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A Deep Uzawa-Lagrange Multiplier Approach for Boundary Conditions in PINNs and Deep Ritz Methods

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Abstract. We introduce a deep learning-based framework for weakly enforcing boundary conditions in the numerical approximation of partial differential equations. Building on existing physics-informed neural network and deep Ritz methods, we propose the Deep Uzawa algorithm, which incorporates Lagrange multipliers to handle boundary conditions effectively. This modification requires only a minor computational adjustment but ensures enhanced convergence properties and provably accurate enforcement of boundary conditions, even for singularly perturbed problems. We provide a comprehensive mathematical analysis demonstrating the convergence of the scheme and validate the effectiveness of the Deep Uzawa algorithm through numerical experiments, including high dimensional, singularly perturbed problems and those posed over non-convex domains.

Keywords:
Physics-informed neural networks,
Deep Ritz method,
Uzawa algorithm,
Lagrange multipliers,
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1 Introduction

The numerical approximation of partial differential equations (PDEs) using artificial neural networks (ANNs) has gained significant attention in recent years [4, 9, 14, 18, 20]. This surge is largely attributed to the success of deep learning in various complex tasks [10, 13]. In the context of solving PDEs, neural network-based methods such as the deep Ritz approach [4], which approximates solutions by minimising the Dirichlet energy, and the physics-informed neural networks (PINNs) [18], which minimise the L^2-norm of the residuals are prominent examples.

Despite their success, a challenge in these methods lies in the enforcement of boundary conditions. While classical numerical methods also face difficulties in this regard, the non-standard nature of neural network approximation spaces makes this issue particularly pronounced. Standard penalty approaches often require large penalty weights to enforce boundary conditions accurately, resulting in ill-conditioned optimisation problems that are difficult to tune and can lead to suboptimal solutions. This issue is particularly

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severe in problems involving singular perturbations or complex domains. Additionally, the practical implementation of boundary conditions in ANN-based methods poses challenges, as accurately capturing boundary data within the neural network's architecture often proves difficult.

To address these challenges, we propose extending the Lagrange multiplier framework from finite elements, as introduced by Babuška [1], to neural network-based PDE solvers. Our work develops a class of algorithms termed Deep Uzawa algorithms, which iteratively solve the resulting saddle point problems to weakly impose boundary conditions. The key innovation lies in adapting Uzawa's algorithm [22] to this context, allowing for efficient iterative approximation of PDEs where boundary conditions are enforced using an augmented Lagrangian formulation. This approach ensures that the algorithmic framework remains stable and accurate due to the coercivity of the energies involved.

The Deep Uzawa methods, Ritz-Uzawa (RitUz) and PINNs-Uzawa (PINNUz), extend existing deep Ritz and PINN frameworks with minimal modifications, making them highly practical for integration into current computational workflows. The theoretical analysis provided includes convergence proofs that demonstrate the iterative schemes' stability at the PDE level. These theoretical guarantees offer a robust foundation for the implementation of the Deep Uzawa algorithms and provide insight into their convergence behaviour. We compare the behaviour of these approaches to the vanilla methods and show that the Deep Uzawa approach achieves comparable or superior performance without relying on tuning penalty parameters.

Numerous methods have been explored for weakly imposing boundary conditions within ANN-based PDE solvers. The deep Ritz method [4] and PINNs [18] form the foundational basis for many current approaches, but both rely on penalty terms for boundary enforcement, which can make optimisation challenging, particularly when large penalties are needed. To address these shortcomings, [14] proposed an adaptation using Nitsche's method [17] from finite element analysis to weakly impose boundary conditions, mitigating conformity issues highlighted in [4]. Similarly, [23] compared traditional Ritz-Galerkin methods with ANN-based approaches, noting the implicit regularisation properties provided by neural networks. Other advancements, such as the penalty-free neural network strategy in [19], have targeted second-order boundary value problems in complex geometries. In high-dimensional settings, [11] explored deep learning approaches for elliptic PDEs with non-trivial boundary conditions, showcasing the flexibility of neural networks in handling such cases.

Our Deep Uzawa method builds on these developments by leveraging a consistent saddle point framework to address the boundary enforcement problem, offering a minor tweak computationally that provably enhances stability and accuracy. The application of Uzawa-type iterations in neural network contexts, as presented in [16], serves as a foundation for our iterative scheme. Our approach provides a structured way to balance the competing objectives of PDE accuracy and boundary condition enforcement, demonstrating improved stability in various numerical experiments, including problems on non-convex domains and high-dimensional geometries.

The rest of the paper is organized as follows: In Section 2, we introduce the notation and fundamental concepts related to Sobolev spaces, which form the basis for the