Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2021-0176

Vol. **31**, No. 3, pp. 966-986
March 2022

An Augmented Lagrangian Deep Learning Method for Variational Problems with Essential Boundary Conditions

Jianguo Huang[1], Haoqin Wang[1] and Tao Zhou[2,*]

[1] *School of Mathematical Sciences, and MOE-LSC, Shanghai Jiao Tong University, Shanghai, China.*
[2] *LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China.*

Received 27 August 2021; Accepted (in revised version) 5 January 2022

Abstract. This paper is concerned with a novel deep learning method for variational problems with essential boundary conditions. To this end, we first reformulate the original problem into a minimax problem corresponding to a feasible augmented Lagrangian, which can be solved by the augmented Lagrangian method in an infinite dimensional setting. Based on this, by expressing the primal and dual variables with two individual deep neural network functions, we present an augmented Lagrangian deep learning method for which the parameters are trained by the stochastic optimization method together with a projection technique. Compared to the traditional penalty method, the new method admits two main advantages: i) the choice of the penalty parameter is flexible and robust, and ii) the numerical solution is more accurate in the same magnitude of computational cost. As typical applications, we apply the new approach to solve elliptic problems and (nonlinear) eigenvalue problems with essential boundary conditions, and numerical experiments are presented to show the effectiveness of the new method.

AMS subject classifications: 65N25, 65N30, 68U99

Key words: The augmented Lagrangian method, deep learning, variational problems, saddle point problems, essential boundary conditions.

1 Introduction

Variational problems play important roles in various industrial and engineering applications, with typical examples including partial differential equations (PDEs) and eigen-

*Corresponding author. *Email addresses:* jghuang@sjtu.edu.cn (J. Huang), wanghaoqin@sjtu.edu.cn (H. Wang), tzhou@lsec.cc.ac.cn (T. Zhou)

value problems. Many classical numerical methods have been developed for such problems, e.g., the finite difference method, the spectral method, and the finite element method. The first two methods are generally used for solving problems over regular domains while the latter one is particularly suitable for problems in irregular domains [6, 11]. In recent years, deep learning based techniques have been widely used to solve a variety of variational problems [9, 14, 16, 18, 23, 24, 28, 32, 35, 39, 40]. Historically, related studies can date back to the 1990s [12, 26]. We also refer the reader to [13] and the references therein for a comprehensive review on machine learning from the perspective of computational mathematics. For such kind of methods, deep neural networks (DNNs) are exploited to parameterize the PDE solutions and appropriate parameters are identified by minimizing an optimization problem formulated from the PDEs. The most significant feature of those methods is that they are mesh-free, and their approximation capacity has been well studied in recent years [3, 15, 19, 21, 33].

For variational problems with natural boundary conditions, one doesn't need to impose these conditions on the admissible functions [16], so that the DNNs can easily be used for approximation. However, for variational problems with essential boundary conditions, these conditions should be imposed on the admissible functions, and this gives rise to a significant difficulty since one cannot enforce the boundary condition in a simple way even at the interpolation nodes for a neural network function. It is worth noting that even in the context of finite element methods, this is also a very tough issue. In fact, one has to use Nitsche's trick [30], developed further by Stenberg [36], to handle this issue. As far as we know, there are two main strategies to overcome the bottleneck in deep learning framework:

- The first strategy is to construct neural network functions that satisfy the essential boundary conditions exactly. For instance, if the boundary condition is given by $u=g$ on the boundary Γ, then we construct the approximate function by

$$\phi(\boldsymbol{x};\boldsymbol{\theta})=\ell(\boldsymbol{x})\psi(\boldsymbol{x};\boldsymbol{\theta})+\bar{g}(\boldsymbol{x}), \tag{1.1}$$

  where $\ell(\boldsymbol{x})$ is a known function such that on Γ it holds $\ell(\boldsymbol{x})=0$, $\bar{g}$ is the extension of g to the whole domain, and $\psi(\boldsymbol{x};\boldsymbol{\theta})$ is another neural network function that is used to approximate the solution in the domain. The main limitation of this approach is that for problems with complex (non-regular) domains, it is in general not easy to find explicit functions ℓ and $\bar{g}$. For details, one can refer to [4] and references therein. It is worth mentioning that based on the formulation (1.1), one can also introduce an additional neural network function on the boundary Γ to approximate g by a least squares approach [34].

- Another strategy is the penalty method, where a penalty term (with a penalty parameter β) is included into the objective functional to enforce the boundary condition [16, 32, 35, 39]. This method is easy to implement. Theoretically, the penalty parameter β should be chosen large enough, however, this may make the optimization problem become ill-conditioned [31]. We also mention the deep Nitsche