Scientific Machine Learning in Geophysical Exploration and Monitoring

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ABSTRACT

Scientific Machine Learning (SciML) emerges at the convergence of traditional scientific computing and machine learning (ML), aiming to leverage the rigor of scientific computing with the adaptability of ML to address shortcomings in data-driven learning within scientific domains. Unlike traditional ML models that struggle with limited, noisy data or the incorporation of scientific knowledge, leading to less reliable or physically implausible results, SciML integrates physical models based on scientific laws with ML techniques, offering enhanced interpretability, robustness, and generalizability from limited datasets. This interdisciplinary field has already started to revolutionize various scientific disciplines, notably improving computational efficiency and accuracy in fluid mechanics, materials science, climatology, etc., by incorporating physical laws into neural networks. A number of advancements have also been made in recent years in the field of geophysical modeling and inversion using emerging SciML paradigms, including physics-informed neural networks (PINNs), Fourier neural operators (FNOs), and Deep Operator Networks (DeepONets). These developments offer a new pathway to address longstanding computational challenges in the field of geophysics. We delve into these strides forward, highlighting the potential impact of such methods and the associated challenges in making these methods mainstream.

PINNs harness the capacity of deep neural networks to serve as universal function approximators, uniquely integrating the governing physical laws, typically represented by partial differential equations (PDEs), directly into their learning process (Raissi et al., 2019). This integration is achieved through a specialized training regimen that incorporates both data-driven loss and physics-based loss. The former assesses the fit between the model's predictions and the observed data, while the latter ensures adherence to the physical principles governing the system. The resultant model not only aligns with observed data but also inherently respects the underlying physics, setting PINNs apart with their ability to produce physically consistent solutions, generalize effectively even from sparse data, and amalgamate different data types.

PINNs have garnered significant attention in geophysics, particularly in modeling seismic travel times and wavefield solutions through forward solvers for the eikonal and wave equations (Smith et al., 2020; Alkhalifah et al., 2021). Early applications demonstrated their potential in surrogate modeling for fast travel time computation and complex seismic wavefield modeling across isotropic and anisotropic Earth approximations. However, challenges such as slow convergence due to neural networks' spectral bias were identified. Innovations like the sine activation function (Song et al., 2022), frequency scaling with neuron splitting (Huang and Alkhalifah, 2022), and Kronecker Neural Networks (Waheed, 2022) have been developed to enhance convergence for high-frequency features. PINNs have also been pivotal in tackling geophysical inverse problems, including full waveform inversion (Song and Alkhalifah, 2021) and travel time tomography (Waheed et al., 2021), benefiting from the addition of the PDE term in the loss function as a physics-informed regularizer. Efforts to improve training efficiency have led to strategies like integrating the data misfit as a hard constraint (Taufik et al., 2023). Despite successes in various applications, challenges in generalizability and the need for re-training with changes in model parameters persist, leading to an interest in neural operators for mapping between function spaces.

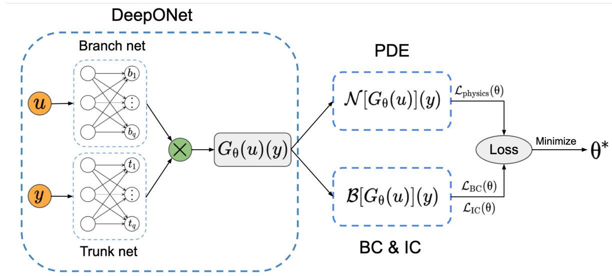

Figure 1: A physics-informed DeepONet architecture for learning the wavefield modeling operator consisting of two subnetworks: the branch net for extracting latent representations of input functions and the trunk net for extracting latent representations of input coordinates at which the output functions are evaluated. The wave equation along with simulated data are used to train the model parameters through a combined loss function.

The advent of neural operators in SciML marks a significant advancement in the construction of surrogate models for physical systems, offering the potential for near-instantaneous simulations. This emerging area promises significant advances, offering the ability to perform simulations quickly for a variety of applications. Neural operators adeptly learn mappings within partial differential equation frameworks, facilitating both data-centric and physics-driven optimizations. FNOs, in particular, have gained attention thanks to their ability to handle complex, high-dimensional problems more efficiently than traditional neural networks (Li et al., 2020). Further advancements, such as DeepONets (Lu et al., 2021) and their physics-informed variants (PI-DeepONets) (Wang et al., 2021), expand these capabilities, offering real-time prediction and robustness in modeling complex systems. Despite these strides, the application of neural operators in geophysics is still in its infancy. Innovations like Fourier-enhanced DeepONets (Zhu et al., 2023) and Enriched DeepONets (Haghighat et al., 2024) underscore the ongoing efforts to achieve higher accuracy and reliability in geophysical problems. In a similar vein, Figure 1 shows an illustration of a PI-DeepONet architecture that could be used to learn the wavefield modeling operator.