Less Emphasis on Hard Regions: Curriculum Learning of PINNs for Singularly Perturbed Convection-Diffusion-Reaction Problems

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Received 18 February 2023; Accepted (in revised version) 17 May 2023.

Abstract. Although physics-informed neural networks (PINNs) have been successfully applied in a wide variety of science and engineering fields, they can fail to accurately predict the underlying solution in slightly challenging convection-diffusion-reaction problems. In this paper, we investigate the reason of this failure from a domain distribution perspective, and identify that learning multi-scale fields simultaneously makes the network unable to advance its training and easily get stuck in poor local minima. We show that the widespread experience of sampling more collocation points in high-loss regions hardly help optimize and may even worsen the results. These findings motivate the development of a novel curriculum learning method that encourages neural networks to prioritize learning on easier non-layer regions while downplaying learning on harder regions. The proposed method helps PINNs automatically adjust the learning emphasis and thereby facilitates the optimization procedure. Numerical results on typical benchmark equations show that the proposed curriculum learning approach mitigates the failure modes of PINNs and can produce accurate results for very sharp boundary and interior layers. Our work reveals that for equations whose solutions have large scale differences, paying less attention to high-loss regions can be an effective strategy for learning them accurately.

AMS subject classifications: 35Q68, 68T07, 68W25

Key words: Physics-informed neural network, convection-diffusion-reaction, boundary layer, interior layer, curriculum learning.

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1. Introduction

Convection-diffusion-reaction problems appear in the modeling of various modern complicated processes, such as fluid flow at high Reynolds numbers [16], drift diffusion in semiconductor device modeling [29], and chemical reactor theory [26]. Very often the size of diffusion is characterized by a parameter ϵ , which could be smaller by several orders of magnitude compared to the size of convection and/or reaction, resulting in narrow boundary or interior layers in which the solution changes extremely rapidly [31]. Classical numerical methods use layer-adapted meshes or introduce carefully designed artificial stability terms to solve these challenging problems [2,4,33,37,38].

In recent years, there has been a surge of interest in applying neural networks in traditional scientific modeling — e.g. partial differential equations, which yields the so-called physics-informed neural networks [5, 10, 11, 14, 17, 18, 21, 23, 30, 34, 35]. The main idea of PINNs is to include physical domain knowledge as soft constraints in the empirical loss function and then use existing machine learning methodologies such as stochastic optimization, to train the model. As an interesting alternative to traditional numerical solvers, PINN has the advantage of flexibility in dealing with high-dimensional PDEs in complicated geometry and easy incorporation of available data information. Moreover, well-trained PINNs can have good generalization ability and can quickly predict solutions outside the computational area.

However, as reflected in some recent studies on the failure modes of PINNs [1, 6-8, 21], it has been found that PINNs can fail to converge to the correct solution even for relatively simple convection-diffusion problems. Approaches to improve the accuracy of PINNs in solving convection-diffusion problems can be broadly classified into two categories. The first category borrows theories and concepts from conventional numerical methods. For example, Mojgani et al. [28] rewrote the original equation into a Lagrangian form on the characteristic curves and then applied a two-branch neural network to solve the reformulated form. However, the approach is only applicable to time-dependent problems and not to steady-state equations. Recently, inspired by the theory of singular perturbation and asymptotic expansions, Arzani et al. [1] used separate neural networks to learn the different levels on the inner and outer layer regions, respectively. The second category emphasizes machine learning techniques, such as the design of loss functions, sample selection, and learning strategies. He et al. [15] used a weighted sum of residual losses and showed that in order to obtain an accurate solution of the advection-dispersion equation, the weights of the initial and boundary conditions should be larger than the PDE residuals. Daw et al. [6] proposed an evolutionary sampling algorithm in which the collocation points evolve gradually with training to prioritize high-loss regions while maintaining a background distribution of uniformly sampled points. Krishnapriyan et al. [21] argued that the PDE-based soft constraints make the loss landscapes difficult to optimize, and proposed a curriculum approach that sets the PINN loss term starting with a simple equation regularization and progressively become more complex as the network gets trained, which suffers from complex training scheme and very long training phase when solving strong singular perturbation problems.