Physics-informed neural networks for the solution of nonlinear PDEs.

Student: Miguel Ángel Cruz Gama

Advisors: Julio Cesar Pérez Sansalvador, Gustavo Rodríguez Gómez

Abstract

The present work is based on Physics-Informed Neural Networks (PINNs). This methodology focuses on approximating a solution by solving initial and boundary value problems defined by ordinary differential equations (ODEs) and partial differential equations (PDEs). This idea, originally proposed in the 1990s by Lagaris et al., integrates knowledge of physical laws directly into the training process of artificial neural networks (ANNs).
The main objective is to construct a test solution to the differential equation consisting of two parts: the first satisfies the initial or boundary conditions and contains no adjustable parameters, while the second is a neural network that does not affect these conditions, with the ANN trained to satisfy the differential equation itself. This approach transforms a constrained optimization problem (imposed by the boundary conditions) into an unconstrained one.

Motivation

Many scientific and engineering applications require the solution of PDEs to describe physical phenomena. Applications can be found in the fields of aerodynamics, geophysics, biophysics, combustion, among others. In some exceptional cases, an analytical solution for PDEs exists, but in the vast majority of applications, some type of numerical approximation is required. In this work, we propose an alternative using PINNs as an approximation function for PDEs. Unlike traditional numerical methods, NNs have the property of being able to approximate any function with sufficient parameters.
Furthermore, these solutions are continuous and derivable throughout the domain, so they do not require discretization.

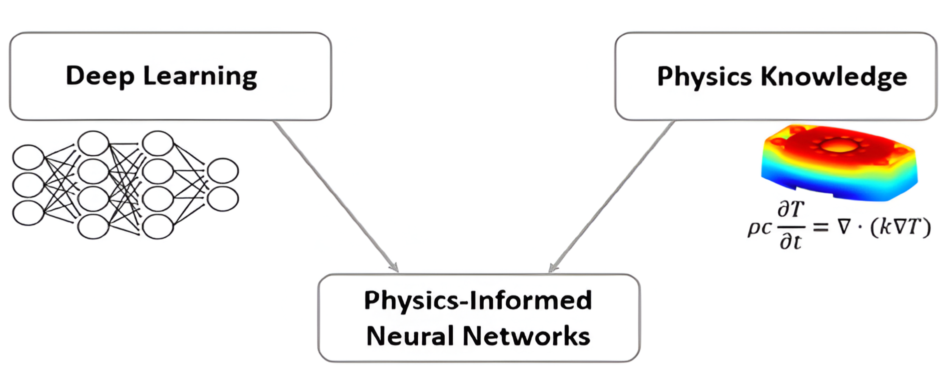


Figure 1. a learning algorithm physics-informed amounts to introducing appropriate observational, inductive or learning biases that can steer the learning process towards identifying physically consistent solutions

Main objetive

The general (preliminary) objective of the work is to design a PINN to approximate the solution of a nonlinear PDE.

Related work

Year	Author	Type of Differential Equation	Characteristic of Differential Equation
1998	Lagaris et al.	ODE's PDE's Systems of Coupled ODEs	• First-order and second-order ODEs for Dirichlet BC's • nonlinear PDE
2019	Raissi et al	nonlinear PDE	• Burgers equation • Nonlinear Schrödinger equation (with complex-valued solutions and periodic boundary conditions)
2021	LU LU et al	PDE's Systems of ODEs	• Poisson's equation (over an L-shaped domain) • EID of Volterra (first order)
2023	Cosmin Anitescu et al	ODE's PDE's	• 1D Steady State Heat Equation (Forward and Inverse Problem) • 2D linear elasticity (direct problem) • 3D Hyperelasticity (direct problem) • Helmholtz equation (inverse complex-valued problem)

The building blocks of a PINN

PINN's can solve differential equations expressed, in the most general form, like:

$$\begin{cases} F(u(z), \gamma) = f(z) & z \in \Omega \\ G(u(z)) = g(z) & z \in \partial\Omega \end{cases}$$

The goal is to predict the solution $u(z)$ of the DE by implementing a NN, giving rise to an approximation

$$u(z) \approx \hat{u}_\theta(z)$$

The NN approximates the solution by searching for parameters, minimizing a loss function.

$$\{\theta, b\}^* = \arg\min_{\{\theta, b\}} \left(w_F \mathcal{L}_{Physics} + w_B \mathcal{L}_{BCs} + w_D \mathcal{L}_{Data} \right)$$

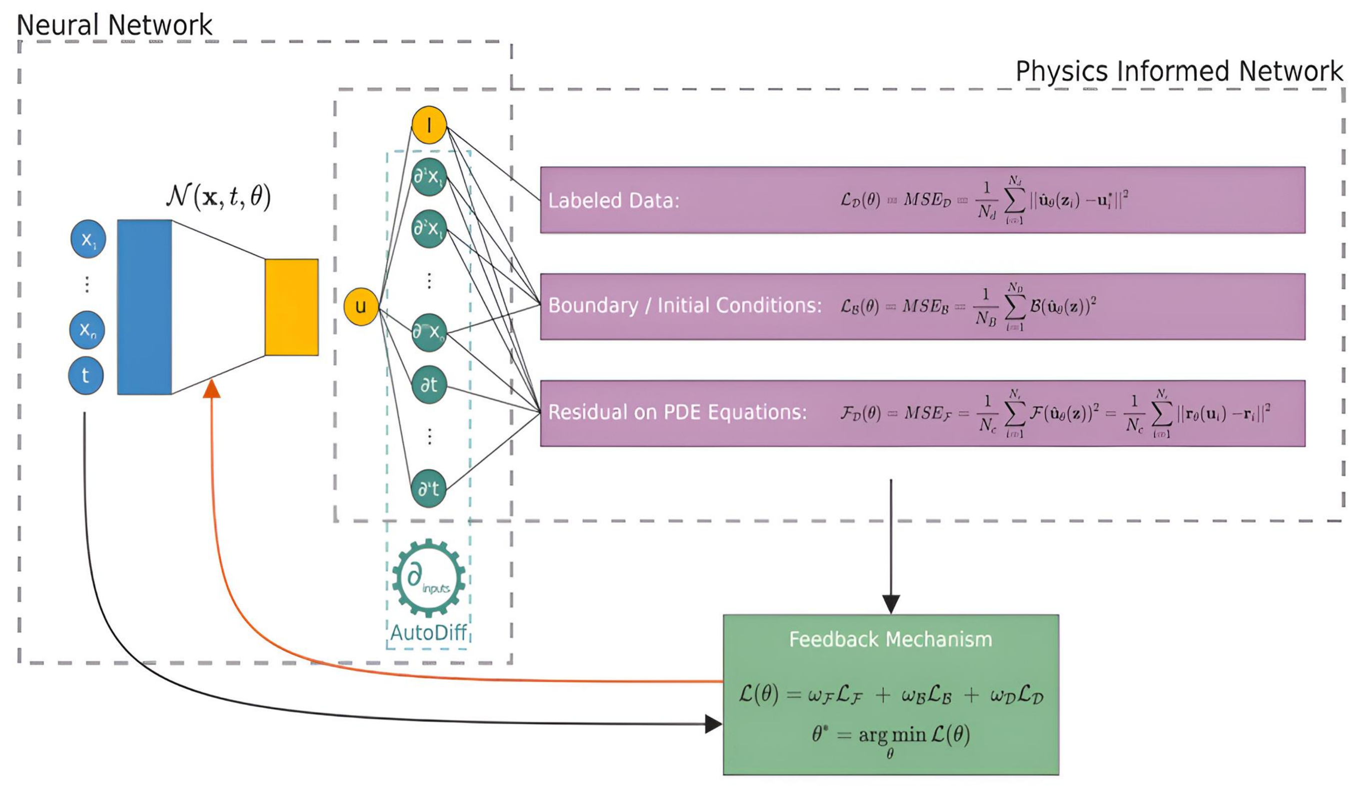


Figure 2. Loss function depends on the differential equations $\mathcal{L}_F$, the boundary conditions $\mathcal{L}_B$ and $\mathcal{L}_D$ loss of data that may be know

Description of the method

The objetive is to solve a PDE in the general form:

$$G(x, \psi(x), \nabla\psi(x), \nabla^2\psi(x)) = 0, \qquad x \in D$$

The problem becomes minimizing the error at these points:

$$\min_\theta \sum_{x_i \in D} \left(G(x_i, \psi_t(x_i, \theta), \nabla\psi_t(x_i, \theta), \nabla^2\psi_t(x_i, \theta)) \right)$$

Where $\psi_t(x_i, \theta)$ it is a test solution parameterized by θ (the weights of the neuronal network).

For Poisson's equation in 2D:

$$\nabla^2\psi(x, y) = f(x, y)$$

With boundary conditions:

$$\begin{cases} \psi(x, 0) = g_0(x) \\ \psi(x, 1) = g_1(x) \end{cases} \text{and} \begin{cases} \psi(0, y) = f_0(y) \\ \psi(1, y) = f_1(y) \end{cases}$$

The test solution is

$$\psi_t(x, y) = A(x, y) + x(1 - x)y(1 - y)N(x, y, \theta)$$

Preliminary results

For the mathematical model that represent the uniform heat distribution in metal rod T(x), given by the differential equation:

$$k\frac{d^2T}{dx^2} + q(x) = 0, x \in [0,1].$$

With $q(x) = 15x - 2, k = 0.5$ and $T(0) = T(1) = 0$.
To adapt the problem to a PINN, a loss function is designed that collects the points within the domain and the initial conditions.

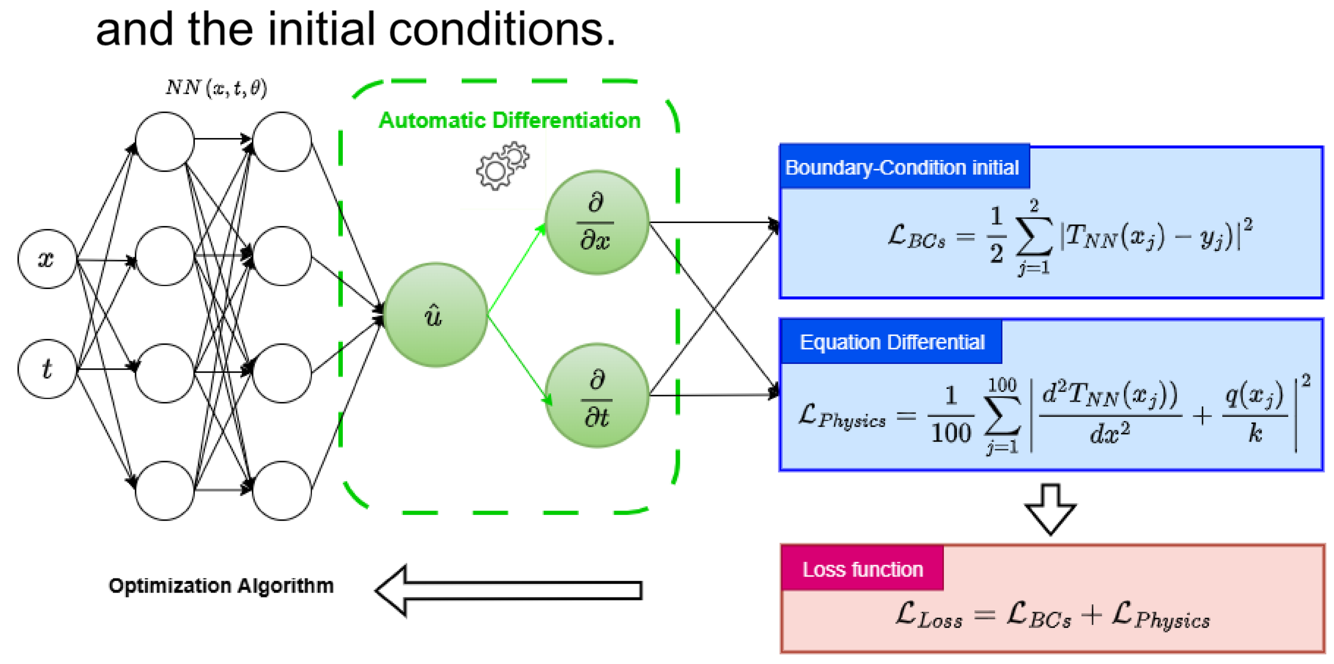
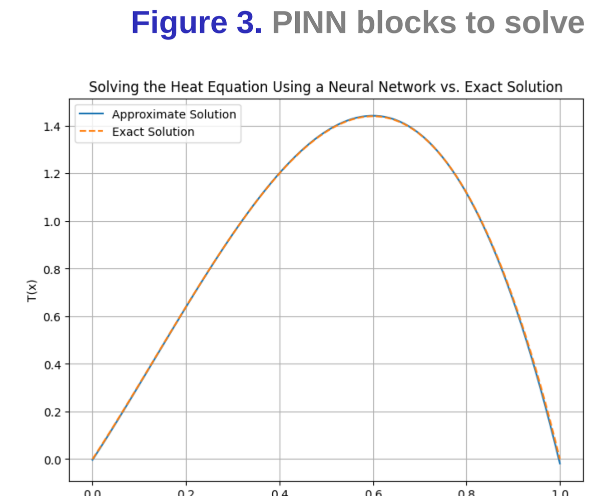
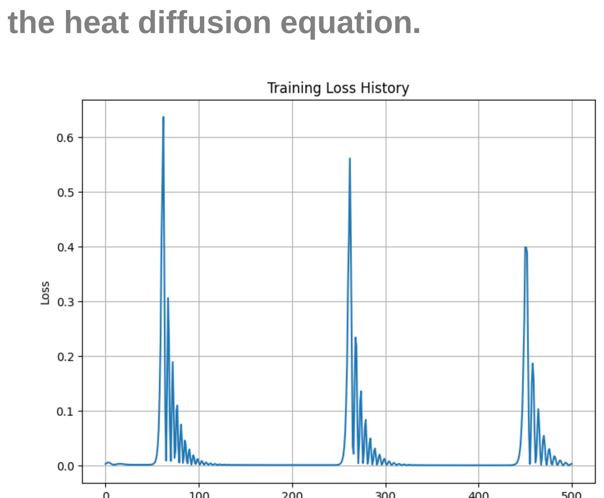


Figure 3. PINN blocks to solve the heat diffusion equation.

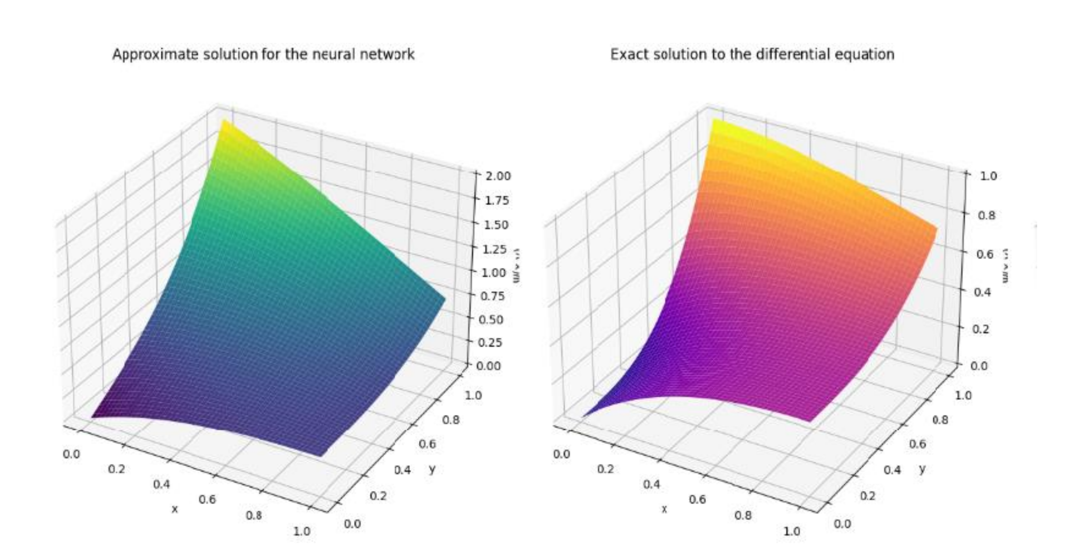




We consider boundary value problems with Dirichlet and Neuman BC's.

$$\nabla^2\Psi(x, y) = e^{-x}(x - 2 + y^3 + 6y)$$

With $x, y \in [0,1]$ and $\Psi(0, y) = y^3, \Psi(1, y) = (1 + y^3)$, $\psi(x, 0) = xe^{-x}$ and $\psi(x, 1) = e^{-x}(x + 1)$



References

1. Anitescu, C., İsmail Ateş, B., Rabczuk, T. (2023). Physics-Informed Neural Networks: Theory and Applications. In: Rabczuk, T., Bathe, KJ. (eds) Machine Learning in Modeling and Simulation. Computational Methods in Engineering & the Sciences. Springer, Cham.
2. M. Raissi, P. Perdikaris, and G. E. Karniadakis. (2019) Physics-informed neural networks: Adeep learning framework for solving forward and inverse problems involving non linear partial differential equations. Journal of Computational Physics, 378:686–707.
3. Lagaris I, Likas A, Fotiadis D. (1998) Artificial neural networks for solving ordinary and partial diferential equations. IEEE Transactions on Neural Network .
4. Lu, L., Meng, X., Mao, Z., & Karniadakis, G. E. (2021). DeepXDE: A Deep Learning Library for Solving Differential Equations. *SIAM Review*, *63*(1), 208–228.