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High Order Deep Neural Network for Solving High Frequency Partial Differential Equations

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Abstract. This paper proposes a high order deep neural network (HOrderDNN) for solving high frequency partial differential equations (PDEs), which incorporates the idea of "high order" from finite element methods (FEMs) into commonly-used deep neural networks (DNNs) to obtain greater approximation ability. The main idea of HOrderDNN is introducing a nonlinear transformation layer between the input layer and the first hidden layer to form a high order polynomial space with the degree not exceeding p, followed by a normal DNN. The order p can be guided by the regularity of solutions of PDEs. The performance of HOrderDNN is evaluated on high frequency function fitting problems and high frequency Poisson and Helmholtz equations. The results demonstrate that: HOrderDNNs($p>1$) can efficiently capture the high frequency information in target functions; and when compared to physics-informed neural network (PINN), HOrderDNNs($p>1$) converge faster and achieve much smaller relative errors with same number of trainable parameters. In particular, when solving the high frequency Helmholtz equation in Section 3.5, the relative error of PINN stays around 1 with its depth and width increase, while the relative error can be reduced to around 0.02 as p increases (see Table 5).

AMS subject classifications: 68T99, 35Q68, 65N99

Key words: Deep neural network, high order methods, high frequency PDEs.

1 Introduction

High frequency problems appear in diverse scientific and engineering applications, such as high frequency Helmholtz equations arising from electromagnetics [28]. Although

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they usually encounter in low-dimensional space, finding numerical solutions of high accuracy to these problems is challenging due to their highly oscillatory nature. To efficiently approximate the high frequency components in the solutions, high order methods such as spectral methods and high order FEMs are often used [7, 13, 15]. However, these traditional numerical methods are mesh-dependent and mesh generation is hard and expensive especially in complex domains.

Recently deep learning based numerical methods for solving partial differential equations (PDEs) have attracted many attentions from scientific computing [1, 5, 8–10, 17, 19, 24]. Several novel methods have been proposed in the framework of Ritz formulation [24], least square formulation [17] and Galerkin formulation [8]. All these approaches yield promising empirical results especially for PDEs defined in irregular domains in high dimensions where classical numerical methods suffer the issues of slow computation, instability and the curse of dimensionality (CoD) [20]. Therefore, DNNs are recognized as potential tools to solve complex PDEs due to their meshless features. However, challenges still exist when DNNs are applied to high frequency problems. One of the most obvious challenges is that they often endow low-frequency components of the target functions with a higher priority during training, while cannot approximate the high frequency components well, which causes the stalling of convergence in the later stage of training. This phenomenon that DNNs have difficulty in capturing high frequency information is named as "F-Principle" by [11, 25] and "spectral bias" by [23]. To overcome this difficulty and obtain the benefits of high order methods in dealing with high frequency components, it is worthwhile to study the introduction of high order idea into commonly-used DNNs to improve their ability to approximate high frequency components.

In this paper, we propose a high order deep neural network, termed HOrderDNN, by incorporating the high order idea from FEMs into commonly-used DNNs. HOrderDNN is described in the framework of PINN and improves the network architecture used in PINN to obtain greater approximation capability, additional efficiency and higher accuracy when fitting high frequency functions and solving high frequency PDEs in complex domains. The key idea of HOrderDNN is to insert a nonlinear transformation layer between the input layer and the first hidden layer, which transforms the inputs that are independent coordinate components and linear with respect to themselves into a set of basis functions from the polynomial space with degree not exceeding p. In this way, any polynomial with degree not greater than p can be reproduced directly. Now the key step of HOrderDNN is to choose an appropriate set of basis functions which define the nonlinear transformation layer. Inspired by the observation in FEMs that the choice of basis functions will affect the condition number of the discrete linear system, we investigate the performances of three different kinds of basis functions, namely, monomial basis functions, Lagrangian basis functions on equidistant nodes and Gauss-Lobatto-Legendre (GLL) nodes. Consider the advantages of GLL nodes in spectral methods [2, 6, 21] and its superior performance in Fig. 3, our final choice is the Lagrangian basis functions on GLL nodes. With this specially designed nonlinear transformation layer, the proposed