HNO: Neural Operators with Hard Constraints to Learn Partial Differential Equations

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Our research investigates the effectiveness of applying hard constraints to neural operators for learning partial differential equations. Machine learning techniques, particularly deep neural networks, have become increasingly prevalent in the study of physical systems. These methods are applied to a variety of scientific investigations, ranging from system identification, such as the discovery of parameters in PDEs, to the learning of complete systems solely from sensory data. While these methods can be computationally expensive and slow to train, once they are trained, their evaluation time is extremely fast. Additionally, their ability to seamlessly integrate the existing algorithms with new data makes them a promising alternative to traditional numerical solvers[1].

Despite the increased use of deep neural networks in scientific machine learning, the accuracy of these models remains a significant challenge. To address this issue, physics-informed neural networks (PINNs) were introduced as a means of combining domain knowledge with data by including the partial differential equation (PDE) in the DNN loss function[2]. This approach removes inadmissible mappings that do not adhere to physics, improving the accuracy of the model. However, the drawback of PINNs is that they are limited to learning only a single instance of a PDE, requiring new training for each new problem encountered.

To overcome this limitation, neural operators were introduced to extend the capabilities of PINNs to function spaces[3]. Neural operators can learn a family of PDEs, and therefore, only require a forward pass for a new PDE instance. By incorporating the knowledge of the function space, neural operators can generalize to new PDEs without the need for retraining, making them a more efficient approach for scientific machine learning.

The primary reason for the accuracy issues in neural operators is also a failure to respect the underlying physical laws. While soft constraints can partially address this problem by adding a physical loss term and increasing its weight, this approach can lead to ill-conditioning and limit the model's ability to learn from data[4]. Hard constraints provide a more effective solution for enforcing physical laws while also preserving the contribution of data to the learning process. In our study, we explore different techniques for applying hard constraints, such as penalty methods and augmented Lagrangian methods, and compare their performance to that of soft constraints for various partial differential equations.

References

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