Is L^2 Loss Always Suitable for Training Physics-Informed Neural Network?

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Outline

1. Introduction
2. Definition of Stability
3. Bounds on the Stability of PINN for HJB Equation
4. New Algorithms
5. Conclusion & Future Direction

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2. Theoretical Analysis for the Validity of PINN

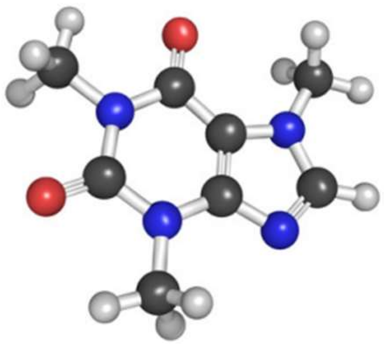
3. Failure of PINN for High Dimensional HJB Equation

4. New Algorithm for High Dimensional HJB Equation

5. Conclusion & Future Direction

Preliminary: Partial Differential Equation

Partial Differential Equation (PDE) is a ubiquitous tool in mathematical modeling of physics, control, and finance.



- Solving PDE is important for understanding these systems.
- Designing an accurate and efficient PDE solver is very challenging.

Formulation of Partial Differential Equation

Partial Differential Equation involves an unknown multi-variable function $u(x)$ and partial derivatives of the unknown function.

$$\begin{cases} \mathcal{L}u(x) = \varphi(x) & x \in \Omega \subset \mathbb{R}^n \\ \mathcal{B}u(x) = \psi(x) & x \in \partial\Omega, \end{cases}$$

$\mathcal{L}$: partial differential operator.
B: boundary condition.

PINN: solving PDE with deep learning

Physics-informed Neural Networks (PINN):

- Solving PDE as a function approximate problem.
- Training an NN to express the PDE solution with L^2 **Physics-Informed Loss**.

$$\begin{cases} \mathcal{L}u(x) = \varphi(x) \\ \mathcal{B}u(x) = \psi(x) \end{cases} \quad \Longrightarrow \quad \begin{aligned} \ell_{\Omega}(u) &= \|\mathcal{L}u(x) - \varphi(x)\|^2_{L^2(\Omega)}, \\ \ell_{\partial\Omega}(u) &= \|\mathcal{B}u(x) - \psi(x)\|^2_{L^2(\partial\Omega)}. \end{aligned}$$

Neural Network: $u_\theta(x)$ with x as the input and θ as the parameters.

PINN is straightforward and successful.

Can we use it to solve **high-dimensional PDEs**?

- Conventional methods fail due to the **curse of dimensionality**.
- Neural networks do well in representing **high-dimensional mappings**.

PINN is straightforward and successful.

Can we use it to solve **high-dimensional PDEs**?

- PINN's **accuracy** is not satisfactory on high-dimensional non-linear PDEs.

Outline

Theoretical Analysis for the Validity of PINN

$$\ell_{\Omega}(u) = \|\mathcal{L}u(x) - \varphi(x)\|_{L^2(\Omega)}^2,$$

$$\ell_{\partial\Omega}(u) = \|\mathcal{B}u(x) - \psi(x)\|_{L^2(\partial\Omega)}^2.$$

- PINN uses L^2 Physics-Informed Loss by default.

  Zero Training Loss ⇔ Learned solution is exactly accurate

- But practically we only obtain **small** but **non-zero** losses.

*Does **a learned solution with a small loss** always corresponds to **a good approximator of the exact solution**?*

A closer look at the learned solution

A learned solution $u_\theta(x)$ is the solution to **a *perturbed* PDE**:

$$\begin{cases} \mathcal{L}u(x) = \varphi(x) + (\mathcal{L}u_\theta(x) - \varphi(x)) & x \in \Omega \subset \mathbb{R}^n \\ \mathcal{B}u(x) = \psi(x) + (\mathcal{B}u_\theta(x) - \psi(x)) & x \in \partial\Omega \end{cases}$$

The scale of the perturbation can be characterized by the **Physics-Informed Loss**:

$$\ell_\Omega(u) = \|\mathcal{L}u(x) - \varphi(x)\|^2_{L^2(\Omega)},$$

$$\ell_{\partial\Omega}(u) = \|\mathcal{B}u(x) - \psi(x)\|^2_{L^2(\partial\Omega)}.$$

Stability of PDEs

The accuracy of PINN is closely related to the ***stability*** of PDE.

In PDE literature, we say an equation is ***stable*** if the solution of the perturbed PDE converges to the exact solution as the perturbations approach zero (measured by certain norm).

$$\begin{cases} \mathcal{L}u(x) = \varphi(x) + (\mathcal{L}u_\theta(x) - \varphi(x)) \\ \mathcal{B}u(x) = \psi(x) + (\mathcal{B}u_\theta(x) - \psi(x)) \end{cases} \quad \Rightarrow \quad \begin{cases} \mathcal{L}u(x) = \varphi(x) \\ \mathcal{B}u(x) = \psi(x) \end{cases}$$

Approximation → Ground truth

Stability of PDEs

$$\begin{cases} \mathcal{L}u(x) = \varphi(x) & x \in \Omega \subset \mathbb{R}^n \\ \mathcal{B}u(x) = \psi(x) & x \in \partial\Omega, \end{cases}$$

[Definition] We say a PDE is (Z_1, Z_2, Z_3)-**stable**, if

$$\|u^*(x) - u(x)\|_{Z_3} = O(\|\mathcal{L}u(x) - \varphi(x)\|_{Z_1} + \|\mathcal{B}u(x) - \psi(x)\|_{Z_2})$$

as $\|\mathcal{L}u(x) - \varphi(x)\|_{Z_1}, \|\mathcal{B}u(x) - \psi(x)\|_{Z_2} \to 0$, where Z_1, Z_2, Z_3 are three Banach spaces and u^* is the exact solution.

- Loss functions corresponding to $||\cdot||_{Z_1}$ and $||\cdot||_{Z_2}$ help to obtain u_θ that is ***provably*** close to the exact solution.

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- PINN training with **L^2 Physics-Informed Loss** is suitable only when a PDE is (L^2, L^2, Z)-stable for some Banach space Z.

$$\ell_\Omega(u) = \|\mathcal{L}u(x) - \varphi(x)\|^2_{L^2(\Omega)},$$

$$\ell_{\partial\Omega}(u) = \|\mathcal{B}u(x) - \psi(x)\|^2_{L^2(\partial\Omega)}.$$

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[Theorem1] (informal) A large class of n-dimensional HJB Equation is $(L^p, L^q, W^{1,1})$-stable if $p>n$, $q>kn$ (k depends on the equation).

[Theorem2] (informal) A large class of n-dimensional HJB Equation is *not* $(L^p, L^q, W^{1,1})$-stable if $p<n/4$.

HJB Equation: **H**amilton-**J**acobi-**B**ellman Equation

- The class of PDE we study is representative in high-dimensional non-linear PDEs. Power-law trading cost in optimal execution problem, Linear-Quadratic-Gaussian control and Merton's portfolio model are all special cases of this form.

$$\begin{cases} \mathcal{L}_{\text{HJB}} u := \partial_t u(x,t) + \frac{1}{2}\sigma^2 \Delta u(x,t) - \sum_{i=1}^{n} A_i |\partial_{x_i} u|^{c_i} = \varphi(x,t) & (x,t) \in \mathbb{R}^n \times [0,T] \\ \mathcal{B}_{\text{HJB}} u := u(x,T) = g(x) & x \in \mathbb{R}^n \end{cases}$$

- We consider $W^{1,1}$-stability here because both u and ∇u is important in application.

Theoretical analysis

[Theorem1] (informal) A large class of n-dimensional HJB Equation is (L^p, L^q, $W^{1,1}$)-stable if $p>n$, $q>kn$ (k depends on the equation).

Theorem 4.3. *For $p, q \geq 1$, let $r_0 = \frac{(n+2)q}{n+q}$. Assume the following inequalities hold for p, q and r_0:*

$$p \geq \max\left\{2, \left(1 - \frac{1}{\bar{c}}\right) n\right\};\ q > \frac{(\bar{c}-1)n^2}{(2-\bar{c})n+2};\ \frac{1}{r_0} \geq \frac{1}{p} - \frac{1}{n}, \tag{7}$$

where $\bar{c} = \max_{1\leq i\leq n} c_i$ in Eq. (6). Then for any $r \in [1, r_0)$ and any bounded open set $Q \subset \mathbb{R}^n \times [0, T]$, Eq. (6) is $(L^p(\mathbb{R}^n \times [0,T]), L^q(\mathbb{R}^n), W^{1,r}(Q))$-stable for $\bar{c} \leq 2$.

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$\mathrm{O}(n)$ $\mathrm{O}(n)$

Theoretical analysis

[Theorem2] (informal) A large class of n-dimensional HJB Equation is *not* $(L^p, L^q, W^{1,1})$-stable if $p<n/4$.

Theorem 4.4. *There exists an instance of Eq. (6), whose exact solution is u^*, such that for any $\varepsilon > 0, A > 0, r \geq 1, m \in \mathbb{N}$ and $q \in \left[1, \frac{n}{4}\right]$, there exists a function $u \in C^\infty(\mathbb{R}^n \times (0,T])$ which satisfies the following conditions:*

- $\|\mathcal{L}_{\mathrm{HJB}} u - \varphi\|_{L^q(\mathbb{R}^n \times [0,T])} < \varepsilon$, $\mathcal{B}_{\mathrm{HJB}} u = \mathcal{B}_{\mathrm{HJB}} u^*$, *and* $\mathrm{supp}(u - u^*)$ *is compact, where* $\mathcal{L}_{\mathrm{HJB}}$ *and* $\mathcal{B}_{\mathrm{HJB}}$ *are defined in Eq. (6).*
- $\|u - u^*\|_{W^{m,r}(\mathbb{R}^n \times [0,T])} > A.$

Theoretical analysis

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Theorem 4.4. *There exists an instance of Eq. (6), whose exact solution is u^*, such that* ***for any*** $\varepsilon > 0, A > 0, r \geq 1, m \in \mathbb{N}$ *and* $p \in \left[1, \frac{n}{4}\right]$, *there* ***exists a function*** $u \in C^\infty(\mathbb{R}^n \times (0,T])$ *which satisfies the following conditions:*

- $\|\mathcal{L}_{\text{HJB}} u - \varphi\|_{L^p(\mathbb{R}^n \times [0,T])} < \varepsilon$, $\mathcal{B}_{\text{HJB}} u = \mathcal{B}_{\text{HJB}} u^*$, *and* $\text{supp}(u - u^*)$ *is compact, where* $\mathcal{L}_{\text{HJB}}$ *and* $\mathcal{B}_{\text{HJB}}$ *are defined in Eq. (6).*
- $\|u - u^*\|_{W^{m,r}(\mathbb{R}^n \times [0,T])} > A$.

- Set $m = 0$, then Sobolev norm becomes L^r-norm.
- The distance between u_θ and u^*, ∇u_θ and ∇u^* could be **arbitrarily large** even though the ***L^2 loss* is small**!

Empirical results (100-dimensional HJB)

Table 6: **Error/loss-vs-time result of original PINN for Eq. (12).**

Iteration	**1000**	**2000**	**3000**	**4000**	**5000**
L^2 Loss	0.098	0.088	0.070	0.584	0.041
L^1 Relative Error	6.18%	5.36%	3.86%	3.94%	3.47%
$W^{1,1}$ Relative Error	17.53%	17.67%	14.83%	14.40%	11.31%

- L^2 loss drops very quickly, while relative error remains high.

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Recap: theoretical analysis

[Theorem1] (informal) A large class of n-dimensional HJB Equation is $(L^p, L^q, W^{1,1})$-stable if $p>n$, $q>kn$ (k depends on the equation).
[Theorem2] (informal) A large class of n-dimensional HJB Equation is *not* $(L^p, L^q, W^{1,1})$-stable if $p<n/4$.

L^2 Loss is not suitable for high-dimensional HJB Equation.

***L^p Loss (p>>1 or $p = \infty$)** can be a better choice!*

Experiments: Naïvely minimizing L^p loss

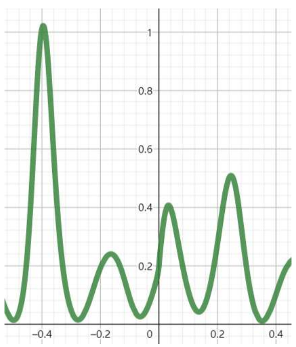
- Naïvely minimizing L^p loss with large but finite p does not lead to satisfactory results.

Method	Error	
	Domain	Boundary
L^4 Loss	2.42%	13.64%
L^8 Loss	53.55%	23.78%
L^{16} Loss	113.24%	80.68%

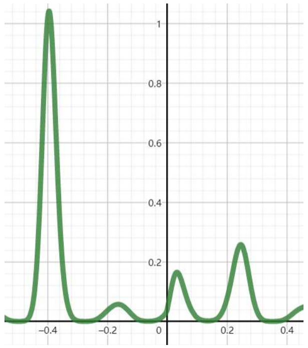
Experiments: Naïvely minimizing L^p loss

- Naïvely minimizing L^p loss with large but finite p does not lead to satisfactory results.
- Possible reasons:

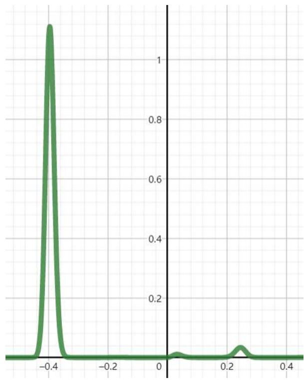
Large p → { Large MC variance → Sampling inefficiency; Stiff landscape → Optimization difficulty }



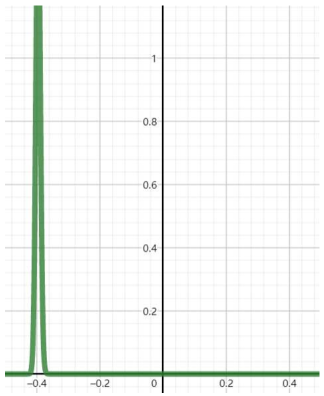
$p = 1$



$p = 2$



$p = 5$



$p = 20$

Minimizing L^∞ Physics-Informed Loss

New training objective: L^∞ Physics-Informed Loss

$$\ell_\infty(u) = \sup_{x \in \Omega} |\mathcal{L}u(x) - \varphi(x)| + \lambda \sup_{x \in \partial\Omega} |\mathcal{B}u(x) - \psi(x)|$$

Algorithm: adversarial-training-like min-max optimization.

- Inner loop: gradient-based methods to obtain data points with large point-wise loss to approximate supremum.
- Outer loop: fix the generated data points and calculate the gradient g to learn the network parameters.

L^∞ training for Physics-Informed Neural Networks

Algorithm 1 L^∞ Training for Physics-Informed Neural Networks

Input: Target PDE (Eq. (1)); neural network u_θ; initial model parameters θ

Output: Learned PDE solution u_θ

Hyper-parameters: Number of total training iterations M; number of iterations and step size of inner loop K, η; weight for combining the two loss term λ

1: **for** $i = 1, \cdots, M$ **do**

2: Sample $x^{(1)}, \cdots, x^{(N_1)} \in \Omega$ and $\tilde{x}^{(1)}, \cdots, \tilde{x}^{(N_2)} \in \partial\Omega$

3: **for** $j = 1, \cdots, K$ **do**

4: **for** $k = 1, \cdots, N_1$ **do**

5: $x^{(k)} \leftarrow \text{Project}_\Omega \left(x^{(k)} + \eta \, \text{sign} \nabla_x \left(\mathcal{L}u_\theta(x^{(k)}) - \varphi(x^{(k)}) \right)^2 \right)$

6: **for** $k = 1, \cdots, N_2$ **do**

7: $\tilde{x}^{(k)} \leftarrow \text{Project}_{\partial\Omega} \left(\tilde{x}^{(k)} + \eta \, \text{sign} \nabla_x \left(\mathcal{B}u_\theta(\tilde{x}^{(k)}) - \psi(\tilde{x}^{(k)}) \right)^2 \right)$

8: $g \leftarrow \nabla_\theta \left(\frac{1}{N_1} \sum_{i=1}^{N_1} \left(\mathcal{L}u_\theta(x^{(i)}) - \varphi(x^{(i)}) \right)^2 + \lambda \cdot \frac{1}{N_2} \sum_{i=1}^{N_2} \left(\mathcal{B}u_\theta(\tilde{x}^{(i)}) - \psi(\tilde{x}^{(i)}) \right)^2 \right)$

9: $\theta \leftarrow \text{Optimizer}(\theta, g)$

10: **return** u_θ

3-7:computing supremum （gradient ascend for data points）

8-9: optimization (gradient descent for NN parameters)

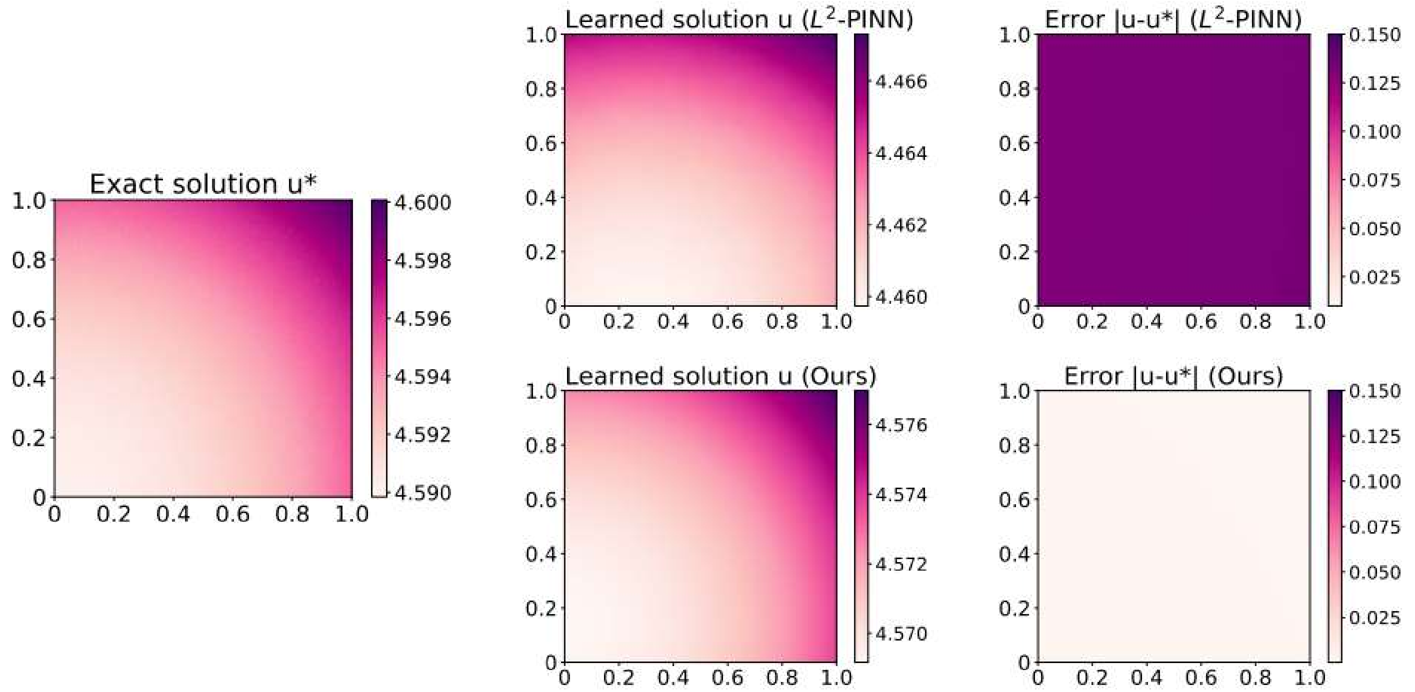
Experiments: High-dimensional HJB Equation

Method	$n = 100$		$n = 250$	
	Domain	Boundary	Domain	Boundary
Original PINN [23]	3.47%	19.59%	6.74%	23.25%
Adaptive time sampling [30]	3.05%	15.37%	7.18%	23.66%
Learning rate annealing [29]	11.09%	17.73%	6.94%	25.10%
Curriculum regularization [15]	3.40%	16.41%	6.72%	22.67%
Adversarial training (ours)	**0.27%**	**0.63%**	**0.95%**	**0.48%**

10x more accurate compared with baseline methods!

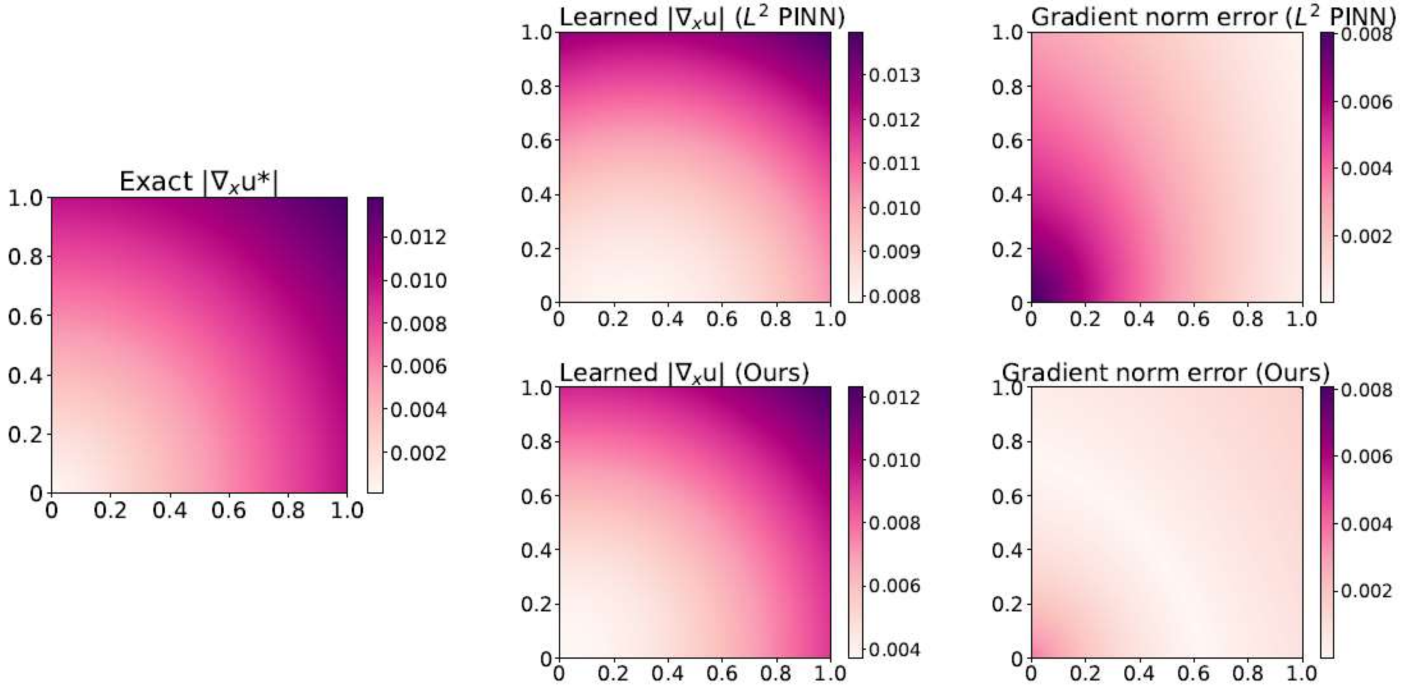
Experiments: High-dimensional HJB Equation

- Visualization of the learned solution of PINN and our method.



Experiments: High-dimensional HJB Equation

- Visualization of the ***gradient*** norm of the learned solution of PINN and our method.



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Conclusion

- In our work, we prove that for general L^p loss function, it is suitable for high dimensional HJB equation only if p is sufficiently large.
- Based on the theoretical results, we propose a novel PINN training algorithm to minimize the L^∞ loss for HJB equation in a similar spirit to adversarial training.


Thanks!
北京大學
PEKING UNIVERSITY
paper can be found at https://arxiv.org/abs/2206.02016