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Solving Bivariate Kinetic Equations for Polymer Diffusion Using Deep Learning

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Abstract. In this paper, we derive a class of backward stochastic differential equations (BSDEs) for infinite-dimensionally coupled nonlinear parabolic partial differential equations, thereby extending the deep BSDE method. In addition, we introduce a class of polymer dynamics models that accompany polymerization and depolymerization reactions, and derive the corresponding Fokker-Planck equations and Feynman-Kac equations. Due to chemical reactions, the system exhibits a Brownian yet non-Gaussian phenomenon, and the resulting equations are infinitely dimensionally coupled. We solve these equations numerically through our new deep BSDE method, and also solve a class of high-dimensional nonlinear equations, which verifies the effectiveness and shows approximation accuracy of the algorithm.

Keywords:
BSDEs,
Deep BSDE method,
Polymer dynamics,
Brownian yet non-Gaussian.

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1 Introduction

In recent years, the diffusion phenomenon with non-Gaussian shape in complex systems has been gradually discovered experimentally, e.g. microbeads in lipid tubes [36], networks [37] or in a matrix of micropillars [4]. More examples include the movement of tracers in colloids, polymeric, and active suspensions [39], and the motion of individuals in heterogeneous populations such as nematodes [20]. This paper develops the deep BSDE method to model and simulate this kind of polymer dynamics.

More concretely, we focus on the diffusion behavior of a class of polymeric microparticles that accompany polymerization and depolymerization chemistry. It is shown that the polymerization and depolymerization of molecules is the natural basis of Brownian yet non-Gaussian diffusion of the center of mass (CM) [1]. The diffusivity D of the CM is affected by the molecular size N, and the molecular size is determined by the chemical reaction and changes randomly, so the diffusivity $D(N(t))$ becomes a stochastic process. Such random diffusivity leads to Brownian yet non-Gaussian diffusion. Further, reference [27] discusses the motion of a polymer in a chemostatted monomer bath while the monomer concentration in the bath changes. Reference [41] derives the Fokker-Planck equations for

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CM and the Feynman-Kac equations through subordination technique [3, 5, 13]. Since the size of the polymer particle is a discrete variable, the resulting equation is of bivariate form

$$\frac{\partial}{\partial t}u(n,x,t) = \mathcal{T}_n u(n,x,t) + \frac{1}{2}\mathrm{Tr}\big(\sigma\sigma^\top(n,x,t)(\mathrm{Hess}_x)u(n,x,t)\big) + \nabla_x u(n,x,t)\cdot\mu(n,x,t) + f\big(t,n,x,u(n,x,t),(\sigma^\top\nabla_x u)(n,x,t)\big) \tag{1.1}$$

with the initial condition $u(n,x,0) = g(n,x)$, here $\mathcal{T}_n$ is an operator with respect to the discrete variable n. If we consider n as a state parameter, then Eq. (1.1) can be seen as an infinite-dimensionally coupled system, the way of coupling depends on the operator $\mathcal{T}_n$.

With the growth of data resources and computing power, deep learning has been becoming an important methodology of our research. In recent years, a large number of deep learning-based partial differential equation (PDE) solvers have been developed, most of which are inspired by traditional methods. But unlike traditional methods, learning-based methods reduce the requirements for meshing and directly use neural networks as basis functions. These improvements allow us to avoid various complex problems encountered by traditional methods when solving PDEs. For example, the deep Ritz method [12] is a deep learning method based on the variational principle, which uses deep learning to solve the variational problem corresponding to PDEs. Least squares-based deep learning methods include deep Galerkin method [34] and physics-informed neural networks [32], which train models by minimizing the squared residuals of PDEs. Physics-informed neural networks also has a discrete-time version, which is based on the Runge-Kutta method. Weak adversarial networks [40] provide a method for solving the weak formulations of high-dimensional partial differential equations through adversarial learning. E *et al.* [11, 18] propose a deep learning method for solving parabolic PDEs based on BSDEs, called the deep BSDE method. References [15, 19] provide posterior estimates of the deep BSDE method.

The main contributions of this paper are as follows. Defining

$$\mathcal{T}_n f(n) = \begin{cases} \alpha(n)\big(f(n+1)-f(n)\big) + \beta(n)\big(f(n-1)-f(n)\big), & n \geq 1, \\ \alpha(0)\big(f(1)-f(0)\big), & n = 0, \end{cases} \tag{1.2}$$

where $\alpha(n)$ and $\beta(n)$ are known functions, we derive the BSDEs of Eq. (1.1) by constructing a stochastic process $X(t)$ coupled with the birth-death process $N(t)$ and extend the deep BSDE method (see Section 2). In addition, we present a class of applications of our new method in solving polymer dynamics problems. Specifically, we model a class of polymer particle diffusion dynamics accompanied by polymerization and depolymerization reactions, and derive the forward (backward) Fokker-Planck equations and the corresponding Feynman-Kac equations (see Section 3). To solve the Feynman-Kac equations, we extend the deep BSDE method to the space of frequency domain (see Section 4). On the aspect of the deep BSDE method, the main distinction of this work from [18] can be summarized as follows:

(i) The process considered in this paper is the coupling of the diffusion process with the jumping one, instead of the pure diffusion process.