Weak Adversarial Network (WAN): A Deep Learning Method for Forward and Inverse Problems with High Dimensional PDEs

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Outline

Motivation

Goal: numerically solve forward and inverse problems with PDEs in high dimensions.

example: elliptic equation in $\Omega \in \mathbb{R}^d$ (arbitrary shape),

$$\begin{cases} -\sum_{i=1}^{d} \partial_i(a_{ij}\partial_j u) = f, & \text{in } \Omega \\ u(x) - g(x) = 0 \quad \text{(Dirichlet)} & \text{on } \partial\Omega \end{cases}$$

Challenge: The computational cost for conventional methods (Finite Difference, Finite Elements, Spectral, and others) becomes intractable when the dimension is high.

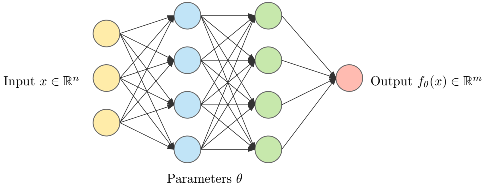
Our Strategies: Leveraging a minimax framework (2-player game strategy) and neural networks.

Neural Networks

Deep neural networks are compositions of multiple simple functions (called layers) so that they can approximate complicated functions. For example:

$$f_\theta(x) = w_K^T l_{K-1} \circ \cdots \circ l_0(x) + b_K,$$

where k-th layer $l_k(z) = \sigma_k(W_k z + b_k)$ with weight $W_k \in \mathbb{R}^{d_{k+1} \times d_k}$ and bias $b_k \in \mathbb{R}^{d_{k+1}}$. Parameters θ are collections of (w_K, b_k, W_k).



Training of neural networks: find the best parameters to minimize a loss function: measuring the success of a task such as approximation.

Neural Networks (NNs) for numerical PDEs

NNs have been used to solve PDEs in the last three decades. Using DNNs for high-dimensional PDEs emerged in the past few years, and there are many more in developments.

- Use NNs to improve the standard methods: Lee-Kang '90, Yentis-Zaghloul '96, Rudd-Ferrari '15, Tompson-Schlachter-Sprechmann-Perlin '17, Suzuki '17, ...
- Use NNs to approximate the solutions directly, and they may be friendly for high-dimensional problems, such as the physics-informed NN (PINN), Ritz Net, backward-forward SDEs: Dissanayake-Phan-Thien '94, Lagaris-Likas-Fotiadis '98, Beck-E-Jentzen '17, Fujii-Takahashi-Takahashi '17, E-Han-Jentzen '17, He-Li-Xu-Zheng '18, Berg-Nystrom '18, Magill-Qureshi-de Haan '18, Cai-Xu '19, Raissi-Perdikaris-Karniadakis '19, ...
- Use NNs with the variational forms of PDEs, and solve PDEs (SPDEs) by optimization: Nabian-Meidani '18, E-Yu '18, Khoo-Lu-Ying '19, Anitescu-Atroshchenko-Alajlan-Rabczuk '19, Yang-Perdikaris '19, ...

WAN formulation

The weak form of the solution, multiple the equation by a test function φ and perform integration by part,

$$\begin{aligned} &\langle \mathcal{A}[u], \varphi \rangle = 0 \\ &\mathcal{B}[u] = 0, \quad \text{on } \partial\Omega \end{aligned}$$

example: for the elliptic equation,

$$\langle \mathcal{A}[u], \varphi \rangle \triangleq \int_\Omega \sum_{i,j=1}^{d} a_{ij} \partial_j u \partial_i \varphi - f \varphi \, \mathrm{d}x$$

Why weak solution?

(a) Classical solution may not exist.

(b) Integral form is friendly to sample-based computation, which is crucial for high dimension problems.

(c) Solution and test function are in a 2-player game, helping to overcome the challenge of lack of data in neural network training.

A minimax problem

Theorem

Suppose u^* satisfies the boundary condition $\mathcal{B}[u^*] = 0$, then u^* is a weak solution if and only if u^* solves the problem

$$\min_{u \in H^1} \max_{\varphi \in H_0^1} |\langle \mathcal{A}[u], \varphi \rangle|^2 / \|\varphi\|_{H^1}^2.$$

Furthermore, u^* satisfies

$$\|\mathcal{A}[u^*]\|_{op} = 0,$$

where

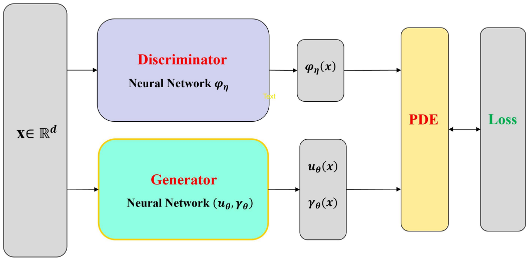
$$\|\mathcal{A}[u]\|_{op} \triangleq \max\{\langle \mathcal{A}[u], \varphi \rangle / \|\varphi\|_{H^1} \mid \varphi \in H_0^1, \varphi \neq 0\},$$

WAN framework

Idea:

- Weak solution $u \in H^1$, approximated by the primary NN u_θ,
- Test function $\varphi \in H_0^1$, approximated by the adversarial NN φ_η.
- Iteratively learn θ to minimize $\|\mathcal{A}[u_\theta]\|_{op}$ with fixed φ_η, and challenges u_θ by maximizing $\langle \mathcal{A}[u_\theta], \varphi_\eta \rangle$ modulus its own norm $\|\varphi_\eta\|_{H^1}$ for every given u_θ .

Weak Adversarial Network



Loss Functions

The lost function used for training (optimization for the parameters) may have many different choices. For example, the following one is used in our computations,

$$\min_{\theta} \max_{\eta} L(\theta, \eta), \quad \text{where} \quad L(\theta, \eta) \triangleq L_{\text{int}}(\theta, \eta) + \alpha L_{\text{bdry}}(\theta),$$

with

$$L_{\text{int}}(\theta, \eta) \triangleq \log |\langle \mathcal{A}[u_\theta], \varphi_\eta \rangle|^2 - \log \|\varphi_\eta\|^2_{H^1},$$

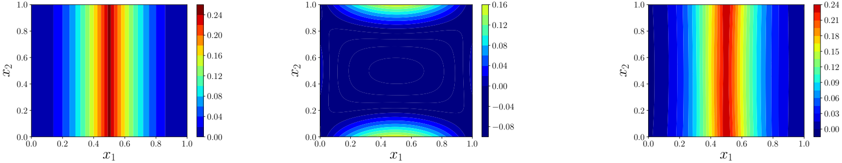
and

$$L_{\text{bdry}}(\theta) \triangleq (1/N_b) \cdot \sum_{j=1}^{N_b} |u_\theta(x_b^{(j)}) - g(x_b^{(j)})|^2.$$

Weak solution v.s. classical solution

$$\begin{cases} \Delta u = 2, & \text{in } \Omega \\ u = g, & \text{on } \partial\Omega \end{cases}$$

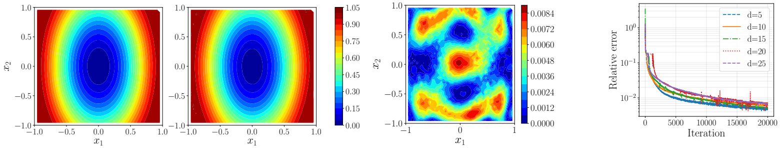
Weak solution exists, but the classical solution doesn't.



(a) True u^* (b) u_s from classical form (c) u_w from weak form

Nonlinear equation ($d = 20$)

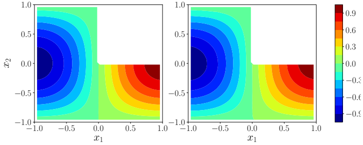
$$\begin{cases} -\nabla \cdot (a(x)\nabla u) + \frac{1}{2}|\nabla u|^2 = f(x) & \text{in} \quad \Omega \triangleq (-1,1)^d, \\ u(x) = g(x) & \text{on} \quad \partial\Omega \end{cases}$$



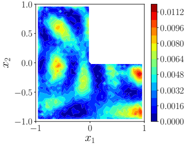
(a) u^* vs u_θ (b) $|u_\theta - u^*|$ (c) Error vs iteration

L-shape domain ($d = 10$)

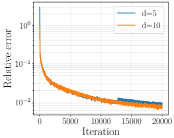
$$
\begin{cases}
-\nabla \cdot (a(x)\nabla u) = f(x) & \text{in} \quad \Omega \triangleq (-1,1)^d \setminus [0,1)^d \\
u(x) = g(x) & \text{on} \quad \partial\Omega
\end{cases}
$$



(a) u^* vs u_θ



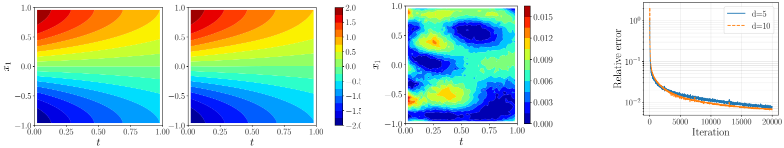
(b) $|u_\theta - u^*|$



(c) Error vs iteration

Time dependent equation ($d = 5$)

$$\begin{cases} u_t - \Delta u - u^2 = f(x,t), & \text{in } \Omega \times [0,T] \\ u(x,t) = g(x,t), & \text{on } \partial\Omega \times [0,T] \\ u(x,0) = h(x), & \text{in } \Omega \end{cases}$$



(a) u^* vs u_θ (b) $|u_\theta - u^*|$ (c) Error vs iteration

Features

- The primary and adversarial NNs are used to train each other. No training data is needed.
- It is flexible in sampling points used to compute the integrals. It fits the frameworks of un-supervised or supervised learning.
- It is mesh-less, basis-less.
- It seeks convergence only in u_θ.
- It is different from existing methods (FEM, Spectral, FDM, Collocation), not Galerkin based, no triangulation, no finite element basis or Fourier basis, no enforcement on selected points.

Inverse problem

Goal: numerically solve inverse problems in high dimensions.

The PDEs in a high-dimension space $\Omega \in \mathbb{R}^d$:

$$\begin{cases} \mathcal{A}[u,\gamma] = 0, & \text{in } \Omega \\ \mathcal{B}[u,\nabla u,\gamma] = 0, & \text{on } \partial\Omega \end{cases} \tag{1}$$

where $\mathcal{A}[u,\gamma]$ may be a second order elliptic differential operator, such as the electrical impedance tomography (EIT) $\mathcal{A}[u,\gamma] = -\nabla\cdot(\gamma\nabla u) - f$, $\mathcal{B}[u,\nabla u,\gamma]$ is the boundary value, u the solution and γ the coefficient function.

The inverse problem: Given the observations of $\mathcal{B}[u,\nabla u,\gamma]$ on $\partial\Omega$, find (u,γ) that satisfies the equation (1).

Challenges: ill-posedness; instability; curse-of-dimensionality. (Alessandrini 1987, Mandache 2001).

Recent deep learning approaches for inverse problems

DNNs have been used for solving inverse problem in the last three decades. Here are partially selected works:

Martin-Choi '15, Tan-Lv-Dong-Takei '18, Yao-Wei-Jiang '19.
Martin-Choi '17, Kang-Min-Ye '17, Jin-Mccann-Froustey-Unser '17, Hamilton-Hauptmann '18, Antholzer-Haltmeier-Schwab '19, Wei-Liu-Chen '19.
Adler-öktem '17, Li-Schwab-Antholzer-Haltmeier '20.
Dadvand-Lopez-Onate '06, Khoo-Ying '18,
Raissi-Perdikaris-Karniadakis '19, Fan-Ying '19,
Jo-Son-Hwang-Kim '19, Bar-Sochen '19, and many more.

The equivalent minimax problem for the inverse problem

Define an operator norm

$$\|\mathcal{A}[u,\gamma]\|_{op} \triangleq \max\{\langle \mathcal{A}[u,\gamma],\varphi\rangle / \|\varphi\|_{H^1} \mid \varphi \in H_0^1, \varphi \neq 0\},$$

Theorem

Suppose (u^*, γ^*) satisfies the boundary condition $\mathcal{B}[u^*, \nabla u^*, \gamma^*] = 0$, then u^* is a weak solution if and only if (u^*,γ^*) solves the problem

$$\min_{u\in H^1,\gamma\in L^2} \max_{\varphi\in H_0^1} |\langle \mathcal{A}[u,\gamma],\varphi\rangle|^2 / \|\varphi\|_{H^1}^2.$$

Furthermore, (u^*, γ^*) satisfies

$$\|\mathcal{A}[u^*,\gamma^*]\|_{op} = 0.$$

WAN framework for inverse problems

Idea:

- Weak solution $u \in H^1$, $\gamma \in L^2$ approximated by the primary NN u_θ and γ_θ respectively.
- Test function $\varphi \in H_0^1$, approximated by the adversarial NN φ_η.
- Iteratively learn θ to minimize $\|\mathcal{A}[u_\theta, \gamma_\theta]\|_{op}$ with fixed φ_η, and challenges u_θ and γ_θ by adjusting φ_η to maximize $\langle \mathcal{A}[u_\theta, \gamma_\theta], \varphi_\eta \rangle / \|\varphi_\eta\|_{H^1}$ for every given $(u_\theta,\, \gamma_\theta)$.

The framework for the inverse problems is almost identical to that for the forward problem.

Theorem

For any $\varepsilon > 0$*, let* $\{\theta_j\}$ *be a sequence of the network parameters in* $(u_\theta, \gamma_\theta)$ *generated by the stochastic gradient descent (SGD) algorithm with integrals in* $\nabla_\theta L(\theta)$ *approximated by sample averages with sample complexities* $N_r, N_b = O(\varepsilon^{-1})$ *in each iteration, then* $\min_{1 \le j \le J} \mathbb{E}[|\nabla_\theta L(\theta_j)|^2] \le \varepsilon$ *after* $J = O(\varepsilon^{-1})$ *iterations.*

- This is the so-called ε-convergence.
- It ensures an approximation to a stationary point only.

Key implementation issues

- Various optimization methods can be used for gradient descent or ascent. We use AdaGrad for the test NN and Adam for solution NN. Auto-differentiation is used to calculate derivatives.

- Use fully-connected feed-forward NNs for both the solution u_θ and the test function φ_η. u_θ has 6 hidden layers with 40 neurons per hidden layer, while φ_η consists of 8 hidden layers with 40 neurons per hidden layer. (Other NN structures can be used as well.)

- Calculate integrals by Monte Carlo method.

- Enforce $\varphi_\eta = 0$ on the boundary by setting $\varphi_\eta = wv_\eta$, where $w = 0$ is pre-selected taking zero on $\partial\Omega$, v_η can be non-zero on the boundary.

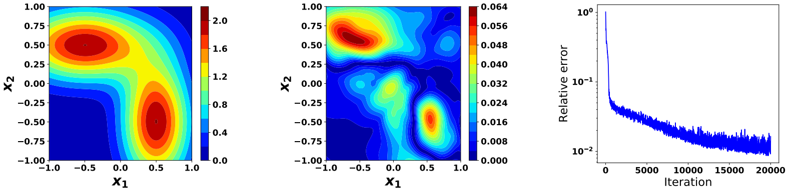
- Other loss functions may work too.

EIT with smooth conductivity (d=5, noise free)

$$-\nabla \cdot (\gamma \nabla u) - f = 0, \quad \text{in } \Omega = (-1,1)^d \qquad (2)$$

$$u - u_b = 0, \; \gamma - \gamma_b = 0, \; \partial_{\vec{n}} u - u_n = 0, \quad \text{on } \partial\Omega \qquad (3)$$

where the conductivity γ is a smooth function. ($N_r = 10^5$, $N_b = 100d$.)

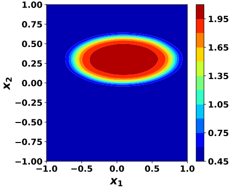


(a) True γ^* (b) $|\gamma^* - \gamma_\theta|$ (c) Error vs iteration

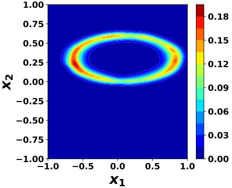
EIT with nearly piecewise conductivity (noise free)

$$-\nabla \cdot (\gamma \nabla u) - f = 0, \quad \text{in } \Omega = (-1,1)^d \tag{4}$$
$$u - u_b = 0,\ \gamma - \gamma_b = 0,\ \partial_{\vec{n}} u - u_n = 0, \quad \text{on } \partial\Omega \tag{5}$$

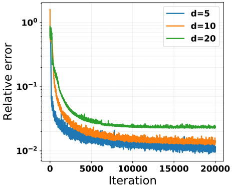
where the conductivity γ is a nearly piecewise function. (For different dimension d, $N_r = 20000d$, $N_b = 100d$.)



(a) True γ^*



(b) $|\gamma^* - \gamma_\theta|$ for $d = 10$



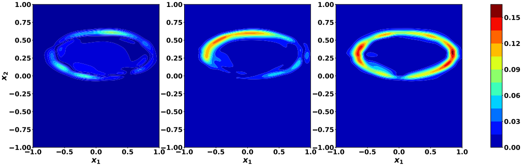
(c) Error vs iteration

EIT with nearly piecewise conductivity (with noise)

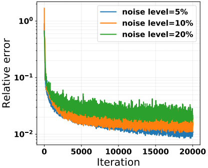
The problem is the same as that defined in (4) and (5),

$$-\nabla \cdot (\gamma \nabla u) - f = 0, \quad \text{in } \Omega = (-1,1)^d$$
$$u - u_b = 0,\ \gamma - \gamma_b = 0,\ \partial_{\vec{n}} u - u_n = 0, \quad \text{on } \partial\Omega$$

where $d = 5$. ($N_r = 20000d$, $N_b = 100d$.)



(a) $|\gamma^* - \gamma_\theta|$ for noise level$= 5\%, 10\%, 20\%$



(b) Error vs iteration

EIT with nonconvex conductivity (d=5, noise free)

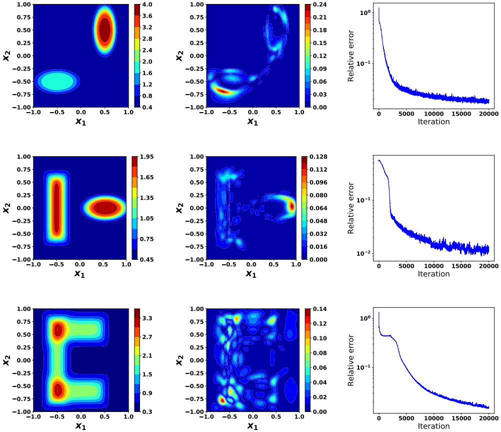
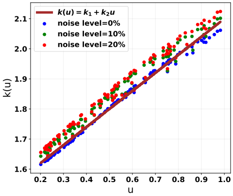


Figure: Left: True γ^*; Middle: $|\gamma^* - \gamma_\theta|$; Right: Error vs iteration

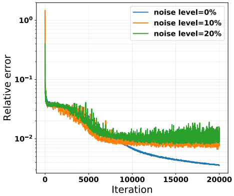
Inverse thermal conductivity problem (d=5, with noise)

$$\partial_t u - \nabla\cdot(\gamma\nabla u) - f = 0, \quad \text{in } \Omega_T = \Omega\times[0,1]$$
$$u - u_i = 0, \quad \text{in } \Omega\times\{0\}$$
$$\nabla u\cdot\vec{n} - u_n = 0,\ u - u_b = 0,\ \gamma - \gamma_b = 0, \quad \text{on } \partial\Omega\times[0,1]$$

where $\gamma(u) = k_1 + k_2 u$ with $k_1 = 1.5$ and $k_2 = 0.6$. ($N_r = 10^5$, $N_b = 100d$.)



(a) $\gamma_\theta(u_\theta)$ vs u_θ



(b) Error vs iteration

Figure: inverse thermal conductivity problem with noise level= 0%, 10%, 20%.

Conclusion and Questions

- A minimax framework for PDEs.
- Using NN in high dimensions.
- A lot of open questions
  - Convergent? Experiments indicate so.
  - Accuracy? Examples are promising.
  - Stability? Seems to be stable, no regularizer is used!
  - Speed? There are rooms to improve.
- Improvement strategies are desirable.

References

- Bao G, Ye X, Zang Y, Zhou H. Numerical Solution of Inverse Problems by Weak Adversarial Networks. Inverse Problems, Vol 36, No. 11, 2020.
- Zang Y, Bao G, Ye X, Zhou H. Weak adversarial networks for high-dimensional partial differential equations. Journal of Computational Physics, Vol 411, 15 June 2020, 109409

Thank you