“Automatic Discovery of Algorithms and Neural Architectures in Scientific Machine Learning”

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Abstract

We will first review deep neural operators, which we will use as foundation models for scientific machine learning tasks. Then, we will design two classes of ultra-fast meta-solvers for linear systems arising after discretizing PDEs by combining neural operators with either simple iterative solvers, e.g., Jacobi and Gauss-Seidel, or with Krylov methods, e.g., GMRES and BiCGStab, using the trunk basis of DeepONet as a coarse preconditioner. The idea is to leverage the spectral bias of neural networks to account for the lower part of the spectrum in the error distribution while the upper part is handled easily and inexpensively using relaxation methods or fine-scale preconditioners. We create a pareto front of optimal meta-solvers using a plurality of metrics, and we introduce a preference function to select the best solver most suitable for a specific scenario. This automation for finding optimal solvers can be extended to neural architectures for predicting time series as well as to nonlinear systems and other setups, e.g. finding the best meta-solver for space-time in time-dependent PDEs.