ChEESE

Artificial Intelligence and Machine Learning for Geosciences

Physics-informed neural networks (PINNs)

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IPGP

Université Paris Cité

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Trained models and physics

$$f_\theta(\mathbf{x}) : \mathbf{x} \rightarrow \mathbf{y}, \qquad \operatorname{argmin}_\theta \mathcal{L}(f_\theta(\mathbf{x}), \mathbf{y})$$

Can I say my model f_θ is physically **accurate**?

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- Respect some invariances.
- Solution of some equation.
- Stable when used in simulations (for IVPs).

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How? Any guesses?

Inductive biases

	Technique	Nature	Instances
1	Data manipulation	Both	Augmentation / post processing
2	Loss function	Approx.	PINNs
3	Architecture	Exact	Basic blocks
4	Free parameters	Exact	

Different techniques to physically constrain a model.

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Different techniques to physically constrain a model.

Many success stories:

- Atmospheric and ocean science (Bolton and Zanna, 2019; Beucler, Pritchard, et al., 2021).
- Weather and climate science (Kashinath et al., 2021; Beucler, Gentine, et al., 2024).
- Any fluid dynamics-based field.
- How about solid earth? See Moseley et al. (2020) for the wave equation in complex media

Solving a PDE: the modern way

Let's say we want to solve a non-linear (time-dependent) PDE.

$$
\begin{aligned}
u_t + \mathcal{N}(u) &= 0 \\
u(t = 0, x) &= g(x) \\
u(t, x = \partial\Omega) &= c(t)
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- Temporal discretization.
- Efficient parallelization of the entire process.

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- Temporal discretization.
- Efficient parallelization of the entire process.
- A couple hundred lines of Python?

PINNs: a powerful revolution

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

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(Huge success in the scientific community ($>$ 11k citations).

- Mesh-free (live in abstract latent space).
- Data-free (but supervised in the strict sense).
- Interpolation capabilities / super-resolution.
- Zero-effort parallelization.

The idea behind PINNs

$$
\begin{aligned}
f_\theta(t,x)_t + \mathcal{N}[f_\theta(t,x)] &= 0 \\
f_\theta(t=0,x) &= g(x) \\
f_\theta(t, x=\partial\Omega) &= c(t)
\end{aligned}
$$

A loss for each prior term

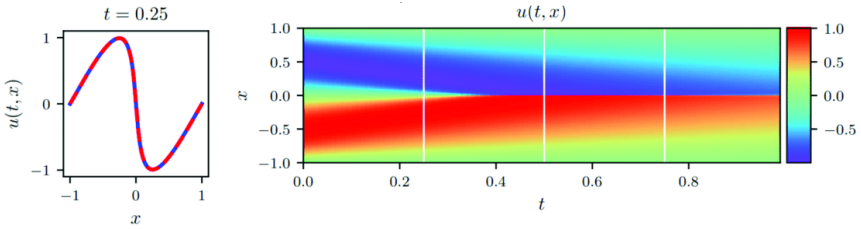
- Boundary conditions loss $\mathcal{L}_{\mathrm{BC}}(f_\theta(t, x=\partial\Omega), c(t))$.
- Initial conditions loss $\mathcal{L}_{\mathrm{IC}}(f_\theta(t=0,x), g(x))$.
- Equation residual loss $\mathcal{L}_{\mathrm{eq}}(f_\theta(t,x)_t + \mathcal{N}[f_\theta(t,x)])$.

The total loss is a sum of each:

$$\mathcal{L} = \mathcal{L}_{\mathrm{BC}} + \mathcal{L}_{\mathrm{IC}} + \mathcal{L}_{\mathrm{eq}}.$$

An illustration with Burgers' equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0$$



Solution of Burgers' equation (Raissi et al., 2019).

- Let's create and train a neural solver for Burgers' equation in the notebook.

Bonus: hybrid modeling

Sometimes the problem is either **too slow** to solve, or contains **some unknown quantities**:

- Model complex phenomena not resolved by the equations (microphysics, clouds, etc.).
- Accelerate simulations by only resolving large scales (sub-grid modeling).
- Probably other instances.

- Keep the physics components with classical numerical methods.
- We can explore an example of sub-grid modeling in the bonus notebook.

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