Solving Time Dependent Fokker-Planck Equations via Temporal Normalizing Flow

Xiaodong Feng, Li Zeng* and Tao Zhou

LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, AMSS, Chinese Academy of Sciences, Beijing, China.

Received 22 March 2022; Accepted (in revised version) 6 May 2022

Abstract. In this work, we propose an adaptive learning approach based on temporal normalizing flows for solving time-dependent Fokker-Planck (TFP) equations. It is well known that solutions of such equations are probability density functions, and thus our approach relies on modelling the target solutions with the temporal normalizing flows. The temporal normalizing flow is then trained based on the TFP loss function, without requiring any labeled data. Being a machine learning scheme, the proposed approach is mesh-free and can be easily applied to high dimensional problems. We present a variety of test problems to show the effectiveness of the learning approach.

AMS subject classifications: 65M75, 65C30, 68T07
Key words: Temporal normalizing flow, Fokker-Planck equations, adaptive density approximation.

1 Introduction

The Fokker-Planck (FP) equations, which describe the time evolution of probability density functions (PDFs) of complex stochastic systems, have been widely used in different fields such as physical and biological modelling [1, 2]. Solving the FP equations numerically has been an important research topic in the past few decades. Generally, there are two main ways to obtain the PDFs of stochastic dynamics: solving the FP equations directly, or evaluating the transition probability density of the associated stochastic differential equations (SDEs). Traditional numerical methods for doing this include the finite element methods [32], the finite difference methods [19], the path integral methods [20], to name just a few. One of the biggest difficulties of these approaches is that either discretization of a high dimensional (unbounded) physical space is needed, or a large number of sample paths via Monte Carlo method [21] should be used.

*Corresponding author. Email addresses: xdfeng@lsec.cc.ac.cn (X. Feng), zengli@lsec.cc.ac.cn (L. Zeng), tzhou@lsec.cc.ac.cn (T. Zhou)
In recent years, machine learning techniques have been widely used to solve partial differential equations (PDEs), see e.g. [45–47] and references therein. Among others, we mention the deep Galerkin method [30], the deep Ritz method [31], and the so-called physics-informed neural networks (PINNs) [3]. These approaches have been widely applied to many realistic problems, such as fluid mechanics [33, 41], high dimensional PDEs (with applications in computational finance) [34, 35], uncertainty quantification [36, 37, 40, 42, 43], to name just a few. Meanwhile, generative models such as generative adversarial networks [10], variational autoencoder [11] and normalizing flow (NF) [12, 25], have also been successfully applied to learn forward and inverse PDEs [8, 22–24]. For instance, physics-informed generative adversarial model was proposed in [18] to tackle high dimensional stochastic differential equations. In [17], normalizing field flow was developed to build surrogate models for uncertainty quantification problems.

As the solution of the Fokker-Planck equation is a probability density function, solving this problem can also be considered as a density estimation problem. This motivates us to propose in this work an adaptive learning scheme based on the normalizing flow. More precisely, our approach relies on modelling the target solutions of the FP equations. Consequently, the temporal normalizing flow is trained based on the TFP loss function (the physics informed residual), without requiring any labeled data. We list in the following the main features and related works of our approach:

- Our approach is an extension of the previous interesting work [5] where only steady state FP equations are investigated. To address time dependent problems, we propose an adaptive density approximation scheme based on temporal normalizing flow.

- Being a machine learning scheme, the proposed approach is mesh-free and can be easily applied to high dimensional problems.

- Our approach is based on PDE-loss functions, and does not need sample paths generated from stochastic differential equations. This is different from previous works such as [4] where sample paths of the corresponding stochastic dynamics are used.

- We present a variety of test problems, including TFP equations with linear or nonlinear drift terms and high dimensional problems, to show the effectiveness of the learning approach.

The remainder of this paper is structured as follows. In Section 2, we provide with some preliminary results. Section 3 provides our adaptive density approximation scheme based on the temporal normalizing flow. In Section 4 we demonstrate the efficiency of our adaptive sampling approach with several numerical experiments. We then give some concluding remarks in Section 5.