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Analysis of the Closure Approximation for a Class of Stochastic Differential Equations

Yunfeng Cai[1], Tiejun Li[1,*], Jiushu Shao[2] and Zhiming Wang[1],

[1] *Laboratory of Mathematics and Applied Mathematics and School of Mathematical Sciences, Peking University, Beijing 100871, China*
[2] *College of Chemistry, Beijing Normal University, Beijing 100875, China*

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Dedicated to Professor Zhenhuan Teng on the occasion of his 80th birthday

Abstract. Motivated by the numerical study of spin-boson dynamics in quantum open systems, we present a convergence analysis of the closure approximation for a class of stochastic differential equations. We show that the naive Monte Carlo simulation of the system by direct temporal discretization is not feasible through variance analysis and numerical experiments. We also show that the Wiener chaos expansion exhibits very slow convergence and high computational cost. Though efficient and accurate, the rationale of the moment closure approach remains mysterious. We rigorously prove that the low moments in the moment closure approximation of the considered model are of exponential convergence to the exact result. It is further extended to more general nonlinear problems and applied to the original spin-boson model with similar structure.

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Key words: Moment closure, spin-boson dynamics, convergence analysis, banded structure.

1. Introduction

In various fields of applied mathematics, the stochastic ordinary differential equations (SODEs) and stochastic partial differential equations (SPDEs) are known to be an effective tool in modeling complicated systems. Examples include chemical reaction networks [11, 16, 19], stochastic hydrodynamics [7, 9, 18], non-equilibrium statistical mechanics [6, 8, 17], and spin-boson dynamics in quantum dissipative systems [15, 20, 24, 25], etc.. Many features of these systems, such as small scale effects and various uncertainties, can be well-described by suitable stochastic dynamics while deterministic modeling either fails or turns out to be too complex. In these systems,

*Corresponding author. *Email addresses:* `yfcai@math.pku.edu.cn` (Y. F. Cai), `wangzm@pku.edu.cn` (Z. M. Wang), `tieli@pku.edu.cn` (T. J. Li), `jiushu@bnu.edu.cn` (J. S. Shao)

the statistical quantities such as the mean, variance and high-order moments are of interest.

The Monte Carlo method with suitable temporal discretization is the most direct and popular method in solving these stochastic dynamical systems, but it may encounter great difficulty such as slow convergence and expensive computational cost. In order to achieve a reliable estimate of the interested statistical quantity, a lot of realizations have to be sampled due to the Monte Carlo half order convergence. This situation could be very severe when the interested random variable has extremely large variance. To overcome these difficulties, some approaches are taken to transform the original system into another deterministic system involving the quantities we are interested in. Some representative works include the polynomial chaos expansion or generalized polynomial chaos expansion (gPC), which utilizes the polynomial spectral representation of the random variables in the probability space [10, 13, 18, 22, 23], and different kinds of moment closure approach in diverse research fields, such as the hyperbolic moment method for the Boltzmann equation [4, 5], moment closure method in stochastic reaction network [12, 14], conditional moment closure method in the turbulent combustion problem [1], and flexible random-deterministic method in solving the spin-boson model [24, 25], etc.. These methods are effective for certain systems.

The moment closure methods share a similarity that the transformed system is described by an infinite number of differential equations. Truncation of the system is needed for numerical computations. Though efficient and accurate for many systems, the rationale of the moment closure approach remains mysterious for most problems. This can be exemplified by the following simple SODE

$$\mathrm{d}X_t = \mu X_t \mathrm{d}t + X_t(W_t + iV_t)\mathrm{d}t + X_t(\mathrm{d}W_t - i\mathrm{d}V_t), \quad X_0 = 1, \tag{1.1}$$

where W_t and V_t are independent standard Wiener processes with mean $\mathbb{E}W_t = 0$ and covariance $\mathbb{E}W_tW_s = t \wedge s$. If we define the generalised moments $x_n(t) = \mathbb{E}X_t(W_t + iV_t)^n$ and derive the relation among $x_n(t)$ according to Eq. (1.1), we get an infinite ODE system as

$$\frac{\mathrm{d}x_n(t)}{\mathrm{d}t} = \mu x_n(t) + 2nx_{n-1}(t) + x_{n+1}(t), \quad n \in \mathbb{N}, \tag{1.2}$$

by noting the important relation $(\mathrm{d}W_t \pm i\mathrm{d}V_t)^2 = 0$. We will also call (1.2) the moment equations of (1.1) although $x_n(t)$ are not the usual moments in probability theory. The final closure approximations share similar structures in different fields. To obtain an implementable scheme, we make truncation at $n = N$, and thus x_{N+1} in the last equation is abandoned. Theoretically, understanding the effectiveness of this moment closure approach is not clear. Note that x_{N+1} is *not* a small number in general, therefore we actually neglect at least an $\mathcal{O}(1)$ quantity in the Nth moment (for some cases, this may be even worse since x_{N+1} might be $\mathcal{O}(N)$ or bigger). This $\mathcal{O}(1)$ error will propagate to the lower moments and the overall solution might be polluted eventually. It is obvious that we can not hope to get the convergence of the high moments, but