Universität Bremen

Center for Industrial Mathematics (ZeTeM)

Faculty 03

Mathematics / Computer science

Deep Learning for Real Life Problems

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Session to start with your own problem

or

work on one of our prepared examples

Template: `.../KoMSO-Workshop/examples/Templates`

Duration: 60 minutes

When to Use DL for PDEs?

Use for

- Parameter studies
- Solving similar problems multiple times
- Extrapolation of data

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Do not use for

- Computing forward solution once [Grossmann et al. 2023]
- Solutions with need of high accuracy

Challenges for PI-Deep Learning

- Accuracy (open problem)
- Convergence (NNs are non-convex)
- Balancing different loss terms (data, initial, boundary, PDE)
- Finding a fitting network architecture
- Different scales
- Choosing the training parameters

Strategies for Better Results

Implement solution features into architecture:

- Hard constrains [Liu et al. 2023]
- **Fourier Features** [Tancik et al. 2020]
- Stiff-PINNs [Ji et al. 2021]
- ...

Fourier Features

- Suppose function $u : [0,1] \to \mathbb{R}$ has high frequencies

$$u(x) \approx \sum_{k=1}^{N} a_k \cos(2\pi kx) + b_k \sin(2\pi kx)$$

- Training **standard PINN** might be difficult

$$\begin{aligned} u_\theta : [0,1] &\longrightarrow \mathbb{R} \\ x &\longmapsto u_\theta(x) \end{aligned}$$

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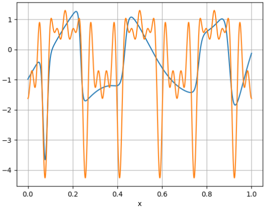
Use Fourier Features as an input:

$$u_\theta : [0,1] \times [0,1]^{2P} \longrightarrow \mathbb{R}$$

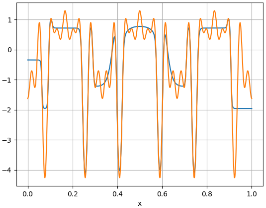
$$z := \begin{pmatrix} x \\ \cos(2\pi x) \\ \sin(2\pi x) \\ \vdots \\ \cos(2\pi Px) \\ \sin(2\pi Px) \end{pmatrix} \longmapsto u_\theta(z) \approx u(x)$$

Fourier Features - Example

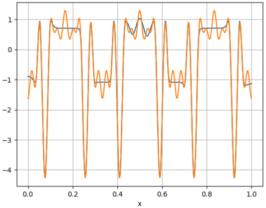
- **Groundtruth:** Orange curve
- **NN Reconstruction:** Blue curve



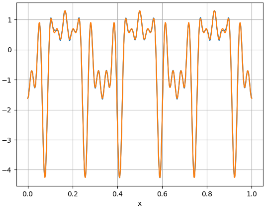
No Fourier Features



2 Fourier Features



4 Fourier Features



8 Fourier Features

Strategies for Better Results

Modify training goal:

- Learning on a **domain decomposition** [Jagtap and Karniadakis 2020]
- Variational formulation [Kharazmi et al. 2019]
- Learn coefficients of basis functions [Moseley et al. 2021]
- ...

Learning on a domain decomposition

Suppose solution

- has important local details or
- behaves differently on local sections

Standard PINN might:

- be inaccurate
- need large network $\rightarrow$ expensive

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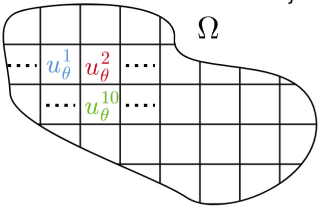
Stitch multiple small PINNs together:

$$u_\theta^k : \Omega_k \rightarrow \mathbb{R}$$

$$\bigcup_k \Omega_k = \Omega$$

$\Omega_k \cap \Omega_j = \emptyset$, for $k \neq j$



Strategies for Better Results

Modify training procedure:

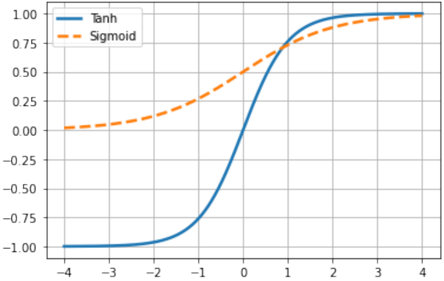
- Include prior knowledge (e.g symmetries)
- Enrich training with data points
- Nondimensionalization [Lin et al. 2021]
- **Normalization** of input and output [Rasht-Behesht et al. 2022]
- Combine Adam and LBFGS [He et al. 2020]
- ...

Normalization

- Scale each input into range $[-1, 1]$
  $\rightarrow$ Most activation functions have interesting behavior around 0
- Also normalize output of network:

$$u_\theta : \Omega \rightarrow [-1, 1]^n$$

  $\rightarrow$ Needs a priori solution bounds!
- Learning of scaling no longer necessary



Literature

- T. G. Grossmann, U. J. Komorowska, J. Latz, C.-B. Schönlieb. *Can Physics-Informed Neural Networks beat the Finite Element Method?*, 2023.
- S. Liu, Z. Hao, C. Ying, H. Su, J. Zhu, Z. Cheng. *A Unified Hard-Constraint Framework for Solving Geometrically Complex PDEs*, 2023.
- M. Tancik, P. P. Srinivasan, B. Mildenhall, S. Fridovich-Keil, N. Raghavan, U. Singhal, R. Ramamoorthi, J. T. Barron, R. Ng. *Fourier Features Let Net- works Learn High Frequency Functions in Low Dimensional Domains*, 2020.
- ...

→ Prepared a small literature collection on Github:

`https://github.com/TomF98/torchphysics/blob/KoMSO-Workshop/examples/literature_collection.pdf`