Investigating the Ability of PINNs to Solve Burgers' PDE near Finite-Time Blowup

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Let $\boldsymbol{u}(\boldsymbol{x}, t)$ be the actual solution

PDE

$$\boldsymbol{u}_t + \mathcal{N}_{\boldsymbol{x}}[\boldsymbol{u}] = 0, \quad \boldsymbol{x} \in D, t \in [0, T]$$

Initial Condition

$$\boldsymbol{u}(\boldsymbol{x}, 0) = h(\boldsymbol{x}), \quad \boldsymbol{x} \in D$$

Boundary Conditions

$$\boldsymbol{u}(\boldsymbol{x}, t) = g(\boldsymbol{x}, t), \quad \boldsymbol{t} \in [0, T], \boldsymbol{x} \in \partial D$$

Physics Informed Neural Nets (PINNs)

Let the neural solution be $\boldsymbol{u}_\theta(\boldsymbol{x}, t)$

Functional Residual

$$\mathcal{R}_{pde}(x, t) := \partial_t \boldsymbol{u}_\theta + \mathcal{N}_{\boldsymbol{x}}[\boldsymbol{u}_\theta(\boldsymbol{x}, t)]$$

Conditional Residual (I.C.)

$$\mathcal{R}_t(x) := \boldsymbol{u}_\theta(\boldsymbol{x}, 0) - h(\boldsymbol{x})$$

Conditional Residual (B.C.)

$$\mathcal{R}_b(x, t) := \boldsymbol{u}_\theta(\boldsymbol{x}, t) - g(\boldsymbol{x}, t)$$

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PINN Loss Function

$$\mathcal{L}(\theta) := \frac{1}{N_{pde}} \sum_{i=1}^{N_{pde}} \mathcal{R}_{pde}(x_r^i, t_r^i)^2 + \lambda_1 \frac{1}{N_t} \sum_{i=1}^{N_t} \mathcal{R}_t(x_t^i)^2 + \lambda_2 \frac{1}{N_b} \sum_{i=1}^{N_b} \mathcal{R}_b(x_b^i, t_b^i)^2$$

Why Physics Informed Neural Nets (PINNs) ?

PINNs have been achieving ever newer feats of solving complicated PDEs numerically while offering an attractive trade-off between **accuracy** and **speed** of inference.

In this work, we investigate the stability of PINNs near finite-time blow-ups from a rigorous theoretical viewpoint.

Why Physics Informed Neural Nets (PINNs) ?

$$\mathcal{E}_G := \|\boldsymbol{u} - \boldsymbol{u}_\theta\|$$

$$\tilde{\mathcal{E}}_T := \left(\sum_{n=1}^{N} w_n |\mathcal{R}_\theta|^p \right)^{1/p}$$

Risk Upperbound (Theorem 2.6)[1]

$$\mathcal{E}_G \leq C_{pde} \tilde{\mathcal{E}}_T + C_{pde} C_{quad}^{\frac{1}{p}} N^{-\frac{\alpha}{p}}$$

It was proven in the above mentioned theorem – for the first time – that one can minimize certain empirical errors to find provably good approximations to any PDE.

The strength of this result lies in its reliance on only **mild conditions** on the PDE.

[1] Mishra and Molinaro, "Estimates on the generalization error of physics-informed neural networks for approximating PDEs".

Why Finite-Time Blow-Ups ?

- Existing studies with PINNs (including studies of its failure modes) focus on cases where the true solution is "nice".

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- A finite-time blow-up – a phenomenon where the solution $\boldsymbol{u}$ becomes infinite at some points as t approaches a certain time $T < \infty$, while the solution is well-defined for all $0 < t < T$, $\sup_{x \in D} |\boldsymbol{u}(\boldsymbol{x}, t)| \to \infty \quad as \quad t \to T^-$
- $\frac{du}{dt} = u^2,\ u(0) = u_0,\ u_0 > 0$ is an ODE whose solution blows-up at $t = \frac{1}{u_0}$

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- $\frac{du}{dt} = u^2,\ u(0) = u_0,\ u_0 > 0$ is an ODE whose solution blows-up at $t = \frac{1}{u_0}$
- There are multiple real-world phenomena whose PDE models have finite-time blow-ups and these singularities are known to correspond to practically relevant processes – such as in chemotaxis models, thermal-runoff models and combustion models.

Why Finite-Time Blow-Ups ?

In a recent experimental studies with PINNs[2], experimental evidence was shown for PINNs potentially **discovering PDE solutions with blow-up** even when their **explicit descriptions are not known**.

[2] Wang et al., *Asymptotic self-similar blow up profile for 3-D Euler via physics-informed neural networks.*

Why Finite-Time Blow-Ups ?

In a recent experimental studies with PINNs[2], experimental evidence was shown for PINNs potentially **discovering PDE solutions with blow-up** even when their **explicit descriptions are not known**.

Here we look to understand this interface from a rigorous viewpoint and show how well the theoretical risk bounds correlate to their experimentally observed values - in certain blow-up situations.

[2] Wang et al., *Asymptotic self-similar blow up profile for 3-D Euler via physics-informed neural networks.*

Why is Burgers' PDE Interesting?

In order to assess the efficacy of PINNs in the vicinity of a blow-up phenomenon, we have chosen a very specific case - that of the Burgers' PDE where analytically exact solutions with finite-time blow-up are known - as is needed for a controlled study!

Burgers' Equation (inviscid)

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = 0$$

Main Results

We analyse the following PDE in the domain $D \subset \mathbb{R}^d$ and $t \in [-\frac{1}{\sqrt{2}} + \delta, \delta]$ for the following initial condition

PDE

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = 0$$

Initial Condition

$$\boldsymbol{u}(t = t_0) = \boldsymbol{u}_{t_0},\ t_0 = -\frac{1}{\sqrt{2}} + \delta$$

(d+1)-Burgers' PDE : Residuals

Let the neural net we aim to train be $\boldsymbol{u}_\theta(\boldsymbol{x}, t) \in \mathbb{R}^d$.

Then the residual terms for this predictor are,

Conditional Residual

$$\mathcal{R}_{\mathrm{t}} := \boldsymbol{u}_\theta(t = t_0) - \boldsymbol{u}(t = t_0)$$

The residual term for the functional loss is

Functional Residual

$$\mathcal{R}_{\mathrm{pde}} := \partial_t \boldsymbol{u}_\theta + (\boldsymbol{u}_\theta \cdot \nabla)\boldsymbol{u}_\theta$$

The L^2 population risk of the predictor that we are interested in is,

$$\int_{\Omega} \|\boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{u}_\theta(\boldsymbol{x}, t)\|_2^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

where $\boldsymbol{u}$ is the exact solution and $\boldsymbol{u}_\theta$ is the neural surrogate.

This definition of L^2-risk measures the distance of the neural surrogate from the true PDE solution.

Theorem 1

Let $\boldsymbol{u} \in C^1(D \times [t_0, T])$ be the unique solution of the $(d+1)-$dimensional Burgers' PDE. Then for any C^1 surrogate solution, say $\boldsymbol{u}_\theta$, the L^2-risk with respect to the true solution is bounded as,

$$\log \left(\int_\Omega \|\boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{u}_\theta(\boldsymbol{x}, t)\|_2^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t \right) \leq \log \left(\frac{C_1 C_2}{4} \right) + \frac{C_1}{\sqrt{2}} \tag{1}$$

where,

$$C_1 = d^2 \|\nabla \boldsymbol{u}_\theta\|_{L^\infty(\Omega)} + 1 + d^2 \|\nabla \boldsymbol{u}\|_{L^\infty(\Omega)}$$

$$C_2 = \int_D \|\mathcal{R}_t\|_2^2 \, \mathrm{d}\boldsymbol{x} + \int_\Omega \|\mathcal{R}_{pde}\|_2^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t + d^2 \|\nabla \boldsymbol{u}_\theta\|_{L^\infty(\Omega)} \int_\Omega \|\boldsymbol{u}_\theta\|_2^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t$$
$$+ d^2 \|\nabla \boldsymbol{u}\|_{L^\infty(\Omega)} \int_\Omega \|\boldsymbol{u}\|_2^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t$$

$$
\begin{aligned}
C_1 &= d^2 \|\nabla \boldsymbol{u}_\theta\|_{L^\infty(\Omega)} + 1 + d^2 \|\nabla \boldsymbol{u}\|_{L^\infty(\Omega)} \\
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&\quad + d^2 \|\nabla \boldsymbol{u}\|_{L^\infty(\Omega)} \int_\Omega \|\boldsymbol{u}\|_2^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t
\end{aligned}
$$

Note the following key points about this bound,

- This can be estimated just by knowing an upper bound on $\|\nabla \boldsymbol{u}\|_{L^\infty(\Omega)}$ and $\|\boldsymbol{u}\|_2$.

(d+1)-Burgers' PDE: An Upper Bound for the L^2−Risk

$$C_1 = d^2 \|\nabla \boldsymbol{u}_\theta\|_{L^\infty(\Omega)} + 1 + d^2 \|\nabla \boldsymbol{u}\|_{L^\infty(\Omega)}$$

$$C_2 = \int_D \|\mathcal{R}_t\|_2^2 \,\mathrm{d}\boldsymbol{x} + \int_\Omega \|\mathcal{R}_{pde}\|_2^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t + d^2 \|\nabla \boldsymbol{u}_\theta\|_{L^\infty(\Omega)} \int_\Omega \|\boldsymbol{u}_\theta\|_2^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$
$$+ d^2 \|\nabla \boldsymbol{u}\|_{L^\infty(\Omega)} \int_\Omega \|\boldsymbol{u}\|_2^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

Note the following key points about this bound,

- This has explicit dependence on the norm of the surrogate (through C_2) and its spatial gradient (through both C_1 and C_2). Hence providing a theoretical foundation for the role of **functional regularization** in PINN training[3].

[3] Wang et al., *Asymptotic self-similar blow up profile for 3-D Euler via physics-informed neural networks.*

In one dimension, for Burgers's PDE we can get a more interesting bound! Towards that we consider working in the domain $x \in [-1, 1]$ and $t \in [-1+\delta, \delta)$, parameterized by δ.

PDE

$$u_t + uu_x = 0$$

Initial Conditions

$$u(x, -1+\delta) = \frac{x}{-2+\delta}$$

Boundary Conditions

$$u(-1, t) = \frac{1}{1-t}$$

$$u(1, t) = \frac{1}{t-1}$$

(1+1)-Burgers' PDE Near Finite-Time Blow Up

In one dimension, for Burgers's PDE we can get a more interesting bound! Towards that we consider working in the domain $x \in [-1, 1]$ and $t \in [-1 + \delta, \delta)$, parameterized by δ.

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$$u_t + uu_x = 0$$

Initial Conditions

$$u(x, -1 + \delta) = \frac{x}{-2 + \delta}$$

Boundary Conditions

$$u(-1, t) = \frac{1}{1 - t}$$

$$u(1, t) = \frac{1}{t - 1}$$

These initial and boundary conditions correspond to an exact solution to the Burgers' PDE i.e. $u(x, t) = \frac{x}{t-1}$

(1+1)-Burgers' PDE Near Finite-Time Blow Up : Residuals

As earlier, for the neural net $u_\theta(x,t)$ attempting to solve this PDE, we define the following residuals,

Conditional Residuals

$$R_{tb,\theta}(x) = u_\theta(x, -1+\delta) - \frac{x}{-2+\delta}$$

$$R_{sb,-1,\theta}(t) = u_\theta(-1, t) - \frac{1}{1-t}, \quad R_{sb,1,\theta}(t) = u_\theta(1, t) - \frac{1}{t-1}$$

Functional Residual

$$R_{int,\theta}(x,t) = \partial_t u_\theta(x,t) + u_\theta(x,t) \cdot \partial_x u_\theta(x,t)$$

Theorem 2

Let $u \in C^1((-1+\delta, \delta) \times (-1,1))$ be the unique solution of the (1+1)-D Burgers' equation for any $k \geq 1$ and $u^* = u_{\theta^*}$ be the neural surrogate. Then the population risk of it is bounded as,

$$\left(\int_{-1+\delta}^{\delta}\int_{-1}^{1} |u(x,t) - u_\theta(x,t)|^2 \, dxdt\right)^{\frac{1}{2}}$$
$$\leq \left[1 + Ce^C\right] \left[\int_{-1}^{1} \mathcal{R}_{tb,\theta^*}(x)dx + \int_{-1+\delta}^{\delta}\int_{-1}^{1} \mathcal{R}^2_{int,\theta^*}(x,t)dxdt\right.$$
$$+ 2C_{2b}\left(\int_{-1+\delta}^{\delta} \mathcal{R}^2_{sb,-1,\theta^*}(t)dt + \int_{-1+\delta}^{\delta} \mathcal{R}^2_{sb,1,\theta^*}(t)dt\right)$$
$$\left. + 2C_{1b}\left(\left(\int_{-1+\delta}^{\delta} \mathcal{R}^2_{sb,-1,\theta^*}(t)dt\right)^{\frac{1}{2}} + \left(\int_{-1+\delta}^{\delta} \mathcal{R}^2_{sb,1,\theta^*}(t)dt\right)^{\frac{1}{2}}\right)\right] \quad (2)$$

where $C = 1 + 2C_{u_x}$, with

$$C_{u_x} = \|u_x\|_{L^\infty} = \left\|\frac{1}{t-1}\right\|_{L^\infty([-1+\delta,\delta])} = \frac{1}{1-\delta}$$

$$C_{1b} = \|u(1,t)\|^2_{L^\infty} = \left\|\frac{1}{1-t}\right\|^2_{L^\infty([-1+\delta,\delta])} = \frac{1}{(1-\delta)^2}$$

$$C_{2b} = \|u_{\theta^*}(1,t)\|_{L^\infty([-1+\delta,\delta])} + \frac{3}{2}\left\|\frac{1}{t-1}\right\|_{L^\infty([-1+\delta,\delta])} = \|u_{\theta^*}(1,t)\|_{L^\infty([-1+\delta,\delta])} + \frac{3}{2}\left(\frac{1}{1-\delta}\right)$$

Even though we set up the initial and boundary conditions to reflect a finite-time singularity, our bound for the L_2 population risk indicates the stability of the PINN risk, defined as,

$$\mathbb{E}[|\mathcal{R}_{int,\theta}|^2] + \mathbb{E}[|\mathcal{R}_{tb,\theta}|^2] + \mathbb{E}[|\mathcal{R}_{sb,-1,\theta}|^2] + \mathbb{E}[|\mathcal{R}_{sb,1,\theta}|^2]$$

The "stability"[4] here means that if this PINN risk is found to be $\mathcal{O}(\epsilon)$ then that would directly imply that the L_2 population risk is also $\mathcal{O}(\epsilon)$.

[4] Wang et al., "Is L^2 Physics Informed Loss Always Suitable for Training Physics Informed Neural Network?"

Experiment and Analysis

(2+1)-Burgers' PDE with Finite-Time Blow Up

Consider solving the $(2+1)-$Burgers' PDE on $t \in [-\frac{1}{\sqrt{2}} + \delta, \delta]$ where $\delta \in [0, \frac{1}{\sqrt{2}})$

Initial Conditions

$$u_{1,t_0} = \frac{(1+\sqrt{2}-2\delta)x_1 + x_2}{2\delta(\sqrt{2}-\delta)} \; ; \; u_{2,t_0} = \frac{x_1 - (1-\sqrt{2}+2\delta)x_2}{2\delta(\sqrt{2}-\delta)}$$

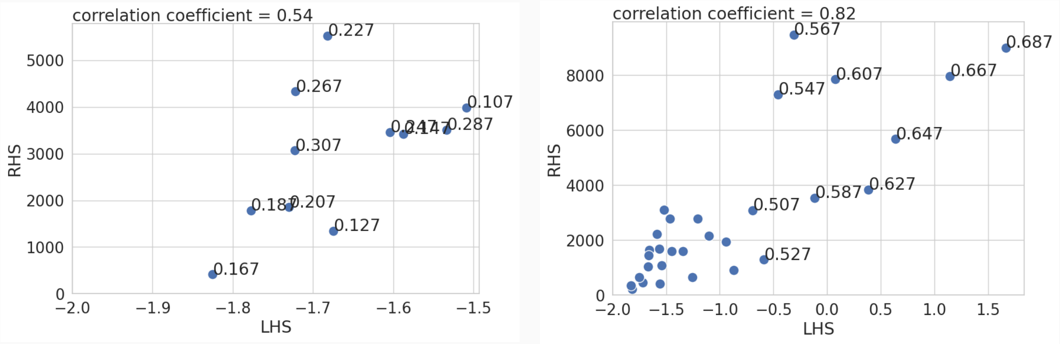
Boundary Conditions

$$u_1(x_1 = 0) = \frac{x_2}{1 - 2 \cdot t^2} \; ; \quad u_1(x_1 = 1) = \frac{1 + x_2 - 2 \cdot t}{1 - 2 \cdot t^2}$$

$$u_2(x_2 = 0) = \frac{x_1}{1 - 2 \cdot t^2} \; ; \quad u_2(x_2 = 1) = \frac{x_1 - 1 - 2 \cdot t}{1 - 2 \cdot t^2}$$

These I.C. and B.C. correspond to this exact solution $u_1 = \frac{x_1 + x_2 - 2x_1 t}{1 - 2t^2}, \; u_2 = \frac{x_1 - x_2 - 2x_2 t}{1 - 2t^2}$

(2+1)-Burgers' PDE with Finite-Time Blow Up : LHS vs RHS Plots for Theorem 1



(a) width=30

(b) width=100

Figure 1: This figure shows the RHS vs LHS plot of Equation (1) from Theorem 1 for different values of δ for PINNs of 2 different widths. (Recall that here the blow up is at $\delta \sim 0.7$)

Future Directions

Generalization Error

$$\mathcal{E}_{gen,\theta} := \frac{1}{N_r}\sum_{i=1}^{N_r} R_{pde,\theta}(x_{ri}, t_{ri}) + \frac{\lambda}{N_0}\sum_{j=1}^{N_0} R_{t,\theta}(x_{0j})$$
$$- \left(\mathbb{E}_{(x_r,t_r)\sim\mathcal{D}_1}[R_{pde,\theta}(x_r, t_r)] + \lambda\mathbb{E}_{x_0\sim\mathcal{D}_2}[R_{t,\theta}(x_0)]\right)$$

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Theorem 3

The worst case data-averaged generalization error can be bounded as,

$$\mathbb{E}_{\substack{(x_{ri},t_{ri})\sim\mathcal{D}_1\forall i\in[N_r]\\ x_{0j}\sim\mathcal{D}_2\forall j\in[N_0]}}\left[\sup_{\theta}\left(\mathcal{E}_{gen,\theta}\right)\right] \leq \frac{C_r}{\sqrt{N_r}} + \lambda\frac{C_0}{\sqrt{N_0}}.$$

Ongoing Work : (1+1)-Burgers

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- This is thus far only for depth-2 neural nets
- tanh activation

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As far as we have checked this is possible the first generalization error bound for solving a non-linear PDE by neural nets.

- Can modifications to the PINN formalism be made to make them more sensitive to the local structure of the solutions and thus help detect the existence of finite-time blow-ups in PDEs?

[5] Wang et al., "Is L^2 Physics Informed Loss Always Suitable for Training Physics Informed Neural Network?"
[6] Gopalani and Mukherjee, "Global Convergence of SGD On Two Layer Neural Nets".

Future Directions

- Can modifications to the PINN formalism be made to make them more sensitive to the local structure of the solutions and thus help detect the existence of finite-time blow-ups in PDEs?
- Are there any PINN losses for the $(d+1)$-dimensional Burgers – or for Navier-Stokes in general – that is "stable"[5], as was shown to be true in our $(1+1)$-dimensional Burgers' PDE setup?

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- Are there any PINN losses for the $(d+1)$-dimensional Burgers – or for Navier-Stokes in general – that is "stable"[5], as was shown to be true in our $(1+1)$-dimensional Burgers' PDE setup?
- Do PINN loss functions for fluid PDEs satisfy the Villani condition[6], thereby establishing that Langevin Monte Carlo can effectively minimize PINN losses?

[5] Wang et al., "Is L^2 Physics Informed Loss Always Suitable for Training Physics Informed Neural Network?"
[6] Gopalani and Mukherjee, "Global Convergence of SGD On Two Layer Neural Nets".