Generalized Neural Closure Models with Interpretability

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Complex dynamical systems are used for predictions in many domains. Because of computational costs, models are truncated, coarsened, or aggregated. As the neglected and unresolved terms become important, the utility of model predictions diminishes. In our recently published work [1], we developed a novel neural delay differential equations (nDDEs) based framework to learn closure parameterizations for known-physics/low-fidelity models using data from high-fidelity simulations or high-resolution data, and increase the long-term predictive capabilities of the original models. The need for the time-delays in these *neural closure models* is rooted in the presence of inherent delays in real-world systems and justified by the Mori-Zwanzig formulation. In the present study, we develop the unified neural partial delay differential equations (nPDDEs) theory which augments low-fidelity models in their partial differential equation (PDE) forms with both Markovian and non-Markovian closure parameterized with neural networks (NNs). The amalgamation of low-fidelity model and NNs in the continuous spatio-temporal space followed with numerical discretization, automatically allows for generalizability to computational grid resolution, boundary conditions, initial conditions, and provide interpretability. We provide adjoint PDE derivations in the continuous form, thus allowing one to implement across differentiable and non-differentiable computational physics codes, different machine learning frameworks, and also allowing for nonuniformly-spaced spatio-temporal training data. We demonstrate the ability of our new framework to discriminate and learn model ambiguity in the advecting shock problem governed by the KdV-Burgers PDE and a biogeochemical-physical ocean acidification model in an interpretable fashion. We also learn the subgrid-scale processes and augment model simplification in those models, respectively. Finally, we analyze computational advantages associated with our new framework.

References

[1] A. Gupta and P. F. J. Lermusiaux. Neural closure models for dynamical systems. *Proceedings of The Royal Society A*, 477(2252):1–29, Aug. 2021.