Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2022-0239

Vol. **33**, No. 5, pp. 1240-1269
May 2023

Investigating and Mitigating Failure Modes in Physics-Informed Neural Networks (PINNs)

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Received 20 September 2022; Accepted (in revised version) 26 March 2023

Abstract. This paper explores the difficulties in solving partial differential equations (PDEs) using physics-informed neural networks (PINNs). PINNs use physics as a regularization term in the objective function. However, a drawback of this approach is the requirement for manual hyperparameter tuning, making it impractical in the absence of validation data or prior knowledge of the solution. Our investigations of the loss landscapes and backpropagated gradients in the presence of physics reveal that existing methods produce non-convex loss landscapes that are hard to navigate. Our findings demonstrate that high-order PDEs contaminate backpropagated gradients and hinder convergence. To address these challenges, we introduce a novel method that bypasses the calculation of high-order derivative operators and mitigates the contamination of backpropagated gradients. Consequently, we reduce the dimension of the search space and make learning PDEs with non-smooth solutions feasible. Our method also provides a mechanism to focus on complex regions of the domain. Besides, we present a dual unconstrained formulation based on Lagrange multiplier method to enforce equality constraints on the model's prediction, with adaptive and independent learning rates inspired by adaptive subgradient methods. We apply our approach to solve various linear and non-linear PDEs.

AMS subject classifications: 65D15, 35E05, 35E15, 68T20, 90C26, 90C29, 90C30, 90C31, 49N15, 90C46, 90C47, 90C90

Key words: Constrained optimization, Lagrangian multiplier method, Stokes equation, convection equation, convection-dominated convection-diffusion equation, heat transfer in composite medium, Lid-driven cavity problem.

1 Introduction

A wide range of physical phenomena can be explained with partial differential equations (PDEs), including sound propagation, heat and mass transfer, fluid flow, and elasticity.

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The most common methods (i.e., finite difference, finite volume, finite element, spectral element) for solving problems involving PDEs rely on domain discretization. Thus, the quality of the mesh heavily influences the solution error. Moreover, mesh generation can be tedious and time-consuming for complex geometries or problems with moving boundaries. While these numerical methods are efficient for solving forward problems, they are not well-suited for solving inverse problems, particularly data-driven modeling. In this regard, neural networks can be viewed as an alternative meshless approach to solving PDEs.

Dissanayake and Phan-Thien [1] introduced neural networks as an alternative approach to solving PDEs. The authors formulated a composite objective function that aggregated the residuals of the governing PDE with its boundary condition to train a neural network model. Independent from work presented in [1], van Milligen et al. [2] also proposed a similar approach for the solution of a two-dimensional magnetohydrodynamic plasma equilibrium problem. Several other researchers adopted the work in [1,2] for the solution of nonlinear Schrodinger equation [3], Burgers equation [4], self-gravitating N body problems [5], and chemical reactor problem [6]. Unlike earlier works, Lagaris et al. [7] proposed to create trial functions for the solution of PDEs that satisfied the boundary conditions by construction. However, their approach is not suitable for problems with complex geometries. It is possible to create many trial functions for a particular problem. But to choose an optimal trial function is a challenging task, particularly for PDEs.

Recently, the idea of formulating a composite objective function to train a neural network model following the approach in [1,2] has found a resurgent interest thanks to the works in [8–10]. This particular way of learning the solution to strong forms of PDEs is commonly referred to as physics-informed neural networks (PINNs) [9]. PINNs employ physics as a regularizing term in their objective function. However, this approach brings forth the challenge of manually adjusting the corresponding hyperparameters. Furthermore, the absence of validation data or prior knowledge of the solution to the Partial Differential Equation (PDE) can render PINNs impracticable. The deep Ritz method has been proposed to solve variational problems arising from PDEs [8]. This method enforces boundary conditions through a hyperparameter that cannot be tuned without validation data or prior knowledge of the solution. Thus, it is not well-suited for solving forward problems. There is a growing interest in using neural networks to learn the solution to PDEs [11–18]. Despite the great promise of PINNs for the solution of PDEs, several technical issues remained a challenge, which we discuss further in Section 2.2. Different from the earlier approaches [1,2,6,9], we recently proposed *physics and equality constrained artificial neural networks* (PECANNs) that are based on constrained optimization techniques. Furthermore, we used a maximum likelihood estimation approach to seamlessly integrate noisy measurement data and physics while strictly satisfying the boundary conditions. In Section 4, we discuss our proposed formulation, constrained optimization problem, and unconstrained dual problem.

Our contribution is summarized as follows: