Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2024-0263

Vol. **38**, No. 5, pp. 1453-1497
November 2025

Adaptive Basis-Inspired Deep Neural Network for Solving Partial Differential Equations with Localized Features

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Received 29 October 2024; Accepted (in revised version) 11 August 2025

Abstract. This paper proposes an Adaptive Basis-inspired Deep Neural Network (ABI-DNN) for solving partial differential equations with localized phenomena such as sharp gradients and singularities. Like the adaptive finite element method, ABI-DNN incorporates an iteration of "solve, estimate, mark, enhancement", which automatically identifies challenging regions and adds new neurons to enhance its capability. A key challenge is to force new neurons to focus on identified regions with limited understanding of their roles in approximation. To address this, we draw inspiration from the finite element basis function and construct the novel Basis-inspired Block (BI-block), to help understand the contribution of each block. With the help of the BI-block and the famous Kolmogorov Superposition Theorem, we first develop a novel fixed network architecture named the Basis-inspired Deep Neural Network (BI-DNN), and then integrate it into the aforementioned adaptive framework to propose the ABI-DNN. Extensive numerical experiments demonstrate that both BI-DNN and ABI-DNN can effectively capture the challenging singularities in target functions. Compared to PINN, BI-DNN attains significantly lower relative errors with a similar number of trainable parameters. When a specified tolerance is set, ABI-DNN can adaptively learn an appropriate architecture that achieves an error comparable to that of BI-DNN with the same structure.

AMS subject classifications: 65M50, 68T99, 35Q68, 35J75

Key words: Adaptive basis-inspired deep neural network, partial differential equations, singularity.

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1 Introduction

Recently, the remarkable success of Deep Neural Networks (DNNs) in data science has motivated numerous researchers to explore their potential in solving Partial Differential Equations (PDEs). Various DNN-based methods have emerged, such as the deep Ritz method (DRM) [1], the Physical Information Neural Network (PINN) [2], and the deep Galerkin method (DGM) [3]. In particular, the PINN introduced by Raissi et al. has attracted much attention due to its ability to embed physical equations into the network architecture, allowing for accurate predictions without the requirement of extensive data. It offers advantages over traditional mesh-based methods, including flexibility with complex geometries, efficiency in handling high-dimensional problems, and ease of implementation. As a result, the PINN has become an increasingly important tool for scientists and engineers seeking to understand better and predict the behavior of complex systems, such as fluid mechanics [4–6], hydrogeophysics [7] and transport phenomena in porous media [8].

Despite their successes, PINNs still face challenges in dealing with complicated PDE problems. For instance, the training of PINNs often encounters difficulties when target solutions involve sharp gradients or discontinuities. Therefore, continuous refinements are conducted from diverse perspectives to further improve the performance of PINNs. For instance, [9–11] proposed various adaptive sampling strategies that automatically adjust collocation points according to the residual of the PDE, the gradient information of the NN or insights derived from them. [12, 13] introduced adaptive activation functions with scalable parameters to enhance convergence rates and solution accuracy. [14, 15] focused on adaptive loss weighting strategies to achieve balanced training. [16] addressed problems with singular solutions by adaptive domain decomposition.

Besides factors explored in the above studies, the choice of neural network architecture, including the number of layers, the number of neurons within each layer, and patterns of connectivity, is also crucial for an accurate scheme [17]. However, network architecture design is often empirical due to a limited understanding of the DNN. Noticing that overly simple architectures might underperform and complex ones might overfit with limited data, designing an appropriately complex architecture is inherently challenging. An attractive idea is to shift from a pre-specified architecture with fixed complexity to an adaptively generated, task-specific network architecture, which is more efficient and suitable for the challenges it addresses. Regrettably, literature on the adaptive network architecture design within PINNs is still limited. A pioneering effort is the Adaptive Network Enhancement (ANE) method [17–19], which starts with a small network and iteratively adds neurons based on the a posteriori estimator until the desired accuracy is reached. However, the ANE method heavily relies on the physical partition generated by the ReLU activation function, and computing the physical partition for a deep network is computationally intensive.

In this paper, we focus on the adaptive design of network architecture and draw inspiration from the adaptive finite element method (AFEM) to propose the Adaptive Basis-