

SOLVING PARTIAL DIFFERENTIAL EQUATIONS WITH MACHINE LEARNING

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ABSTRACT

Advancements in deep learning are starting to impact various scientific fields, but the full potential of these techniques for data-driven discoveries is yet to be achieved. A hindrance to reaching this potential is that current methods often don't cater to the needs of scientific users. General-purpose algorithms that are created for common machine learning (ML) applications like image or natural language processing cannot be easily applied to scientific data and require significant modifications for specific tasks. Scientific machine learning (SciML), an emerging discipline, seeks to address domain-specific data challenges (solid mechanics, biomechanics and fluid mechanics to name a few) and extract insights from scientific data sets through innovative methodological solutions. The development of neural operators (deep operator network, DeepONet) has revolutionized high-dimensional nonlinear regression by shifting the focus from function regression to operator regression, opening up new possibilities in the field of computational engineering. For black box systems, training of neural operators is data-driven only [1] but if the governing equations are known they can be incorporated into the loss function during training to develop physics-informed neural operators [2]. Additionally, to ease the training time of the neural operators to handle high-dimensional data, extension of the vanilla DeepONet is proposed which integrates the neural operator with an autoencoder model [3]. Furthermore, to improve the predictive performance of the operator models for scenarios with sparse labelled datasets, an operator level transfer learning model [4] is developed. The developed framework leverages information from a model trained on a source domain with sufficient labeled data and transfers it to a different but closely related target domain for which only a small amount of training data is available. This framework is applicable for task-specific learning of partial differential equations (PDEs) under multiple domains that are heterogeneous but subtly correlated. Through numerous high-dimensional benchmark examples, we have established the superiority of neural operators in the domain of computational engineering.

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