INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 21, Number 5, Pages 697–715

© 2024 Institute for Scientific
Computing and Information
doi: 10.4208/ijnam2024-1028

DEEP SURROGATE MODEL FOR LEARNING GREEN'S FUNCTION ASSOCIATED WITH LINEAR REACTION-DIFFUSION OPERATOR

JUNQING JIA, LILI JU, AND XIAOPING ZHANG*

Abstract. In this paper, we present a deep surrogate model for learning the Green's function associated with the reaction-diffusion operator in rectangular domain. The U-Net architecture is utilized to effectively capture the mapping from source to solution of the target partial differential equations (PDEs). To enable efficient training of the model without relying on labeled data, we propose a novel loss function that draws inspiration from traditional numerical methods used for solving PDEs. Furthermore, a hard encoding mechanism is employed to ensure that the predicted Green's function is perfectly matched with the boundary conditions. Based on the learned Green's function from the trained deep surrogate model, a fast solver is developed to solve the corresponding PDEs with different sources and boundary conditions. Various numerical examples are also provided to demonstrate the effectiveness of the proposed model.

Key words. Reaction-diffusion operator, Green's function, surrogate model, deep learning, fast solver.

1. Introduction

With the rapid development and great success of deep learning technology in computer vision, natural language processing and other fields, it has also shown an increasing impact in the field of scientific computing, especially in the numerical solution of partial differential equations (PDEs) [1, 2, 3]. The use of neural networks to solve PDEs has been investigated in several early works, e.g., [4, 5], recent advances in deep learning techniques have further stimulated new explorations in this direction.

Representative methods of interest are the physics-informed neural network (PINN) [3], the deep Galerkin method (DGM) [6] and the deep Ritz method (DRM) [1]. All these methods model the mapping from space and/or time variables to the system states with a fully connected neural network. Their differences mainly lie in the construction of loss functions. The loss functions of PINN and DGM are expressed as a weighted sum of PDE residuals at randomly selected interior points as well as solution errors at initial/boundary points. This idea also has been extended to solve inverse problems [3], fractional differential equations [7], stochastic differential equations and uncertainty qualification [8, 9, 10] and other applications. DRM [1] designs loss function using the variational form of PDEs, requiring numerical integrations to train the network. Related works have subsequently emerged [11, 12, 13, 14]. Meanwhile, the solution of parameterized PDEs is also receiving increasing attention. For example, PINNs with special treatments are used to solve parameterized PDEs involving point sources in [15] and [16]; the meta-learning methods coupled with PINNs are developed to solve parameterized PDEs with different boundary conditions and domain shapes in [17] and [18].

Received by the editors on August 9, 2023 and, accepted on January 27, 2024.
2000 *Mathematics Subject Classification.* 34B27, 65N99.
*Corresponding author.

In theoretical research and engineering applications of various PDEs, including Poisson, Helmholtz and wave equations, the use of Green's function is significant. Having obtained the associated Green's function of the given differential operator, the Green's function method is used to precisely determine the solution of the corresponding PDE, which is explicitly expressed in an integral form, with the integral kernel based on the Green's function. Green's function is, in reality, a solution of the corresponding PDE with a point source subject to the homogeneous Dirichlet boundary condition. Such a problem can also be regarded as the solution of a parametrized PDE, where the location of the point source is the parameter.

However, the Green's function in a general domain typically lacks an analytic form. Therefore, we must approximate the Green's function numerically, which has led to increased attention on corresponding numerical methods in recent decades. Fortunately, the rapid development of deep learning techniques and their powerful expressive capability have introduced a potentially novel method for computing Green's function. Supervised learning methods, such as those proposed by [19] and [20], have been suggested to learn the Green's function. However, using these methods requires a considerable amount of labeled training data, which can be acquired by repeatedly solving PDEs through traditional numerical methods beforehand. The process of preparing training data consumes expensive computational resources. In addition, since these methods are purely data-driven, their generalization ability is usually restricted by the dataset coverage. In contrast, certain physics-driven models also have been proposed to compute Green's function, including GF-Net [21] and BI-GreenNet [22]. GF-Net [21] extends the PINN structure [3] to solve PDEs stipulated by Green's function. Moreover, these models utilize certain special techniques, such as the smoothness of the Dirac delta function and domain decomposition approach to optimize the network training process. BI-GreenNet [22] introduces a novel framework for computing Green's function, which leverages the fundamental solution, boundary integral method and neural networks to achieve high accuracy levels.

All of the above methods are solely based on neural networks. In the past decades, traditional numerical methods, such as finite difference, finite element and finite volume methods, have been extensively studied for solving PDEs, especially with point sources, to compute Green's function. A plausible approach is to develop a model to compute Green's function by leveraging the benefits of both traditional methods and neural networks. In this context, we propose to use the U-Net architecture to develop a deep surrogate model for learning the Green's function of the linear reaction-diffusion operator on a rectangular domain, and to design a novel loss function, inspired by traditional numerical methods, which helps train the deep surrogate model efficiently.

The remaining sections of the paper are organized as follows. In Section 1.1, we briefly introduce the problem setting, including the reaction-diffusion equation, its Green's function as well as the Green's representation formula. Section 2 presents and discusses the deep surrogate model for learning the Green's function of the linear reaction-diffusion operator on a rectangular domain. This section includes the network architecture, data generation, loss function and training strategy. In Section 3 we present a fast solver based on the proposed deep surrogate model to solve the corresponding PDEs. Extensive numerical experiments and comparisons are provided in Section 4 to demonstrate the outstanding performance of the proposed method, including some ablation studies and the application of the deep surrogate