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Project: Operator learning for periodic systems with partially hidden physics

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1 Project Description

Engineers increasingly rely on system modeling, like engine control or digital twins of factories. Traditionally, these models are based on physical principles derived from understanding the processes involved. However, complex systems, resource constraints, or incomplete knowledge can limit this approach. Data-driven models offer an alternative, but neglecting valuable physics knowledge hinders model interpretability and broader applicability. Recent advances in Scientific Machine Learning (SciML) [1] like the hidden physics models (HPM) [4] can address this space of deficient equations by bringing together physics and data and bridging the gap between these two approaches; cf figure 1. First introduced for neural networks, this methodology can be extended to Gaussian processes as well as sparse and symbolic regression [2]. Below is a schematic of the HPM.

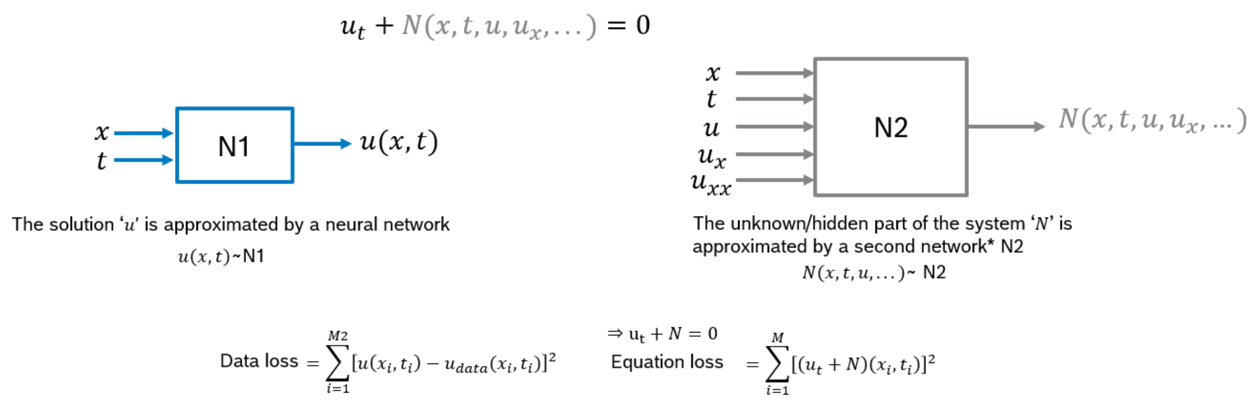

Figure 1: Hidden physics model: The parameters of $N1$ and $N2$ have to be optimized to minimize the cost function which is a sum of the equation and data loss. After training, $N1$ represents the solution state and the hidden part of the system $N2$.

As the model cannot be trained for all possible configurations, model generalizability poses an important challenge directly impacting the potential in model deployment. In operator learning, instead of individual functions, operators on function spaces are learned. Hence, a neural operator can trained to predict a function depending on parametrization of the problem configuration. Fourier neural operators (FNO) [3] are one example of operator learning where the neural operator is formulated on Fourier space. This opens a whole new perspective on on finding periodic operators, which are ubiquitous in real life. In this work, we explore the combination of HPMs with the generalization properties of operator learning via the use of Fourier neural operator architectures.

Tasks

- Familiarize with a machine and deep learning software[1] to carry out this project
- Implement HPM and FNO models
- Combine HPM and FNOs, and test them on synthetic data sets
- Apply the developed framework to real world data from Bosch

Requirements

- Expertise in machine learning and deep learning
- Basic knowledge of numerical methods for partial differential equations (e.g., FEM) for data generation
- Programming with Python

[1] For example, PyTorch or TensorFlow

Contact

If you are interested in this project and/or have further questions, please contact Alexander Heinlein, a.heinlein@tudelft.nl, and Birupaksha Pal, birupaksha.pal@in.bosch.com.

References

[1] N. Baker, F. Alexander, T. Bremer, A. Hagberg, Y. Kevrekidis, H. Najm, M. Parashar, A. Patra, J. Sethian, S. Wild, and K. Willcox. Brochure on Basic Research Needs for Scientific Machine Learning: Core Technologies for Artificial Intelligence. Technical report, USDOE Office of Science (SC) (United States), Dec. 2018. URL `https://www.osti.gov/biblio/1484362`.

[2] S. L. Brunton, J. L. Proctor, and J. N. Kutz. Discovering governing equations from data by sparse identification of nonlinear dynamical systems. *Proceedings of the National Academy of Sciences of the United States of America*, 113(15):3932–3937, 2016. ISSN 0027-8424. doi: 10.1073/pnas.1517384113. URL `https://mathscinet.ams.org/mathscinet-getitem?mr=3494081`.

[3] Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, and A. Anandkumar. Fourier Neural Operator for Parametric Partial Differential Equations, May 2021. URL `http://arxiv.org/abs/2010.08895`. arXiv:2010.08895 [cs, math].

[4] M. Raissi and G. E. Karniadakis. Hidden physics models: machine learning of nonlinear partial differential equations. *Journal of Computational Physics*, 357:125–141, 2018. ISSN 0021-9991. doi: 10.1016/j.jcp.2017.11.039. URL `https://mathscinet.ams.org/mathscinet-getitem?mr=3759415`.