Novel deep learning approaches for learning scientific simulations

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Abstract

Over the past few years, computer simulation has gained immense importance in various fields, including engineering and core sciences, where many applications rely on the predictive capabilities of computational models. However, some of these applications, such as biomedical simulations for surgical training or support, demand computationally efficient or even real-time solutions. Traditional methods for solving non-linear problems, such as the finite element method (FEM), often prove too computationally expensive to be practical in such scenarios.

In this regard, deep learning approaches have been increasingly applied to accelerate conventional numerical simulations in recent years. However, as the size and complexity of the problems increase, their performance efficiency tends to diminish. In order to address these issues, we propose a novel geometric deep-learning framework for performing supervised learning on graph-structured data. Our approach is based on the Multi-Channel Aggregation (MAg) operation, which efficiently handles non-linear regression tasks on graph-structured data. We combine the MAg operation with novel clique-based graph pooling layers to create a graph U-Net architecture, called MAgNET [1]. This architecture is robust and can handle arbitrary complex meshes, while scaling efficiently with problem size.

We validate the performance of MAgNET by learning on numerically generated non-linear finite element datasets [2] and by comparing its performance to state-of-the-art attention-based architecture, Perceiver IO [3], and convolutional neural network U-Net framework [4].

Keywords: Non-linear FEM, deep learning, graph U-Net, CNN U-NET, Perceiver IO, Surrogate modeling

References

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