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HRW: Hybrid Residual and Weak Form Loss for Solving Elliptic Interface Problems with Neural Network

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Abstract. Deep learning techniques for solving elliptic interface problems have gained significant attentions. In this paper, we introduce a hybrid residual and weak form (HRW) loss aimed at mitigating the challenge of model training. HRW utilizes the functions residual loss and Ritz method in an adversary-system, which enhances the probability of jumping out of the local optimum even when the loss landscape comprises multiple soft constraints (regularization terms), thus improving model's capability and robustness. For the problem with interface conditions, unlike existing methods that use the domain decomposition, we design a Pre-activated ResNet of ResNet (PRoR) network structure employing a single network to feed both coordinates and corresponding subdomain indicators, thus reduces the number of parameters. The effectiveness and improvements of the PRoR with HRW are verified on two-dimensional interface problems with regular or irregular interfaces. We then apply the PRoR with HRW to solve the size-modified Poisson-Boltzmann equation, an improved dielectric continuum model for predicting the electrostatic potentials in an ionic solvent by considering the steric effects. Our findings demonstrate that the PRoR with HRW accurately approximates solvation free-energies of three proteins with irregular interfaces, showing the competitive results compared to the ones obtained using the finite element method.

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1. Introduction

As one application, the deep neural networks for solving partial differential equations (PDEs) have received extensive attentions recently for their simplicity in construction and success in various applications [18]. Dating back to the early 1990s, Lagaris *et al.* [13] proposed a single layer feed-forward neural network, in which the governing equations and the boundary conditions are taken as loss functions. Then Isaac and Aristidis [14] proposed a decomposition method to decompose the trial solution into the sum of the neural network and the initial or boundary condition to strictly meet the physical constraints. Recently, extending the single layer neural network in [13] to multiple layers and adding the difference of observation samples into the loss function, Karniadakis proposed the physical information neural network (PINN) [11, 16], and gave a series of improvements to solve the forward and inverse problems [27]. E *et al.* [3] extended the Ritz method to the field of deep learning, and used the variational form to obtain the weak solution of the Poisson equation, convergence analysis of which can be found in [2]. Wang *et al.* [19, 20] incorporated scientific theory on the basis of controlling equation constraints to avoid unreasonable predictions in fluid simulation and subsurface geological inversion. The above methods are all soft constraints in essence, Chen *et al.* [1] proposed Hard constraint projection (HCP) to integrate the discrete form of the governing equation into the activation function of the output layer in neural networks. Through this approach, the predicted results of the neural network adhere rigorously to the physical constraints by being projected onto the constrained hyperplane. As for the non-symmetric PDEs with no energy functional available to characterize the weak solution, the deep Galerkin method [17] utilizes the integral form of the residual as a loss function, effectively reducing the derivative order and providing a viable means to resolve high-order problems.

All of these mentioned methods were proposed for PDEs without interface conditions. Considering the elliptic interface problem, Wang *et al.* [21] used two shallow neural networks to approximate the boundary conditions and the differential equations for solving elliptic interface problems with high-contrast coefficients. Based on the domain decomposition idea, some improved deep learning methods [5, 7, 23] were proposed using different formulations of the loss functions. To approximate the solution to the given interface problem, the present research proposes utilizing two or more neural networks, in contrast to a single network, to simulate the solution within each subdomain. Subsequently, the networks are interlinked by enforcing the interface conditions from different subdomains to derive the final solution. To be able to better capture the solution in each subdomain, the deep learning methods based on the domain decomposition idea have acceptable solution accuracy (about 10^{-2}). Of course, using better network structure [25], appropriately determining the hyper-parameters such as the coefficients of the various terms in the loss function [22] and using the adaptive technique [4] would enhance the solution accuracy. To further improve the accuracy, Lai *et al.* [9] augmented one coordinate variable into the input vector, and used only one network with one hidden layer to solve the elliptic interface problem with discon-