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A Label-Free Hybrid Iterative Numerical Transferable Solver for Partial Differential Equations

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Abstract. In scientific computing, traditional numerical methods for partial differential equations (PDEs), such as finite difference method and finite element method, often need to solve (large-scale) linear systems of equations. It is known that classical iterative solvers, such as Jacobi iteration and Gauss-Seidel iteration, have the smoothing property, i.e. the high-frequency part of the solution can be efficiently captured while the low-frequency part cannot. Multigrid offers a general methodology that utilizes the smoothing property of iterative solvers in a hierarchical manner. Meanwhile, machine learning-based methods for PDEs, such as deep operator network and Fourier neural operator, show the spectral bias, i.e. the low-frequency part of the solution can be efficiently captured while the high-frequency part cannot. The recently developed hybrid iterative numerical transferable solver (HINTS) offers an alternative choice that combines the advantages of classical iterative solvers on fine grids and operator learning methods on coarse grids. In this work, we propose a label-free HINTS for PDEs with the following features: (1) the training of the operator learning component is totally label-free, i.e. we do not need solutions to a given problem, which are typically obtained by classical solvers, (2) the resolution of the operator learning component is far coarser than that of the linear system of equations to be solved, (3) the success of label-free HINTS depends on whether the high-frequency component of the solution is captured on fine grids or not. Numerical experiments, including Possion equation in two and three dimensions, Hemholtz equation in two and three dimensions, anisotropic diffusion equation in two dimensions, are conducted to demonstrate the features of the proposed method. Based on these results, we conclude that the label-free HINTS provides a valuable addition for solving linear systems of equations arising from numerical PDEs.

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1 Introduction

Solving partial differential equations has been an important tool for understanding various physical and natural phenomena. Well-developed numerical methods, such as the finite difference method [12], the finite element method [8], and the spectral method [20], have been widely used in applications. It is a common observation that these methods' precision and convergence hinge significantly on the granularity of the grid employed. Coarser grids yield less accurate results, while finer grids require escalated computational expenditures.

Conventional iterative methods, such as Jacobi iteration and Gauss-Seidel iteration, are employed to solve the resulting linear systems of equations. As the mesh size h reduces, the number of iterations increases significantly in order to achieve good convergence. Precisely, to achieve a fixed tolerance, the number of iterations needed scales like $\mathcal{O}(h^{-2})$ with respect to h, since conventional iterative methods are effective in capturing the high-frequency components of the solution but ineffective for the low-frequency components [2]. A prevalent remedy for this challenge is the adoption of the multigrid method. The key idea behind this is to employ conventional iterative methods on a hierarchy of grids such that both high-frequency and low-frequency components can be captured simultaneously. Therefore, to achieve the same tolerance, the number of iterations needed in multigrid is $\mathcal{O}(1)$, independent of h.

In recent years, an increasing number of studies have adopted deep learning methodologies to solve PDEs. Physically informed neural networks (PINNs) [9, 19, 21] represent a notable paradigm, incorporating physical constraints during neural network training to enable unsupervised learning. Deep operator network (DeepONet) [6, 7, 15–17], grounded in the universal approximation theorem [4], excels in learning mappings between function spaces to address specific classes of PDEs. Drawing inspiration from Green's function method, Fourier neural operator [13] introduces a novel approach by parameterizing the integral kernel in Fourier space, yielding an efficient expression structure. These breakthroughs not only pave the way for efficient and effective solutions to PDEs but also, akin to PINN, DeepONet, and Fourier neural operator (FNO) [10,14,22,25] achieve unsupervised learning by integrating physical constraints into the neural network training process. One interesting property of deep neural networks is the spectral bias, i.e. the low-frequency component of a function is easier to learn [18, 23].

To address the challenges inherent in traditional numerical methods, [24] introduced a data-driven operator learning paradigm into the iterative framework, unveiling the hybrid iterative numerical transferable solver. This algorithm, marked by an alternating