

# Center for Industrial Mathematics (ZeTeM)

Mathematics / Computer science

Faculty 03

# Outlook: DeepONets

Janek Gödeke, Tom Freudenberg Bremen, 21.07.2023

Learned PDEs for single parameter

a) For fixed  $D \in \mathbb{R}$  solve parachute example:

$$\begin{cases} \partial_t^2 u(t) &= D(\partial_t u(t))^2 - g \text{ for } t \in [0,3] \\ u(0) &= H \\ \partial_t u(0) &= 0 \end{cases}$$

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$$\Delta \partial_t u = D \Delta_x u$$
 in  $\Omega \times I_t$ 

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!! Bonus exercises: PINNs can solve for multiple  $D \in [D_{min}, D_{max}]$ 

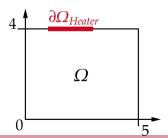
$$u_{\theta}(D, x, t) \approx u_{D}(x, t)$$

Learned PDE for single parameter function

Room-with-heater example

$$\partial_t u(x,t) = D\Delta_x u(x,t)$$
 for  $(x,t) \in \Omega \times I_t$   $u(x,t) = h(t)$  for  $(x,t) \in \partial\Omega_{Heater} \times I_t$ 

• Fixed temperature function h(t) of the heater

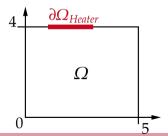


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- If solution for different  $\tilde{h}(t)$  is desirable ...
- ... start new training with PINNs :(

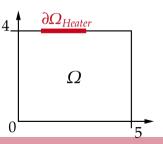


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- **Goal:** Solve PDE for many  $\tilde{h}(t)$  with ONE network





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# Simpler Example for Illustration

• Goal: For multiple functions  $f:[0,1] \to \mathbb{R}$  use single NN to solve

$$\begin{cases} u^{(1)}(x) &= f(x) \text{ for } x \in [0, 1] \\ u(0) &= 0 \end{cases}$$

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- **Second goal:** After training on  $f_1, f_2...$ , want good performance on test set
- → Want NN that learns the mapping

$$\mathcal{A}: f \mapsto u_f$$
 "f is mapped to corr. solution  $u_f$ "

**Problem:** Inputs of NNs can only be vectors in  $\mathbb{R}^m$ , but  $\mathcal{A}$  receives a function!



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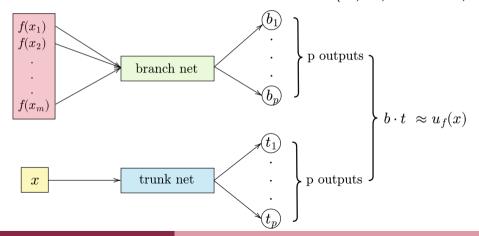
- 🔽 Idea:
  - Fix points  $x_1, ..., x_m$  in domain of f
  - Consider NNs of the form

$$u_{\theta}: \mathbb{R}^m \times [0,1] \longrightarrow \mathbb{R}$$
$$\left(f(x_1), f(x_2), ..., f(x_m), x\right) \longmapsto u(x)$$

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## DeepONets - Divide and Conquer

(Lu, Jin, Karniadakis; 2019)



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# DeepONets - Construction Steps

#### **Construction of DeepONet**

$$u_{\theta}: \mathbb{R}^m \times [0, 1] \longrightarrow \mathbb{R}$$
  
 $\Big(f(x_1), f(x_2), ..., f(x_m), x\Big) \longmapsto b \cdot t \approx u(x)$ 

• Choose and **fix** sample points  $x_1, ..., x_m$  for f

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- Set number p of output neurons of branch/trunk
   → Outputs b, t ∈ R<sup>p</sup> of branch/trunk nets must have same size!

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- Set number p of output neurons of branch/trunk  $\rightarrow$  Outputs  $b, t \in \mathbb{R}^p$  of branch/trunk nets must have same size!
- Build architecture of branch/trunk net, e.g. fully-connected

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## DeepONets - Train with Data

#### **Train the DeepONet**

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- Data: Consider Parameter-solution tuples (f, u<sub>f</sub>)
- Data points look like  $f(x_1), ..., f(x_m)$  and  $u_f(\tilde{x}_1), ..., u_f(\tilde{x}_k)$

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- Data: Consider Parameter-solution tuples (f, u<sub>f</sub>)
- Data points look like  $f(x_1), ..., f(x_m)$  and  $u_f(\tilde{x}_1), ..., u_f(\tilde{x}_k)$
- Loss function for single tuple  $(f, u_f)$ :

$$\frac{1}{K} \sum_{i=1}^{K} \left\| u_{\theta}(f(x_1), ..., f(x_m), \tilde{x}_j) - u_{f}(\tilde{x}_j) \right\|^2$$

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- Time dependent D "=" parachute is opening and closing while falling
- ullet Analytic solution is unknown o employ classical schemes to create training data
- Trained with TorchPhysics



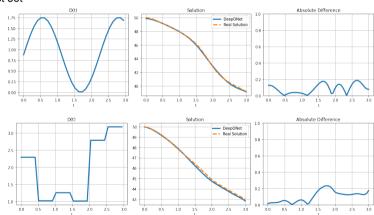
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### DeepONet - Parachute Example

Evaluation on test set

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### **DeepONet Properties**

Mesh-independent

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- Once trained: evaluation for given parameters fast
- Good generalization for unseen data
- Multiple parameter functions → multiple branch net

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- Mesh-independent
- Once trained: evaluation for given parameters fast
- Good generalization for unseen data
- Multiple parameter functions  $\rightarrow$  multiple branch net
- Needs lot of data for training:
  - Expensive and time consuming to obtain
  - Physics-informed DeepONets
- May need problem specific adaptions
- Often trial and error for finding good parameters

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### The End

Thank you for participating! :)

Thanks to Tom for his support!