Universität
Bremen

Center for Industrial
Mathematics (ZeTeM)
Faculty 03
Mathematics / Computer science

Deep Learning for PDE based Forward and Inverse Problems

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Topics

1. Basics of Deep Learning and physics informed approaches
2. TorchPhysics: a software for PI-Deep Learning
3. Application study to inverse problems

Basics of Deep Learning

What is a Neural Network (NN)?

- Parameterized function

$$\begin{aligned} u : \Theta \times \mathbb{R}^n &\longrightarrow \mathbb{R}^m \\ (\theta, x) &\longmapsto u(\theta, x) \end{aligned}$$

  parameter space $\Theta \subseteq \mathbb{R}^p$

- **Notation:** $u_\theta(x) := u(\theta, x)$

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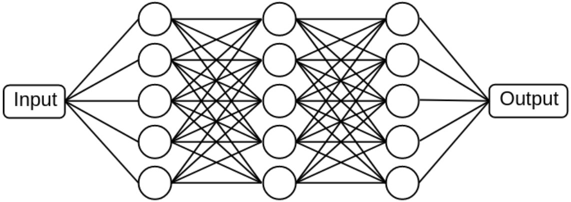
Fully Connected NN:



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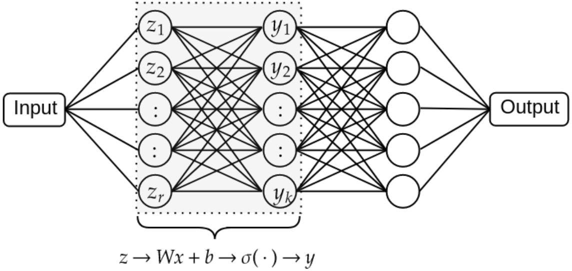
Fully Connected NN:



- Weight matrix $W \in \mathbb{R}^{k \times r}$ and bias $b \in \mathbb{R}^k$ belong to parameters θ
- Activation function $\sigma : \mathbb{R} \to \mathbb{R}$ applied coordinate-wise

Universal Approximation Theorem[1]

Theorem (Hornik, 1989)

Let $K \subset \mathbb{R}^n$ be compact and consider a continuous function

$$f : K \subset \mathbb{R}^n \to \mathbb{R}^m.$$

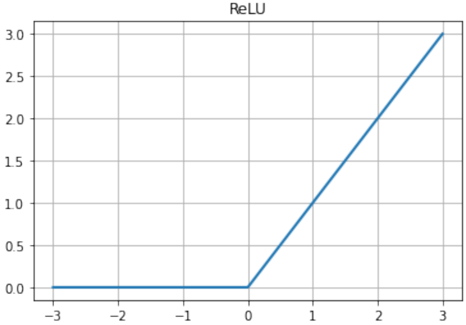
For each error ε ***there exists*** *a NN u_θ with N hidden neurons and* ***"specific"*** *activations that uniformly approximates f, i.e.*

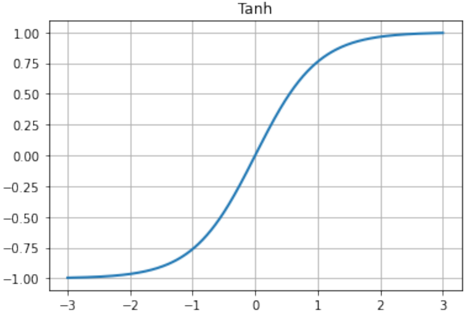
$$\|f(x) - u_\theta(x)\| < \varepsilon \quad \text{for every} \quad x \in K.$$

[1] Hornik: *Multilayer Feedforward Networks are Universal Approximators*, 1989

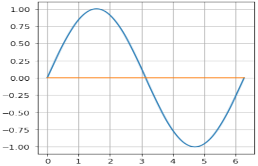
"Specific" activations

For example:

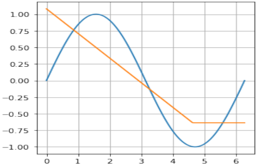




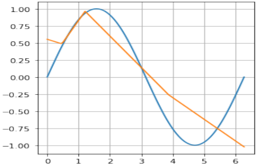
Example of Approximation Properties



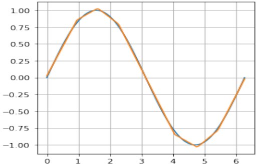
(a) 1 layer with 1 neuron



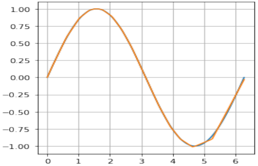
(b) 1 layer with 2 neurons



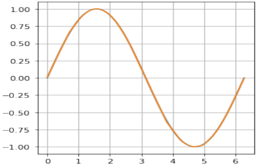
(c) 1 layer with 5 neurons



(d) 1 layer with 10 neurons



(e) 1 layer with 50 neurons



(f) 1 layer with 100 neurons

Motivation: Why Deep Learning for DEs?

Parameter identification/optimization problems

$\rightarrow$ Iterative algorithms: Solve many **similar** PDEs

$\rightarrow$ Classical methods like FDM or FEM: Time-consuming

$\rightarrow$ Replace by trained NN

$\rightarrow$ Less time-consuming

DL for DEs: Data-Driven Approach

- For example, Harmonic Oscillator: $\begin{cases} \partial_t^2 u(t) = -\lambda u(t) \\ u(0) = u_0,\ \partial_t u(0) = 0 \end{cases}$
- Generate/obtain data $\{\tilde{u}_j, t_j, \lambda_j\}_{j=1}^N$, with $\tilde{u}_j \approx u(t_j; \lambda_j)$
- Initialize a neural network $u_\theta : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$
- Train u_θ by minimizing

$$\mathcal{L}(\theta_i) = \frac{1}{N} \sum_{j=1}^{N} \left| u_{\theta_i}(t_j, \lambda_j) - \tilde{u}_j \right|^2 \quad \text{(Mean-Squared-Error)}$$

with gradient descent: $\theta_{i+1} = \theta_i - \eta \nabla_\theta \mathcal{L}(\theta_i)$

Problems of Data-Driven Approach

- Deep Learning generally needs lot of data
- Obtaining data of solution u is complicated
  - Through multiple experiments
  - Solving the equation with classical methods

  → Expensive and time consuming

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💡 Encode physical laws/PDEs into DL approaches?

→ **Physics-informed neural networks (PINNs)**

→ Plug neural network into the differential equation

Physics-Informed Neural Networks (PINNs)

PINNs[2] - Main Idea

- Find solution $\mathbf{u} : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ of

$$\begin{aligned} \mathcal{N}[\mathbf{u}](x) &= 0, \text{ for } x \in \Omega, \\ \mathcal{B}[\mathbf{u}](x) &= 0, \text{ for } x \in \partial\Omega. \end{aligned}$$

- E.g. $\Omega = [0,1] \times [0,1], \mathbf{u} : \mathbb{R}^2 \to \mathbb{R}$

$$\begin{aligned} \mathcal{N}[\mathbf{u}](x) &= \Delta \mathbf{u}(x) - f(x), \text{ for } x \in \Omega, \\ \mathcal{B}[\mathbf{u}](x) &= \mathbf{u}(x) - u_0, \qquad \text{ for } x \in \partial\Omega. \end{aligned}$$

[2] Raissi, Perdikaris and Karniadakis: *Physics-informed neural networks: [...]*, 2019

PINNs - Main Idea

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- Sample points $x_i^{\mathcal{N}} \in \Omega$ and $x_j^{\mathcal{B}} \in \partial\Omega$
- Train network $\mathbf{u}_\theta$ that minimizes the PDE-loss

$$\frac{1}{N_{\mathcal{N}}} \sum_{i=1}^{N_{\mathcal{N}}} \left\| \mathcal{N}[\mathbf{u}_\theta](x_i^{\mathcal{N}}) \right\|^2 + \frac{1}{N_{\mathcal{B}}} \sum_{j=1}^{N_{\mathcal{B}}} \left\| \mathcal{B}[\mathbf{u}_\theta](x_j^{\mathcal{B}}) \right\|^2$$

Physics-Informed Loss: We need to ...

- Compute differential operator $\mathcal{N}$ of NN u_θ, e.g. Laplacian Δu_θ
  - $\rightarrow$ Compute the derivatives of a neural network
  - $\rightarrow$ Generally possible with basics math operations

Physics-Informed Loss: We need to ...

- Compute differential operator $\mathcal{N}$ of NN u_θ, e.g. Laplacian Δu_θ
  - $\rightarrow$ Compute the derivatives of a neural network
  - $\rightarrow$ Generally possible with basics math operations
- Consider $u_\theta : \mathbb{R} \rightarrow \mathbb{R}$, with $u_\theta(x) = \sigma(W_2\sigma(W_1 x + b_1) + b_2)$, then:

$$\partial_x u_\theta(x) = \partial_x\sigma(W_2\sigma(W_1 x + b_1) + b_2)[W_2^T \partial_x\sigma(W_1 x + b_1) W_1]$$
$$\partial_x^2 u_\theta(x) = \dots$$

$\rightarrow$ Derivatives contain the same network parameters $\theta = (W_1, b_1, W_2, b_2)$

Parameter Studies

Realization with PINNs

- Many applications involve solving the same PDE with different parameters $c \in \mathbb{R}^d$:

$$\mathcal{N}[\mathbf{u}_c, c](x) = 0, \text{ for } x \in \Omega,$$

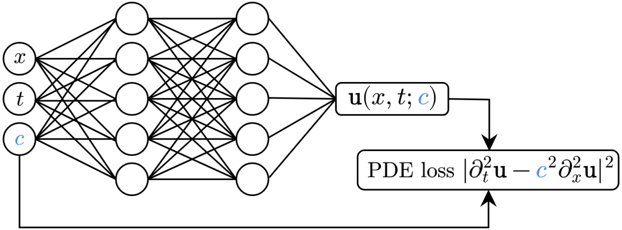
- For example:

Parameter-dependent wave equation:

$$\begin{cases} \partial_t^2 u = c^2\, \partial_x^2 u, & \text{in } I_x \times I_t, \\ u = 0 & \text{in } \partial I_x \times I_t, \\ \partial_t u(\cdot, 0) = 0 & \text{in } I_x, \\ u(\cdot, 0) = \sin(x) & \text{in } I_x, \end{cases}$$

Parameter Studies with PINNs

Solving the same PDE for many different choices of c

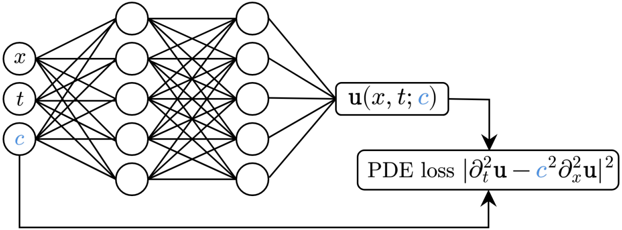


Method:

- Include parameter(s) as additional input(s) to the PINN
- Training: Sample parameter range together with function domain

Parameter Studies with PINNs

Solving the same PDE for many different choices of c

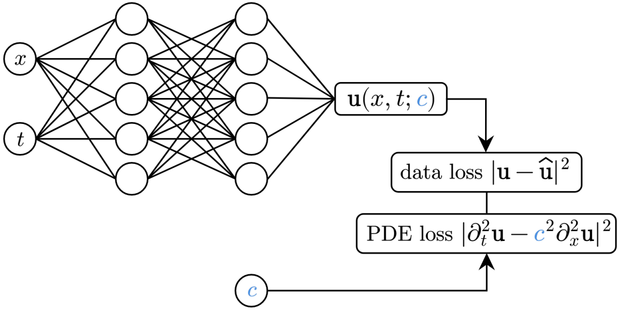


Result:

- Inference of solution for new parameter by a forward pass to the trained network
- Very little additional effort in evaluation of the network
- Increased amount of training points necessary

Parameter Identification with PINNs

Finding the c that leads to given solution data $\{\hat{u}_i\}$



Method:

- Include parameter(s) as learnable parameter(s)
- Training: Incorporate data loss in training
  $\rightsquigarrow$ Goal: Find a solution that fits data and solves PDE for the optimized parameter

TorchPhysics

Initiation of TorchPhysics

BOSCH

- 2021: Robert Bosch GmbH got interested in PINNs
- Technical applications:
  Car parts, electronics, injection molding, etc.

©factum

[a] Paszke et al., *PyTorch: An Imperative Style [...]*, 2019

Initiation of TORCHPHYSICS

- 2021: Robert Bosch GmbH got interested in PINNs
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- Main Developers: Nick Heilenkötter & Tom Freudenberg

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- Technical applications:
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- Student project: Deep Learning library for PDEs
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- Open-Source on GitHub
- Build upon PyTorch[a]

[a] Paszke et al., *PyTorch: An Imperative Style [...]*, 2019

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What is needed for a PINN library?

We need...

- to create different types of domains
- a way to sample points in a given domain
- to be able to define different network architectures
- implement the need differential equations and boundary conditions as training conditions

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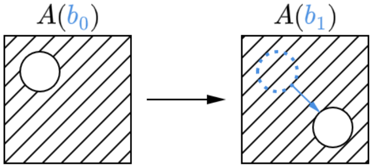
Domains

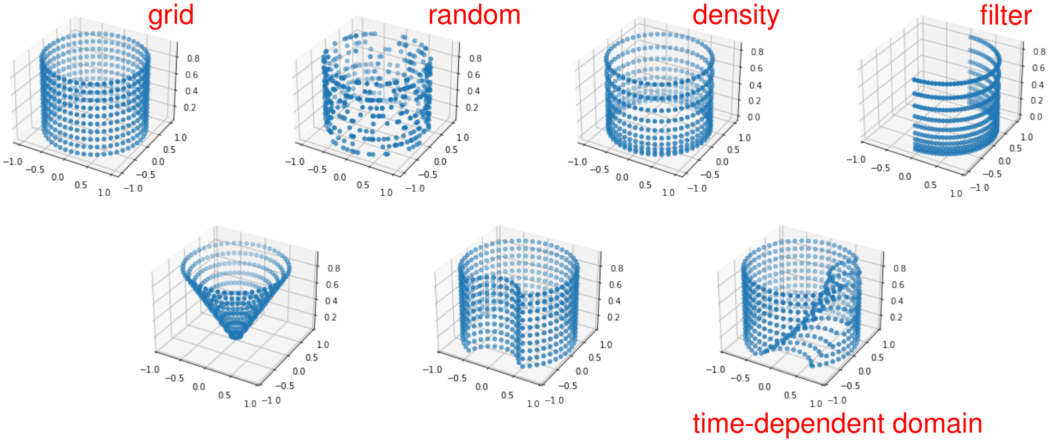
- Basic geometries implemented:
  - `Point, Interval, Parallelogram, Circle, ...`
- Complex domains via logical operators:

- Domains can depend on variables of other domains (e.g. time-dependent)



PointSampler

Flexible domain sampling

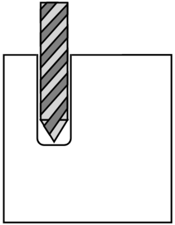


Applications

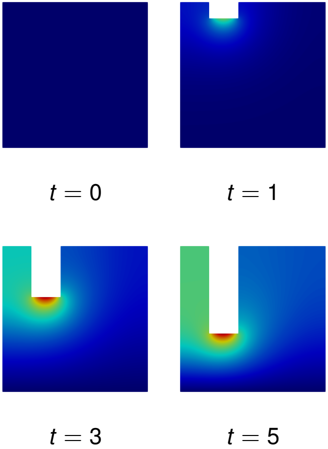
Temperature in a drilling process

- Drilling problem:

$$
\begin{aligned}
\partial_t u(x,t) - \kappa \Delta u(x,t) &= 0, && \text{in } \Omega(t),\\
u(x,0) &= 0, && \text{in } \Omega(0),\\
u(x,t) &= 0, && \text{on } \Gamma_D,\\
\kappa \nabla u(x,t) \cdot n &= f, && \text{on } \Gamma_N(t).
\end{aligned}
$$



- L^2–difference to FEM $\sim$7 %

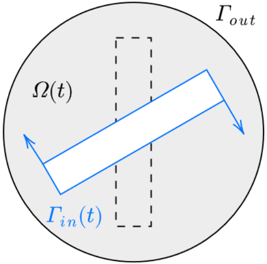


Applications

PINNs for Temperature–Navier–Stokes example

Bar heats up and rotates within some fluid:

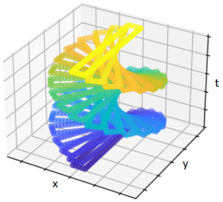
$$
\begin{aligned}
\partial_t u + (u \cdot \nabla) u &= \nu \Delta u - \nabla p, && \text{in } \Omega(t),\\
\nabla \cdot u &= 0, && \text{in } \Omega(t),\\
\partial_t T + u \cdot \nabla T &= \lambda \Delta T, && \text{in } \Omega(t),\\
u(0,\cdot), p(0,\cdot), T(0,\cdot) &= 0, 0, 270 && \text{in } \Omega(0),\\
u, T &= (0,0), 270, && \text{on } \Gamma_{\text{out}},\\
u, T &= u_{\text{in}}(t), T_{\text{in}}(t), && \text{on } \Gamma_{\text{in}}.
\end{aligned}
$$

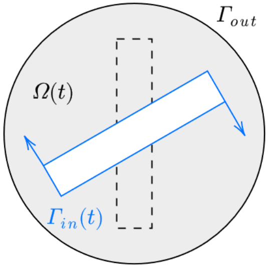


Time-Dependent Domain

Implementation inside TorchPhysics

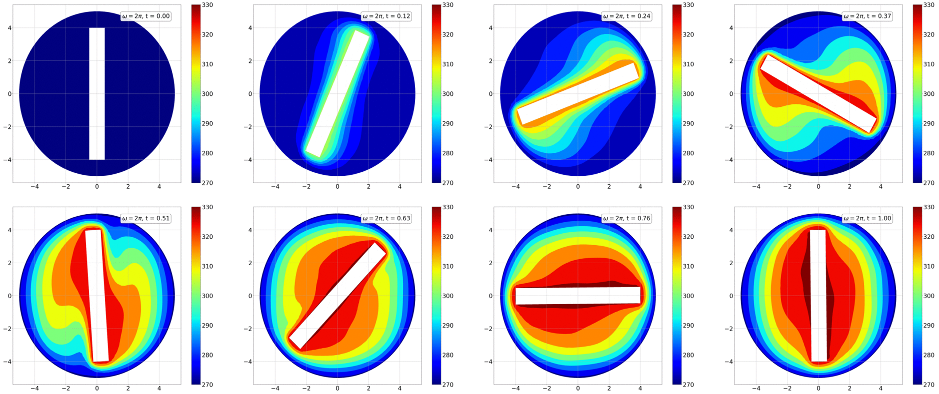
```
def corner1(t):
    return rotation_matrix(t) * start_position_1

bar    = tp.domains.Parallelogram(X, corner1, corner2, corner3)
circle = tp.domains.Circle(X, center, radius)

omega  = circle - bar
```





Applications

Learned Temperature Field



Advantages of PINNs

Compared to classical methods

- (usually) Grid/mesh independent, therefore more flexible & saving is usually more memory efficient
- General approach for different kinds of differential equations, especially nonlinear
- Learning parameter dependencies, useful for parameter studies
- Extension to optimization- & inverse problems easy to implement
- Interpolation and extrapolation of data

Disadvantages of PINNs
Compared to classical methods

- No convergence theory
- Error not arbitrarily small
- Sometimes optimal minimum difficult to find, poor convergence
- Much slower for single computation of forward solutions
- Often trial and error for finding good parameters

Application to Inverse Problems

Operator Learning

First natural idea

- Many problems include function valued parameters $f : \mathbb{R}^d \to \mathbb{R}^m$
- **Goal**: Learn operator on function set F

$$\begin{aligned} \Phi_\theta : \mathbb{R}^n \times F &\longrightarrow \mathbb{R}^m \\ (x, f) &\longmapsto u_f(x) \end{aligned}$$

- **Problem**: Inputs of NN has to be discrete

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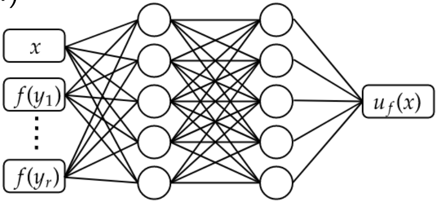
- **Idea**: Discretize f on $y_1, \dots, y_r \in \mathbb{R}^d$



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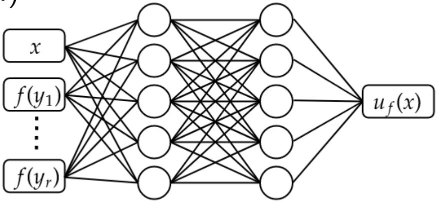
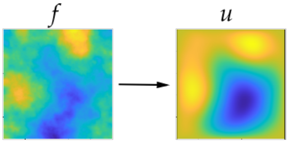
- **Problem**: Inputs of NN has to be discrete
- **Idea**: Discretize f on $y_1, \ldots, y_r \in \mathbb{R}^d$
- Many $f(y_i)$-inputs versus $x \to$ **Imbalance**



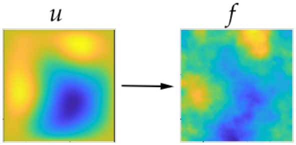
Operator Learning

State of the art

- Keep idea of discrete $f(y_i)$-inputs, change network architecture:
  - **DeepONet** [Lu et al. (2019)] - Divide and Conquer
  - **Fourier Neural Operator** (FNO) [Li et al. (2020)] - Discrete Fourier transform
  - **PCANN** [Bhattacharya et al. (2020)] - Principle component analysis
- Generally data-driven, but with physics informed extensions



Forward mapping



Inverse mapping

Operator Learning

For inverse problems

- Usually the mapping $u \mapsto f$ is unstable under noisy data u^δ
- **Idea**: Learn forward operator Φ_θ and use it in Tikhonov scheme

$$\min_{f \in F} \|\Phi_\theta(f) - u^\delta\|^2 + \alpha R(f)$$

[3] Nganyu et al., *Deep Learning Methods for Partial Differential Equations [...]*, 2023

Operator Learning

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$$\min_{f \in F} \|\Phi_\theta(f) - u^\delta\|^2 + \alpha R(f)$$

- We studied[3]:
  - Performance of different methods for forward and inverse problem
  - Influence of noise in the inverse problem
- Training: 1000 data pairs (f, u_f), Testing: 5000 additional data pairs

[3] Nganyu et al., *Deep Learning Methods for Partial Differential Equations [...]*, 2023

Forward Problem

- Consider Darcy flow equation

$$
\begin{aligned}
-\nabla \cdot (f \nabla u) &= 1, \quad \text{in } (0,1)^2 \\
u &= 0, \quad \text{on } \partial(0,1)^2
\end{aligned}
$$

Forward Problem

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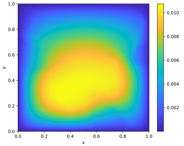
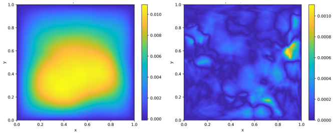
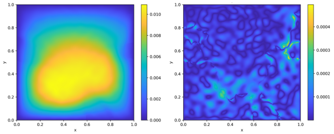


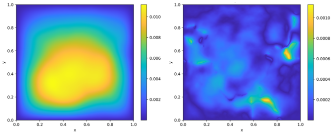
Ground Truth



(a) DeepONet



(b) FNO



(c) PCANN

Forward Problem

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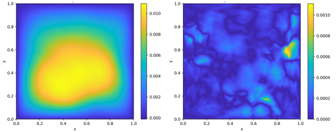
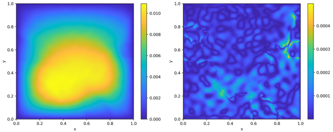
\end{aligned}
$$

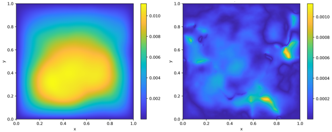
	Rel. L^2 error	Evaluation time [s]
DeepONet	0.029	0.001
FNO	0.011	0.017
PCANN	0.025	0.611



(a) DeepONet



(b) FNO



(c) PCANN

Inverse Problem

Without noise

- Consider Darcy flow equation

$$
\begin{aligned}
-\nabla \cdot (f \nabla u) &= 1, \quad \text{in } (0,1)^2 \\
u &= 0, \quad \text{on } \partial(0,1)^2
\end{aligned}
$$

Inverse Problem

Without noise

- Consider Darcy flow equation

$$
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-\nabla \cdot (f \nabla u) &= 1, \quad \text{in } (0,1)^2 \\
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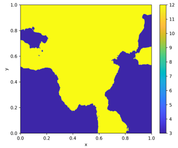
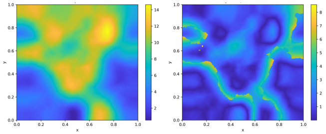
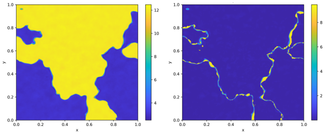


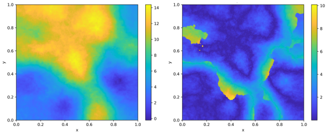
Ground Truth



(a) DeepONet



(b) FNO



(c) PCANN

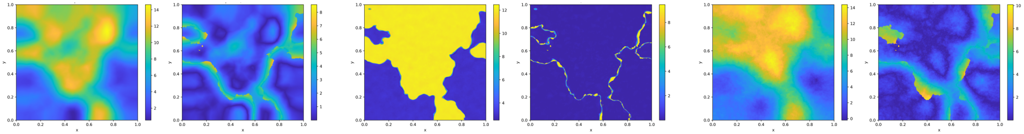
Inverse Problem

Without noise

- Consider Darcy flow equation

$$-\nabla \cdot (f \nabla u) = 1, \quad \text{in } (0,1)^2$$
$$u = 0, \quad \text{on } \partial(0,1)^2$$

	Rel. L^2 error	Evaluation time [s]
DeepONet	0.222	0.001
FNO	0.093	0.016
PCANN	0.098	0.154



(a) DeepONet (b) FNO (c) PCANN

Inverse Problem

With noise

- Three different training strategies:
  1) $u \mapsto f$, with noise-free data
  2) $u \mapsto f$, with noisy data of the same noise level
  3) $f \mapsto u$ and then Tikhonov for the inverse problem
- Always evaluate on noisy data u^δ
- Only demonstrate FNO

Inverse Problem
With noise

- Three different training strategies:
  1) $u \mapsto f$, with noise-free data
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- Always evaluate on noisy data u^δ
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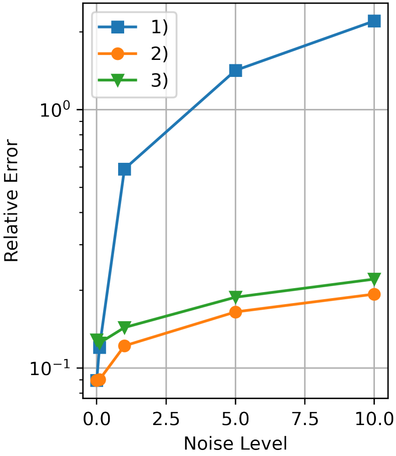
$\rightarrow$ Tikhonov helpful if noise level not previously known



Summary

- DL for differential equations is useful for parameter studies, control/inverse problems, and data extrapolation
- Disadvantages are sometimes poor convergence and not arbitrarily small error
- TorchPhysics is a open source framework that allows simple implementation of many different problems
- Use of learned forward operator in classical Tikhonov speeds up the computation