Improving Data-Driven Systems with Differential Equations – Approaches and Open Problems

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MaritimeMET Workshop: Role of Metrology for Greener Shipping
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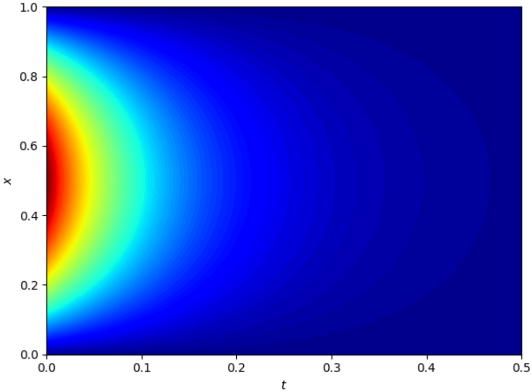
Motivation: Heat Equation



Task: Find approximation $u_\theta(x, t)$ to the true $u(x, t)$

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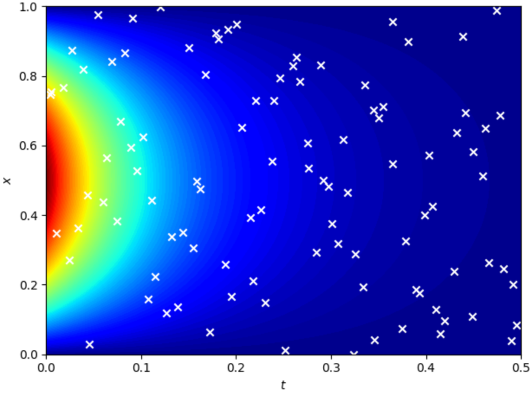
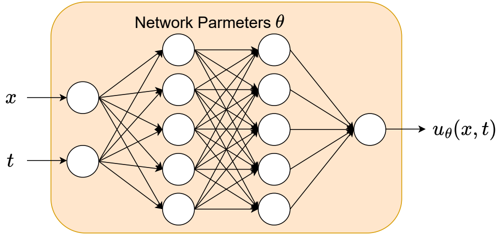


Task: Find approximation $u_\theta(x, t)$ to the true $u(x, t)$

Vanilla NN

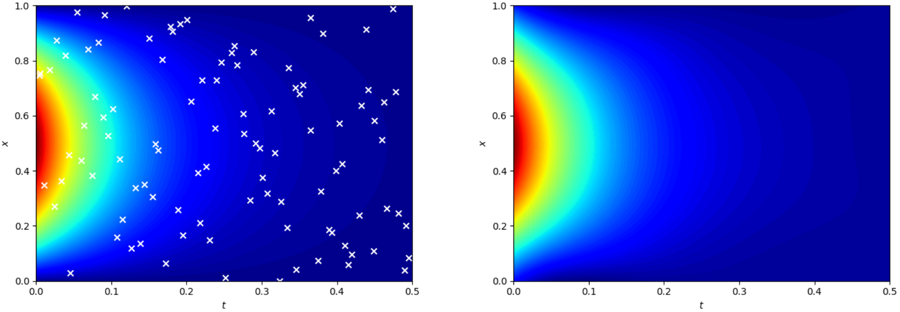


- $\mathcal{D} = \{(x_i, t_i, u_i = u(x_i, t_i))\}_{i=1,\dots,N}$
- MLP 20-20, tanh
- squared error loss $\ell(u, u_\theta) = (u - u_\theta)^2$
- Adam optimizer

$$\theta^\bullet \in \operatorname*{argmin}_{\theta \in \Theta} \frac{1}{|\mathcal{D}|} \sum_{(x_i, t_i, u_i) \in \mathcal{D}} \|u_i - u_\theta(x_t, t_i)\|^2$$

Vanilla NN (cont'd)

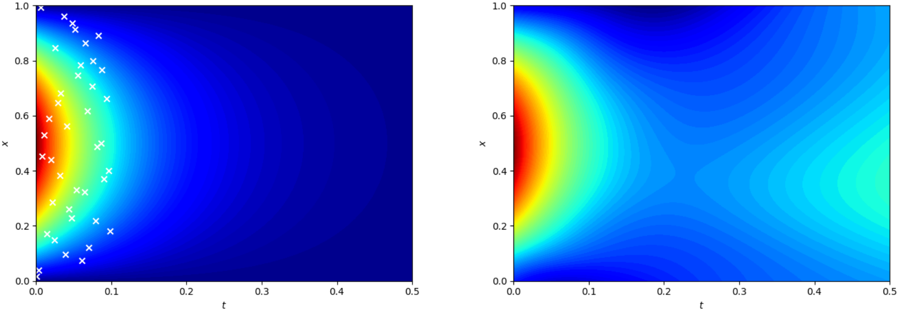
$\mathcal{D}$ from $\Omega = [0, 0.5] \times [0, 1]$, $|\mathcal{D}| = 100$



Rel. L2-Error: ≈2-3%

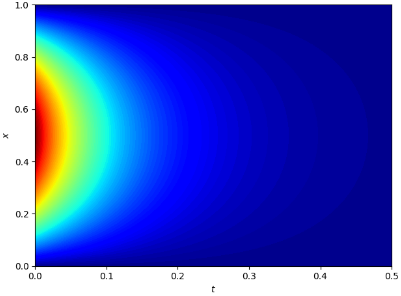
Vanilla NN (cont'd)

$\mathcal{D}$ from $[0, 0.1] \times [0, 1]$, $|\mathcal{D}| = 40$



Rel. L2-Error: ≈60-80%

Heat Equation Revisited



- Governing equation:

$$\frac{\partial}{\partial t}u(x,t) - \frac{\partial^2}{\partial x^2}u(x,t) = 0$$

- Initial condition:

$$u(x,0) = \sin(\pi x)$$

- Boundary conditions:

$$u(0,t) = u(1,t) = 0$$

Physics-Informed Neural Networks (PINNs)

Idea: Ensure that u_θ satisfies the differential equation on the whole computational domain Ω

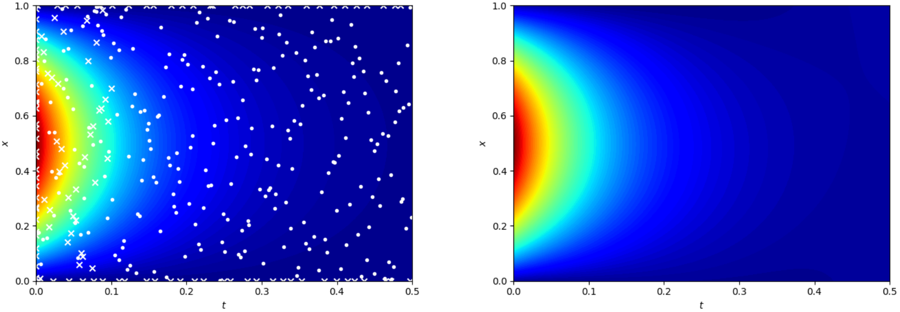
- sample *collocation points* $\mathcal{C}$ from Ω
- add regularization term that penalizes if u_θ violates physics at $\mathcal{C}$
- implement via automatic differentiation

$$\theta^\bullet \in \underset{\theta\in\Theta}{\operatorname{argmin}} \frac{1}{|\mathcal{D}|} \sum_{(x_i,t_i,u_i)\in\mathcal{D}} \left\|u_i - u_\theta(x_t, t_i)\right\|^2 + \lambda \frac{1}{|\mathcal{C}|} \sum_{(x_i,t_i)\in\mathcal{C}} \left\|u_{\theta,t}(x_i, t_i) - u_{\theta,xx}(x_i, t_i)\right\|^2$$

M. Raissi & al. "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations". Journal of Computational Physics 378:686-707, (2023)

PINNs (cont'd)

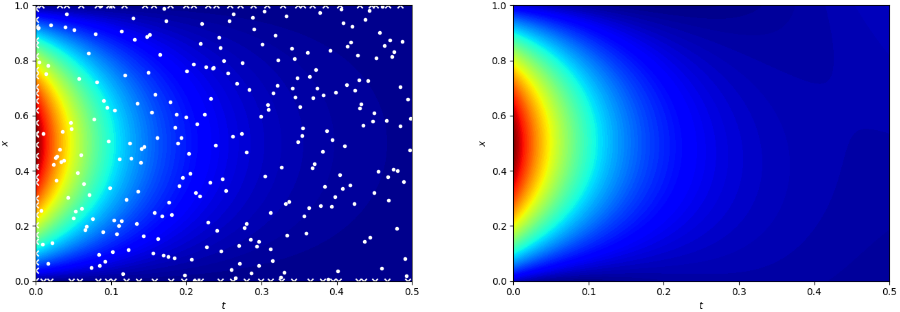
$\mathcal{D}$ from $[0, 0.1] \times [0, 1]$ + IC/BC, $|\mathcal{D}| = 100$, $|\mathcal{C}| = 250$, $\lambda = 1$



Rel. L2-Error: $\approx$1.5%

PINNs (cont'd)

$\mathcal{D}$ from IC/BC, $|\mathcal{D}| = 60$, $|\mathcal{C}| = 250$, $\lambda = 1$



Rel. L2-Error: $\approx$5%

PINNs – Preliminary Summary

- PINNs are the “epitome” of physics-informed machine learning
- surrogate model for partial/ordinary differential equations
- physics information included in a regularization term
- can be used
  - to solve differential equations (replace classical solvers)
  - to solve inverse problems, e.g., determine parameters of the ODE/PDE
  - in hybrid settings, e.g., learning pressure field from velocity field

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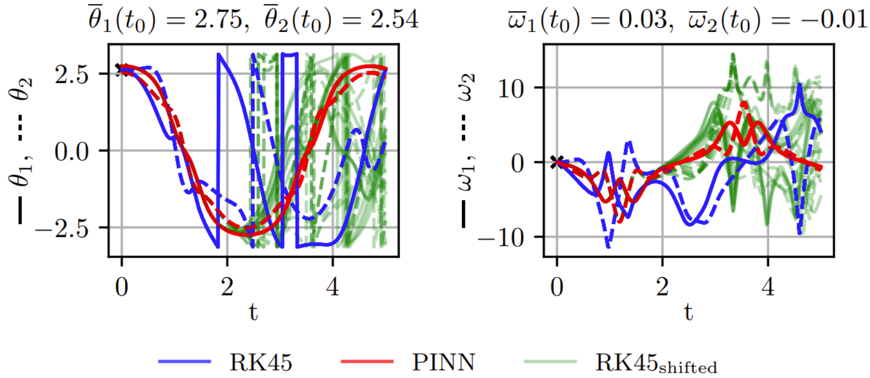
PINNs can improve extrapolation performance of neural surrogates u_θ if there is little or no data.

But training PINNs is hard...

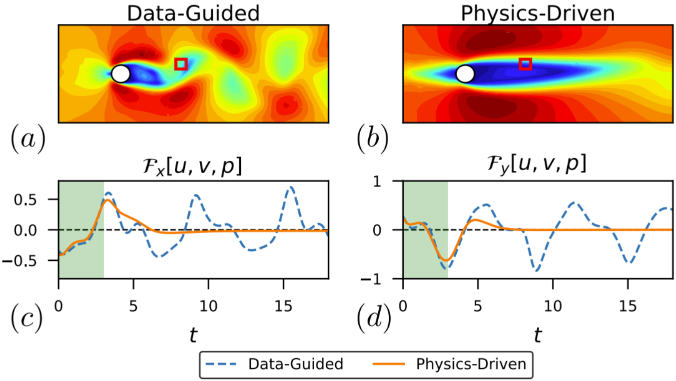
PINNs – Training Troubles



© Sophie Steger

S. Steger & al. "How PINNs cheat: Predicting chaotic motion of a double pendulum". DLDE Workshop @ NeurIPS (2022)

PINNs – Training Troubles



F. M. Rohrhofer & al. "On the Role of Fixed Points of Dynamical Systems in Training Physics-Informed Neural Networks". TMLR 1/2023

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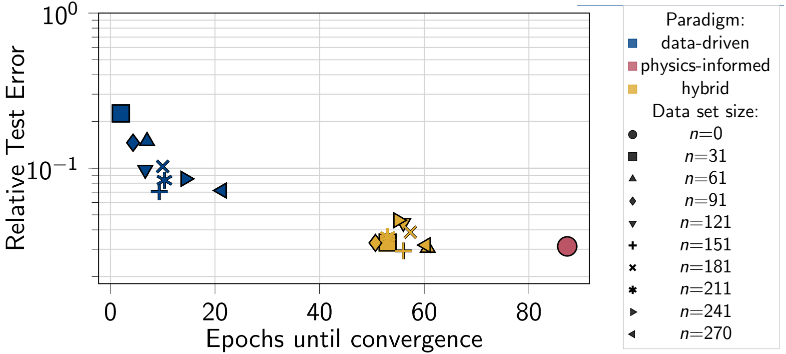

M. Wellenhof-Karner & al. “Data and Modeling Assumptions in Physics-Informed Operator Learning”. Differentiable Systems and Scientific Machine Learning Workshop @ EurIPS (2025)

Remedies?

- **Training schemes**: loss weighting, collocation point weighting, domain decomposition, curriculum learning, adaptive activation functions, ensemble/Bayesian approaches, hard-encoded IC/BCs,. . .
- **Model parameterization**: include prior knowledge about u in the inductive bias of the NN (characteristics-informed NNs, etc.)
- **Domain-Decomposition, Linearization, and ELMs**: no backpropagation, regularized linear least-squares.

U. Braga-Neto, "Characteristics-Informed Neural Networks for Forward and Inverse Hyperbolic Problems". arXiv (2023)
F. M. Rohrhofer & al., "Approximating families of sharp solutions to Fisher's equation with physics-informed neural networks". Computer Physics Communications 307:109422 (2025)
S. Anderson & al., "ELM-FBPINNs: An Efficient Multilevel Random Feature Method". arXiv (2024)

Conclusions

- machine learning should use knowledge, not only data
- physics-informed machine learning is domain and application specific
- PINNs can utilize differential equations, but
  - must be adapted to the respective problem
  - suffer from training instabilities
  - require a larger number of computations for training
- **energy-performance trade-off** of physics-informed machine learning is still poorly understood

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Thanks!