Gaussian Processes and Kernel Methods

for Solving Nonlinear PDEs and Inverse Problems

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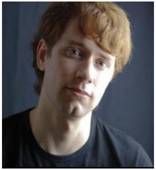

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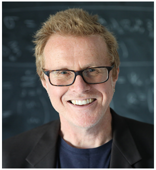

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Solving PDEs/Inverse Problems

Traditional numerical methods designed by experts

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

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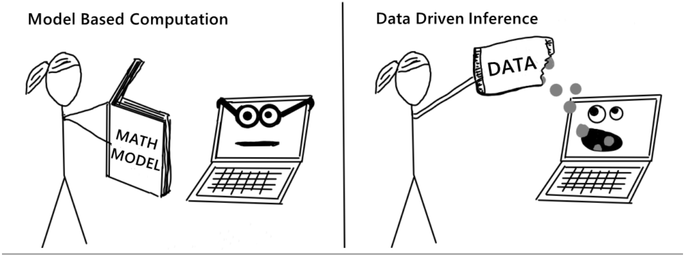

Machine learning methods aiming for automation

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

Our Focus: 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], ...

This talk

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

Outline

Outline

The Methodology

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 $f, g : \Omega \to \mathbb{R}$.
- Assume PDE has a unique strong/classical solution $u^\star$.

The Methodology for A Nonlinear Elliptic PDE

1. Choose a kernel $K : \overline{\Omega} \times \overline{\Omega} \to \mathbb{R}$ (Choose the prior $\mathcal{GP}(0, K)$)
   - Corresponding RKHS $\mathcal{U}$ with norm $\|\cdot\|_K$
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")

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

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

How to Solve: Introducing Slack Variables

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

$$\Updownarrow$$

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

How to Solve: Inner optimization

A linear inner problem

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

- Notations for kernel vectors and matrices

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

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

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

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

How to Solve: Finite Dimensional Representation

Representer Theorem

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

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

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

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

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

Outline

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

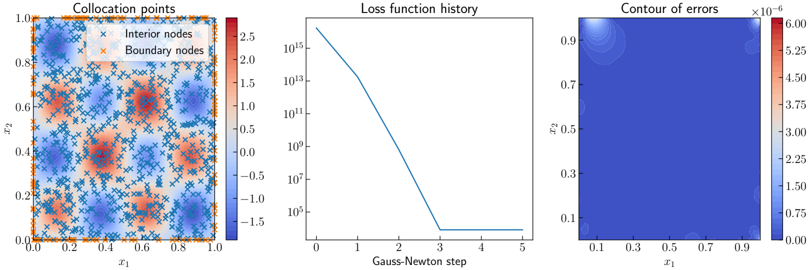

Figure: $N_{\text{domain}} = 900, N_{\text{boundary}} = 124$

Convergence Study

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

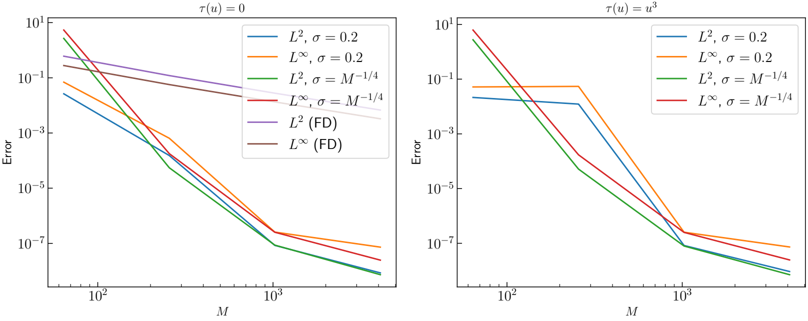

Figure: Fast convergence, since the solution is smooth

Outline

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 $u(\mathbf{x}_j^{\mathrm{data}}) = o_j + \mathcal{N}(0, \gamma^2), 1 \leq j \leq N_{\mathrm{data}}$

$$\begin{aligned} \underset{u,a}{\text{minimize}} \quad & \|u\|_K^2 + \|a\|_K^2 + \frac{1}{\gamma^2}\sum_{j=1}^{N_{\mathsf{data}}} |u(\mathbf{x}_j^{\mathsf{data}}) - o_j|^2 \\ \text{constraint} \quad & -\nabla \cdot (\exp(a)\nabla u)(\mathbf{x}_m^{\mathrm{int}}) = 1 \text{ for some } \mathbf{x}_m^{\mathrm{int}} \in (0,1)^2 \\ & u(\mathbf{x}_m^{\mathrm{bd}}) = 0 \text{ for some } \mathbf{x}_m^{\mathrm{bd}} \in \partial(0,1)^2 \end{aligned}$$

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

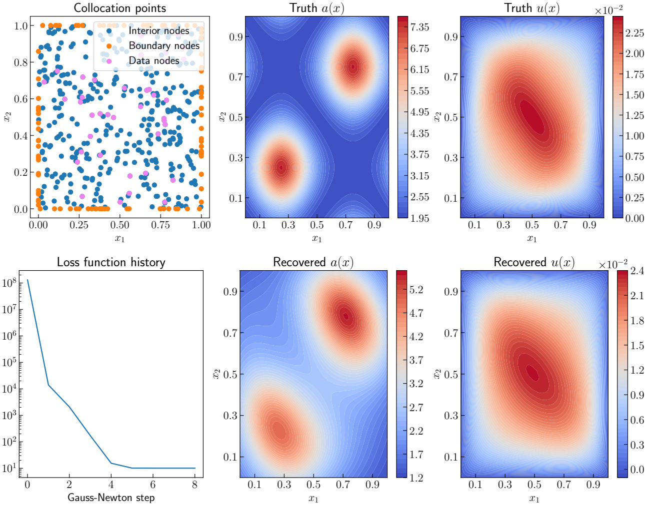

Figure: $N_{\text{domain}} = 400, N_{\text{boundary}} = 100, N_{\text{data}} = 50$

Other Examples of Nonlinear and Parametric PDEs

Reported in [Chen, Hosseni, Owhadi, Stuart 2021], [Batlle, Chen, Hosseni, 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-Amperè 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 $> 10^6$ collocation points

Thank You

Gaussian processes and kernel methods for

- **Solving nonlinear PDEs and inverse problems**
  - General computational framework for both
  - Convergence guarantee when kernel selected properly
  - Fast convergence using sequential quadratic programming

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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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

Convergence Theory for Solving PDEs

Convergence of the minimizer $u^\dagger$ to the truth $u^\star$

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

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

Assumptions:

- K is chosen so that
  - $\mathcal{U} \subseteq H^s(\Omega)$ for some $s > s^*$ where $s^* = d/2 +$ 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 $t \in (s^*, s)$

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

Burgers' Equation

- $\partial_t u + u\partial_x u - 0.001\partial_x^2 u = 0, \quad \forall (x,t) \in (-1,1) \times (0,1]$
- $\Delta t = 0.02, \rho = 4$, solve to $t = 1$

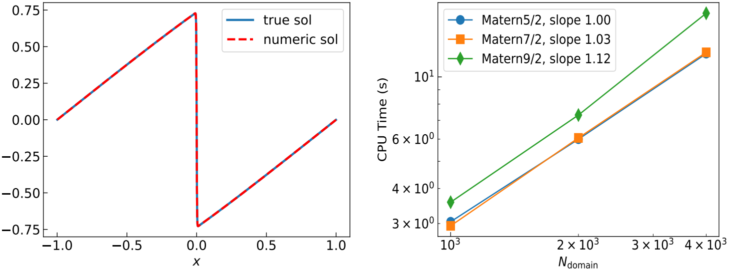

Figure: Run 2 linearization steps at each time step

Monge-Ampère Equation

- Equation: $\det(D^2u) = f$ in $(0,1)^2$
- Truth $u(\mathbf{x}) = \exp\big(0.5((x_1 - 0.5)^2 + (x_2 - 0,5)^2)\big)$
- Matérn kernel with $\nu = 5/2$, lengthscale 0.3

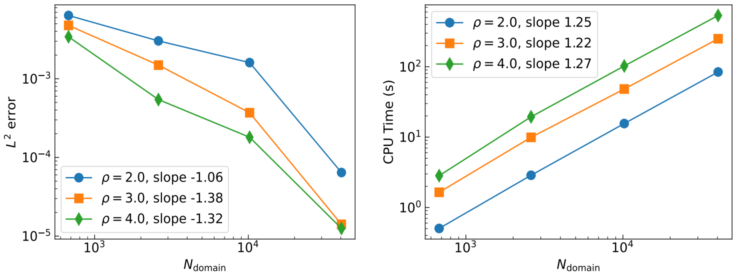

Figure: Run 3 linearization steps with initial guess $1/2\|\mathbf{x}\|^2$. Accuracy floor due to finite ρ