Learning methods for solving PDEs

ANNs

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations.
M. Raissi, P.Perdikaris, G.E. Karniadakis, JCP 2019

Model reduction and neural networks for parametric PDEs.
K. Bhattacharya, B. Hosseini, N. B. Kovachki, and A. M. Stuart. arXiv preprint:2005.03180, 2020.

GPs

Gamblets: Bayesian Numerical Homogenization. H. Owhadi. SIAM MMS, 2015.
Multigrid with rough coefficients and Multiresolution operator decomposition from Hierarchical Information Games. H. Owhadi, SIREV, 2017
Operator adapted wavelets, fast solvers, and numerical homogenization from a game theoretic approach to numerical approximation and algorithm design. H. Owhadi and C. Scovel. Cambridge University Press, Cambridge Monographs on Applied and Computational Mathematics, 2019

Time dependent: Numerical Gaussian processes for time-dependent and nonlinear partial differential equations M Raissi, P Perdikaris, GE Karniadakis, SISC 2018

Probabilistic numerics: Cockayne, C. Oates, T. Sullivan, and M. Girolami, 2017
RBF collocation methods: R. Schaback and H. Wendland, 2006
Interplays with numerical approximation: Sard, Larkin, Diaconis, Suldin, Kimeldorf and Wahba

GPs: **More theoretically well-founded and with a long history of interplays with numerical approximation but were limited to linear/quasi-linear/time-dependent PDEs**

Generalization of GP methods to arbitrary nonlinear PDEs

Solving and Learning Nonlinear PDEs with Gaussian Processes. 2021.
Y. Chen, B. Hosseini, H. Owhadi, AM. Stuart.
(https://arxiv.org/abs/2103.12959, JCP)

Properties

- Provably convergent for forward problems
- Interpretable and amenable to numerical analysis
- Solve forward and inverse problems
- Inherit the complexity of SOA solvers for dense kernel matrices
- Could be used to develop a theoretical understanding of PINNs

A simple prototypical non-linear PDE

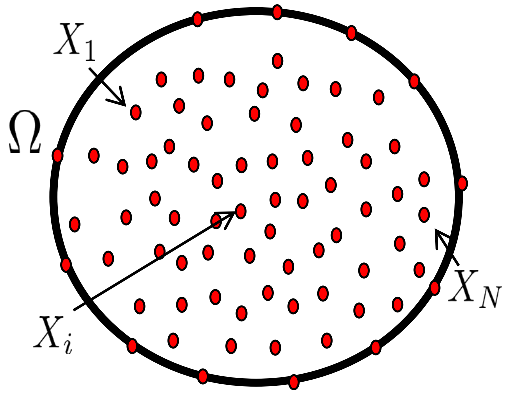
$$\begin{cases} -\Delta u^\dagger + \tau(u^\dagger) = f, & x \in \Omega, \\ u^\dagger = g, & x \in \partial\Omega, \end{cases}$$

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

τ: Such that the PDE has a unique strong solution

Generalizes to arbitrary non-linear PDEs

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



The method

$K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$: Given kernel.

$X_1, \ldots, X_N$: Collocation points on Ω and $\partial\Omega$

Approximate $u^\dagger$ with the minimizer u of

$$\begin{cases} \text{Minimize} & \|u\|_K^2 \\ \text{subject to} & -\Delta u(X_i) + \tau(u(X_i)) = f(X_i), \quad X_i \in \Omega, \\ \text{and} & u(X_i) = g(X_i), \quad X_i \in \partial\Omega, \end{cases}$$

Theorem

Assume that

- K is chosen so that
  - $\mathcal{H} \subset H^s(\Omega)$ for some $s > s^*$, where $s^* = \frac{d}{2} +$ order of PDE (order of PDE$= 2$)
  - $u^\dagger \in \mathcal{H}$
- Fill distance of $\{X_1, \ldots, X_N\}$ goes to zero as $N \to \infty$

Then, as $N \to \infty$

- $u \to u^\dagger$ pointwise in $\bar{\Omega}$
- $u \to u^\dagger$ in $H^t(\Omega)$ for $t < s$

$\mathcal{H}$: RKH space defined by kernel K

Implementation

$$\begin{cases} \text{Minimize} & \|u\|_K^2 \\ \text{subject to} & -\Delta u(X_i) + \tau(u(X_i)) = f(X_i), \quad X_i \in \Omega, \\ \text{and} & u(X_i) = g(X_i), \quad X_i \in \partial\Omega, \end{cases}$$

⇕

$$\begin{cases} \min_{z^{(1)},z^{(2)}} \begin{cases} \min_u \|u\|_K^2 \\ \text{s.t. } u(X_i) = z_i^{(1)} \text{ and } -\Delta u(X_i) = z_i^{(2)} \end{cases} \\ z_i^{(2)} + \tau(z_i^{(1)}) = f(X_i) \text{ for } X_i \in \Omega \\ z_i^{(1)} = g(X_i) \text{ for } X_i \in \partial\Omega \end{cases}$$

⇕

Reduction theorem

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

$$\begin{cases} \min_{z^{(1)},z^{(2)}} z^T K(\phi,\phi)^{-1} z \\ z_i^{(2)} + \tau(z_i^{(1)}) = f(X_i) \text{ for } X_i \in \Omega \\ z_i^{(1)} = g(X_i) \text{ for } X_i \in \partial\Omega \end{cases}$$

$$z = (z^{(1)}, z^{(2)})$$

$$\phi = (\phi^{(1)}, \phi^{(2)})$$

$$\phi_i^{(1)} = \delta_{X_i}$$

$$\phi_i^{(2)} = \delta_{X_i} \circ \Delta$$

$$\big(K(x,\phi)\big)_i = \int K(x,y)\phi_i(y)\,dy$$

$$\big(K(\phi,\phi)\big)_{i,j} = \int \phi_i(x)K(x,y)\phi_j(y)\,dx\,dy$$

$$\begin{cases} \min_{z^{(1)},z^{(2)}} z^T K(\phi,\phi)^{-1} z \\ z_i^{(2)} + \tau(z_i^{(1)}) = f(X_i) \text{ for } X_i \in \Omega \\ z_i^{(1)} = g(X_i) \text{ for } X_i \in \partial\Omega \end{cases}$$

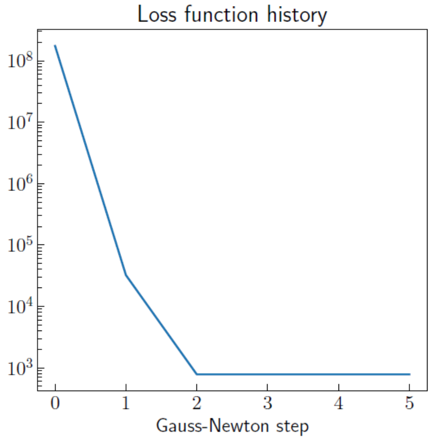
Eliminate $z^{(2)}$

$$\min_{z^{(1)}} \left(z_i^{(1)}, g(X_i), f(X_i) - \tau(z_i^{(1)})\right)^T K(\phi,\phi)^{-1} \left(z_i^{(1)}, g(X_i), f(X_i) - \tau(z_i^{(1)})\right)$$

Gauss-Newton Iteration

$$z_i^{(1),n+1} = z_i^{(1),n} + \delta z_i^{(1),n}$$

$$\min_{\delta z^{(1)}} Z^T K(\phi,\phi)^{-1} Z^T$$



$$Z = \left(z_i^{(1),n} + \delta z_i^{(1),n}, g(X_i), f(X_i) - \tau(z_i^{(1),n}) - \delta z_i^{(1),n} \nabla\tau(z_i^{(1),n})\right)$$

Converges in 2 to 7 steps

Inherits the complexity of fast linear solvers for $K(\phi,\phi)$

[Schäfer, Katzfuss and O., 2020]: $\mathcal{O}\left(N \log^{2d}(\frac{N}{\epsilon})\right)$ complexity

Gauss-Newton Iteration ⟺ Successive linerization of the PDE

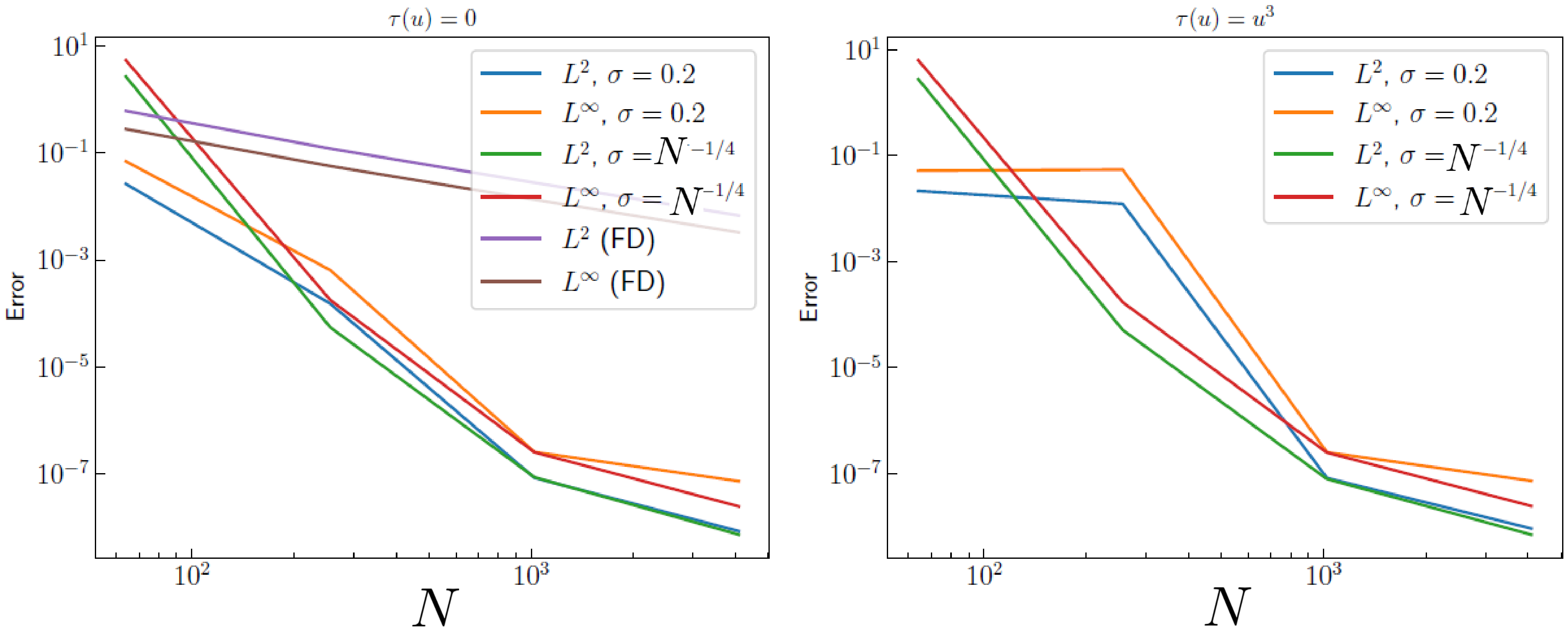
$$\begin{cases} -\Delta u^\dagger + \tau(u^\dagger) = f, & x \in \Omega, \\ u^\dagger = g, & x \in \partial\Omega, \end{cases}$$

$$u^{n+1} = u^n + \delta u^n$$

Given u^n solve for δu^n

$$\begin{cases} -\Delta(u^n + \delta u^n) + \tau(u^n) + \delta u^n \nabla\tau(u^n) = f, & x \in \Omega, \\ u^n + \delta u^n = g, & x \in \partial\Omega, \end{cases}$$

Numerical experiments



$$K(x, x') = \exp\left(-\frac{|x - x'|^2}{\sigma^2}\right)$$

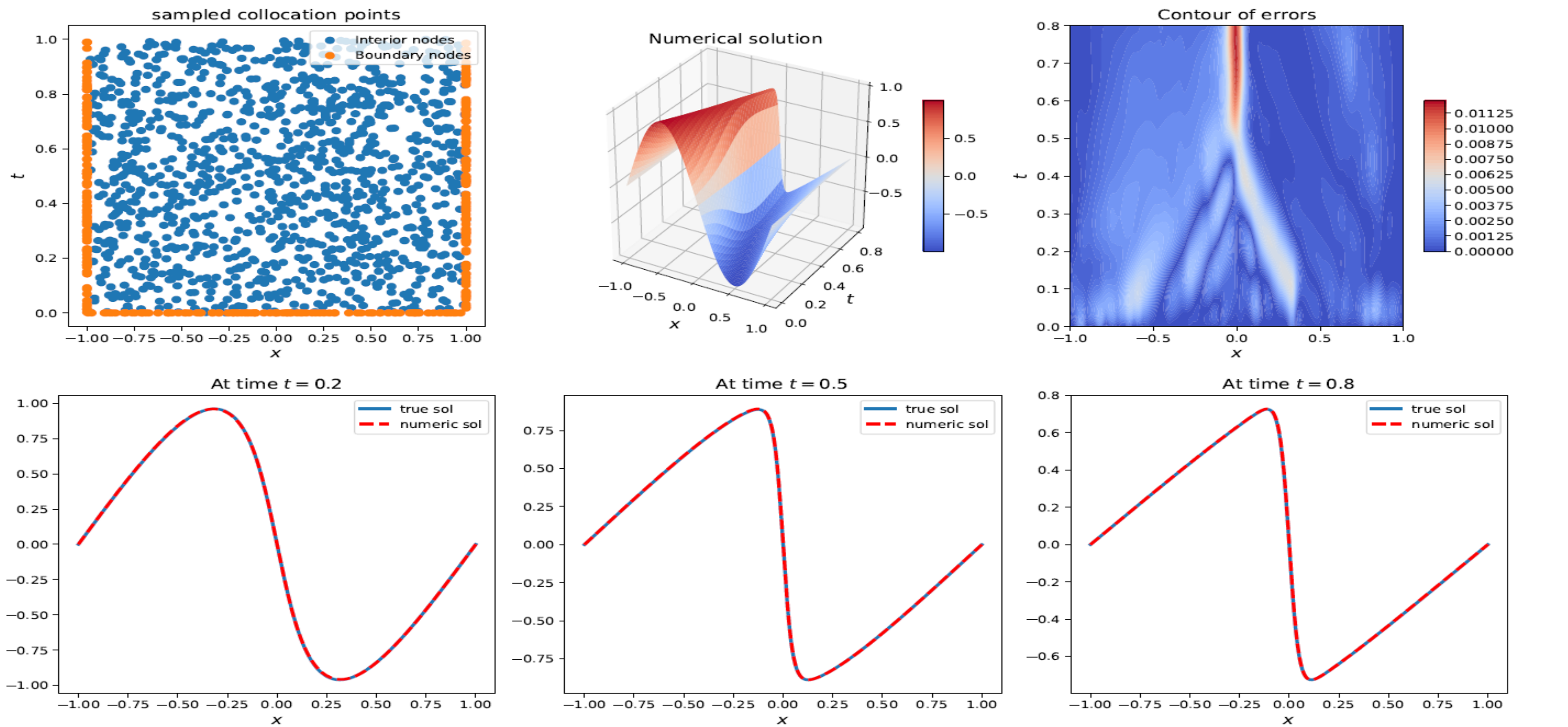
FD: Finite difference

Burger's

$$\partial_t u + u\partial_s u - \nu\partial_s^2 u = 0, \qquad \forall (s,t) \in [-1,1] \times [0,\infty),$$
$$u(s,0) = -\sin(\pi x),$$
$$u(-1,t) = u(1,t) = 0.$$

$$K\big((x,t),(x',t')\big) = \exp\big(-20|x-x'|^2 - 3|t-t'|^2\big)$$

N	600	1200	2400	4800
L^2 error	1.75e-02	7.90e-03	8.65e-04	9.76e-05
L^∞ error	6.61e-01	6.39e-02	5.50e-03	7.36e-04

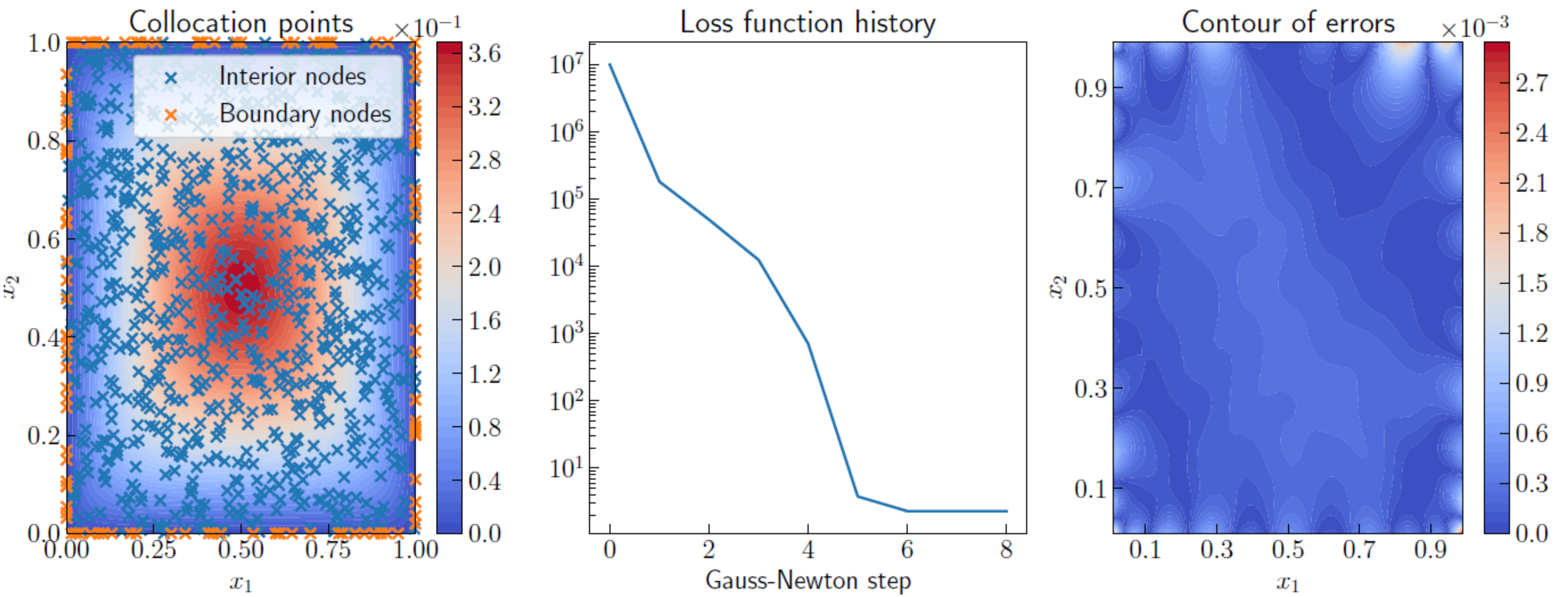


Eikonal

$$\begin{cases} \|\nabla u(x)\|^2 = f(x)^2 + \epsilon \Delta u(x), & \forall x \in \Omega\,, \\ u(x) = 0, & \forall x \in \partial\Omega\,, \end{cases}$$

$$K(x, x') = \exp\left(-\frac{|x-x'|^2}{\sigma^2}\right)$$

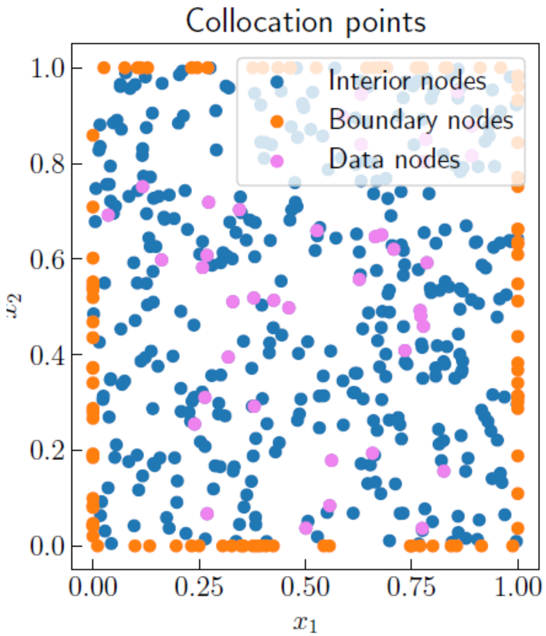
N	1200	1800	2400	3000
L^2 error	3.7942e-04	1.3721e-04	1.2606e-04	1.1025e-04
L^∞ error	5.5768e-03	1.4820e-03	1.3982e-03	9.5978e-04



Inverse Problem

$$\begin{cases} -\operatorname{div}\left(\exp(a)\nabla u\right)(x) = f(x), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega. \end{cases}$$

a, u: Unknown. u observed at pink points.
Problem: Recover a and u.



$$\begin{cases} \text{Minimize} & \|u\|_K^2 + \|a\|_\Gamma^2 \\ \text{subject to} & -\operatorname{div}\left(\exp(a)\nabla u\right)(X_i) = f(X_i), \quad X_i \in \Omega, \\ \text{and} & u(X_i) = Y_i, \quad (X_i, Y_i) \text{ is data point}, \\ \text{and} & u(X_i) = 0, \quad X_i \in \partial\Omega, \end{cases}$$

Inverse Problem

$$\begin{cases} -\operatorname{div}\left(\exp(a)\nabla u\right)(x) = f(x), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega. \end{cases}$$

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