Sticking a ‘PINN’ in It: A Physics-Informed Neural Network Approach to PDEs

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Abstract

Recent successes in neural networks have greatly encouraged their use in solving classical problems in applied mathematics, as the networks allow for rapid prototyping with usable estimations. This holds especially true in areas involving high dimensional partial differential equations (PDEs), such as quantum physics and fluid dynamics. Here, we present a neural network architecture, the physics-informed neural network (PINN), and implement a specific method, the continuous time approach.

Background

We describe the PINN approach for approximating the solution

$$u : [0,T] \times \mathcal{D} \to \mathbb{R} \quad (\star)$$

of an evolution equation

$$\partial_t u(t,x) + \mathcal{N}[u](t,x) = 0, \qquad (t,x) \in (0,T] \times \mathcal{D}, \qquad (1a)$$

$$u(0,x) = u_0(x), \qquad x \in \mathcal{D}, \qquad (1b)$$

where $\mathcal{N}$ is a differential operator acting on $u, \mathcal{D} \subset \mathbb{R}^d$ a bounded domain, T denotes the final time and $u_0 : \mathcal{D} \to \mathbb{R}$ the prescribed initial data. Based on the literature review conducted, we restrict our discussion to the Dirichlet case and define

$$u(t,x) = u_b(t,x), \quad (t,x) \in (0,T] \times \partial\mathcal{D}, \qquad (1c)$$

where $\partial\mathcal{D}$ denotes the boundary of the domain $\mathcal{D}$ and $u_b : (0,T] \times \partial\mathcal{D} \to \mathbb{R}$ the given boundary data. The method constructs a neural network approximation $u_\theta(t,x) \approx u(t,x)$ of the solution of (1), where $u_\theta : [0,T] \times \mathcal{D} \to \mathbb{R}$ denotes a function realized by a neural network with parameters θ.

Continuous Time Approach

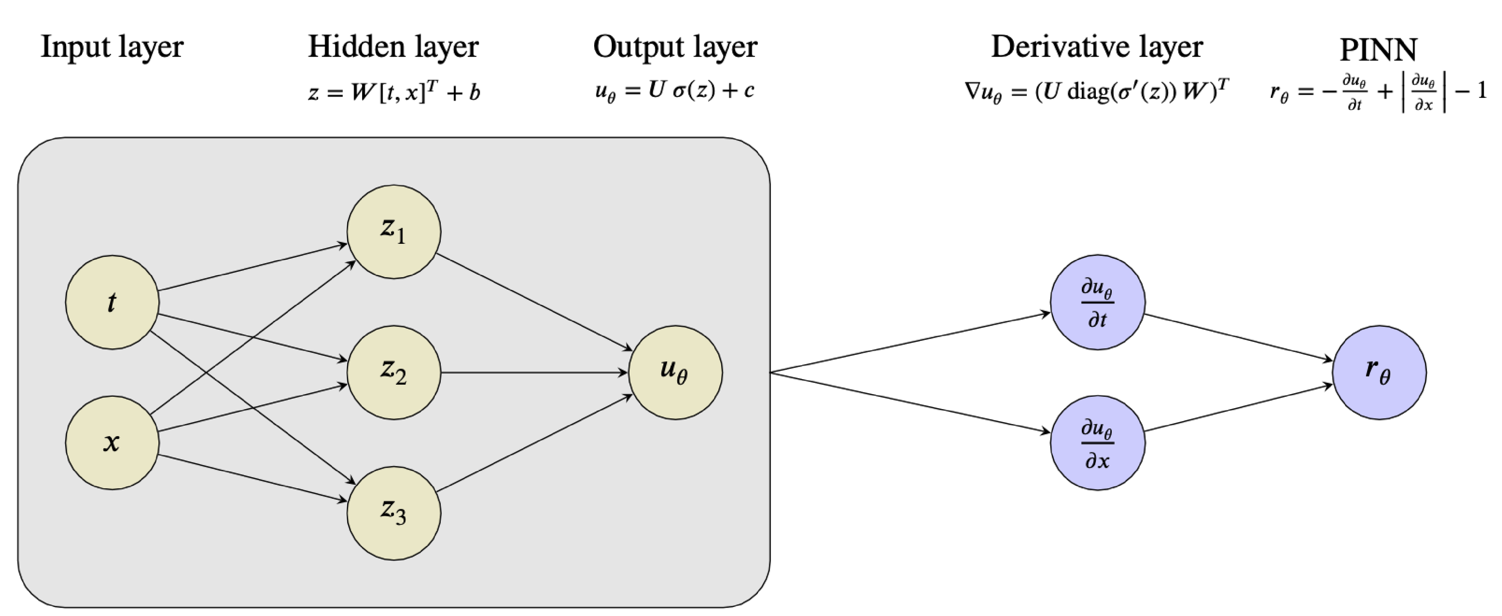


Figure 1) Neural network architecture of the PINN approach

The (strong) residual of a given neural network approximation of $(\star)$ with respect to the PINN approach above is

$$r_\theta(t,x) := \partial_t u_\theta(t,x) + \mathcal{N}[u_\theta](t,x) \qquad (2)$$

These networks are compositions of alternating affine linear $W^\ell \cdot + b^\ell$ and nonlinear functions $\sigma^\ell(\cdot)$ called activations, i.e.,

$$u_\theta(z) := W^L \sigma^L \left(W^{L-1} \sigma^{L-1} \left(\cdots \sigma^1 \left(W^0 z + b^0 \right) \cdots \right) + b^{L-1} \right) + b^L,$$

where W^ℓ and b^ℓ are weight matrices and bias vectors, and $z = [t,x]^T$.

PINN Approach

For the solution of the PDE (1) now proceeds by minimization of the loss functional

$$\phi_\theta(X) := \phi_\theta^r(X^r) + \phi_\theta^0\left(X^0\right) + \phi_\theta^b\left(X^b\right), \qquad (3)$$

where X denotes the collection of training data and the loss function ϕ_θ contains the following terms:

The Mean Squared Residual

$$\phi_\theta^r(X^r) := \frac{1}{N_r} \sum_{i=1}^{N_r} |r_\theta(t_i^r, x_i^r)|^2$$

in a number of collocation points $X^r := \left\{(t_i^r, x_i^r)\right\}_{i=1}^{N_r} \subset (0,T] \times \mathcal{D}$, where r_θ is the physics-informed neural network (2),

The Mean Squared Misfit *w.r.t* Initial and Boundary Conditions

$$\phi_\theta^0\left(X^0\right) := \frac{1}{N_0} \sum_{i=1}^{N_0} \left| u_\theta\left(t_i^0, x_i^0\right) - u_0\left(x_i^0\right) \right|^2 \quad \text{and} \quad \phi_\theta^b\left(X^b\right) := \frac{1}{N_b} \sum_{i=1}^{N_b} \left| u_\theta\left(t_i^b, x_i^b\right) - u_b\left(t_i^b, x_i^b\right) \right|^2$$

in a number of points $X^0 := \left\{(t_i^0, x_i^0)\right\}_{i=1}^{N_0} \subset \{0\} \times \mathcal{D}$ and $X^b := \left\{\left(t_i^b, x_i^b\right)\right\}_{i=1}^{N_b} \subset (0,T] \times \partial\mathcal{D}$, where u_θ is the neural network approximation of the solution $u : [0,T] \times \mathcal{D} \to \mathbb{R}$.

Example: Heat Equation

A classical problem in the domain of PDEs, the heat equation governs the temperature distribution of a rod of length l :

$$u_t = k u_{xx} \qquad (t,x) \in \mathbb{R}^+ \times (0,l)$$

$$u(t,0) = u(t,l) = 0 \qquad t \geq 0$$

$$u(0,x) = f(x) \qquad x \in (0,l).$$

If k, called the conductivity is a constant the rod is isotropic; if $k = k(x)$ it is anisotropic or heterogeneous medium.

Application

For the fitting, we choose $k = 1, l = \pi$, and $f(x) = \sin(3x)$ for the application of the PINN.

We assume that the collocation points X_r as well as the points for the initial time and boundary data X_0 and X_b are generated by random sampling from a uniform distribution. $(N = 10,000)$

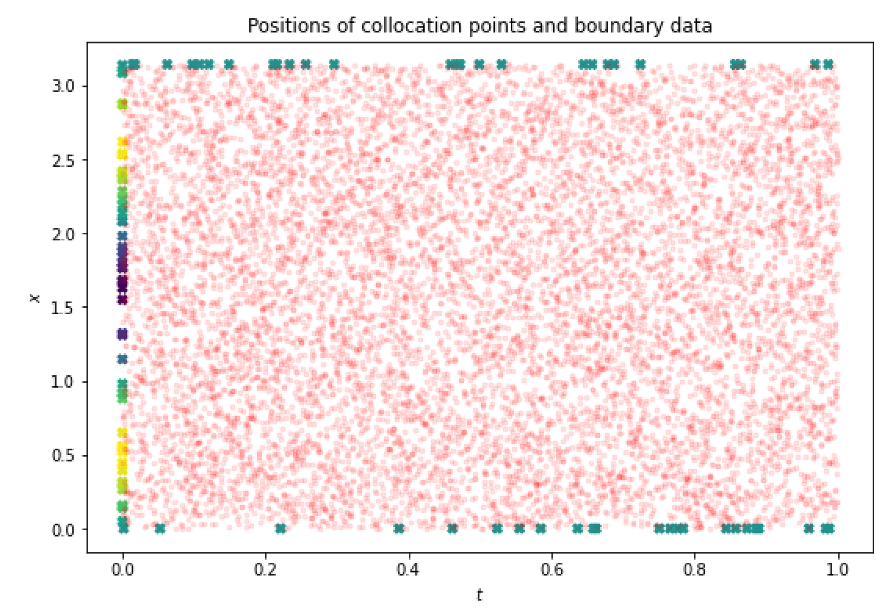
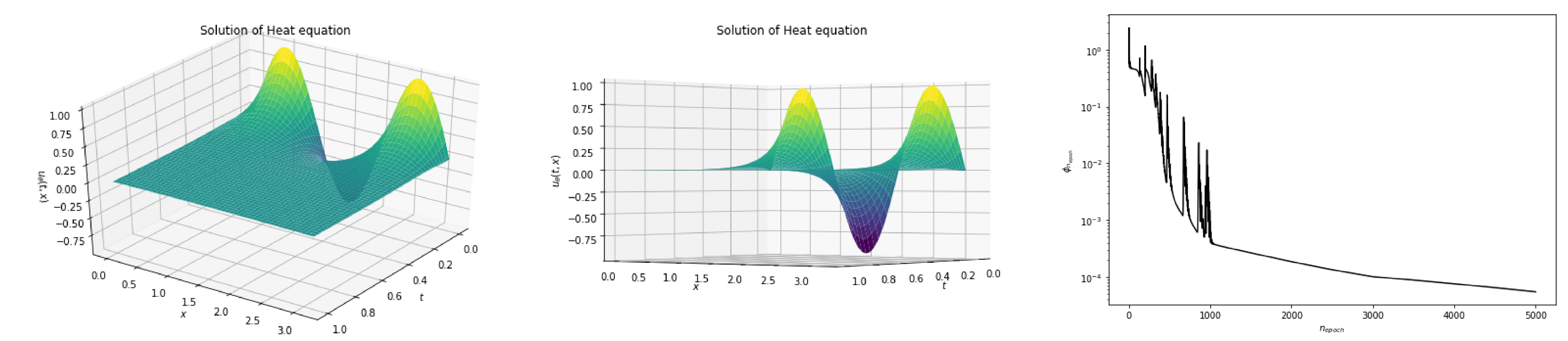


Figure 2) Plot of the collocation points $(N = 10,000)$

PINN Approximation and Evolution of Loss



(a) View 1 (b) View 2 (c) Loss

Test

The chosen problem can be solved via separation of variables. The idea is to assume the solution $u = u(t,x)$ can be written as

$$u(t,x) = F(t)G(x)$$

If we compute the corresponding partial derivatives and replace in the PDE, we get

$$\frac{F'(t)}{F(t)} = \frac{G''(x)}{G(x)}$$

The only way this equality is true for all t and x is if

$$F'(t) = \lambda F(t) \quad \text{and} \quad G''(x) = \lambda G(x)$$

The boundary condition becomes

$$G(0) = G(\pi) = 0$$

We can easily solve this ordinary differential equations. By considering the cases $\lambda > 0, \lambda = 0$ and $\lambda < 0$, we conclude $\lambda = -n^2, n \in \mathbb{N}$ and (up to constants)

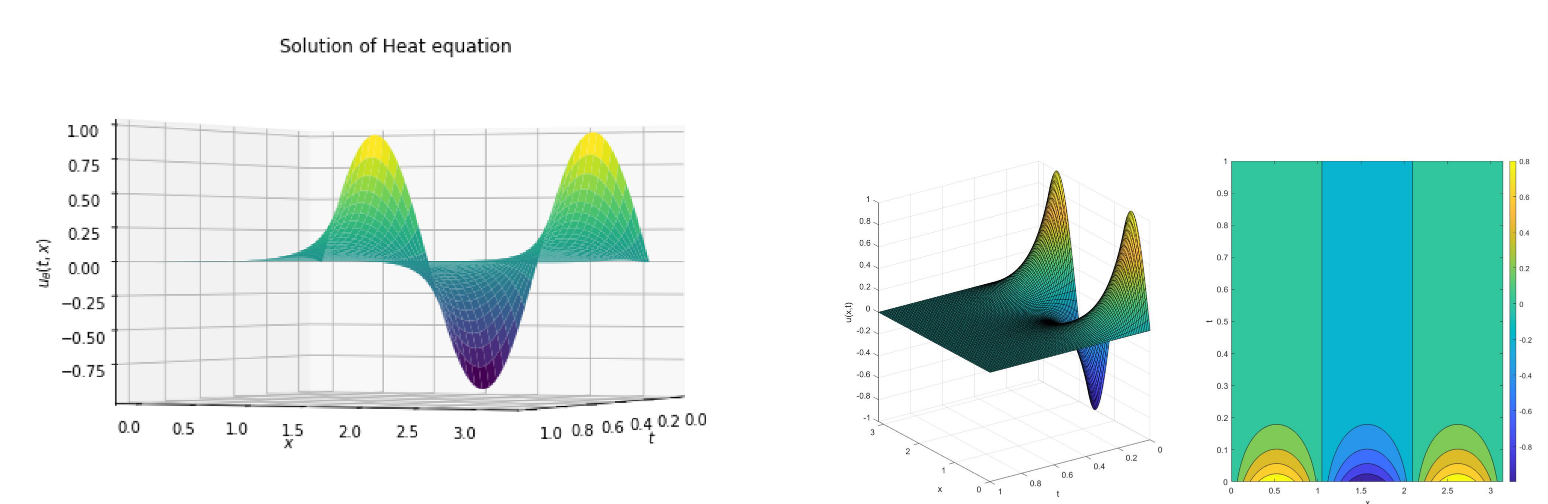
$$F(t) = \exp\left(-n^2 t\right) \quad \text{and} \quad G(x) = \sin(nx)$$

Since the equation is linear, by the principle of superposition $u(t,x) = \sum_{n=1}^{\infty} c_n \exp\left(-n^2 t\right) \sin(nx)$

Finally, since $u(0,x) = \sin(3x) = \sum_{n=1}^{\infty} c_n \sin(nx)$ with $c_3 = 1$ and $c_n = 0$ if $n \neq 3$. Hence,

$$u(t,x) = \exp(-9t)\sin(3x)$$

True Solution



(a) PINN (b) True Solution

References

[1] Jan Blechschmidt Oliver Ernst. Three ways to solve partial differential equations with neural networks — a review. *GAMM-Mitteilungen*, 44(2), 2021.

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