

A scalable adversarial learning approach using natural gradients for solving partial differential equations

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NPDG algorithm

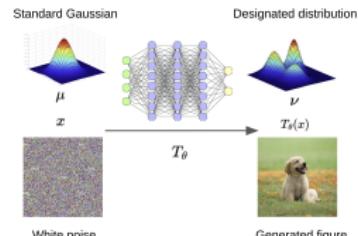
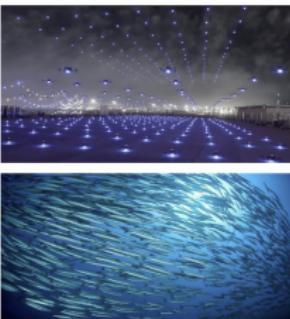
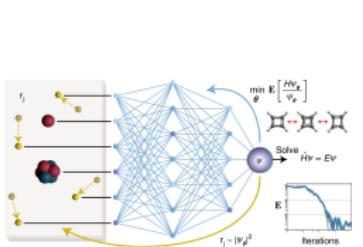
Convergence analysis

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Summary & Future plans

Computing high-dimensional PDEs

- Growing demand for solving high-dimensional partial differential equations (PDEs) across diverse fields¹:



- Due to *curse of dimensionality*, classical numerical methods face challenges.

¹ J. Hermann, Z. Schätle, F. Noé. Deep-neural-network solution of the electronic Schrödinger equation.

Nature Chemistry, 2020.

Deep learning algorithms for PDEs

□ Solving specific PDE:

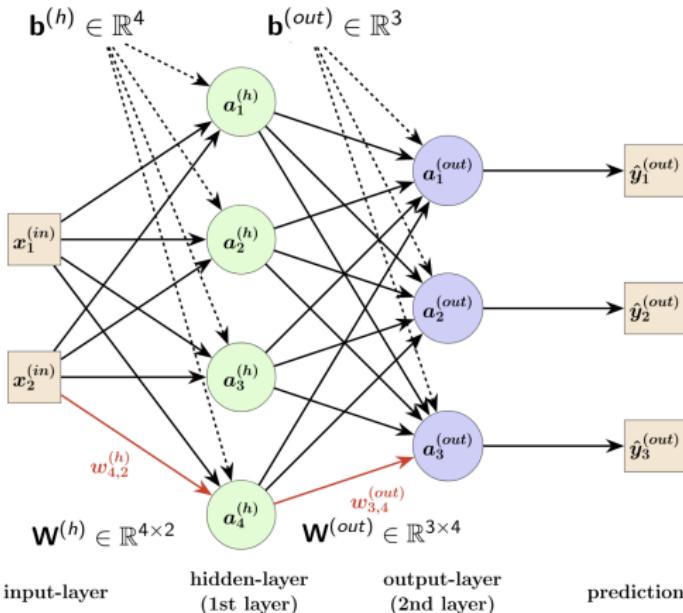
- Minimizing residue:
 - Physics-informed neural networks (**PINNs**) [Raissi, et al. 2019], etc.
- Variational formula:
 - The Deep Ritz method (**DeepRitz**) [Yu, et al. 2017], etc.
- Adversarial training:
 - Weak adversarial networks (**WANs**) [Zang, et al. 2020], etc.
 - Residual-attention-based approach [McCleny, et al. 2020], etc.
- Backward SDE (BSDE) [Han, et al. 2017], etc.
- And many more...

□ Operator learning:

- Deep Operator Network [Lu, et al. 2021], Fourier Neural Operator [Li, et al. 2021], In-context operator learning [Yang, et al. 2023], etc.
- Multi-Operator Multimodal learning [Liu, et al. 2023][Zhang, et al. 2024], etc.

What is a Neural Network?

A fully connected neural network: Multilayer Perceptron (MLP)



$$\text{MLP: } f_\theta(\cdot) : \mathbb{R}^2 \rightarrow \mathbb{R}^3.$$

- Input: $\mathbf{x}^{(in)} \in \mathbb{R}^2$,
- $\mathbf{a}^{(h)} = \sigma(\mathbf{W}^{(h)}\mathbf{x}^{(h)} + \mathbf{b}^{(h)})$,
- $\mathbf{a}^{(out)} = \sigma(\mathbf{W}^{(out)}\mathbf{a}^{(h)} + \mathbf{b}^{(out)})$,
- Output: $f_\theta(\mathbf{x}^{(in)}) = \mathbf{a}^{(out)}$.

σ : nonlinear activation function.

Parameter:

$$\theta = (\mathbf{W}^{(h)}, \mathbf{b}^{(h)}, \mathbf{W}^{(out)}, \mathbf{b}^{(out)}).$$

¹ <https://www.geo.fu-berlin.de/en/v/soga-r/index.html>

Solving PDEs via deep learning

- Poisson equation:

$$-\Delta u = f, \text{ on } \Omega, \quad u = g, \text{ on } \partial\Omega. \quad (1)$$

Assume $\Omega \subset \mathbb{R}^d$ is a bounded open region.

Suppose (1) admits a unique solution u_* .

- We substitute $u(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}$ with a neural network $u_\theta(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}$ with trainable parameter $\theta \in \Theta \subset \mathbb{R}^m$.
- How we compute for an approximation solution $u_\theta(\cdot)$ of (1)?
 - Propose a loss function $L(\theta)$ that quantifies the discrepancy between u_θ and u_* .
 - Optimize $L(\theta)$ w.r.t. θ .

Paradigm of deep learning PDE solver

Algorithm Paradigm of deep learning PDE solver

Require: Given the PDE, neural network u_θ , the loss function $L(\theta)$.

- 1: Initialize the parameters θ , of the neural network(s) $u_\theta(\cdot)$.
- 2: **for** $iter = 1$ to N_{iter} **do**
- 3: Apply Monte-Carlo algorithm to approximate $L(\theta)$,
- 4: Apply auto-differentiation to evaluate $\nabla_\theta L(\theta)$,
- 5: Apply the optimizer with stepsize τ_u to update θ .
- 6: **end for**

Ensure: $u_\theta(\cdot)$

- We mainly focus on $L(\theta)$ and the optimizer in this research.
- u_θ : MLP, ResNet, Exhausted Learning Machine, Tensor NN, KAN, etc.
samples: Uniform, Adaptive, etc.

Key ingredients of a deep learning PDE solver

► Loss function $L(\theta)$

- PINN: Minimize L^2 norm of residue.

$$\begin{aligned} L(\theta) &= \int_{\Omega} | -\Delta u_{\theta} - f|^2 d\mu + \lambda \int_{\partial\Omega} |u_{\theta} - g|^2 d\mu_{\partial\Omega} \\ &= \| -\Delta(u_{\theta} - u_*) \|_{L^2(\Omega)}^2 + \lambda \| u_{\theta} - u_* \|_{L^2(\partial\Omega)}^2. \end{aligned}$$

Pathologies due to high differential order².

- DeepRitz: Optimize the energy functional,

$$\begin{aligned} L(\theta) &= \int_{\Omega} \frac{1}{2} \|\nabla u_{\theta}\|^2 - f u_{\theta} d\mu + \lambda \int_{\partial\Omega} |u_{\theta} - g|^2 d\mu_{\partial\Omega} \\ &= \|\nabla(u_{\theta} - u_*)\|_{L^2(\Omega)}^2 + \text{Const} + \lambda \| u_{\theta} - u_* \|_{L^2(\partial\Omega)}^2. \end{aligned}$$

Only applicable to PDEs with the variational formulas.

²Y. Park, C. Song, and M. Kang. Beyond Derivative Pathology of PINNs: Variable Splitting Strategy with Convergence Analysis. JMLR, 2024

Key ingredients of a deep learning PDE solver

► Loss function $L(\theta)$ (continued)

- WAN: introduce a test function $\varphi_\eta \in H_0^1(\Omega)$, integration by parts yields

$$\begin{aligned} L(\theta, \eta) &= 2 \log \left| \left\langle -\Delta u_\theta - f, \frac{\varphi_\eta}{\|\varphi_\eta\|} \right\rangle \right| + \lambda \|u_\theta - g\|_{L^2(\partial\Omega)} \\ &= \log \left(\frac{\langle \nabla(u_\theta - u_*), \nabla \varphi_\eta \rangle^2}{\|\varphi_\eta\|^2} \right) + \lambda \|u_\theta - u_*\|_{L^2(\partial\Omega)}^2. \end{aligned}$$

We consider

$$\inf_{\theta} \sup_{\eta} L(\theta, \eta).$$

Versatile scheme. But a challenging saddle point problem involving neural networks!

Key ingredients of a deep learning PDE solver

► Optimizer

- First order optimizers:
 - Basic: Stochastic Gradient Descent (SGD)
 - Accelerated: Nesterov method...
 - With per-parameter learning rates: AdaGrad, RMSProp, **Adam**,... **Fast but usually suffers from strong fluctuations.**
- Second order optimizers:
 - Quasi-Newton: **L-BFGS** method. **Unstable in training.**
 - **Natural gradient** method[Amari, 1998]. Broad applications.
Fast convergence, robust w.r.t. random batch training

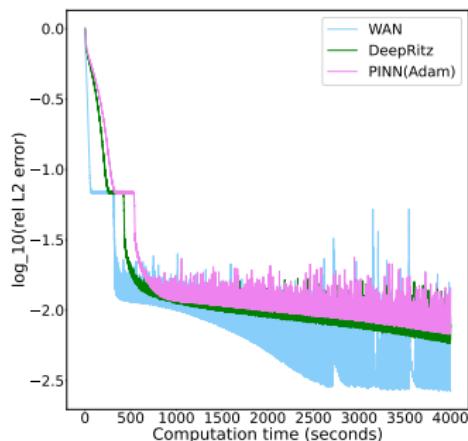
Performances of existing methods

Relative L^2 error vs. wall clock time(s).

- **Sampling:** uniform sampler on Ω and $\partial\Omega$;
- **NN architecture:** Multilayer Perceptron (MLP);

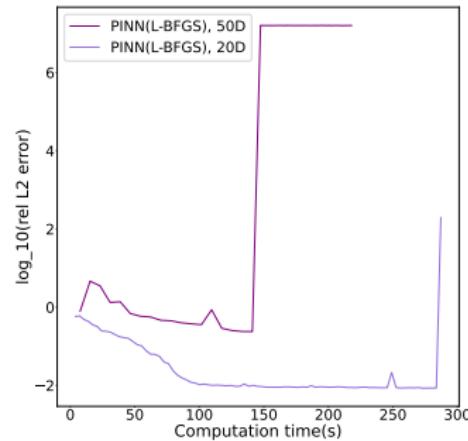
PINN/DeepRitz/WAN + Adam

50D, Poisson equation



PINN + L-BFGS

PINN with L-BFGS (20D 50D)



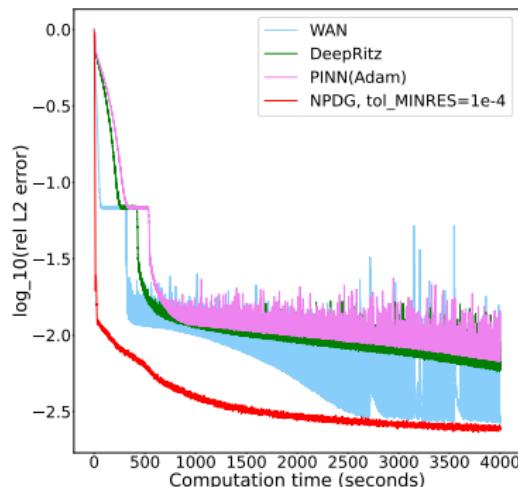
Performances of existing methods

Relative L^2 error vs. wall clock time(s).

- Sampling: uniform sampler on Ω and $\partial\Omega$;
- NN architecture: Multilayer Perceptron (MLP);

**Proposed algorithm:
Stability, Efficiency, Versatility.**

50D, Poisson equation



Related works

Various preconditioned deep-learning PDE-solver

- Multigrid-augmented method: [Azulay, et al. 2022]
- Domain decomposition strategy: [Kopaničáková]
- Incomplete LU preconditioning: [Liu, et al. 2024]
- Gauss-Newton for variational problems: [Hao, et al. 2024]
- **Natural gradient** method for PINNs (Distilling the Hessian for the residual functional for preconditioning):
 - Direct forming and inverting the precondition matrix via least square problem: [Müller, et al. 2023];
 - Utilizing K-FAC approximation: [Dangel, et al. 2024].
- And many more...

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Novel scheme: Adversarial learning scheme + Natural gradient ⇒ Natural Primal-Dual Gradient (NPDG)

Let us derive the algorithm for the Poisson equation:

$$-\Delta u = f, \text{ on } \Omega, \quad u = g, \text{ on } \partial\Omega. \quad (2)$$

- Denote the functional

$$\mathcal{F} : H^2(\Omega) \rightarrow L^2(\Omega) \times L^2(\partial\Omega), \quad u \mapsto (-\Delta u - f, \mathcal{B}u - g),$$

where \mathcal{B} denotes the trace operator.

- It suffices to solve the root-finding problem $\mathcal{F}(u) = 0$.
- This can be reformulated as:

$$\inf_{u \in H^2(\Omega)} \frac{1}{2} \|\mathcal{F}(u)\|_{\mathbb{L}^2}^2 := \frac{1}{2} (\|-\Delta u - f\|_{L^2(\Omega)}^2 + \|\mathcal{B}u - g\|_{L^2(\partial\Omega)}^2).$$

$$\mathbb{L}^2 := L^2(\Omega) \times L^2(\partial\Omega)$$

A saddle point scheme

- Recall Legendre transform: $\frac{1}{2}\|\cdot\|_{\mathbb{L}^2}^2 = \sup_{v \in \mathbb{L}^2} \langle \cdot, v \rangle_{\mathbb{L}^2} - \frac{1}{2}\|v\|_{\mathbb{L}^2}^2$.
- We formulate

$$\begin{aligned} \inf_{u \in H^2(\Omega)} \sup_{\substack{\varphi \in L^2(\Omega), \\ \psi \in L^2(\partial\Omega)}} \mathcal{E}_0(u, \varphi, \psi) &:= \langle \mathcal{F}(u), (\varphi, \psi) \rangle_{\mathbb{L}^2} - \frac{1}{2}\|(\varphi, \psi)\|_{\mathbb{L}^2}^2 \\ &= \langle -\Delta u - f, \varphi \rangle_{L^2(\Omega)} + \langle u - g, \psi \rangle_{L^2(\partial\Omega)} - \frac{1}{2}\|(\varphi, \psi)\|_{\mathbb{L}^2}^2. \end{aligned}$$

- $H_0^1(\Omega)$ is dense in $L^2(\Omega)$, fix $\varphi \in H_0^1(\Omega)$,

$$\begin{aligned} \inf_{u \in H^2(\Omega)} \sup_{\substack{\varphi \in H_0^1(\Omega), \\ \psi \in L^2(\partial\Omega)}} \mathcal{E}_0(u, \varphi, \psi) &:= \int_{\Omega} \nabla u \cdot \nabla \varphi - f \varphi dx + \int_{\partial\Omega} (u - g) \psi d\sigma \\ &\quad - \frac{1}{2} \left(\int_{\Omega} \varphi^2 dx + \int_{\partial\Omega} \psi^2 d\sigma \right). \end{aligned}$$

Leveraging Primal-Dual Hybrid Gradient (PDHG)¹ algorithm

$$\begin{bmatrix} \varphi_{n+1} \\ \psi_{n+1} \end{bmatrix} = \operatorname{argmin}_{\substack{\varphi \in H_0^1(\Omega) \\ \psi \in L^2(\partial\Omega)}} \left\{ \frac{1}{2\tau_\varphi} (\|\varphi - \varphi_n\|_{L^2(\Omega)}^2 + \|\psi - \psi_n\|_{L^2(\partial\Omega)}^2) - \mathcal{E}_0(u_n, \varphi, \psi) \right\},$$

$$\begin{bmatrix} \tilde{\varphi}_{n+1} \\ \tilde{\psi}_{n+1} \end{bmatrix} = \begin{bmatrix} \varphi_{n+1} \\ \psi_{n+1} \end{bmatrix} + \omega \left(\begin{bmatrix} \varphi_{n+1} \\ \psi_{n+1} \end{bmatrix} - \begin{bmatrix} \varphi_n \\ \psi_n \end{bmatrix} \right),$$

$$u_{n+1} = \operatorname{argmin}_{u \in H^2(\Omega)} \left\{ \frac{1}{2\tau_u} (\|u - u_n\|_{L^2(\Omega)}^2 + \|\mathcal{B}u - \mathcal{B}u_n\|_{L^2(\partial\Omega)}^2) + \mathcal{E}_0(u, \tilde{\varphi}_{n+1}, \tilde{\psi}_{n+1}) \right\}.$$

- Proximal Grad Ascent + Extrapolation + Proximal Grad Descent.
- τ_φ, τ_u : stepsizes, ω : extrapolation coefficient.
- Successful applications on conservation laws, reaction-diffusion equations³, etc. (1D, 2D)

¹ M. Zhu, T. Chan. An efficient primal-dual hybrid gradient algorithm for total variation image restoration. UCLA CAM Report, 2008.

A. Chambolle, T. Pock. A first-order primal-dual algorithm for convex problems with applications to imaging. JMIV, 2011.

³ Shu Liu, Siting Liu, Stanley Osher, Wuchen Li. A first-order computational algorithm for reaction-diffusion type equations via primal-dual hybrid gradient method. JCP, 2023.

III-conditioned problem and its preconditioning

Experience gained from classical methods:

- Solve Poisson equation on $\Omega = [0, 1]$ with finite difference scheme.
Suppose Ω is discretized into $N_x + 1$ subintervals.

- Denote $A = \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \in \mathbb{R}^{N_x \times N_x}$ as discrete Laplace.

- Root-finding problem $Au - b = 0$.
- Assoc. saddle point problem: $\min_u \max_p \left\{ p^\top (Au - b) - \frac{1}{2} \|p\|^2 \right\}$.
- PDHG algorithm yields the convergence rate $\sqrt{1 - \frac{c}{\kappa(A)^2}} = 1 - \mathcal{O}\left(\frac{1}{N_x^4}\right)$
($\kappa(A) = \mathcal{O}(N_x^2)$). **Very slow convergence!**
- Remedy:** Find an easy-to-invert precondition matrix $M \approx A$ and consider $M^{-1}Au - M^{-1}b = 0$.

Introduce preconditioning

- PDHG algorithm suffers from the ill-conditioning of $\mathcal{F}(u)$.
- How do we apply the precondition operator, say, Δ^{-1} to $\mathcal{F}(u)$? How to realize the computation? 🤔
Seems intractable.
- 💡 Preconditioning on metric terms of the proximal steps:

$$\|u - u_n\|_{L^2(\Omega)}^2 \quad \text{replaced by} \quad \|\mathcal{M}_u u - \mathcal{M}_u u_n\|_{L^2(\Omega)}^2.$$

$$\|\varphi - \varphi_n\|_{L^2(\Omega)}^2 \quad \text{replaced by} \quad \|\mathcal{M}_\varphi \varphi - \mathcal{M}_\varphi \varphi_n\|_{L^2(\Omega)}^2.$$

\mathcal{M}_u , \mathcal{M}_φ are precondition operators for u , φ .

- How to pick \mathcal{M}_u , \mathcal{M}_φ ?

Key idea:

- Recall u_* is the solution to (2), and $-\Delta u_* = f$,

$$\begin{aligned} \langle \mathcal{F}(u), (\varphi, \psi) \rangle_{\mathbb{L}^2} &= \int_{\Omega} (-\Delta u - f)\varphi \, dx + \int_{\partial\Omega} (u - g)\psi \, d\sigma \\ &= \int_{\Omega} (\nabla u - \nabla u_*) \cdot \nabla \varphi \, dx + \int_{\partial\Omega} (\mathcal{B}u - \mathcal{B}u_*)\psi \, d\sigma. \\ &= \left\langle \underbrace{\begin{pmatrix} \nabla u \\ \mathcal{B}u \end{pmatrix}}_{\mathbf{u}} - \underbrace{\begin{pmatrix} \nabla u_* \\ \mathcal{B}u_* \end{pmatrix}}_{\mathbf{u}_*}, \underbrace{\begin{pmatrix} \nabla \varphi \\ \psi \end{pmatrix}}_{\Phi} \right\rangle_{\mathbb{L}^2} \end{aligned}$$

- We modify $\mathcal{E}_0(u, \varphi, \psi)$ as:

$$\begin{aligned} \mathcal{E}(u, \varphi, \psi) &:= \langle \mathcal{F}(u), (\varphi, \psi) \rangle_{\mathbb{L}^2} - \frac{1}{2} \left(\int_{\Omega} \|\nabla \varphi\|^2 \, dx + \int_{\partial\Omega} \psi^2 \, d\sigma \right) \\ &= \langle \mathbf{U} - \mathbf{U}_*, \Phi \rangle_{\mathbb{L}^2} - \frac{1}{2} \|\Phi\|_{\mathbb{L}^2}^2. \end{aligned}$$

- $\|\mathbf{U} - \mathbf{U}_n\|_{\mathbb{L}^2}^2 = \|\nabla u - \nabla u_n\|_{L^2(\Omega)}^2 + \|\mathcal{B}u - \mathcal{B}u_n\|_{L^2(\partial\Omega)}^2$.
- This motivates us to pick $\mathcal{M}_u = \nabla$, and similarly, $\mathcal{M}_\varphi = \nabla$.

PDHG with preconditioning

The preconditioned PDHG for solving (2) yields

$$\begin{bmatrix} \varphi_{n+1} \\ \psi_{n+1} \end{bmatrix} = \operatorname{argmin}_{\substack{\varphi \in H_0^1(\Omega) \\ \psi \in L^2(\partial\Omega)}} \left\{ \frac{1}{2\tau_\varphi} (\|\nabla \varphi - \nabla \varphi_n\|_{L^2(\Omega)}^2 + \|\psi - \psi_n\|_{L^2(\partial\Omega)}^2) - \mathcal{E}(u_n, \varphi, \psi) \right\},$$

$$\begin{bmatrix} \tilde{\varphi}_{n+1} \\ \tilde{\psi}_{n+1} \end{bmatrix} = \begin{bmatrix} \varphi_{n+1} \\ \psi_{n+1} \end{bmatrix} + \omega \left(\begin{bmatrix} \varphi_{n+1} \\ \psi_{n+1} \end{bmatrix} - \begin{bmatrix} \varphi_n \\ \psi_n \end{bmatrix} \right),$$

$$u_{n+1} = \operatorname{argmin}_{u \in H^2(\Omega)} \left\{ \frac{1}{2\tau_u} (\|\nabla u - \nabla u_n\|_{L^2(\Omega)}^2 + \|\mathcal{B}u - \mathcal{B}u_n\|_{L^2(\partial\Omega)}^2) + \mathcal{E}(u, \tilde{\varphi}_{n+1}, \tilde{\psi}_{n+1}) \right\}.$$

- The algorithm is at functional level.
- Set $u = u_\theta$, $\varphi = \varphi_\eta$, $\psi = \psi_\xi$ as neural networks.
- Instead of updating u, φ, ψ , we update parameters $\theta \in \mathbb{R}^{m_\theta}$, $\eta \in \mathbb{R}^{m_\eta}$, $\xi \in \mathbb{R}^{m_\xi}$.

PDHG with preconditioning

Preconditioned PDHG for neural networks

$$\begin{bmatrix} \eta^{n+1} \\ \xi^{n+1} \end{bmatrix} = \operatorname{argmin}_{\substack{\eta \in \Theta_\eta \\ \xi \in \Theta_\xi}} \left\{ \frac{1}{2\tau_\varphi} (\|\nabla \varphi_\eta - \nabla \varphi_{\eta^n}\|_{L^2(\Omega)}^2 + \|\psi_\xi - \psi_{\xi^n}\|_{L^2(\partial\Omega)}^2) - \mathcal{E}(u_{\theta^n}, \varphi_\eta, \psi_\xi) \right\},$$

$$\begin{bmatrix} \tilde{\varphi}^{n+1} \\ \tilde{\psi}^{n+1} \end{bmatrix} = \begin{bmatrix} \varphi_{\eta^{n+1}} \\ \psi_{\xi^{n+1}} \end{bmatrix} + \omega \left(\begin{bmatrix} \varphi_{\eta^{n+1}} \\ \psi_{\xi^{n+1}} \end{bmatrix} - \begin{bmatrix} \varphi_{\eta^n} \\ \psi_{\xi^n} \end{bmatrix} \right),$$

$$\theta^{n+1} = \operatorname{argmin}_{\theta \in \Theta_\theta} \left\{ \frac{1}{\tau_u} (\|\nabla u_\theta - \nabla u_{\theta^n}\|_{L^2(\Omega)}^2 + \|\mathcal{B}u_\theta - \mathcal{B}u_{\theta^n}\|_{L^2(\partial\Omega)}^2) + \mathcal{E}(u_\theta, \tilde{\varphi}^{n+1}, \tilde{\psi}^{n+1}) \right\}.$$

- The algorithm is at functional level.
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PDHG with preconditioning

Preconditioned PDHG for neural networks

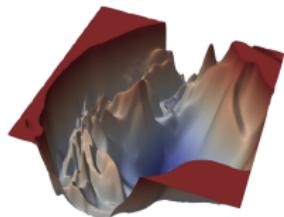
$$\begin{aligned} \begin{bmatrix} \eta^{n+1} \\ \xi^{n+1} \end{bmatrix} &= \operatorname{argmin}_{\eta, \xi} \left\{ \frac{1}{2\tau_\varphi} \underbrace{\left(\|\nabla \varphi_\eta - \nabla \varphi_{\eta^n}\|_{L^2(\Omega)}^2 + \|\psi_\xi - \psi_{\xi^n}\|_{L^2(\partial\Omega)}^2 \right)}_{d_2^2((\eta, \xi), (\eta^n, \xi^n))} - \mathcal{E}(u_{\theta^n}, \varphi_\eta, \psi_\xi) \right\}, \\ \begin{bmatrix} \tilde{\varphi}^{n+1} \\ \tilde{\psi}^{n+1} \end{bmatrix} &= \begin{bmatrix} \varphi_{\eta^{n+1}} \\ \psi_{\xi^{n+1}} \end{bmatrix} + \omega \left(\begin{bmatrix} \varphi_{\eta^{n+1}} \\ \psi_{\xi^{n+1}} \end{bmatrix} - \begin{bmatrix} \varphi_{\eta^n} \\ \psi_{\xi^n} \end{bmatrix} \right), \\ \theta^{n+1} &= \operatorname{argmin}_\theta \left\{ \frac{1}{2\tau_u} \underbrace{\left(\|\nabla u_\theta - \nabla u_{\theta^n}\|_{L^2(\Omega)}^2 + \|\mathcal{B}u_\theta - \mathcal{B}u_{\theta^n}\|_{L^2(\partial\Omega)}^2 \right)}_{d_1^2(\theta, \theta^n)} + \mathcal{E}(u_\theta, \tilde{\varphi}^{n+1}, \tilde{\psi}^{n+1}) \right\}. \end{aligned}$$

- The algorithm is at functional level.
- Set $u = u_\theta$, $\varphi = \varphi_\eta$, $\psi = \psi_\xi$ as neural networks.
- Instead of updating u, φ, ψ , we update parameters $\theta \in \mathbb{R}^{m_\theta}, \eta \in \mathbb{R}^{m_\eta}, \xi \in \mathbb{R}^{m_\xi}$.

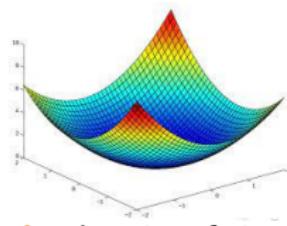
Key idea:

$$-\mathcal{E} = -\mathcal{E}(u_\theta, \varphi_\eta, \psi_\xi)$$

$$-\mathcal{E} = -\langle \mathbf{U}_\theta - \mathbf{U}_*, \Phi_{\eta, \xi} \rangle_{\mathbb{L}^2} + \frac{1}{2} \|\Phi_{\eta, \xi}\|_{\mathbb{L}^2}^2$$



(η, ξ) 's point of view⁴.



$\Phi_{\eta, \xi}$'s point of view.

The intrinsic distance between (η, ξ) and (η^n, ξ^n) should be induced by

$$d_2((\eta, \xi), (\eta^n, \xi^n)) = \|\Phi_{\eta, \xi} - \Phi_{\eta^n, \xi^n}\|_{\mathbb{L}^2}^2,$$

rather than ℓ^2 distance $\|(\eta, \xi) - (\eta^n, \xi^n)\|_2$.

⁴

H. Li, Z. Xu, G. Taylor, C. Studer, T. Goldstein. Visualizing the Loss Landscape of Neural Nets. Advances in neural information processing systems, 2018.

Natural Gradient Descent

- The update of θ^{n+1} :

$$\theta^{n+1} = \operatorname{argmin}_{\theta \in \mathbb{R}^{m_\theta}} \left\{ \frac{1}{2\tau_u} (\textcolor{blue}{d}_1^2(\theta, \theta^n) + \mathcal{E}(u_\theta, \tilde{\varphi}_{n+1}, \tilde{\psi}_{n+1})) \right\}.$$

- The *time-explicit* scheme:

$$\theta^{n+1} = \theta^n - \tau_u \underbrace{\mathbf{M}_p(\theta^n)^\dagger \nabla_{\theta} \mathcal{E}(u_{\theta^n}, \tilde{\varphi}_{n+1}, \tilde{\psi}_{n+1})}_{\text{Nature Gradient}},$$

$\mathbf{M}_p(\theta^n)$ is induced by:

$$d_1^2(\theta, \theta^n) = \|\nabla u_\theta - \nabla u_{\theta^n}\|_{L^2(\Omega)}^2 + \|\mathcal{B} u_\theta - \mathcal{B} u_{\theta^n}\|_{L^2(\partial\Omega)}^2 \approx (\theta - \theta^n)^\top \mathbf{M}_p(\theta^n) (\theta - \theta^n).$$

$$(\mathbf{M}_p(\theta))_{ij} = \int_{\Omega} \frac{\partial}{\partial \theta_i} \nabla u_\theta(x) \cdot \frac{\partial}{\partial \theta_j} \nabla u_\theta(x) dx + \int_{\partial\Omega} \frac{\partial u_\theta(y)}{\partial \theta_i} \frac{\partial u_\theta(y)}{\partial \theta_j} d\sigma.$$

NPDG algorithm

We update ξ^{n+1} and θ^{n+1} by similar techniques. This yields the **Natural Primal-Dual Gradient** (NPDG) algorithm.

$$\begin{bmatrix} \eta^{n+1} \\ \xi^{n+1} \end{bmatrix} = \begin{bmatrix} \eta^n \\ \xi^n \end{bmatrix} + \tau_\varphi \begin{bmatrix} \textcolor{orange}{M_d}(\eta^n)^\dagger \nabla_\eta \mathcal{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n}) \\ \textcolor{orange}{M}_{bdd}(\xi^n)^\dagger \nabla_\xi \mathcal{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n}) \end{bmatrix},$$
$$\begin{bmatrix} \tilde{\varphi}_{n+1} \\ \tilde{\psi}_{n+1} \end{bmatrix} = \begin{bmatrix} \varphi_{\eta^{n+1}} \\ \psi_{\xi^{n+1}} \end{bmatrix} + \omega \left(\begin{bmatrix} \varphi_{\eta^{n+1}} \\ \psi_{\xi^{n+1}} \end{bmatrix} - \begin{bmatrix} \varphi_{\eta^n} \\ \psi_{\xi^n} \end{bmatrix} \right),$$
$$\theta^{n+1} = \theta^n - \tau_u \textcolor{blue}{M_p}(\theta^n)^\dagger \nabla_\theta \mathcal{E}(u_{\theta^n}, \tilde{\varphi}_{n+1}, \tilde{\psi}_{n+1}).$$

- More general cases:

$$\mathcal{L}u + \mathcal{N}u = f \text{ on } \Omega, \quad \mathcal{B}u = g \text{ on } \partial\Omega,$$

in which linear operator \mathcal{L} splits as $\textcolor{orange}{D}_d^* \widetilde{\mathcal{L}} \textcolor{blue}{D}_p$. We pick $\mathcal{M}_u = \textcolor{blue}{D}_p$, $\mathcal{M}_\varphi = \textcolor{orange}{D}_d$ and apply the NPDG algorithm.

- Monge-Ampère equation arising from L^2 Optimal Transport problem.

Implementation

- Computation of $\nabla_{\eta} \mathcal{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n})$:
 - Monte-Carlo Approximation + Auto-Differentiation
- Evaluation of Natural Gradient $M_d(\eta^n)^\dagger \nabla_{\eta} \mathcal{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n})$:
 - ! $M_d(\eta^n)$ is prohibitively **expensive** to compute.
 - Krylov subspace iteration: **MINRES** (Minimal residual) method: Only requires **matrix-vector** multiplication.
 - **Matrix-vector** multiplication $M_d(\eta^n)\mathbf{v}$ can be efficiently computed using auto-differentiations.

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Time-continuous NPDG algorithm

- **NPDG flow:** time-continuous version of the NPDG algorithm:

$$\begin{aligned}\dot{\eta}_t &= M_d(\eta_t)^\dagger \frac{\partial}{\partial \eta} \mathcal{E}(u_{\theta_t}; \varphi_{\eta_t}, \psi_{\xi_t}), \\ \dot{\xi}_t &= M_{bdd}(\xi_t)^\dagger \frac{\partial}{\partial \xi} \mathcal{E}(u_{\theta_t}, \varphi_{\eta_t}, \psi_{\xi_t}), \\ \dot{\theta}_t &= -M_p(\theta_t)^\dagger \frac{\partial}{\partial \theta} \mathcal{E}(u_{\theta_t}; \varphi_t + \gamma \dot{\varphi}_t, \psi_t + \gamma \dot{\psi}_t),\end{aligned}$$

as $\tau_u, \tau_\varphi \rightarrow 0$ and $\omega \tau_\varphi \rightarrow \gamma > 0$.

- Consider the linear equation:

$$\mathcal{L}u = f, \text{ on } \Omega, \quad \mathcal{B}u = g, \text{ on } \partial\Omega, \tag{3}$$

$\mathcal{L} = \mathcal{D}_d^* \tilde{\mathcal{L}} \mathcal{D}_p$. (For example, $-\Delta = (\nabla)^* \text{ Id } \nabla$.)

Suppose (3) admits unique classical solution u_* .

- Apply NPDG flow with $\mathcal{M}_\varphi = \mathcal{D}_d$, $\mathcal{M}_u = \mathcal{D}_p$.

A posteriori convergence analysis of NPDG flow⁵

- Suppose $\{(\theta_t, \eta_t, \xi_t)\}_{0 \leq t \leq T}$ solves the NPDG-flow.
- Denote $\tilde{\kappa}$ as the condition number of $\tilde{\mathcal{L}}$ w.r.t. L^2 norm.
- Assume α, β_1, β_2 describe the approximation quality of tangent subspaces spanned by neural networks $u_\theta, \varphi_\eta, \psi_\xi$.

Suppose $\alpha + \beta_1 < \frac{1}{\tilde{\kappa}^2}$, $\beta_2 < 1$, if γ further satisfies

$$\left(\frac{1}{\tilde{\kappa}^2} - (\alpha + \beta_1) \right) \cdot (1 - \beta_2) > \frac{((1 + \beta_1)\gamma + \beta_2 + \alpha|1 - \gamma|)^2}{4\gamma}.$$

There exists $r > 0$ depending on $\tilde{\kappa}$, such that, for $0 \leq t \leq T$,

$$\|\mathcal{M}_u(u_{\theta_t} - u_*)\|_{L^2(\Omega)}^2 + \|\mathcal{B}(u_{\theta_t} - u_*)\|_{L^2(\partial\Omega)}^2 \leq 2C_0 \exp(-rt).$$

⁵

S. Liu, S. Osher, W. Li. A Natural Primal-Dual Hybrid Gradient Method for Adversarial Neural Network Training on Solving Partial Differential Equations. arXiv:2411.06278, 2024.

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Elliptic equation with variable coefficients $d = 20$

- We consider:

$$-\nabla \cdot (\kappa(x) \nabla u(x)) = f(x), \quad u(y) = g(y) \text{ on } \partial\Omega.$$

- $\Omega = [-1, 1]^d$ with even dimension d .
- $\kappa(x) = \frac{x^\top \Lambda x + 1}{2}$, with $\Lambda = \text{diag}(\lambda_0, \lambda_1, \dots, \lambda_0, \lambda_1)$, $\lambda_0 = 1, \lambda_1 = 4$.
- $f(x) = -\frac{\text{Tr}(\Lambda^{-1})}{2}(x^\top \Lambda x + 1) - \|x\|^2$, $g(y) = \frac{1}{2}y^\top \Lambda^{-1}y$.
- The solution $u_*(x) = \frac{1}{2}x^\top \Lambda^{-1}x$.
- Pick u, φ, ψ as MLPs with hidden dimension 256, number of hidden layers 4, and $\text{softplus}(\cdot)^6$ activation function.
- $\mathcal{M}_p = \nabla$, $\mathcal{M}_d = \nabla$.

⁶ $\text{softplus}(x) = \frac{1}{\beta} \log(1 + \exp(\beta x))$, $\beta = \frac{1}{4}$.

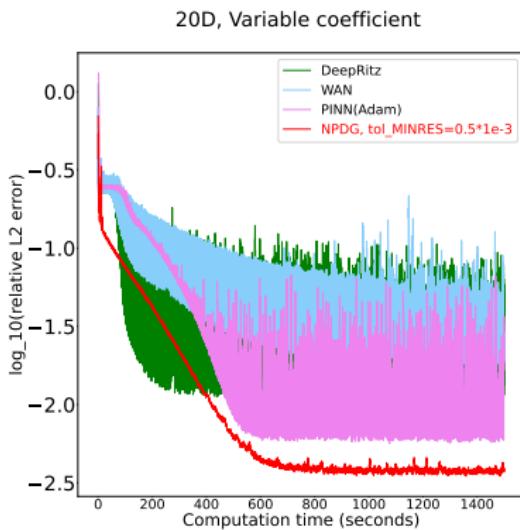


Figure: Plots of relative L^2 error vs. wall clock time(s), comparing NPDG with PINN, DeepRitz, and WAN.

- **Fix NN architecture** as MLP and use the **same sample size** for all tested methods.

Performance comparison on different types of PDEs

- Fix NN architecture as MLP. Use the same sample size.
- We test PINN, DeepRitz, and WAN using different learning rates and present the *optimal* performance.

Equation	δ	d	PINN(Adam)	Deep Ritz	WAN	NPDG
Poisson $-\Delta u = f$	0.005	10D	44.83	43.45	51.65	40.98
		20D	160.82	183.49	460.12	110.42
		50D	1989.06	1452.29	2117.24	821.24
VarCoeff $-\nabla \cdot (\kappa \nabla u) = f$	0.005	10D	—	—	—	281.26
		20D	—	—	—	998.09
		50D	—	—	—	13731.33
Nonlinear Elliptic $\frac{1}{2} \ \nabla u\ ^2 + V = \Delta u$	0.05	5D	—	N.A.	—	1894.89

Figure: GPU time (s) required to reach relative L^2 accuracy δ when different methods are applied to PDEs with different dimensions posed with Dirichlet boundary condition. (“—” the accuracy is never achieved; “N.A.” method is not applicable.)

Monge-Ampère equation arising from L^2 -OT problem

- ρ_0, ρ_1 – probability density functions.
- Monge-Ampère equation:

$$|\det(D^2u(x))| = \frac{\rho_0(x)}{\rho_1(\nabla u(x))}, \quad \rho_0 dx - a.e., \quad u \text{ is convex on } \mathbb{R}^d.$$

- L^2 Optimal Transport (OT) problem (Monge problem):

$$\min_{T: \mathbb{R}^d \rightarrow \mathbb{R}^d, T_\sharp \mu = \nu} \int_{\mathbb{R}^d} \|T(x) - x\|^2 d\mu. \quad \mu = \rho_0 dx, \quad \nu = \rho_1 dx$$

Fact: OT map $T_* = \nabla u_*$, with u_* solves the Monge-Ampère equation.

To compute $T_* = \nabla u_*$, apply **NPDG** algorithm to the **primal-dual** problem assoc. with the L^2 OT problem.

OT from Gaussian to Gaussian mixture in \mathbb{R}^{50}

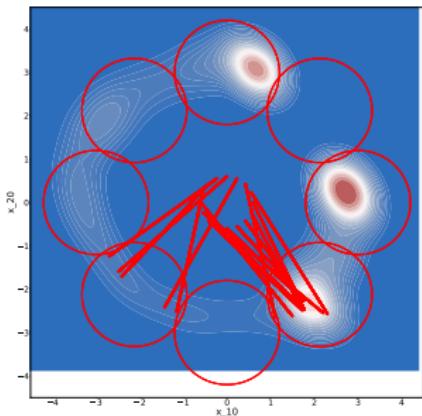
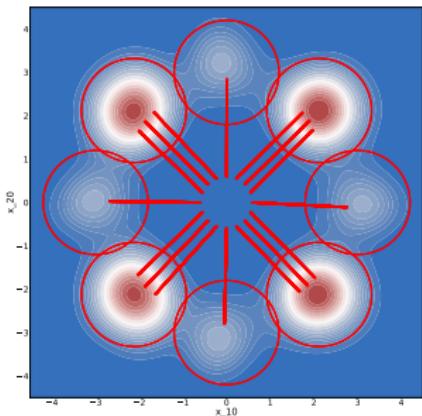


Figure: Plots of the pushforwarded density $T_{\theta} \# \rho_0$ by Kernel Density Estimation (KDE). **Left:** NPDG method; **Right:** Primal-Dual algorithm using Adam⁷. **Red lines** indicate the computed OT map $T_{\theta}(\cdot)$.

⁷

Jiaojiao Fan*, Shu Liu*, Shaojun Ma, Haomin Zhou, Yongxin Chen. Neural Monge Map estimation and its applications. TMLR, 2023

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Summary of the research

NPDG = Adversarial training of NNs + Natural Gradients.

- Adversarial training:
 - Computational efficiency: lower order of differentiation.
 - Versatility: Applicable to PDEs possessing saddle point scheme.
- Natural Gradient:
 - Respect the mathematical nature: PDE-informed precondition.
 - Fast & Stable convergence.

On-going & future plans

Ongoing: improvements of NPDG algorithm:

- Jacobi-free method: Finite difference instead of auto-differentiation.
- Kronecker-Factored Approximate Curvature (KFAC) method for more efficient evaluation of natural gradient⁸.

⁸ Felix Dangel, Johannes Müller, and Marius Zeinhofer. Kronecker-Factored Approximate Curvature for Physics-Informed Neural Networks. NeurIPS, 2024.

NPDG: Efficient scientific machine learning (SciML) paradigm.

Large-scale saddle point/constrained optimization problems:

- Enhancing the training of Generative Adversarial Networks (GANs).
- Optimal Transport (Monge) problem with general cost⁹.
- High-dimensional Mean-Field Control problems.

⁹ Jiaojiao Fan*, Shu Liu*, Shaojun Ma, Haomin Zhou, Yongxin Chen. Neural Monge Map estimation and its applications. TMLR, 2023

Reference:

Shu Liu, Stanley Osher, Wuchen Li. A Natural Primal-Dual Hybrid Gradient Method for Adversarial Neural Network Training on Solving Partial Differential Equations. arXiv:2411.06278, 2024.

We welcome any comments and suggestions.

Thank you!