

A Kolmogorov High Order Deep Neural Network for High Frequency Partial Differential Equations in High Dimensions

Yaqin Zhang^{1,2,†}, Ke Li^{3,†}, Zhipeng Chang⁴, Xuejiao Liu²,
Yunqing Huang^{1,*} and Xueshuang Xiang^{2,*}

¹ School of Mathematics and Computational Science, Xiangtan University,
Xiangtan 411105, China.

² Qian Xuesen Laboratory of Space Technology, China Academy of Space Technology,
Beijing 100094, China.

³ Information Engineering University, Zhengzhou 450001, China.

⁴ School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China.

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Abstract. This paper proposes a Kolmogorov high order deep neural network (K-HOrderDNN) for solving high-dimensional partial differential equations (PDEs), which improves the high order deep neural networks (HOrderDNNs). HOrderDNNs have been demonstrated to outperform conventional DNNs for high frequency problems by introducing a nonlinear transformation layer consisting of $(p+1)^d$ basis functions. However, the number of basis functions grows exponentially with the dimension d , which results in the curse of dimensionality (CoD). Inspired by the Kolmogorov Superposition Theorem (KST), which expresses a multivariate function as superpositions of univariate functions and addition, K-HOrderDNN utilizes a HOrderDNN to efficiently approximate univariate inner functions instead of directly approximating the multivariate function, reducing the number of introduced basis functions to $d(p+1)$. We theoretically demonstrate that CoD is mitigated when target functions belong to a dense subset of continuous multivariate functions. Extensive numerical experiments show that: for high-dimensional problems ($d=10, 20, 50$) where HOrderDNNs($p > 1$) are intractable, K-HOrderDNNs($p > 1$) exhibit remarkable performance. Specifically, when $d=10$, K-HOrderDNN($p=7$) achieves an error of $4.40E-03$, two orders of magnitude lower than that of HOrderDNN($p=1$) (see Table 10); for high frequency problems, K-HOrderDNNs($p > 1$) can achieve higher accuracy with fewer parameters and faster convergence rates compared to HOrderDNNs (see Table 8).

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[†]These two authors contributed equally to this work.

^{*}Corresponding author. Email addresses: huangyq@xtu.edu.cn (Y. Huang), xiangxueshuang2023@163.com (X. Xiang)

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1 Introduction

In recent years, deep learning methods for solving partial differential equations (PDEs) have attracted widespread attention [1]. A series of novel methods, such as the deep Ritz method (DRM) [2], Physical Information Neural Networks (PINNs) [3,4], the deep Galerkin method (DGM) [5] and Weak Adversarial Neural Networks (WAN) [6], have been proposed and demonstrated the vast potential of deep neural networks (DNNs) in solving various PDEs. The basic idea of these methods is reformulating a PDE problem as an optimization problem and training a DNN to approximate the solution of the PDE by minimizing the corresponding loss function. Compared to traditional mesh-dependent methods such as Finite Element Methods (FEMs), these deep learning-based numerical methods show great flexibility and potential for solving complex PDEs defined in high dimensions and irregular domains. Unfortunately, challenges still exist despite their early success, especially when dealing with high-frequency problems. As revealed by frequency principle or spectral bias [7,8], PINNs exhibit different learning behaviours among different frequencies, with low-frequency components being prioritized and high-frequency components hard to capture, ultimately leading to difficulties in achieving stable training and accurate predictions in high-frequency problems.

To address this challenge, a series of extensions to the vanilla PINN have been proposed to boost the performance of PINNs from various aspects, such as PhaseDNN [9], MscaledDNN and its variants [10–12], cFPCT-DNN [13], PIRBN [14], etc. In particular, [15] develops the High Order Deep Neural Network (HOrderDNN), which incorporates high order idea from FEMs into conventional neural networks by introducing a nonlinear transformation layer determined by high order basis functions. As demonstrated in [15], HOrderDNN(p) can directly reproduce polynomials in $\mathcal{Q}_p(\mathbb{R}^d)$, efficiently capture the high frequency information in target functions, and obtain greater approximation capability, additional efficiency and higher accuracy in solving high frequency problems compared to PINN. Furthermore, [16] develops HOrderDeepDDM by combining HOrderDNN with the domain decomposition method for solving high frequency interface problems. However, with the powerful approximation capability in HOrderDNN, there are also some limitations. Specifically, the nonlinear transformation layer incorporated in HOrderDNN requires $(p+1)^d$ tensor product basis functions to reproduce any multivariate polynomial function $f(x) \in \mathcal{Q}_p(\mathbb{R}^d)$. As the dimension d increases, the number of basis functions $(p+1)^d$ grows exponentially, resulting in HOrderDNN suffering the curse of dimensionality (CoD).

In this paper, we continue this line of research for solving high frequency problems and propose a Kolmogorov high order deep neural network, named K-HOrderDNN, to address the issue of CoD in HOrderDNN. Drawing inspiration from the famous Kolmogorov Superposition Theorem (KST), we reconstruct the nonlinear transform layer