Hands-on Physics Informed Neural Networks

Tutorial@MAGNET4Cardiac7T Spring School 2025

7th April 2025

Cecília Coelho,
Institute for Artificial Intelligence(HSU-AI),
Helmut Schmidt University Hamburg, Germany
cecilia.coelho@hsu-hh.de

Requirements: *Python, Pytorch, Numpy, Matplotlib, Deepxde, Scipy, Jupyter Notebooks*

Notebook available at: github.com/CeciliaCoelho/PINNsTutorialMAGNET4Cardiac7T

1 Differential Equations Basics

Problem 1: Numerical solution of a simple ODE using the explicit Euler method

The differential equation $\frac{df(t)}{dt} = e^t$ with initial condition $f(0) = 1$ has the exact solution $f(t) = e^t$. Approximate the solution to this initial value problem between 0 and 1 in increments of 0.1 using the *Explicit Euler Formula*. Plot the difference between the approximated solution and the exact solution.

(a) Play with the *solver*, *model parameters* and the *number of mesh elements*.

Problem 2: Logistic Growth of a Population of Organisms

Consider a population of organisms that follows a logistic growth. The population size $P(t)$ at time t is governed by the following differential equation:

$$P'(t) = rP(t)\left(1 - \frac{P(t)}{K}\right), \quad P(t_0) = 100, \tag{1}$$

where r is the growth rate, and K is the carrying capacity of the environment. Consider $r = 0.1, K = 1000$. Also, consider a mesh of 200 points.

(a) First, try to implement $P'(t) = rP(t)$.

(b) Play with the *solver*, *model parameters* and the *number of mesh elements*.

(c) Now try to implement $P'(t) = rP(t)\left(1 - \frac{P(t)}{K}\right)$.

2 Physics-Informed Neural Networks

2.1 Data-driven Solution

Problem 3: 1D Burger's Equation with Dirichlet Boundary Conditions

Consider the 1D Burger's Equation with Dirichlet boundary conditions and $\lambda_1 = 1, \lambda_2 = \frac{0.01}{\pi}$:

$$\begin{aligned} \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \frac{0.01}{\pi}\frac{\partial^2 u}{\partial x^2} = 0, \quad x \in [-1,1], t \in [0,1], \\ u(0,x) = -\sin(\pi x), \\ u(t,-1) = u(t,1) = 0. \end{aligned}$$

(a) What happens if we change the number of training points inside the domain?

(b) What about in the initial and boundary conditions?

Problem 4: Data-driven Solution - Lotka-Volterra

Use PINNs to approximate the solution of the following Lotka-Volterra problem to know how the population of rabbits and foxes change over time in a system:

$$\begin{aligned} \frac{dr}{dt} = \frac{R}{U}(2Ur - 0.04U^2 rf), \quad \frac{df}{dt} = \frac{R}{U}(0.002U^2 rf - 1.06Uf), \\ r(0) = \frac{100}{U}, \quad f(0) = \frac{15}{U} \end{aligned}$$

with $U = 200$ and $R = 20$.

(a) Define function.

(b) Define ODE.

(c) Define domain and NN.

(d) What happens if we change the number of training points inside the domain?

(e) What about in the initial and boundary conditions?

Problem 5: Helmholtz equation over a 2D square domain

The Helmholtz equation is widely used in physics and engineering to describe wave propagation phenomena. In this exercise, we solve the following Helmholtz equation:

$$-u_{xx} - u_{yy} - k_0^2 u = f, \quad \Omega = [0,1]^2$$

with Dirichlet boundary conditions:

$$u(x,y) = 0, \quad (x,y) \in \partial\Omega$$

and a source term:

$$f(x,y) = k_0^2 \sin(k_0 x)\sin(k_0 y).$$

For

$$k_0 = 2\pi n$$

with

$$n = 2$$

, the exact solution is:

$$u(x,y) = \sin(k_0 x)\sin(k_0 y).$$

We will use the following parameters for this problem:

- Domain: $[0,1]^2$
- Wavenumber: $k_0 = 2\pi n$, where $n = 2$
- Boundary conditions: Dirichlet $u(x,y) = 0$ on $\partial\Omega$
- Source term: $f(x,y) = k_0^2 \sin(k_0 x)\sin(k_0 y)$

(a) Implement a PINN to solve the Helmholtz equation over a 2D square domain using PyTorch.

2.2 Data-driven Discovery

Problem 6: Diffusion Equation

We will solve an inverse problem for the diffusion equation with an unknown parameter C:

$$\frac{\partial y}{\partial t} = C\frac{\partial^2 y}{\partial x^2} - e^{-t}(\sin(\pi x) - \pi^2 \sin(\pi x)), \quad x \in [-1,1], \quad t \in [0,1] \tag{2}$$

with the initial condition

$$y(x,0) = \sin(\pi x) \tag{3}$$

and the Dirichlet boundary condition

$$y(-1,t) = y(1,t) = 0. \tag{4}$$

The reference solution is

$$y = e^{-t}\sin(\pi x). \tag{5}$$

(a) What happens if we change the number of training points inside the domain?

(b) What about in the initial and boundary conditions?

Problem 7: Study Case 1 - Lorenz System

Use PINNs to discover σ, ρ, β for the following Lorenz system:

$$\frac{dx}{dt} = \sigma(y - x), \quad \frac{dy}{dt} = x(\rho - z) - y, \quad \frac{dz}{dt} = xy - \beta z, \quad t \in [0, 3]$$
$$x(0) = -8, \quad y(0) = 7, \quad z(0) = 27.$$

(a) Define unknown variables.

(b) Define Lorenz system.

(c) Define domain with initial and boundary conditions.

Problem 8: Logistic Growth of a Population of Organisms

We aim to solve the following diffusion equation:

$$\frac{\partial y}{\partial t} = C\frac{\partial^2 y}{\partial x^2} - e^{-t}(\sin(\pi x) - \pi^2 \sin(\pi x)), \quad x \in [-1, 1], t \in [0, 1]$$

with the initial condition:

$$y(x, 0) = \sin(\pi x)$$

and Dirichlet boundary conditions:

$$y(-1, t) = y(1, t) = 0.$$

The reference solution is given by:

$$y(x, t) = e^{-t} \sin(\pi x).$$

In this inverse problem, we will identify the unknown parameter C using observations at specific points.
We will use the following parameters for this problem:

- Domain: $x \in [-1, 1]$, $t \in [0, 1]$
- Unknown parameter: C, initialized as $C = 2.0$
- Boundary conditions: Dirichlet ($y(-1, t) = y(1, t) = 0$)
- Initial condition: $y(x, 0) = \sin(\pi x)$
- Source term: $f(x, t) = e^{-t}(\sin(\pi x) - \pi^2 \sin(\pi x))$

(a) Implement a PINN to solve an inverse problem for the diffusion equation, where the parameter C is unknown and must be identified.

2.3 Extra: Study case 3 - PINNs for a 1D Blood Flow in a Vessel

Problem 9: The problem

In this exercise, we will use Physics-Informed Neural Networks (PINNs) to solve a forward problem for blood flow in a vessel. We consider a 1D vessel where blood flow is governed by a simplified version of the Navier-Stokes equation, specifically the Hagen-Poiseuille flow equation:
$\frac{d^2u}{dx^2} = -1$
where: $u(x)$ is the velocity profile of the blood flow, x is the position along the vessel, the right-hand side -1 represents a constant pressure gradient driving the flow.
We assume no-slip boundary conditions, meaning that the velocity at both ends of the vessel is zero:
$u(0) = 0, \quad u(L) = 0$

(a) Define PDE Task: Define the differential equation for blood flow (simplified Navier-Stokes).

(b) Geometry Task: Define geometry (1D vessel of length L).

(c) Boundary Conditions Task: no-slip condition at vessel walls.

(d) Define the problem.

(e) Create the NN.

(f) Training and plot the results.

Recommended Resources

- Tutorial slides: github.com/CeciliaCoelho/PINNsTutorialMAGNET4Cardiac7T
- Deepxde library documentation: deepxde.readthedocs.io/en/latest/index.html
- Lu, Lu, et al. "DeepXDE: A deep learning library for solving differential equations." SIAM review 63.1 (2021): 208-228.
- Raissi, Maziar, Paris Perdikaris, and George E. Karniadakis. "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations." Journal of Computational physics 378 (2019): 686-707.