theorem

Every minimizer u^\dagger can be represented as

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

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

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

- $F : \mathbb{R}^N \rightarrow \mathbb{R}^M$ encodes PDE on collocation points
- \mathbf{y} encodes PDE boundary and RHS data
- We can solve the optimization by sequential quadratic programming (equivalent to Gauss-Newton)

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Numerical Experiments: Elliptic PDEs

- Equation with $\tau(u) = u^3$, $d = 2$

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

- Kernel: $K(\mathbf{x}, \mathbf{y}; \sigma) = \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{2\sigma^2}\right)$, $\sigma = 0.2$

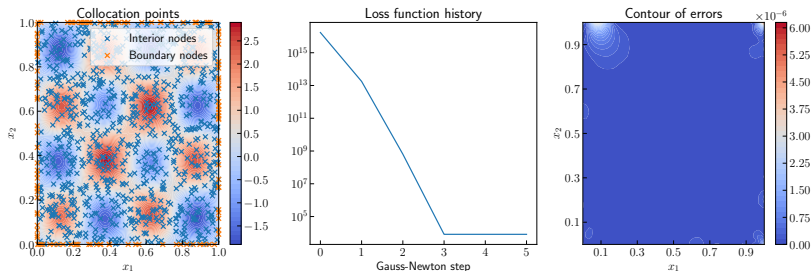


Figure: $N_{\text{domain}} = 900$, $N_{\text{boundary}} = 124$

Convergence Study

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

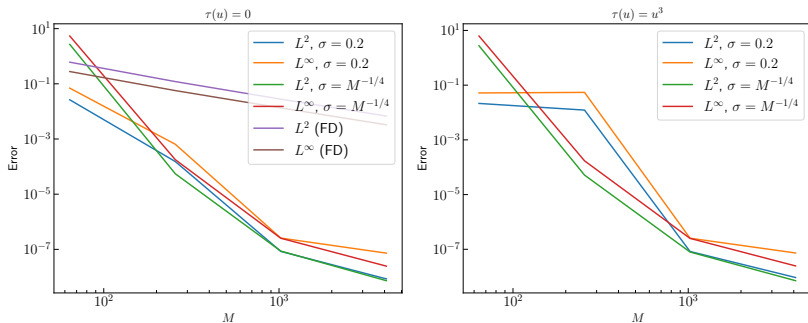


Figure: Fast convergence, since the solution is smooth

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Darcy Flow Example

Darcy Flow inverse problems

- Equation: $-\nabla \cdot (\exp(a)\nabla u) = 1$ in Ω , and $u = 0$ on $\partial\Omega$
- Unknown functions a, u
- Measurement data $u(\mathbf{x}_j^{\text{data}}) = o_j + \mathcal{N}(0, \gamma^2), 1 \leq j \leq N_{\text{data}}$

$$\underset{u, a}{\text{minimize}} \quad \|u\|_K^2 + \|a\|_K^2 + \frac{1}{\gamma^2} \sum_{j=1}^{N_{\text{data}}} |u(\mathbf{x}_j^{\text{data}}) - o_j|^2$$

$$\begin{aligned} \text{constraint} \quad & -\nabla \cdot (\exp(a)\nabla u)(\mathbf{x}_m^{\text{int}}) = 1 \text{ for some } \mathbf{x}_m^{\text{int}} \in (0, 1)^2 \\ & u(\mathbf{x}_m^{\text{bd}}) = 0 \text{ for some } \mathbf{x}_m^{\text{bd}} \in \partial(0, 1)^2 \end{aligned}$$

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

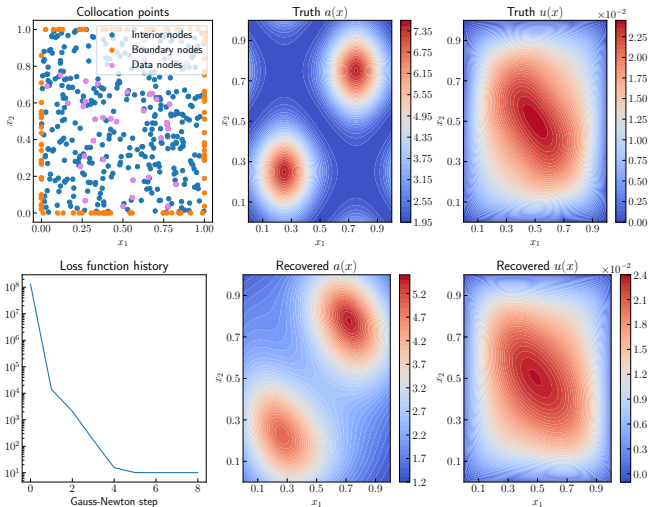


Figure: $N_{\text{domain}} = 400, N_{\text{boundary}} = 100, N_{\text{data}} = 50$

Other Examples of Nonlinear and Parametric PDEs

Reported in [Chen, Hosseini, Owhadi, Stuart 2021], [Batlle, Chen, Hosseini, Owhadi, Stuart 2023], [Chen, Owhadi, Schäfer 2023]

- Burgers' equations: $u_t + uu_x = \nu u_{xx}$
- Regularized Eikonal equations: $|\nabla u|^2 = f^2 + \epsilon \Delta u$
- Hamilton-Jacobi equations: $(\partial_t + \Delta)V(x, t) - |\nabla V(x, t)|^2 = 0$
- Parametric elliptic equations: $\nabla_x \cdot (a(x, \theta) \nabla_x u(x, \theta)) = f(x)$
- Monge-Ampère equations: $\det(D^2 u) = f$

Overall observations:

- The method is fast and achieves high accuracy with $10^3 - 10^4$ collocation points, if the solution is relatively **smooth** and **Matérn/Gaussian kernels** are chosen
- For more challenging cases, **kernel learning** can be used to adapt the kernel to the solution. **Sparse Cholesky factorization** algorithms can be applied to address $> 10^5$ collocation points

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Summary

Gaussian processes and kernel methods

- **Solving PDEs and inverse problems**
 - General computational framework for both
 - Convergence guarantee when kernel selected properly
 - Fast convergence using sequential quadratic programming
- **Kernel learning and sparse Cholesky factorization**
 - Adapt the kernel to the solution
 - Scale to massive collocation points
 - Future works: adaptive sampling of the points

Thank You

Relevant papers

- Yifan Chen, Bamdad Hosseini, Houman Owhadi, and Andrew M. Stuart. Solving and learning nonlinear PDEs with Gaussian processes. JCP, 2021.
- Yifan Chen, Houman Owhadi, Florian Schaefer. Sparse Cholesky Factorization for Solving Nonlinear PDEs via Gaussian Processes. arxiv: 2304.01294, 2023.
- Pau Batlle, Yifan Chen, Bamdad Hosseini, Houman Owhadi, Andrew M. Stuart. Error Analysis of Kernel/GP Methods for Nonlinear and Parametric PDEs. arxiv: 2305.04962, 2023.

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Convergence Theory for Solving PDEs

Convergence of the minimizer u^\dagger to the truth u^*

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

Asymptotic convergence [Chen, Hosseni, Owhadi, Stuart 2021]

Assumptions:

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

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

- Convergence rates obtained when stability of the PDE is further assumed [Batlle, Chen, Hosseni, Owhadi, Stuart 2023]