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

Shu Liu (UCLA), Stanley Osher (UCLA), Wuchen Li (U of SC)

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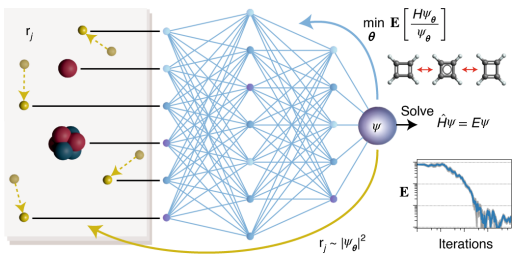
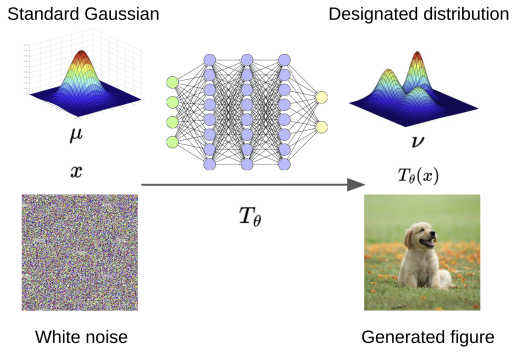
Computing high-dimensional PDEs

- Growing demand for solving high-dimensional partial differential equations (PDEs) across diverse fields[1]:





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

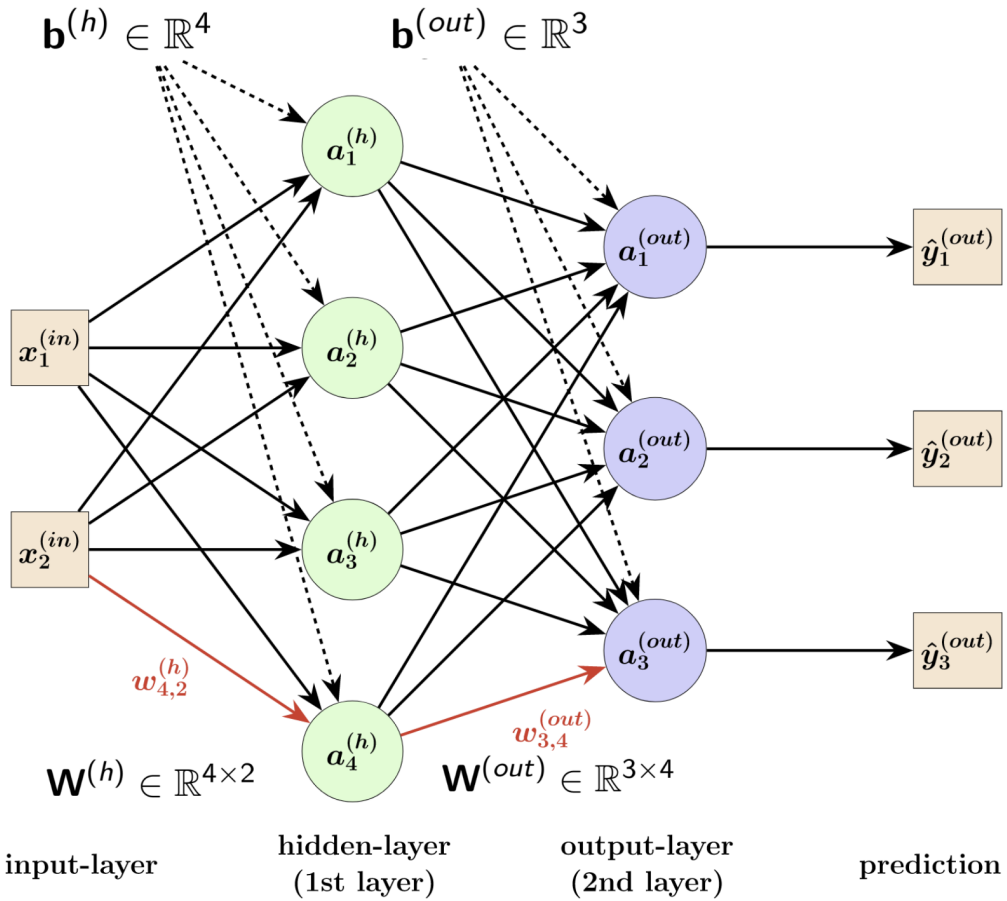
[1] J. Hermann, Z. Schätzle, F. Noé. Deep-neural-network solution of the electronic Schrödinger equation. Nature Chemistry, 2020.

Deep learning algorithms for PDEs

- **Solving specific PDE**:
  - Minimizing residue:
    - Physics-informed neural networks (**PINN**s) [Raissi, et al. 2019], etc.
  - Variational formula:
    - The Deep Ritz method (**DeepRitz**) [Yu, et al. 2017], etc.
  - Adversarial training:
    - Weak adversarial networks (**WAN**s) [Zang, et al. 2020], etc.
    - Residual-attention-based approach [McClenny, et al. 2020], etc.
  - And many more...
- Operator learning:
  - Deep Operator Network [Lu, et al. 2021], training DeepONet [Lee, et al. 2023], 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]...

What is a Neural Network?

A fully connected neural network: Multilayer Perceptron (MLP)



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

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

σ: nonlinear activation function.

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

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

Solving PDEs using deep learning

- Poisson equation:

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

  Assume $\Omega \subset \mathbb{R}^d$ is a bounded open region.
  Suppose (1) admits a unique solution u_*.

- Substitute $u(\cdot) : \mathbb{R}^d \to \mathbb{R}$ with neural network $u_\theta(\cdot) : \mathbb{R}^d \to \mathbb{R}$.
- Find an approximation solution $u_\theta(\cdot)$:
  - Propose a loss function $L(\theta)$ that quantifies the discrepancy between u_θ and u_*.
  - Optimize $L(\theta)$ w.r.t. θ.

Loss function

- Loss function $L(\theta)$
  - PINN: Minimize L^2 norm of residue.

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

Pathologies due to high order differential operator[2].

  - DeepRitz: Optimize the energy functional,

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

Only applicable to PDEs with the variational formulas.

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

Loss function

- Loss function $L(\theta)$ (continued)
  - Adversarial learning (Weak Adversarial Network):
    Introduce a test function $\varphi_\eta \in H_0^1(\Omega)$, integration by parts yields

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

We consider

$$\inf_\theta \sup_\eta \; L(\theta,\eta).$$

Versatility

Challenging saddle point problem involving neural networks!

Optimizer

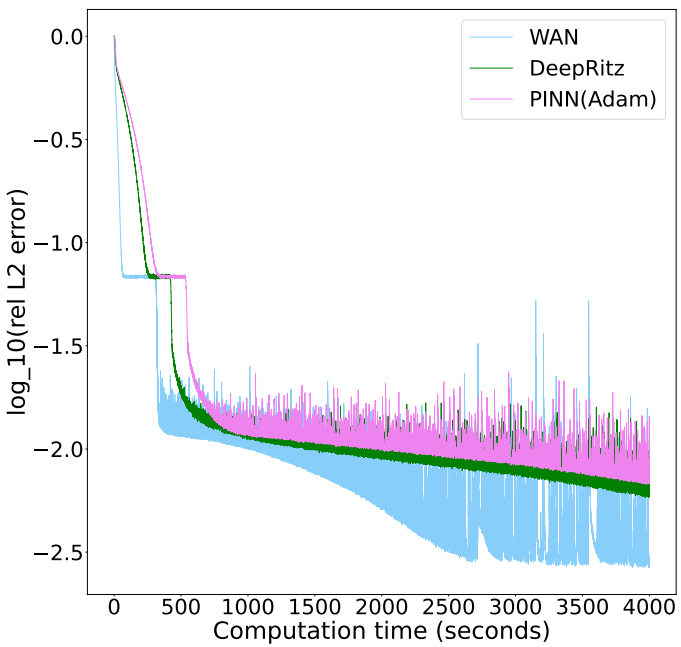
- Optimizer for large-scale machine learning problems
  - First order optimizers:
    - Basic: Stochastic Gradient Descent (SGD).
    - With per-parameter learning rates: AdaGrad [Duchi, et al. 2011], RMSProp [Tieleman, et al. 2012], **Adam** [Kingma, et al. 2014],... Suffer from strong fluctuations.
  - Second order optimizers:
    - Hessian-free method. [Martens, 2010]
    - Quasi-Newton: **L-BFGS** method. [Liu, et al. 1989] Unstable using random batches.

Performances of existing methods

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

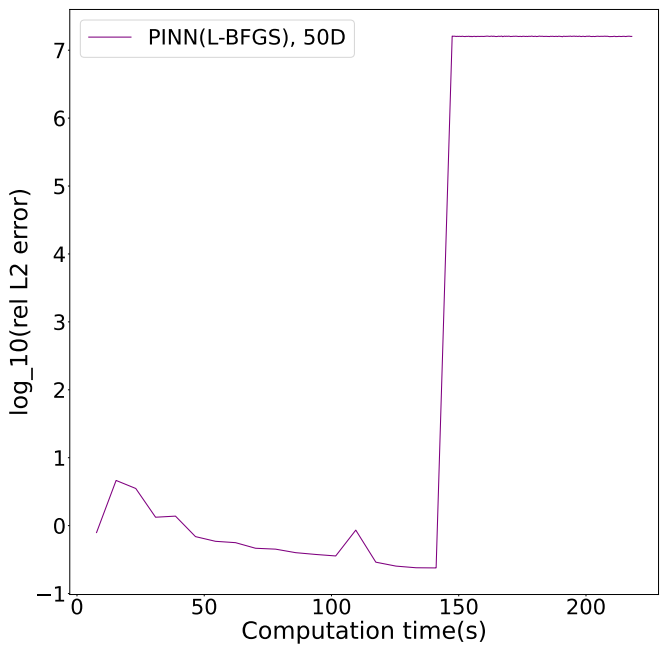
PINN/DeepRitz/WAN (Adam)

50D, Poisson equation



PINN (L-BFGS)

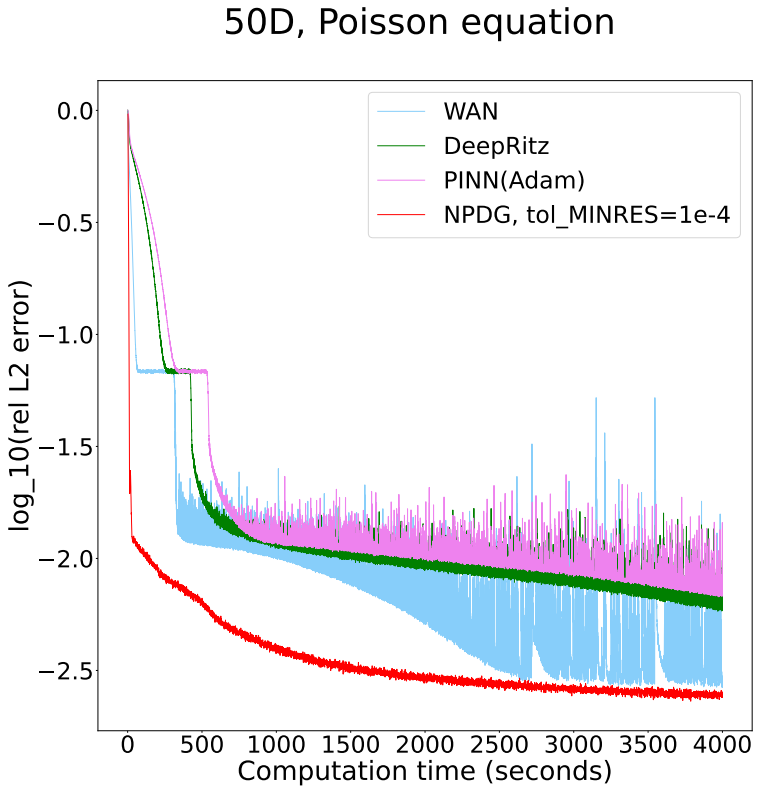
50D, Poisson equation



Performances of existing methods

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

Proposed algorithm: **Versatile, Efficient, Stable.**



Related works: Preconditioning on Deep PDE solver

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 + Preconditioned gradients

New loss functional + Operator-informed preconditioning

Natural Primal-Dual Gradient (NPDG) method

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Let us derive the algorithm for the Poisson equation:

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

- Denote u_* as the unique classical solution.
- Consider ($\mathcal{B}$ denotes the trace operator.)

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

- It suffices to solve the root-finding problem $\mathcal{F}(u) = 0$.
- This can be reformulated as: (Denote $\mathbb{L}^2 := L^2(\Omega) \times L^2(\partial\Omega)$.)

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

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

$$\inf_{u\in H^2(\Omega)} \sup_{\substack{\varphi\in L^2(\Omega),\\ \psi\in L^2(\partial\Omega)}} \mathscr{E}_0(u,\varphi,\psi) := \langle \mathcal{F}(u), (\varphi,\psi)\rangle_{\mathbb{L}^2} - \frac{1}{2}\|(\varphi,\psi)\|_{\mathbb{L}^2}^2$$

$$= \langle -\Delta u - f, \varphi\rangle_\Omega + \langle u - g, \psi\rangle_{\partial\Omega} - \frac{1}{2}\|(\varphi,\psi)\|_{\mathbb{L}^2}^2.$$

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

$$\inf_{u\in H^2(\Omega)} \sup_{\substack{\varphi\in H_0^1(\Omega),\\ \psi\in L^2(\partial\Omega)}} \mathscr{E}_0(u,\varphi,\psi) := \int_\Omega \nabla u\cdot\nabla\varphi - f\varphi dx + \int_{\partial\Omega}(u-g)\psi d\sigma$$

$$- \frac{1}{2}\left(\int_\Omega \varphi^2 dx + \int_{\partial\Omega}\psi^2 d\sigma\right).$$

Leveraging Primal-Dual Hybrid Gradient (PDHG)[1] algorithm

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

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

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- Proximal Grad Ascent + Extrapolation + Proximal Grad Descent.
- τ_φ, τ_u: stepsizes, ω: extrapolation coefficient.
- Successful applications on finite difference schemes for conservation laws, reaction-diffusion equations[3], etc. (1D, 2D)

[1] M. Zhu, T. Chan. An efficient primal-dual hybrid gradient algorithm for total variation image restoration. A. Chambolle, T. Pock. A first-order primal-dual algorithm for convex problems with applications to imaging.

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Ill-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 $\sqrt{1 - \frac{c}{\kappa(A)^2}} = 1 - \mathcal{O}(\frac{1}{N_x^4})$ ($\kappa(A) = \mathcal{O}(N_x^2)$). **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

- How do we apply the precondition operator, say, Δ^{-1} to $\mathcal{F}(u)$? How to realize the computation? 🤔
- Seems impractical.

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- 💡 Preconditioning on metric terms of the proximal steps:

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

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

$\mathcal{M}_u$, $\mathcal{M}_\varphi$ are precondition operators for u, φ.

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  $\mathcal{M}_u$, $\mathcal{M}_\varphi$ are precondition operators for u, φ.
- How to pick $\mathcal{M}_u$, $\mathcal{M}_\varphi$?

Key idea:

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

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

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

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

- $\|\mathbf{U} - \mathbf{U}_n\|^2_{\mathbb{L}^2} = \|\nabla u - \nabla u_n\|^2_{L^2(\Omega)} + \|\mathcal{B}u - \mathcal{B}u_n\|^2_{L^2(\partial\Omega)}$.
- Pick $\mathcal{M}_u = \nabla$. Similarly, $\mathcal{M}_\varphi = \nabla$.

PDHG with preconditioning

The preconditioned PDHG for solving (2) yields

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

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- 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

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

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

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$$\begin{bmatrix} \eta^{n+1} \\ \xi^{n+1} \end{bmatrix} = \underset{\eta,\xi}{\operatorname{argmin}} \left\{ \frac{1}{2\tau_\varphi} \overbrace{\left(\|\nabla\varphi_\eta - \nabla\varphi_{\eta^n}\|^2_{L^2(\Omega)} + \|\psi_\xi - \psi_{\xi^n}\|^2_{L^2(\partial\Omega)} \right)}^{d_2^2((\eta,\xi),(\eta^n,\xi^n))} - \mathscr{E}(u_{\theta^n}, \varphi_\eta, \psi_\xi) \right\},$$

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

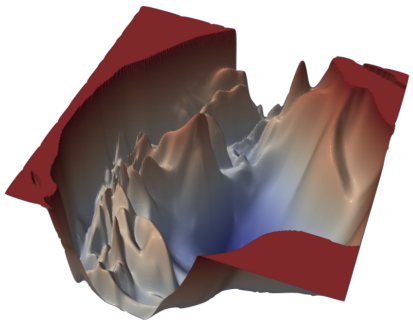
$$\theta^{n+1} = \underset{\theta}{\operatorname{argmin}} \left\{ \frac{1}{2\tau_u} \underbrace{\left(\|\nabla u_\theta - \nabla u_{\theta^n}\|^2_{L^2(\Omega)} + \|\mathcal{B}u_\theta - \mathcal{B}u_{\theta^n}\|^2_{L^2(\partial\Omega)} \right)}_{d_1^2(\theta,\theta^n)} + \mathscr{E}(u_\theta, \widetilde{\varphi}^{n+1}, \widetilde{\psi}^{n+1}) \right\}.$$

- 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 $\theta \in \mathbb{R}^{m_\theta}, \eta \in \mathbb{R}^{m_\eta}, \xi \in \mathbb{R}^{m_\xi}$.

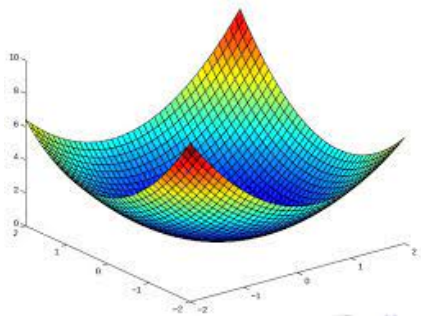
Key idea:

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

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



(η, ξ)'s point of view[4].



$\mathbf{\Phi}_{\eta,\xi}$'s point of view.

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

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

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

Recall that $\mathbf{\Phi}_{\eta,\xi} = (\nabla \varphi_\eta^\top, \psi_\xi)^\top$.

[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}:

$$\theta^{n+1} = \underset{\theta \in \mathbb{R}^{m_\theta}}{\operatorname{argmin}} \left\{ \frac{1}{2\tau_u} d_1^2(\theta, \theta^n) + \mathscr{E}(u_\theta, \widetilde{\varphi}_{n+1}, \widetilde{\psi}_{n+1}) \right\}.$$

- The *time-explicit* scheme: Natural gradient descent.[5]

$$\theta^{n+1} = \theta^n - \tau_u \underbrace{M_p(\theta^n)^\dagger \frac{\partial}{\partial \theta} \mathscr{E}(u_{\theta^n}, \widetilde{\varphi}_{n+1}, \widetilde{\psi}_{n+1})}_{\textbf{Nature Gradient}}.$$

$M_p(\theta^n)$ is induced by:

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

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

[5] S. Amari. Natural Gradient Works Efficiently in Learning, 1998.

NPDG algorithm

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

$$\begin{bmatrix} \eta^{n+1} \\ \xi^{n+1} \end{bmatrix} = \begin{bmatrix} \eta^{n} \\ \xi^{n} \end{bmatrix} + \tau_\varphi \begin{bmatrix} M_d(\eta^n)^\dagger \frac{\partial}{\partial \eta} \mathscr{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n}) \\ M_{bdd}(\xi^n)^\dagger \frac{\partial}{\partial \xi} \mathscr{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n}) \end{bmatrix},$$

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$$\theta^{n+1} = \theta^n - \tau_u M_p(\theta^n)^\dagger \frac{\partial}{\partial \theta} \mathscr{E}(u_{\theta^n}, \widetilde{\varphi}_{n+1}, \widetilde{\psi}_{n+1}).$$

Natural Grad Ascent + Extrapolation + Natural Grad Descent

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Natural Grad Ascent + Extrapolation + Natural Grad Descent

NPDG algorithm

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$$\theta^{n+1} = \theta^n - \tau_u M_p(\theta^n)^\dagger \frac{\partial}{\partial \theta} \mathscr{E}(u_{\theta^n}, \widetilde{\varphi}_{n+1}, \widetilde{\psi}_{n+1}).$$

- More general cases:

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

- Monge-Ampère equation arising in L^2 Optimal Transport problems.

NPDG algorithm

$$\begin{bmatrix} \eta^{n+1} \\ \xi^{n+1} \end{bmatrix} = \begin{bmatrix} \eta^{n} \\ \xi^{n} \end{bmatrix} + \tau_\varphi \begin{bmatrix} M_d(\eta^n)^\dagger \frac{\partial}{\partial \eta} \mathscr{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n}) \\ M_{bdd}(\xi^n)^\dagger \frac{\partial}{\partial \xi} \mathscr{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n}) \end{bmatrix},$$

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$$\theta^{n+1} = \theta^n - \tau_u M_p(\theta^n)^\dagger \frac{\partial}{\partial \theta} \mathscr{E}(u_{\theta^n}, \widetilde{\varphi}_{n+1}, \widetilde{\psi}_{n+1}).$$

Evaluate the natural gradient $M_d(\eta^n)^\dagger \frac{\partial}{\partial \eta} \mathscr{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n})$:

- ⚠ $M_d(\eta^n)$ is prohibitively **expensive** to compute.

  4-layer MLP with hidden dim 100 has more than 30000 parameters!

- How to solve $M_d(\eta^n)\vec{v} = \frac{\partial}{\partial \eta} \mathscr{E}(u_{\theta^n}, \varphi_{\eta^n}, \psi_{\xi^n})$?
  Krylov subspace method: only requires matrix-vector multiplication.

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Time-continuous NPDG algorithm

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

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

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

- Consider the linear equation:

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

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

  Suppose (3) admits unique classical solution u_*.

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

Convergence analysis of NPDG flow[6]

- Suppose $\{(\theta_t, \eta_t, \xi_t)\}_{0\le t\le T}$ solves the NPDG-flow.
- Denote $\widetilde{\kappa}$ as the condition number of $\widetilde{\mathcal{L}}$ 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 $\alpha + \beta_1 < \frac{1}{\widetilde{\kappa}^2}$, $\beta_2 < 1$, if γ further satisfies

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

There exists $r > 0$ depending on $\widetilde{\mathcal{L}}$, the hyperparameters $\gamma, \alpha, \beta_1, \beta_2$, such that, for $0 \le t \le T$,

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

[6] 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 $\Lambda = \mathrm{diag}(\lambda_0, \lambda_1, \ldots, \lambda_0, \lambda_1)$, $\lambda_0 = 1, \lambda_1 = 4$.
  - $f(x) = -\frac{\mathrm{Tr}(\Lambda^{-1})}{2}(x^\top \Lambda x + 1) - \|x\|^2$, $g(y) = \frac{1}{2} y^\top \Lambda^{-1} y$.
  - 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 $\mathrm{softplus}(\cdot)$[7] activation function.

- $\mathcal{M}_p = \nabla$, $\mathcal{M}_d = \nabla$.

[7] $\mathrm{softplus}(x) = \frac{1}{\beta} \log(1 + \exp(\beta x))$, $\beta = \frac{1}{4}$.

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

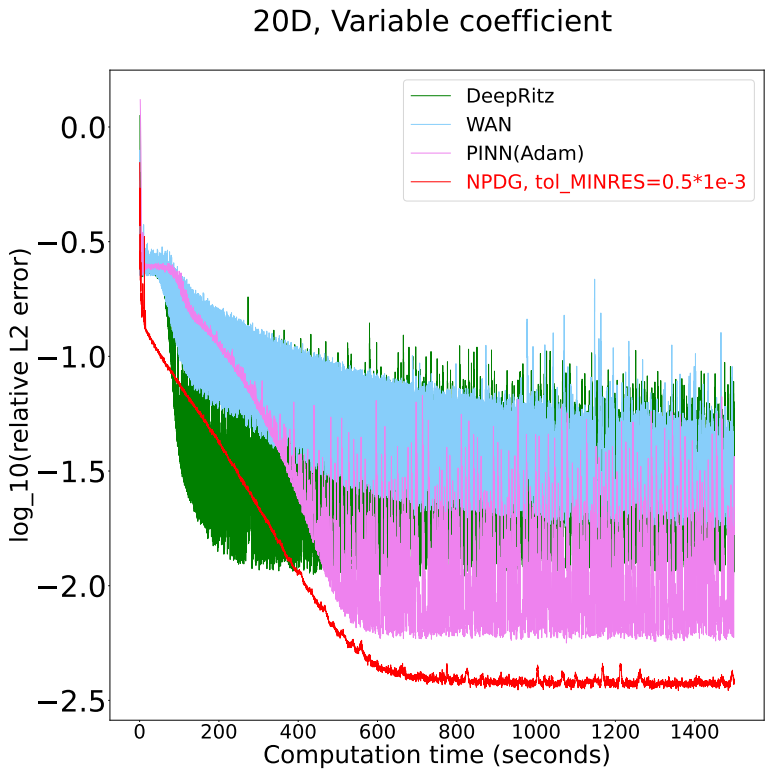

Figure: Plots of relative L^2 error vs. wall clock time(s), comparing NPDG with PINN, DeepRitz, and WAN.

Performance comparison on different types of PDEs

- Fix NN architecture as MLP. Use the same sample size.

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:

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

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

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

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 $\mathbb{R}^{50}$

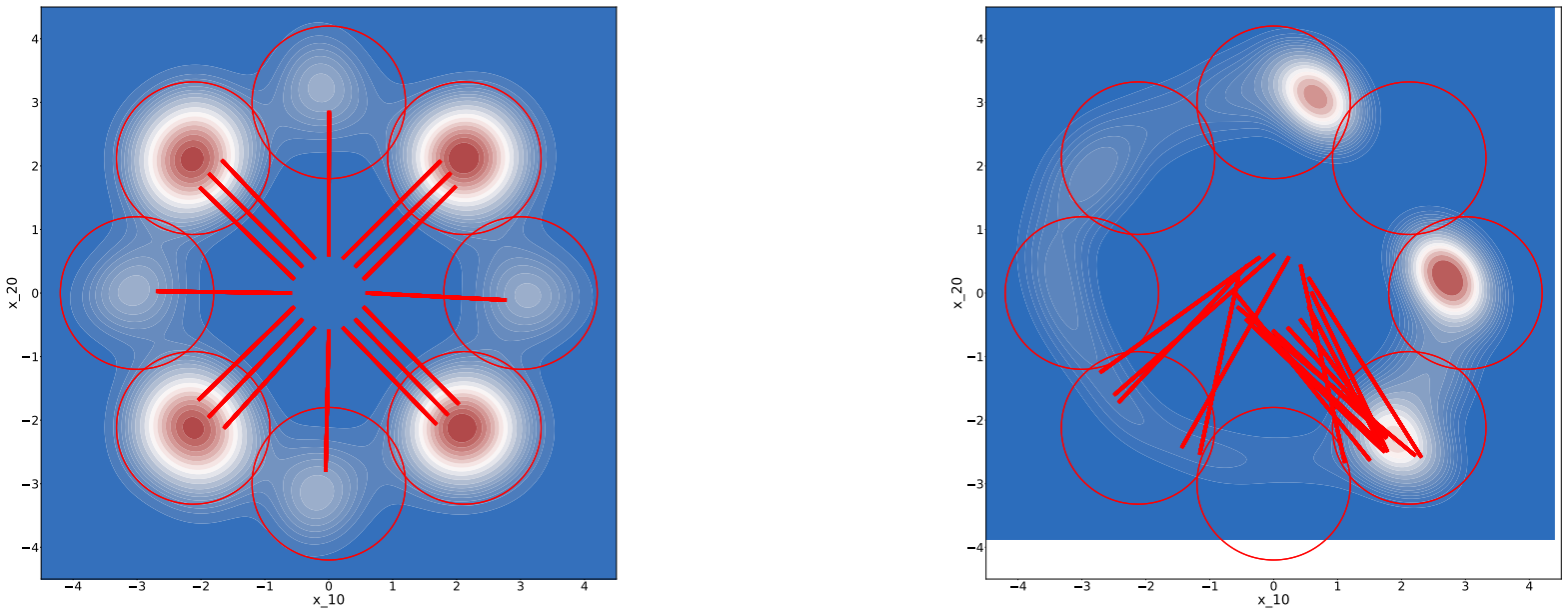

Figure: Plots of the pushforwarded density $T_{\theta\sharp}\rho_0$ by Kernel Density Estimation (KDE). **Left**: NPDG method; **Right**: Primal-Dual algorithm using Adam. Red lines indicate the computed OT map $T_\theta(\cdot)$.

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Summary of the research

NPDG = Adversarial neural nets training + Natural gradients.

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

• Shu Liu, Siting Liu, Stanley Osher, Wuchen Li. A first-order computational method for Reaction-Diffusion type equations via Primal-Dual Hybrid Gradient method. JCP, 2023.
• Shu Liu, Xinzhe Zuo, Stanley Osher, Wuchen Li. Numerical analysis of a first-order computational algorithm for reaction-diffusion equations via the primal-dual hybrid gradient method. arXiv 2401.14602, 2024.
• 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!

A Saddle Point Scheme of OT (Monge) problem

- OT (Monge) problem is a constrained optimization problem.
- Introduce Lagrange multiplier $\varphi \in \mathcal{C}_b(\mathbb{R}^d)$ to the constraint

$$T_\sharp \mu = \nu.$$

- We derive the saddle point scheme for solving the OT problem/Monge-Ampère equation:

$$\sup_{\varphi \in \mathcal{C}_b(\mathbb{R}^d)} \inf_{T \in \mathcal{M}(\mathbb{R}^d, \mathbb{R}^d)} \mathscr{E}(T, \varphi). \tag{4}$$

$$\mathscr{E}(T, \varphi) = \int_{\mathbb{R}^d} \frac{1}{2} \|x - T(x)\|^2 \rho_0(x) dx + \int_{\mathbb{R}^d} \varphi(T(x)) \rho_0(x) dx - \int_{\mathbb{R}^d} \varphi(x) \rho_1(x) dx.$$

- Consistency[8]: saddle point $(T_\star, \varphi_\star)$ of (4) yields OT map T_*, i.e. $T_\star(\cdot) = T_*(\cdot)$–$\mu$ a.s.

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

Set T, φ as neural networks $T_\theta : \mathbb{R}^d \to \mathbb{R}^d$, $\varphi_\eta : \mathbb{R}^d \to \mathbb{R}$.

$$\begin{aligned}
\eta^{n+1} &= \eta^n + \tau_\varphi M_d(\eta^n)^\dagger \frac{\partial}{\partial \eta} \mathscr{E}(T_{\theta^n}, \varphi_{\eta^n}), \\
\widetilde{\varphi}_{n+1} &= \varphi_{\eta^{n+1}} + \omega(\varphi_{\eta^{n+1}} - \varphi_{\eta^n}), \\
\theta^{n+1} &= \theta^n - \tau_T M_p(\theta^n)^\dagger \frac{\partial}{\partial \theta} \mathscr{E}(T_{\theta^n}, \widetilde{\varphi}_{n+1}).
\end{aligned}$$

We define $M_p(\theta)$, $M_d(\eta)$ as

$$\begin{aligned}
M_p(\theta) &= \int_{\mathbb{R}^d} \frac{\partial T_\theta(x)}{\partial \theta}^\top \frac{\partial T_\theta(x)}{\partial \theta} \rho_0(x)\, dx, \\
M_d(\eta;\theta) &= \int_{\mathbb{R}^d} \frac{\partial}{\partial \eta}(\nabla \varphi_\eta(T_\theta(x)))^\top \frac{\partial}{\partial \eta}(\nabla \varphi_\eta(T_\theta(x)))\rho_0(x)\, dx.
\end{aligned}$$

Hint: Dual variable φ should live in $H^1(\mathbb{R}^d)$.