Physics Informed Machine Learning for Solving PDEs

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Numerical PDE Lecture 02

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Quick Recap

Last time

How to solve a simple Heat Equation with Dirichlet BC

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- Separation of Variables (Heavy dependence of IC/BC)

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  - Regular domain, exponential growth for dimension

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- Physics Informed Neural Networks

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Physics Informed Machine Learning

Overview

Hybrid method

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- Traditional Methods

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  - Special Properties (Conservation, TVD, shock detection, etc.)

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  - Mesh-free, no time integration

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- Machine Learning
  - Mesh-free, no time integration
  - Auto-interpolation, auto-differentiation
  - Data assimilation

Data Assimilation

Missing IC/BC[1]

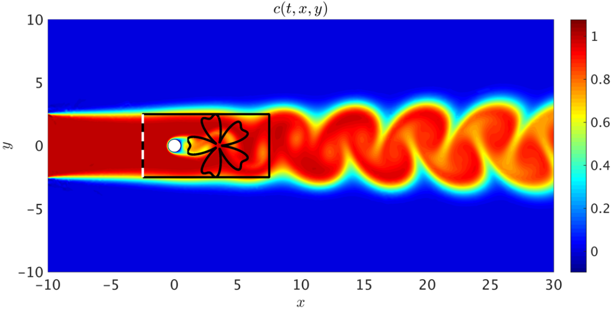

Figure: $2D$ Flow Past a Circular Cylinder.

[1] "Hidden Fluid Mechanics: A Navier-Stokes Informed Deep Learning Framework for Assimilating Flow Visualization Data", 2020.

Data Assimilation

HFM, cont.

$$
\begin{aligned}
c_t + uc_x + vc_y + wc_z - \mathrm{Pec}^{-1}(c_{xx} + c_{yy} + c_{zz}) &= 0,\\
d_t + ud_x + vd_y + wd_z - \mathrm{Pec}^{-1}(d_{xx} + d_{yy} + d_{zz}) &= 0,\\
u_t + uu_x + vu_y + wu_z + p_x + \mathrm{Re}^{-1}(u_{xx} + u_{yy} + u_{zz}) &= 0,\\
v_t + uv_x + vv_y + wv_z + p_y + \mathrm{Re}^{-1}(v_{xx} + v_{yy} + v_{zz}) &= 0,\\
w_t + uw_x + vw_y + ww_z + p_z + \mathrm{Re}^{-1}(w_{xx} + w_{yy} + w_{zz}) &= 0,\\
u_x + v_y + w_z &= 0
\end{aligned}
$$

With observation of c, d.

Other Forms of NN Solver

References

- DeepONet: "Learning Nonlinear Operators for Identifying Differential Equations based on the Universal Approximation Theorem of Operators", 2020.

Other Forms of NN Solver

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- LSNN: "Deep Least-squares Methods: an Unsupervied Learning-based Numerical Methods for Solving Elliptic PDEs", 2020.

Other Forms of NN Solver

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- LSNN: "Deep Least-squares Methods: an Unsupervied Learning-based Numerical Methods for Solving Elliptic PDEs", 2020.
- CVPINN: "Thermodynamically Consistent Physics-informed Neural Networks for Hyperbolic Systems", 2020.

Weaknesses

Multi-Object Losses[2]

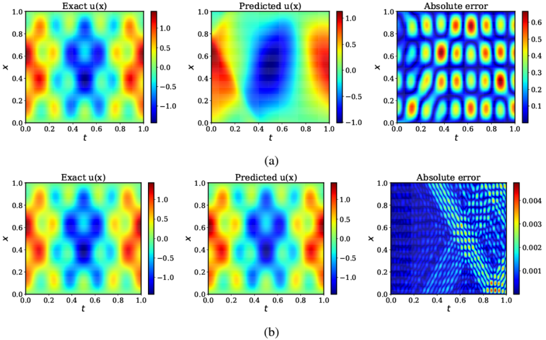


Figure: $1D$ Wave Equation ($u_{tt} = ku_{xx}$).

[2] "When and Why PINNs Fail to Train: a Neural Tanget Kernel Perspective", 2020.

Weaknesses

No Time Marching[3]

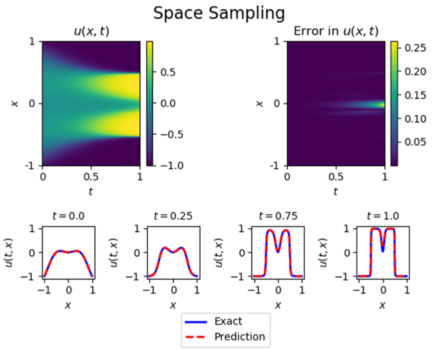
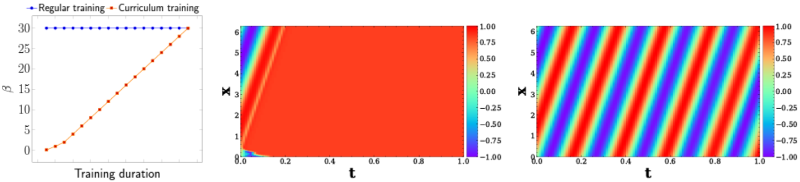


Figure: $1D$ Allen-Chan Equation.

[3] "Solving Allen-Cahn and Cahn-Hilliard Equations using the Adaptive Physics Informed Neural Networks", 2020.

Weakness

No Time Marching[4]



(a) *Curriculum regularization schematic*

(b) *Regular training PINN solution for $\beta = 30$*

(c) *Curriculum training PINN solution for $\beta = 30$*

Figure: $1D$ Transport Equation.

[4] "Characterizing Possible Failure Modes in Physics-informed Neural Networks", 2021.

Weaknesses

No Time Marching[5]

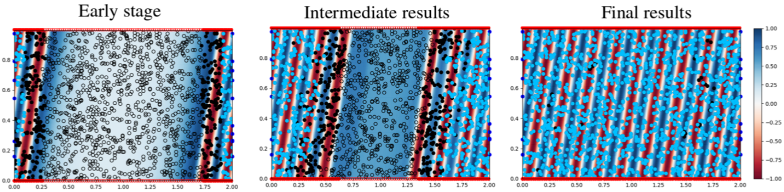


Figure: $1D$ Transport Equation.

[5] "Improved Training of Physics-informed Neural Networks with Model Ensembles", 2022.

Weaknesses

Shock Capturing[6]

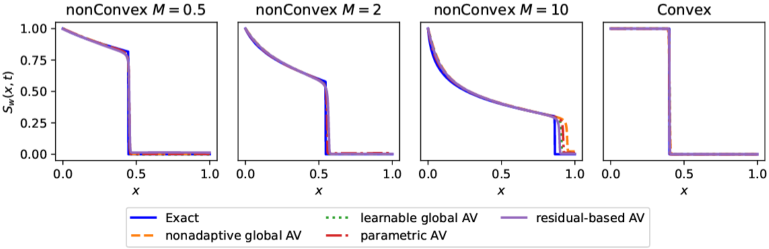


Figure: $1D$ Buckey-Leverett Equation.

[6] "Physics-informed Neural Networks with Adaptive Localized Artificial Viscosity", 2022.

Important References

Gaussian Processes for Machine Learning

Two books

- Gaussian Processes for Machine Learning, Rasmussen and Williams, 2006
- Operator-Adapted Wavelets, Fast Solvers, and Numerical Homogenization: from a Game Theory Approach to Numerical Approximation and Algorithm Design, Owhadi, 2019.

PIGP

Many Kinds

1 : "Machine Learning of Linear Differential Equations using Gaussian Processes", 2017.

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2 : “Numerical Gaussian Processes for Time-Dependent and Nonlinear Partial Differential Equations”, 2018.

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4 : "AutoIP: A United Framework to Integrate Physics into Gaussian Processes", 2022.

5 : Bayesian Numerical PDE, 2023.

GP for Linear PDEs

Approach One[7]

Consider

$$\mathcal{L}_{\mathbf{x}} u(\mathbf{x}) = f(\mathbf{x}), \quad \mathcal{L}_{\mathbf{x}} \text{ is a linear differential operator.}$$

[7] Reference [1].

GP for Linear PDEs

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Examples

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Examples

- For $\Delta_{\mathbf{x}} u(\mathbf{x}) = f(\mathbf{x})$ (Laplace Equation), $\mathcal{L}_{\mathbf{x}} = \Delta_{\mathbf{x}}$.

[7] Reference [1].

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- For $\Delta_{\mathbf{x}} u(\mathbf{x}) = f(\mathbf{x})$ (Laplace Equation), $\mathcal{L}_{\mathbf{x}} = \Delta_{\mathbf{x}}$.
- For $\partial_t u(\mathbf{x}) + c\partial_x u(\mathbf{x}) = f(\mathbf{x})$ (Linear Advection), $\mathcal{L}_{\mathbf{x}} = \partial_{x_1} + c\partial_{x_2}$ where $x_1 = t$ and $x_2 = x$ and $\mathbf{x} = (x_1, x_2)$.

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- For $\partial_t u(\mathbf{x}) - k\partial_x^2 u(\mathbf{x}) = f(\mathbf{x})$ (Heat Equation), $\mathcal{L}_{\mathbf{x}} = \partial_{x_1} - k\partial_{x_2}^2$.

[7] Reference [1].

GP for Linear PDEs

Approach One, cont.

GP Prior

If $u(\mathbf{x}) \sim \mathcal{N}(0, K_{uu}(\mathbf{x}, \mathbf{x}'; \theta))$, then

$$f(\mathbf{x}) \sim \mathcal{N}(0, K_{ff}(\mathbf{x}, \mathbf{x}'; \theta))$$

and

$$K_{ff}(\mathbf{x}, \mathbf{x}'; \theta) = \mathcal{L}_{\mathbf{x}} \mathcal{L}_{\mathbf{x}'} K_{uu}(\mathbf{x}, \mathbf{x}'; \theta).$$

Here θ is the hyper-parameter for the GP.

GP for Linear PDEs

Approach One, cont.

Problem Statement

Given

$$\mathbf{y}_u = u(\mathbf{X}_u) + \epsilon_u \quad \text{and} \quad \mathbf{y}_f = f(\mathbf{X}_f) + \epsilon_f$$

where $\epsilon_u \sim \mathcal{N}(0, \sigma_u^2 \mathrm{Id}_u)$ and $\epsilon_f \sim \mathcal{N}(0, \sigma_f^2 \mathrm{Id}_f)$, how can we find the θ?

GP for Linear PDEs

Approach One, cont.

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Given

$$\mathbf{y}_u = u(\mathbf{X}_u) + \epsilon_u \quad \text{and} \quad \mathbf{y}_f = f(\mathbf{X}_f) + \epsilon_f$$

where $\epsilon_u \sim \mathcal{N}(0, \sigma_u^2 \mathrm{Id}_u)$ and $\epsilon_f \sim \mathcal{N}(0, \sigma_f^2 \mathrm{Id}_f)$, how can we find the θ?

Find θ such that $-\log(P(\mathbf{y}\Big|\theta, \sigma_u^2, \sigma_f^2))$ is minimized

GP for Linear PDEs

Approach One, cont.

Here

$$-\log(P(\mathbf{y}\Big|\theta, \sigma_u^2, \sigma_f^2)) = \frac{1}{2}\log(\big|K\big|) + \frac{1}{2}\mathbf{y}^\top K^{-1}\mathbf{y} + \frac{N}{2}\log(2\pi),$$

where

$$\mathbf{y} = \begin{bmatrix}\mathbf{y}_u \\ \mathbf{y}_f\end{bmatrix} \quad \text{and} \quad \mathbf{y}\Big|\theta, \sigma_u^2, \sigma_f^2 \sim \mathcal{N}(0, K),$$

GP for Linear PDEs

Approach One, cont.

$$K = \begin{bmatrix} K_{uu}(\mathbf{X}_u, \mathbf{X}_u; \theta) + \sigma_u^2 \mathrm{Id}_u & K_{uf}(\mathbf{X}_u, \mathbf{X}_f; \theta) \\ K_{fu}(\mathbf{X}_f, \mathbf{X}_u; \theta) & K_{ff}(\mathbf{X}_f, \mathbf{X}_f; \theta) + \sigma_f^2 \mathrm{Id}_f \end{bmatrix}.$$

Moreover

$$K_{uf}(\mathbf{x}, \mathbf{x}'; \theta) = \mathcal{L}_{\mathbf{x}'} K_{uu}(\mathbf{x}, \mathbf{x}'; \theta) \quad \text{and} \quad \theta)$$

and

$$K_{fu}(\mathbf{x}, \mathbf{x}'; \theta) = \mathcal{L}_{\mathbf{x}} K_{uu}(\mathbf{x}, \mathbf{x}').$$

The minimizater is found using L-BFGS.

GP for Linear PDEs

Approach One, cont.

Next?

How to predict?

GP for Linear PDEs

Approach One, cont.

Next?

How to predict?

Use the fact that

$$u(\mathbf{x})\Big|\mathbf{y} \sim \mathcal{N}(\bar{u}(\mathbf{x}), s_u^2(\mathbf{x}))$$

and

$$f(\mathbf{x})\Big|\mathbf{y} \sim \mathcal{N}(\bar{f}(\mathbf{x}), s_f^2(\mathbf{x})),$$

GP for Linear PDEs

Approach One, cont.

Where

$$\bar{u}(\mathbf{x}) = \mathbf{q}_u^\top K^{-1}\mathbf{y}, \quad s_u^2(\mathbf{x}) = K_{uu}(\mathbf{x},\mathbf{x}) - \mathbf{q}_u^\top K^{-1}\mathbf{q}_u,$$
$$\mathbf{q}_u^\top(\mathbf{x}) = \begin{bmatrix} K_{uu}(\mathbf{x},\mathbf{X}_u) & K_{uf}(\mathbf{x},\mathbf{X}_f) \end{bmatrix}.$$

and

$$\bar{f}(\mathbf{x}) = \mathbf{q}_f^\top K^{-1}\mathbf{y}, \quad s_f^2(\mathbf{x}) = K_{ff}(\mathbf{x},\mathbf{x}) - \mathbf{q}_f^\top K^{-1}\mathbf{q}_f,$$
$$\mathbf{q}_f^\top(\mathbf{x}) = \begin{bmatrix} K_{fu}(\mathbf{x},\mathbf{X}_u) & K_{ff}(\mathbf{x},\mathbf{X}_f) \end{bmatrix}.$$

GP for Linear PDEs

Conclusion

Summary

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- Clean implementation.

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- Easy to train.

GP for Linear PDEs

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- Clean implementation.
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- Uncertainty quantification.

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- Differentiation is done on the kernel function.

GP for Linear PDEs

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Summary

- Clean implementation.
- Easy to train.
- Uncertainty quantification.
- Differentiation is done on the kernel function.

But

- Only for linear PDEs.
- Application when there are data for u and f.

GP for Time-dependent PDEs

Approach Two[8]

Consider

$$u_t = \mathcal{L}_{\mathbf{x}} u, \quad \mathbf{x} \in \Omega, \quad t \in [0, T].$$

[8] Reference [2].

GP for Time-dependent PDEs

Approach Two[8]

Consider

$$u_t = \mathcal{L}_{\mathbf{x}} u, \quad \mathbf{x} \in \Omega, \quad t \in [0, T].$$

Via the explicit Euler scheme for u_t, we end up with

$$u^n = u^{n-1} + \Delta t \mathcal{L}_{\mathbf{x}} u^{n-1} = \mathcal{B}_x(\Delta t) u^{n-1},$$

Here

$$u^n(\mathbf{x}) = u(t_n, \mathbf{x}).$$

[8] Reference [2].

GP for Time-dependent PDEs

Approach Two, cont.

Put on a Gaussian Process prior on u^{n-1}, i.e.

$$u(t_{n-1}, \mathbf{x}) \sim \mathcal{N}(0, K_{uu}^{n-1,n-1}(\mathbf{x}, \mathbf{x}'; \theta)),$$

GP for Time-dependent PDEs

Approach Two, cont.

Put on a Gaussian Process prior on u^{n-1}, i.e.

$$u(t_{n-1}, \mathbf{x}) \sim \mathcal{N}(0, K_{uu}^{n-1,n-1}(\mathbf{x}, \mathbf{x}'; \theta)),$$

then

$$\begin{bmatrix} u(t_n, \mathbf{x}) \\ u(t_{n-1}, \mathbf{x}) \end{bmatrix} \sim \mathcal{N}(0, \begin{bmatrix} K_{uu}^{n,n} & K_{uu}^{n,n-1} \\ k_{uu}^{n-1,n} & K_{uu}^{n-1,n-1} \end{bmatrix}).$$

GP for Time-dependent PDEs

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- Able to handle time-dependent PDE.

GP for Time-dependent PDEs

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- No need to have observation data inside the computational domain (start out from IC/BC).

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- Applicable to other numerical integration schemes (even implicit).

GP for Time-dependent PDEs

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Summary

- Able to handle time-dependent PDE.
- No need to have observation data inside the computational domain (start out from IC/BC).
- Applicable to other numerical integration schemes (even implicit).

But

- Different numerical integration schemes would require different $\mathcal{B}_x(\Delta t)$.
- For nonlinear PDEs, need to linearize it using u^{n-1}.

PIGP for Nonlinear PDE

Approach Three[9]

A Simple Nonlinear Elliptic PDE Problem

Consider $\Omega \subset \mathbb{R}^d$ ($d \geq 1$, open and bounded) with Lipshitz boundary $\partial\Omega$, and for $u^* : \Omega \to \mathbb{R}$ satisfying

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

Here $f : \Omega \to \mathbb{R}$, $g : \partial\Omega \to \mathbb{R}$, and $\tau : \mathbb{R} \to \mathbb{R}$ are given continuous functions.

[9]Reference [3].

PIGP for Nonlinear PDE

Approach Three, cont.

The PIGP method finds the approximation to u^* from the following

$$\min_{u \in \mathcal{U}} \left|u\right|_K, \quad \text{s.t.}$$
$$-\Delta u(\mathbf{x}_m) + \tau(u(\mathbf{x}_m)) = f(\mathbf{x}_m), \quad m = 1, \ldots, M_\Omega$$
$$u(\mathbf{x}_m) = g(\mathbf{x}_m), \quad m = M_\Omega + 1, \ldots, M.$$

PIGP for Nonlinear PDE

Approach Three, cont.

The PIGP method finds the approximation to u^* from the following

$$
\begin{aligned}
&\min_{u \in \mathcal{U}} \left|u\right|_K, \quad \text{s.t.} \\
&-\Delta u(\mathbf{x}_m) + \tau(u(\mathbf{x}_m)) = f(\mathbf{x}_m), \quad m = 1, \dots, M_\Omega \\
&u(\mathbf{x}_m) = g(\mathbf{x}_m), \quad m = M_\Omega + 1, \dots, M.
\end{aligned}
$$

Here

- $\mathcal{U}$ is a RKHS (Reproducing Kernel Hilbert Space) associated with K and the RKHS norm is $\left|\cdot\right|_K$.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Moreover

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Moreover

- A non-degenerate, symmetric, and positive definite kernel function $K : \bar{\Omega} \times \bar{\Omega} \to \mathbb{R}$.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Moreover

- A non-degenerate, symmetric, and positive definite kernel function $K : \bar{\Omega} \times \bar{\Omega} \to \mathbb{R}$.
- K is chosen so that $\mathcal{U} \in C^2(\Omega) \cap C(\bar{\Omega})$.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Moreover

- A non-degenerate, symmetric, and positive definite kernel function $K : \bar{\Omega} \times \bar{\Omega} \to \mathbb{R}$.
- K is chosen so that $\mathcal{U} \in C^2(\Omega) \cap C(\bar{\Omega})$.
- $1 \leq M_\Omega < M < \infty$ with $\mathbf{x}_1, \ldots, \mathbf{x}_{M_\Omega} \in \Omega$ and $\mathbf{x}_{M_\Omega+1}, \ldots, \mathbf{x}_M \in \partial\Omega$.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Moreover

- A non-degenerate, symmetric, and positive definite kernel function $K : \bar{\Omega} \times \bar{\Omega} \to \mathbb{R}$.
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- $1 \leq M_\Omega < M < \infty$ with $\mathbf{x}_1, \ldots, \mathbf{x}_{M_\Omega} \in \Omega$ and $\mathbf{x}_{M_\Omega+1}, \ldots, \mathbf{x}_M \in \partial\Omega$.
- A minimier $u^\dagger$ can be interpreted as a MAP estimator of a GP $\xi \sim \mathcal{N}(0, \mathcal{K})$ ($\mathcal{K}$ is the integral operator with kernel K).

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Finite Dimensional Representation

$$z_m^{(1)} = u(\mathbf{x}_m) \quad \text{and} \quad z_m^{(2)} = -\Delta u(\mathbf{x}_m),$$

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Finite Dimensional Representation

$$z_m^{(1)} = u(\mathbf{x}_m) \quad \text{and} \quad z_m^{(2)} = -\Delta u(\mathbf{x}_m),$$

Define

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Finite Dimensional Representation

$$z_m^{(1)} = u(\mathbf{x}_m) \quad \text{and} \quad z_m^{(2)} = -\Delta u(\mathbf{x}_m),$$

Define

- $\phi_m^{(1)} = \delta_{\mathbf{x}_m}$ and $\phi_m^{(2)} = \delta_{\mathbf{x}_m} \circ (-\Delta)$ where $\delta_{\mathbf{x}}$ is the Dirac delta function centered at $\mathbf{x}$.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

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$$z_m^{(1)} = u(\mathbf{x}_m) \quad \text{and} \quad z_m^{(2)} = -\Delta u(\mathbf{x}_m),$$

Define

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- $\mathbf{z} = \left[(\mathbf{z}^{(1)})^\top \quad (\mathbf{z}^{(2)})^\top \right]$ where $\mathbf{z}^{(i)}$ is the concatenation of $z_m^{(i)}$ for $i = 1, 2$ respectively.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

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- $\phi = \left[(\phi^{(1)})^\top \quad (\phi^{(2)})^\top\right]$ where $\phi^{(i)}$ is the concatenation of $\phi_m^{(i)}$ for $i = 1, 2$ respectively.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Furthermore

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Furthermore

- $\Theta(\mathbf{x}, \phi)$ is the $(M + M_\Omega)$-dim vector with entries $\int K(\mathbf{x}, \mathbf{x}')\phi_m(\mathbf{x}')\, d\mathbf{x}'$.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Furthermore

- $\Theta(\mathbf{x}, \phi)$ is the $(M + M_\Omega)$-dim vector with entries $\int K(\mathbf{x}, \mathbf{x}')\phi_m(\mathbf{x}')\,d\mathbf{x}'$.
- $\Theta(\phi, \phi)$ is the $(M + M_\Omega) \times (M + M_\Omega)$ matrix with entries $\int K(\mathbf{x}, \mathbf{x}')\phi_m(\mathbf{x})\phi_n(\mathbf{x}')\,d\mathbf{x}d\mathbf{x}'$.

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Furthermore

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Thus

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

and

$$\left|u\right|_K^2 = \mathbf{z}^\top\Theta(\phi, \phi)^{-1}\mathbf{z}$$

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Define

$$F(\mathbf{z}) = \begin{cases} z_m^{(2)} + \tau(z_m^{(1)}), & m = 1, \dots, M_\Omega \\ z_m^{(1)}, & m = M_\Omega + 1, \dots, M \end{cases}$$

and

$$\mathbf{y} = \begin{cases} f(\mathbf{x}_m), & m = 1, \dots, M_\Omega \\ g(\mathbf{x}_m), & m = M_\Omega + 1, \dots, M \end{cases}$$

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

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The original optimal recovery problem becomes

$$\min_{\mathbf{z} \in \mathbb{R}^{M+M_\Omega}} \mathbf{z}^\top \Theta(\phi, \phi)^{-1} \mathbf{z}, \quad \text{s.t.} \quad F(\mathbf{z}) = \mathbf{y}.$$

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Or the regularized version

$$\min_{\mathbf{z}\in\mathbb{R}^{M+M_\Omega}} \mathbf{z}^\top \Theta(\phi,\phi)^{-1}\mathbf{z} + \frac{1}{\beta^2}\left|F(\mathbf{z}) - \mathbf{y}\right|^2_{\mathbb{R}^{M+M_\Omega}}.$$

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Or the regularized version

$$\min_{\mathbf{z}\in\mathbb{R}^{M+M_\Omega}} \mathbf{z}^\top \Theta(\phi,\phi)^{-1}\mathbf{z} + \frac{1}{\beta^2}\left|F(\mathbf{z}) - \mathbf{y}\right|^2_{\mathbb{R}^{M+M_\Omega}}.$$

- Choosing a proper β?

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Or the regularized version

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- Choosing a proper β?
- Why does β have to be a scalar?

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

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$$\min_{\mathbf{z}\in\mathbb{R}^{M+M_\Omega}} \mathbf{z}^\top \Theta(\phi,\phi)^{-1}\mathbf{z} + \frac{1}{\beta^2}\left|F(\mathbf{z}) - \mathbf{y}\right|^2_{\mathbb{R}^{M+M_\Omega}}.$$

- Choosing a proper β?
- Why does β have to be a scalar?
- Somewhat easier than the constrained problem

PIGP for Nonlinear PDE

Nonlinear Elliptic PDEs, cont.

Or the regularized version

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- Choosing a proper β?
- Why does β have to be a scalar?
- Somewhat easier than the constrained problem
- But the constrained problem can be reduced further

PIGP for Nonlinear PDE

Numerical Tests

We take

- $d = 2$, $\Omega = (0, 1)^2$, $\tau(u) = 0$ or u^3, and $g(\mathbf{x}) = 0$.
- $u^*(\mathbf{x}) = \sin(\pi x_1)\sin(\pi x_2) + 4\sin(4\pi x_1)\sin(4\pi x_2)$, and find $f(\mathbf{x})$ accordingly.
- Gaussian kernel

$$K(\mathbf{x}, \mathbf{x}'; \sigma) = \exp\left(-\frac{\left|\mathbf{x} - \mathbf{x}'\right|^2_{\ell_2(\mathbb{R}^d)}}{2\sigma^2}\right).$$

- Special care of Θ.
- $M = 1024$ and $M_\Omega = 900$ and $\sigma = M^{-\frac{1}{4}}$.
- $\eta = 10^{-5}$ and $\beta = 10^{-5}$.

PIGP for Nonlinear PDE

A Simple Heat Equation

Recall

$$u_t(t,x) = \lambda u_{xx}(t,x), \quad (t,x) \in (0,T] \times [0,L]$$
$$u(0,x) = f(x), \quad u(t,0) = 0, \quad u(t,L) = 0.$$

so $(\mathbf{x} = (t,x))$

$$z_m^{(1)} = u(\mathbf{x}_m), \quad z_m^{(2)} = u_t(\mathbf{x}_m), \quad \text{and} \quad z_m^{(3)} = u_{xx}(\mathbf{x}_m).$$

Here

$$\phi_m^{(1)} = \delta_{\mathbf{x}_m}, \quad \phi_m^{(2)} = \delta_{\mathbf{x}_m} \circ \frac{\partial}{\partial t}, \quad \text{and} \quad \phi_m^{(3)} = \delta_{\mathbf{x}_m} \circ \frac{\partial^2}{\partial x^2}.$$

PIGP for Nonlinear PDE

A Simple Heat Equation, cont.

Thus

$$
\begin{aligned}
\text{PDE}: & 0 * z_m^{(1)} + z_m^{(2)} - \lambda z_m^{(3)} = 0, \\
\text{BC}: & z_m^{(1)} = \begin{cases} f(x_m), & \mathbf{x}_m \in \{0\} \times [0, L] \\ 0, & \mathbf{x}_m \in [0, T] \times \{0\} \\ 0, & \mathbf{x}_m \in [0, T] \times \{L\} \end{cases}
\end{aligned}
$$

PIGP for Nonlinear PDE

A Simple Heat Equation, cont.

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\end{aligned}
$$

Demo

PIGP for Nonlinear PDE

Conclusion

PIGP can even handle

$$\left|\nabla u(\mathbf{x})\right|^2 = f(\mathbf{x})^2 + \epsilon\Delta u(\mathbf{x}), \quad \text{Eikonal PDE}$$

and

$$u_t + uu_x = \nu u_{xx}, \quad \text{Viscous Burgers}$$

Summary:

PIGP for Nonlinear PDE

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Summary:

- Smaller number of “collocation” points

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- Uncertainty quantification
- $\Omega \subset \mathbb{R}^d$ with $d \gg 1$ and irreuglar.

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PIGP for Nonlinear PDE

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Summary:

- Smaller number of "collocation" points
- Uncertainty quantification
- $\Omega \subset \mathbb{R}^d$ with $d \gg 1$ and irreuglar.
- Auto-interpolation and auto-differentiation
- However, heavy dependence on kernel

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Deep Learning Software

How to install them

- Python
  - TensorFlow: https://www.tensorflow.org/
  - PyTorch: https://pytorch.org/
  - JAX: https://jax.readthedocs.io/en/latest/
- Julia: SciML package https://sciml.ai/
- MATLAB
- Google Colab or Amazon AWS (Microsft? IBM?)

They can work with

- CPU (Slow!!)
- GPU (CUDA or M1/M2 Chips)

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Physics Informed Machine Learning

Conclusion

We have shown

- Solving a heat equation, viscous Burgers, and RTE using PINN.
- Solving elliptic PDEs, a heat equation, viscous Burgers, Eikonal using PIGP.
- Both methods have their own strength and weaknesses: auto-interpolation, mesh-less, etc.

Thank You!