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Uncertainty Quantification with Physics-Informed Generative Process Distributions for the Linear Diffusion Equation

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Abstract. We propose a novel diffusion-based generative model for solving linear stochastic diffusion equations, while enabling uncertainty quantification (UQ). By embedding the governing physical laws into the generative process, our approach establishes a mapping between control parameters and solutions across the latent space of the diffusion model. This ensures that the generated solutions satisfy the underlying physical constraints. Additionally, our method overcomes the limitation of conventional diffusion models, which struggle to generate accurate solutions for new control terms, and achieves superior accuracy compared to traditional data-driven operator learning techniques. Furthermore, by sampling different noise realizations and analyzing variations in the generated solutions, we efficiently capture solution diversity, enabling simultaneous prediction and comprehensive UQ. Experimental results demonstrate that our method outperforms deep operator networks and variational inference-based deep operator networks in both accuracy and confidence estimation.

AMS subject classifications: 68T07, 65C20

Key words: Diffusion model, uncertainty quantification, linear diffusion equation, physics-informed.

1. Introduction

The diffusion operator is used to model the transport and distribution of energy or pressure in the complex system. It has broad applications in chemistry, biology, and environmental science. In financial modeling, variants of the diffusion equation, such as the Fokker-Planck equation, are employed to characterize asset price dynamics [33,44].

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Solving the diffusion equation enables quantitative analysis of these diffusion processes, offering theoretical foundations for optimizing pollutant control, designing drug delivery systems, and predicting financial market behavior. In practical applications, the diffusion equation often involves dynamic and uncertain parameters. For example, in pollutant dispersion studies, the diffusion coefficient may depend on environmental temperature, pressure, and medium properties, and dynamically varies with these parameters [21]. Moreover, in the porous media or biological tissues, the inhomogeneity of microstructures and fluid-dynamic effects render experimental measurements of the diffusion coefficient highly challenging. These challenges not only complicate model validation but also introduce substantial uncertainty. Therefore, developing methods to solve diffusion equations containing uncertain terms while effectively quantifying the effects of these uncertainties is crucial for advancing numerical algorithms and enhancing practical applications in environmental management, biomedical engineering, and related fields.

In the last decades, various methods have been proposed to solve partial differential equations (PDEs) and analyze its uncertainties, including the orthogonal polynomial Galerkin projection method [22, 37], stochastic collocation methods [26, 38, 45], and polynomial chaos methods [23]. Due to the limitations of these approaches in high-dimensional problems, interpolation techniques such as least squares interpolation [4, 5] and radial basis function interpolation [15] have been developed. Although these methods offer high theoretical accuracy, their iterative processes often incur substantial computational costs, limiting their practical efficiency. To address these challenges, data-driven and learning-based solvers have emerged [14, 34, 36]. Bayesian physics-informed neural networks (BPINNs) [40], which integrate Bayesian NNs [18] with physics-informed NNs [27], incorporate physical constraints to enable both simulation and uncertainty quantification in physical systems [24, 25]. However, BPINNs face limitations in generalization. Alternative UQ methods for PDEs solvers include ensemble-based NNs [1, 11, 19, 30] and approaches relying on independently trained NNs within the evidential framework [31, 41]. While these methods enhance robustness under uncertainty, independently trained NNs may suffer from insufficient information sharing, and the evidential framework can introduce computational complexity and model instability. Compared to traditional methods, machine learning approaches offer significant advantages in UQ, including improved handling of complex scenarios, data-driven adaptability, and computational efficiency, particularly in high-dimensional settings [13, 20, 35, 42]. However, incorporating physical constraints often increases computational costs. Therefore, further advancements in UQ methods are necessary to enhance accuracy while reducing computational overhead [17].

Diffusion models are increasingly being employed as generative models for solving PDEs and performing UQ. With their probabilistic generative framework and high-resolution output capabilities, diffusion models naturally capture uncertainties in data distributions. Their application to PDEs solving and UQ has gained traction due to their ability to generate detailed and realistic solutions. However, traditional diffusion models are predominantly data-driven [12, 29] and lack explicit enforcement of physi-