Hands-on Physics-Informed Neural Networks

Tutorial@MAGNET4Cardiac7T

Availability of the Materials

All material can be found at github.com/CeciliaCoelho/PINNsTutorialMAGNET4Cardiac7T, including the slides, hands-on exercises and a jupyter notebook with the coding examples and hands-on that will be used.

Building PINNs

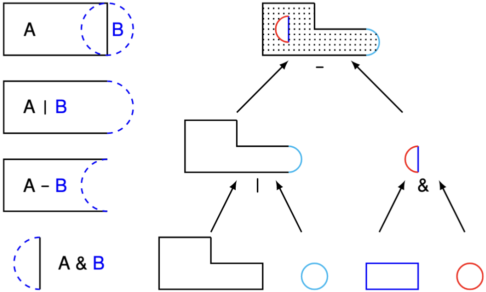
Solving or discovering PDEs with DeepXDE involves specifying:

- Geometry domain;
- Time domain;
- PDE equations;
- Boundary/initial conditions;
- Constraints;
- Training data;
- Neural network architecture;
- Training hyperparameters.

Building PINNs - Available geometries:

Primitive: interval, triangle, rectangle, polygon, disk, ellipse, star, cuboid, sphere, hypercube, hypershpere and point cloud.

Other geometries can be built using the primitive ones and 3 boolean operators: union, difference and intersection.




```
dde.geometry.geometry.Geometry(dim, bbox, diam)
```

Lu Lu et al. "DeepXDE: A deep learning library for solving differential equations". In: *SIAM review* 63.1 (2021), pp. 208–228

Building PINNs - Available boundary conditions:

Standard: Dirichlet, Neumann, Robin and periodic.

General.

```
dde.icbc.boundary_conditions.BC(geom, on_boundary, ...)
dde.icbc.IC(geom, func, ...)
```

Building PINNs - Data:

```
dde.data.TimePDE(geomtime, pde, [bc, ic], num_domain=, num_boundary=, num_initial=)
dde.data.PDE(geom, pde, [bc, ic], num_domain=, num_boundary=)
```

Review: Data-Driven Solution

Start: PINN Algorithm

Construct neural network $\hat{u}(t, x; \boldsymbol{\theta})$

Specify training sets N_u and N_{PDE}

Define loss function using L^2 norm

Train network to optimize $\boldsymbol{\theta}$

End: Estimated parameters $\boldsymbol{\theta}^*$

Review: Data-Driven Discovery

Start: Inverse PINN Algorithm

↓

Construct neural network $\hat{u}(t, x; \boldsymbol{\theta}, \boldsymbol{\lambda})$ with unknown PDE parameters $\boldsymbol{\lambda}$

↓

Specify training sets N_u, N_{PDE} and N_{data}

↓

Define loss function using L^2 norm

↓

Train network to optimize $\boldsymbol{\theta}$ and infer $\boldsymbol{\lambda}$

↓

End: Estimated parameters $\boldsymbol{\lambda}^*$

Hands-On Data-Driven Solution

In the lecture we saw an example on the 1D-Burger's equation. Use it and:

- What happens if we change the number of training points inside the domain? What about in the inital and boundary conditions?
- 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:

$$\frac{dr}{dt} = \frac{R}{U}(2Ur - 0.04U^2 rf), \quad \frac{df}{dt} = \frac{R}{U}(0.002U^2 rf - 1.06Uf),$$

$$r(0) = \frac{100}{U}, \quad f(0) = \frac{15}{U}$$

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

In the lecture we saw an example on the 1D-Burger's equation. Use it and:

- What happens if we change the number of training points inside the domain? What about in the inital and boundary conditions?
- Use PINNs to discover σ, ρ, β for the following Lorenz system:

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

The true values are 10, 15, and $\frac{8}{3}$, respectively.

Study Case - PINNs for the 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, for a wave number $k_0 = 2\pi n$, with $n = 2$, we will 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: $f(x,y) = k_0^2 \sin(k_0 x)\sin(k_0 y)$.
Note that the exact solution is: $u(x,y) = \sin(k_0 x)\sin(k_0 y)$.

Its now time for you to do it by yourselves!

Study Case 2 - PINNs inverse problem for the diffusion equation

We aim to solve the following diffusion equation with an unknown parameter C:

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

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.

Its now time for you to do it by yourselves!

Study Case 3 - PINNs for 1D Blood Flow in a Vessel

Blood flow in arteries can be modelled using simplified 1D fluid dynamics equations.
We consider 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:
$u(0) = 0, \quad u(L) = 0$

Its now time for you to do it by yourselves!

Cecília Coelho
Professorship Computer Science in Mechanical Engineering
Institute for Artificial Intelligence
Helmut Schmidt University / University of the Federal Armed Forces Hamburg
Holstenhofweg 85, 22043 Hamburg
tel.: 040 / 6541-2440
email: cecilia.coelho@hsu-hh.de