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Solving Time-Dependent Parametric PDEs by Multiclass Classification-Based Reduced Order Model

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Abstract. In this paper, we propose a network model, the multiclass classification-based reduced order model (MC-ROM), for solving time-dependent parametric partial differential equations (PPDEs). This work is inspired by the observation of applying the deep learning-based reduced order model (DL-ROM) [14] to solve diffusion-dominant PPDEs. We find that the DL-ROM has a good approximation for some special model parameters, but it cannot approximate the drastic changes of the solution as time evolves. Based on this fact, we classify the dataset according to the magnitude of the solutions and construct corresponding subnets dependent on different types of data. Then we train a classifier to integrate different subnets together to obtain the MC-ROM. When subsets have the same architecture, we can use transfer learning techniques to accelerate offline training. Numerical experiments show that the MC-ROM improves the generalization ability of the DL-ROM both for diffusion- and convection-dominant problems, and maintains the DL-ROM's advantage of good approximation ability. We also compare the approximation accuracy and computational efficiency of the proper orthogonal decomposition (POD) which is not suitable for convection-dominant problems. For diffusion-dominant problems, the MC-ROM has better approximation accuracy than the POD in a small dimensionality reduction space, and its computational performance is more efficient than the POD's.

AMS subject classifications: 68T07, 35M13, 93A30

Key words: Parametric partial differential equation, reduced order model, deep learning, generalization ability, classification, computational complexity.

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1 Introduction

Partial differential equation (PDE) is a fundamental mathematical model in scientific and engineering computation. It is urgent to develop a numerical approach for solving PDEs. The approach requires the following properties: high fidelity, generalization ability (being available to different PDE, different initial-boundary condition, model parameters, and so on), computational efficiency (being expected to achieve the optimal $\mathcal{O}(N)$ computational complexity). The approach is in terms of computational PDE model. Parametric PDEs (PPDEs) are one of the most important PDEs. Many scientific and engineering problems, such as control, optimization, inverse design, uncertainty quantification, Bayesian inference can be described by PPDEs with computational domains, initial-boundary conditions, source terms, and physical properties as parameters. However, numerically solving PPDEs usually requires expensive computational costs mainly due to multi-query and real-time computing. Therefore, designing a computational PDE model that meets the above characteristics for the PPDEs has important applications. However, it is also a challenge in scientific and engineering computation.

The projection-based linear reduced order model (ROM) [15,23] is an effective way to improve the computational efficiency of numerically solving PPDEs. ROM can be divided into offline and online stages. The offline stage constructs a low-dimensional subspace to approximate the solution manifold using obtained high fidelity numerical solutions. The computational tasks on the offline stage are usually expensive. The online stage obtains an approximated solution for a new given model parameter based on the low-dimensional subspace. The proper orthogonal decomposition (POD) method is a popular algorithm for constructing linear ROM and is effective for many questions, such as computational fluid dynamics and structural analysis [5,31]. However, the POD method still has some weaknesses, such as (i) it requires to construct a relatively high-dimensional subspace to obtain an acceptable numerical solution; (ii) it needs relatively expensive reduction strategies; and (iii) it has the intrinsic difficulty to handle physical complexity, etc. To overcome these difficulties, a non-intrusive and data-driven nonlinear reduced-order model based on deep learning (or neural network) has been developed [24,26].

Using the neural network as an ansatz to solve PDE can be traced back to the late 1990s [27]. In recent years, with the evolution of the computational power, the explosive development of deep learning has again attracted much attention of the community of scientific computing. Due to the great expressivity of neural network [13], the neural-network PDE solver achieves some breakthroughs in solving a single PDE, especially high-dimensional PDE [18,41,46]. Using neural networks to solve PPDEs has also been attracted much attention. The idea is to apply neural networks to learn the parameter to solution mapping. The main works can be divided into two parts based on the steady-state and time-dependent PPDEs. Firstly, the works on steady-state PPDEs can be divided into supervised learning [39,43] and unsupervised learning [10,50]. Secondly, since time-dependent PPDEs also involve time variables, the requirements for its generaliza-