Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2020-0219

Vol. **29**, No. 5, pp. 1365-1384
May 2021

Deep Nitsche Method: Deep Ritz Method with Essential Boundary Conditions

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Received 5 November 2020; Accepted (in revised version) 13 January 2021

Abstract. We propose a new method to deal with the essential boundary conditions encountered in the deep learning-based numerical solvers for partial differential equations. The trial functions representing by deep neural networks are non-interpolatory, which makes the enforcement of the essential boundary conditions a nontrivial matter. Our method resorts to Nitsche's variational formulation to deal with this difficulty, which is consistent, and does not require significant extra computational costs. We prove the error estimate in the energy norm and illustrate the method on several representative problems posed in at most 100 dimension.

AMS subject classifications: 65N30, 65M12, 41A46, 35J25

Key words: Deep Nitsche Method, Deep Ritz Method, neural network approximation, mixed boundary conditions, curse of dimensionality.

1 Introduction

Recently there has been a surge of interests in solving partial differential equations by deep learning-based numerical methods [6,11,12,16,17,19,25,29,32,33,40,41,44–46], and we refer to [15] for a review for this direction. These methods allow for the compositional construction of new approximation sets from various neural networks. Such constructions are usually free of a mesh so that they are in essence *meshless methods* [5]. The trial functions in the approximation sets are in general non-interpolatory, which makes the implementation of the essential boundary conditions not an easy task. There are two

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main approaches to handle the essential boundary conditions in deep learning-based numerical methods. One is the conforming method, which exploits a supplementary neural network to make the functions in the trial set satisfy the boundary conditions *exactly*. This is the approach firstly proposed in [30, 31] and recently further developed in [6, 29]. The conforming method usually involves an accurate evaluation of the distance function or a cut-off function, which is not easy for domain with complicated boundary geometry; see, e.g., [6]. Another one is the penalty method, which is a very general concept and belongs to the so-called nonconforming method [17, 40, 41, 45, 46]. An additional surface term is introduced into the variational formulation to enforce the boundary conditions. However, great care has to be taken to balance the different terms in the functional framework. Otherwise, this may cause problems for the existence and uniqueness of the solution [2, 8]. Moreover, the penalty method usually leads to a sub-optimal rate of convergence as shown in [3] for finite element methods and as shown in [5] for the generalized finite element methods and meshless methods.

Compared to the penalty method, the Lagrange multiplier method treats the essential boundary conditions as a constraint in the minimization. This technique has been used to deal with the essential boundary conditions in finite element method [4] and wavelet method [13]. The optimal rate of convergence may be achieved if the approximation function spaces are chosen properly, which relies on the so-called inf-sup condition [4,13]. The Lagrange multiplier method may also be used to enforce boundary conditions in the neural-network based method provided that the resulting constrained minimization problem can be efficiently solved.

An efficient method for imposing the essential boundary conditions has been proposed by Nitsche in the early 1970's [38] in the finite element method. It was quite unknown for many years, and was revived in [42] by STENBERG. He revealed the interesting relation between Nitsche's method and certain stabilized Lagrangian multiplier methods. More recent efforts on Nitsche's method have been devoted to deal with the elliptic interface problems and the unfitted mesh problems; we refer to [10] for a review of the progress in this direction. In the context of the meshless method, Nitsche's idea has been proved to be an efficient approach to deal with the essential boundary conditions in the framework of a particle partition of unity method [23] as well as the generalized finite element method [35].

In this work, we incorporate the idea of Nitsche into the framework of Deep Ritz Method [17] to deal with the essential boundary conditions. This new algorithm is called Deep Nitsche Method. It also imposes the boundary conditions in a nonconforming way as the penalty method. In contrast to the penalty method, this method is consistent if the exact solution is smooth enough. The method is based on the energy formulation of Nitsche [38], which does not involve a Lagrange multiplier. Hence we need not solve a constrained minimization problem, and the stochastic gradient descent (SGD) method may be used to solve the resulting minimization problem. To analyze the method, we exploit Nitsche's energy formulation instead of the Euler-Lagrange equations associated with the minimization problem, which in general does not exist for the deep Nitsche