Regularized Conditionally Parameterized Graph Neural Networks for Parametric Non-intrusive Model Reduction in Complex Flows

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The idea of creating predictive models using partial knowledge about the governing equations has encouraged the development of model reduction methods based on system identification, operator inference and neural networks. Despite the undeniable popularity of neural networks however, extending their application beyond classic problems has been challenging in the context of fluid dynamics for two reasons: inability to generalize to complex grids and mesh topology changes, and difficulty in capturing high-order terms with an affordable training cost. The conditionally parameterized graph neural network (CP-GNet) is a discretization-independent reduced-order model that easily adapts to mesh complexities. Unlike the standard neural networks in which the weight matrices are constant, the weights in CP-GNet are functions of the input parameters, allowing the trained model to change and adapt to geometric and operating conditions during prediction. Conditional parameterization of the weights, along with incorporation of the knowledge about discretization of the governing equations, enables CP-GNet to more efficiently capture the nonlinearities. In this work, we demonstrate that in complex reactive flow problems, the long-term predictive performance of CP-GNet suffers from numerical instabilities that cannot be controlled by regularization methods commonly used in the context of neural networks. Therefore, we use the evolve-filter-relax method originally developed for stabilization of numerical schemes in the finite elements approach. We show that adaptive filtering and relaxation of the CP-GNet solution improves its long-term predictive performance in complex problems. The results indicate that the mature regularization toolbox that supports numerical schemes in computational fluid dynamics contains an underrated potential for improvement of predictive accuracy in neural network-based models.