ICLR 2024 Workshop on AI4Differential Equations

Learning Iterative Algorithms to solve PDEs

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Motivation

➡ *Problem statement*

$$\mathcal{N}(u;\gamma) = f \quad \text{in } \Omega, \qquad \mathcal{B}(u) = g \quad \text{on } \partial\Omega.$$

Solve parametric equations with varying parameters (γ), forcing terms (f) or initial/boundary conditions (g) on a given domain Ω with boundary $\partial\Omega$.

➡ *Hypothesis*

✦ We assume access to a dataset of pairs composed of the PDE data (γ, f, g) and the associated solution u on a grid.

➡ *Relation to existing works*

✦ Physics-Informed Neural Networks [1] models the solution u as a Neural Network and uses the residual of the PDE as optimization criteria. Each PDE needs a full training of the solution.

✦ Neural Operators [2] focus on learning the solution operator directly through a single neural network pass using large amount of data.

References

[1] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics

[2] Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Fourier neural operator for parametric partial differential equations, 2020

Framework

➡ *Build an iterative method to solve PDEs with no data*

$$\theta^{k+1} = \mathcal{A}(\theta^k;\ \mathcal{L}_{\text{PDE}}, \gamma, f, g)$$

Ansatz

$$u_\theta(x) = \sum_{i=0}^{N} \theta_i \psi_i(x)$$

B-splines, Fourier, polynomials...

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Physics-Informed criteria

$$\mathcal{L}_{\text{PDE}} = \mathcal{L}_{\text{Res}} + \lambda \mathcal{L}_{\text{BC}},$$

$$\mathcal{L}_{\text{Res}} = \sum_{x_j \in \Omega} |\mathcal{N}(u_\theta;\gamma)(x_j) - f(x_j)|^2,$$

$$\mathcal{L}_{\text{BC}} = \sum_{x_j \in \partial\Omega} |\mathcal{B}(u_\theta)(x_j) - g(x_j)|^2$$

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Update Algorithm

$$\theta^{k+1} = \theta^k - \eta \mathcal{F}_\varrho(\nabla \mathcal{L}_{\text{PDE}}(\theta^k), \gamma, f, g)$$

Gradient descent, Adam...

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➡ *Training based on data*

$$\mathcal{L}_{\text{DATA}} = \frac{1}{M} \sum_{i=1}^{M} ||u_{\theta_L} - u_i||$$

= *Hybrid solver for PDEs*

Algorithm 1: Inference

Data: $\theta^0 \in \mathbb{R}^n$, PDE (γ, f, g)
Result: $\theta^L \in \mathbb{R}^n$
for *k = 0...L-1* **do**
  $\theta^{k+1} = \theta^k - \mathcal{F}_{\varrho^*}(\nabla \mathcal{L}(\theta^k, \gamma, f, g), \gamma, f, g)$
end
return θ_L

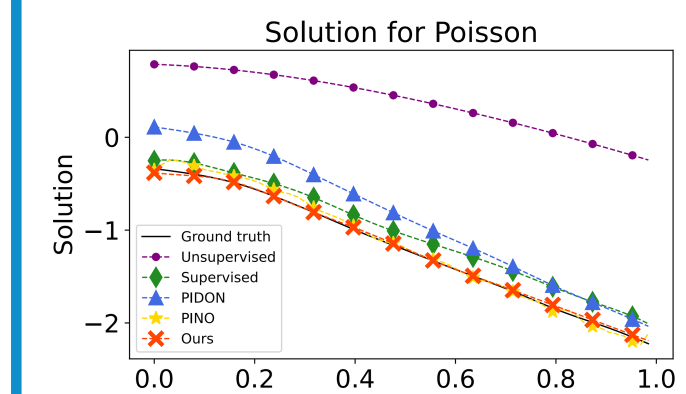
Results

➡ *Training*

	Baseline	1d Helmholtz	1d Poisson	1d + time Advection	2d Darcy-Flow
Unsupervised	*PINNs*	4.26e-1	2.33	2.26e-1	2.31e-1
Supervised	*NN*	9.04e-2	1.09e-1	1.27e-1	7.54e-3
Hybrid	*PIDON*	4.67e-1	8.84e-2	2.26e-1	4.46e-2
	PINO	4.78e-1	5.83e-3	**1.83e-4**	2.80e-2
	Ours	**1.10e-2**	**1.76e-3**	8.40e-3	**6.21e-3**

Table 1: Results - metrics in MSE on the test set.

🡅 Numerical comparison with baselines



🡄 Comparison of trajectories on Poisson

➡ *Test-time Optimization*

5 steps to compute the solution