Physics-Guided Machine Learning: A Novel Neural Network-Based Approach for Inverse Problems

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Problem description

Inverse problems are at the core of uncovering the unseen and interpreting the unknown. Our focus is on inverse problems governed by partial differential equations (PDEs). In this context, the forward problem involves solving the initial-boundary value problem (IBVP) given known problem parameters along with initial and boundary conditions. Conversely, the inverse problem aims to identify the problem parameters, initial conditions, and/or boundary conditions based on available information about the solution, such as measurement data. Inverse problems are important in numerous real-world applications and research fields, including forecasting extreme weather events for natural disaster management, reconstructing subsurface geological structures for sustainable energy storage, decoding medical imaging data for accurate diagnostics, and enhancing remote sensing for environmental monitoring. These problems are inherently challenging due to their ill-posed nature, where solutions may be non-unique, exhibit instability, and be highly sensitive to noisy or sparse data.

Research objective

In this project, you will explore fundamental aspects of inverse problems and develop a neural network-based solution framework using advanced physics-guided machine learning. As a starting point, you will work with physics-informed neural networks (PINNs) [2, 1], which solve PDE-based problems using a neural network model. The loss function in the training process incorporates physical laws (PDEs) as priors, guiding the network's learning process. By defining the unknown parameters of the inverse problem as trainable variables, the PINN model can automatically learn these parameters during training. This makes PINNs particularly well-suited for solving PDE-constrained inverse problems without a strict separation between the forward and inverse solution stages.

As a next step, you will explore a more general and flexible approach, as illustrated in Figure 1. Rather than solving a single, fixed inverse problem—i.e., computing the unknown parameters $\mathbf{X}^{(t)}$ for a specific set of observations $\mathbf{Z}^{(t)}$—you will train a neural network capable of learning the underlying structure of the inverse problem itself. This means the network will be trained to map observation data to the corresponding solutions across a range of different inverse problems, instead of being restricted to a single instance. As a result, once the inverse model has been trained, it will be able to solve the inverse problem efficiently for varying observation data $\mathbf{Z}^{(t)}$, providing a more generalizable and scalable solution framework.

Success in this thesis project will push the boundaries of computational methods for solving PDE-constrained inverse problems, with potential applicability extending to non-PDE-based problems as well. The outcomes could make significant contributions to fields such as climate

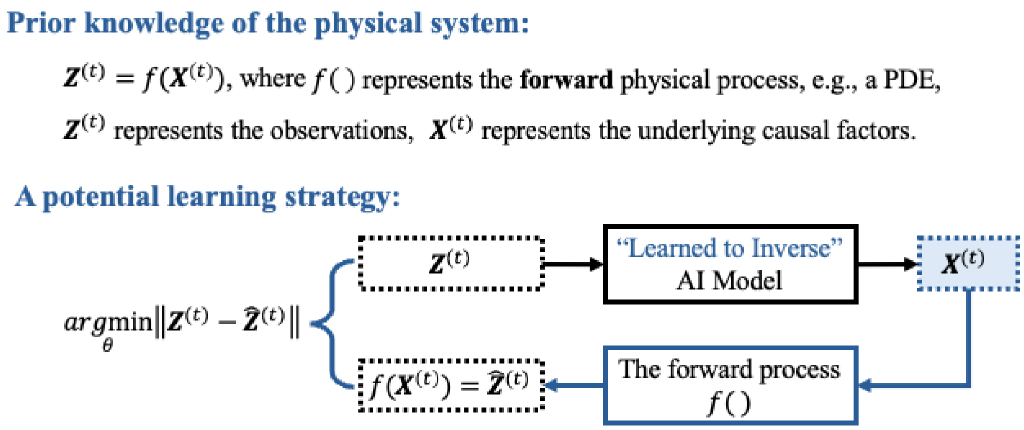

Figure 1: Illustration of the potential learning strategy.

science, energy sustainability, healthcare, and environmental monitoring, helping to develop solutions for some of the most pressing global challenges.

Requirements for candidates

- Experience in programming with Python
- Good expertise in machine learning and deep learning
- Basic knowledge of numerical methods for partial differential equations

References

[1] G. E. Karniadakis, I. G. Kevrekidis, L. Lu, P. Perdikaris, S. Wang, and L. Yang, *Physics-informed machine learning*, Nature Reviews Physics, 3 (2021), pp. 422–440. Number: 6 Publisher: Nature Publishing Group.

[2] M. Raissi, P. Perdikaris, and G. E. Karniadakis, *Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, Journal of Computational Physics, 378 (2019), pp. 686–707.