STOCHASTIC RUNGE–KUTTA METHOD FOR STOCHASTIC DELAY DIFFERENTIAL EQUATIONS

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ABSTRACT

Random effect and time delay are inherent properties of many real phenomena around us, hence it is required to model the system via stochastic delay differential equations (SDDEs). However, the complexity arises due to the presence of both randomness and time delay. The analytical solution of SDDEs is hard to be found. In such a case, a numerical method provides a way to solve the problem. Nevertheless, due to the lacking of numerical methods available for solving SDDEs, a wide range of researchers among the mathematicians and scientists have not incorporated the important features of the real phenomena, which include randomness and time delay in modeling the system. Hence, this research aims to generalize the convergence proof of numerical methods for SDDEs when the drift and diffusion functions are Taylor expansion and to develop a stochastic Runge–Kutta for solving SDDEs. Motivated by the relative paucity of numerical methods accessible in simulating the strong solution of SDDEs, the numerical schemes developed in this research is hoped to bridge the gap between the evolution of numerical methods in ordinary differential equations (ODEs), delay differential equations (DDEs), stochastic differential equations (SDEs) and SDDEs. The extension of numerical methods of SDDEs is far from complete. Rate of convergence of recent numerical methods available in approximating the solution of SDDEs only reached the order of 1.0. One of the important factors of the rapid progression of the development of numerical methods for ODEs, DDEs and SDEs is the convergence proof of the approximation methods when the drift and diffusion coefficients are Taylor expansion that had been generalized. The convergence proof of numerical schemes for SDDEs has yet to be generalized. Hence, this research is carried out to solve this problem. Furthermore, the derivative-free method has not yet been established. Hence, development of a derivative–free method with 1.5 order of convergence, namely stochastic Runge–Kutta, to approximate the solution of SDDEs with a constant time lag, $r > 0$, is also included in this thesis.

ABSTRAK

Kesan rawak dan masa lengahan adalah ciri-ciri yang dipunyai oleh kebanyakan fenomena di sekeliling kita. Maka fenomena ini perlu dimodelkan menggunakan persamaan pembezaan stokastik lengahan (SDDEs). Walaubagaimanapun, kerawakan dan masa lengahan menyebabkan persamaan pembezaan bertambah rumit. Penyelesaian analitik SDDEs sukar untuk dicari. Bagi kes tersebut, kaedah berangka menyediakan cara untuk menyelesaikan masalah yang terlibat. Namun, disebabkan oleh kekurangan kaedah-kaedah berangka yang sedia ada untuk menyelesaikan SDDEs, ramai penyelidik dari kalangan ahli matematik dan saintis tidak memasukkan ciri-ciri penting fenomena nyata iaitu kesan rawak dan masa lengahan dalam memodelkan sistem tersebut. Maka, kajian ini bertujuan untuk mengitlakkan pembuktian penumpuan kaedah-kaedah berangka SDDEs apabila fungsi hanyutan dan resapan merupakan pengembangan Taylor dan membangunkan kaedah berangka stokastik Runge–Kutta untuk menyelesaikan SDDEs. Dimotivasikan oleh kekurangan relatif kaedah-kaedah berangka yang boleh diakses dalam simulasi penyelesaian kukuh SDDEs, skema-skema berangka yang dibangunkan diharap dapat merapatkan jurang di antara perkembangan kaedah-kaedah berangka persamaan pembezaan biasa (ODEs), persamaan pembezaan lengahan (DDEs), persamaan pembezaan stokastik (SDEs) dan SDDEs. Perkembangan kaedah-kaedah berangka SDDEs adalah jauh ketinggalan. Kadar penumpuan kaedah-kaedah berangka yang boleh didapati kini bagi menghampirkan penyelesaian SDDEs hanya mencapai peringkat 1.0. Salah satu daripada faktor-faktor penting perkembangan pesat pembangunan kaedah-kaedah berangka untuk ODEs, DDEs dan SDEs ialah pembuktian penumpuan kaedah-kaedah penghampiran apabila pekali-pekali hanyutan dan resapan merupakan kembangan Taylor yang telah diitlakkan. Pembuktian penumpuan kaedah-kaedah berangka SDDEs masih belum diitlakkan. Maka, kajian ini dijalankan untuk menyelesaikan masalah tersebut. Tambahan pula, kaedah bebas terbitan belum pernah dibangunkan. Maka, pembangunan kaedah bebas terbitan dengan kadar penumpuan 1.5, iaitu stokastik Runge–Kutta, untuk menghampirkan penyelesaian SDDEs dengan masa lengahan malar, $r > 0$, juga telah dimuatkan di dalam tesis ini.

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LIST OF SYMBOLS/ABBREVIATIONS/NOTATIONS

a.s.	–	Almost surely or with probability one
DDEs	–	Delay differential equations
EM	–	Euler–Maruyama
$\mathrm{E}(X)$	–	Expected value of X
f_α	–	Partial derivative with respect to α
f'	–	First derivative
f''	–	Second derivative
$f^{(k)}$	–	k–th derivative
MS	–	Mean–square
ODEs	–	Ordinary differential equations
r	–	Time delay
RK	–	Runge–Kutta
RMSE	–	Root mean square error
t	–	Time
T	–	Terminal time
SDEs	–	Stochastic differential equations
SDDEs	–	Stochastic delay differential equations
SRK	–	Stochastic Runge–Kutta
SRK2	–	2–stage stochastic Runge–Kutta
SRK4	–	4–stage stochastic Runge–Kutta
$\mathrm{Var}(X)$	–	Variance of X
$W(t)$	–	Wiener process

X	–	Random variable or stochastic process
x_{max}	–	Maximum cell concentration
YE1	–	Control medium
YE2	–	Medium of yeast and NH_4Cl
YE	–	Medium of yeast and NH_4NO_3
$\mathcal{B}$	–	*Borel* sets
$\Im$	–	Complex number
$\mathcal{F}$	–	σ–field or σ–algebra
$\mathcal{R}$	–	Remainder
$\Re$	–	Real number
Δ	–	Step size
μ_{max}	–	Maximum specific growth rate
$\emptyset$	–	Empty set
Ω	–	Sample space
σ	–	Diffusion coefficient
$\sigma(\mathcal{C})$	–	the σ–algebra generated by $\mathcal{C}$
$\subseteq$	–	Subset or is included in
$\subset$	–	Subset
$\in$	–	Element
$\cap$	–	Intersection
$\cup$	–	Union
$(\cdot)^T$	–	Transpose
$\int \circ dW(t)$	–	Stratonovich integral

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CHAPTER 1

INTRODUCTION

1.1 Background

Modeling of physical phenomena and biological system via ordinary differential equations (ODEs) and stochastic differential equations (SDEs) had been intensively researched over the last few decades. In both types of equations, the unknown functions and their derivatives are evaluated at the same instant time, t. However, many of the natural phenomena do not have an immediate effect from the moment of their occurrence. The growth of a microbe, for example, is non–instantaneous but responds only after some time lag $r > 0$. Generally, many systems in almost any area of science, for which the principle of causality, i.e. the future state of the system is independent of the past states and is determined solely by the present, does not apply. A crucial point with delay equations is the dynamics of the systems differ dramatically if the corresponding characteristic equations involve time delay. Therefore, ODEs and SDEs which are simply depending on the present state will be better of should the model incorporate time delay. Such phenomenon can then be modeled via delay differential equations (DDEs) for deterministic setting and stochastic delay differential equations (SDDEs) for their stochastic counterpart. However, DDEs are inadequate to model the process with the presence of random effects. Thus, the dynamical systems whose evolution in time is governed by uncontrolled fluctuations as well as the unknown function is depending on its history can be modeled via SDDEs.

Most of the SDDEs do not have an explicit solution. Hence, there is a need for the development of reliable and efficient numerical integrators for such problems. The research on numerical methods for SDDEs is still new. Among the recent works are of Baker [1], Baker and Buckwar [2], Buckwar [3], Küchler and Platen [4], Hu *et al.* [5], Hofmann and Muller [6] and Kloeden and Shardlow [7]. Euler scheme for SDDEs was introduced by Baker [1] and Baker and Buckwar [2]. The derivation of numerical solutions for SDDEs from stochastic Taylor expansions with time delay showed a strong order of convergence of 1.0 was studied by Küchler and Platen [4]. Hu *et al.* [5] introduced Itô formula for tame function in order to derive the same order of convergence but with a different scheme. They provide the convergence proof of Milstein scheme to the solution of SDDEs with the presence of anticipative integrals in the remainder term. Moreover, Hofmann and Muller [6] presented an approximation of double stochastic integral involving time delay and introduce the modification of Milstein scheme. The convergence proof of Euler–Maruyama method for SDDEs was provided in Baker [1]. Baker and Buckwar [2] and Buckwar [3] provided the convergence proof of discrete time approximations of SDDEs in a general way. Meanwhile, Hu *et al.* [5] and Kloeden and Shardlow [7] prepared the proof of the order of convergence for Milstein scheme. Later work on numerical method for SDDEs can be found in Kloeden and Shardlow [7]. They improved the convergence proof of Milstein scheme presented in [5] by avoiding the used of anticipative calculus and anticipative integrals in the remainder term. Hence, the convergence proof of Milstein scheme in [7] is much simpler than the convergence proof expounded in [5]. The proof of the order of convergence of Taylor methods of SDEs had been generalized by Milstein [8]. Theorem 1.1 on page 12 in the book of Milstein [8] showed this result, which underlying the significant development of numerical methods from stochastic Taylor expansion that occurred in the SDEs. However, the proof is not yet generalized in SDDEs. It is quite natural now to ask, can the convergence proof of numerical methods for SDDEs when the drift function, f and diffusion function, g are Taylor expansion be generalized?

Stochastic delay differential equation is a stochastic generalization of DDEs, which is systematically treated in Mohammed [9]. In fact, SDDEs generalize both DDEs and SDEs. Therefore, numerical analysis of DDEs and SDEs provide some bearing on the problems regarding the SDDEs which is of concern here. The derivation of numerical methods for solving SDDEs found in the literature up to the date are based on stochastic Taylor expansion. As the order increases, the complexity of implementing those numerical methods can become more complicated as one needs to compute more partial derivatives of the drift and diffusion functions. To overcome the above-mentioned difficulty, it is natural to look for a derivative-free method for solving the problem at hand. Among the references therein, we realize that there is no derivative-free method such as stochastic Runge–Kutta (SRK) to facilitate the approximation of the strong solution to SDDEs. Moreover, the approximation schemes to the solution for SDDEs in the literature up to the date do not achieve the order of convergence higher than 1.0. Conversely, evolutionary works on the numerical method in SDEs are much more advance. Until now, most researchers have ignored both delay and stochastic effects because of the difficulty in approximation of the solution due to the involvement of multiple stochastic integrals with time delay. However, both of them cannot be neglected as many natural phenomena involve random disturbances as well as non–instantaneous effects. It is now natural to ask the question, is it possible for us to extend the pioneering work of Runge–Kutta (RK) over the last few decades to approximate the solution of SDDEs.

Thus, this research proposes to generalize the convergence proof of numerical methods of SDDEs when the drift and diffusion functions are Taylor approximation as well as to develop SRK for SDDEs. SRK method is a derivative-free method, hence it does not require the computation of derivative for drift and diffusion functions. The method proposed in this research having the order of convergence of 1.5, improves the convergence rate of numerical approximation of SDDEs arising from the literature so far. Moreover, both time delay and stochastic extensions of a mathematical model for bio–process engineering is considered. In this research, the system of batch fermentation involving the growth of the microbe and solvent production of acetone and butanol is highlighted. The simulated result of the mathematical model is approximated using the newly developed SRK method of order 1.5.

1.2 Problem Statement

As mentioned earlier in the previous section, most of the SDDEs do not have analytical solution, and numerical method provides a tool in handling this problem. Baker *et al.* [10] modified RK of ODE to approximate DDE. It was emphasized by Bellen and Zennaro [11] that the main difficulty arising from the numerical integration of DDEs is the discontinuity. Obviously, the discontinuity may occur in DDEs because of the initial function, $\Phi(t)$ specified on the entire interval $[t_0 - r, t_0]$, instead of the use of initial values problem in ODEs. The term t_0 corresponds to the starting time of the process. In fact, Baker *et al.* [10] had verified that Runge–Kutta methods are natural candidates for solving DDEs because they can be easily modified to handle discontinuities. On the other hand, SDE was taken care by the SRK. It is a derivative-free method with the order of convergence of at least 2.0 for SDEs with additive noise and 1.5 if the corresponding SDEs is multiplicative. Further advantages of implementing the RK methods for ODEs and DDEs and the SRK methods for SDEs, are they are stable and easy to adapt for variable step–size. The investigation of stability and variable step–size adaptation of RK (for ODEs and DDEs) and SRK (for SDEs) methods was prepared by Butcher [12] and Hairer *et al.* [13] for ODEs, Baker *et al.* [10] and Bellen and Zennaro [11] for DDEs and Rumelin [14], Burrage and Burrage [15] and Burrage [16] for SDEs.

RK and SRK methods of ODEs and SDEs respectively have difficulties in achieving high accuracy at reasonable cost. To overcome the disadvantage of the methods in maintaining a particular order, Butcher [12] developed rooted–trees theory so that these order conditions of RK methods can be expressed using trees. Then, Burrage [16] extending the Butcher's rooted–trees theory to the area of stochastic. This theory allowed us to compute the order of RK and SRK methods for ODEs and SDEs respectively in an easy way. The suitability and efficiency of employing RK in DDE and SRK in SDE motivate us to explore the applicability of this method in approximating the solution of SDDE. To the best of our knowledge, the literature on SRK for SDDE has not been found. The exploration of numerical approximation to the strong solution of SDDEs is just relied on the truncating of stochastic Taylor expansions, up to 1.0 order of accuracy. Accordingly, the Euler–Maruyama and Milstein schemes had been proposed to apply them in practice or to study their properties. Indeed, the implementation of Taylor method in differential equations leads to complexity, as it requires the computation of the derivative in drift and diffusion functions should a high-order method is needed. Since no effort has been made to derive the derivative-free method with the convergence rate greater than 1.0 and specifically stochastic Runge–Kutta with time delay, we propose to derive SRK for SDDE in this research as well as to approximate the strong solution of SDDE via this method. Obviously, when constructing a numerical method of differential equations, the rate of convergence between the true and numerical solutions is one of the important features to be considered. The key to the rapid progress of numerical methods in handling SDEs is the convergence proof of the corresponding methods when the drift and diffusion coefficients are Taylor expansion had been generalized. It was Milstein [8] who proved in a more general way of numerical methods of SDEs when the drift and diffusion functions are Taylor expansion. However, the later is not yet discovered in SDDEs, hence it is the aim of this research to provide the convergence proof of Taylor methods of SDDEs in a more general way. Therefore, the main research questions are set up as;

(i) Will the convergence proof of numerical methods of SDDEs when the drift and diffusion coefficients are Taylor approximations be generalized?

(ii) What is the SRK scheme for SDDEs?

(iii) Will the general 4–stage stochastic Runge–Kutta (SRK4) for SDDE be a more efficient tool in approximating the solution of SDDE?

Problem (i) is covered in Chapter 4, whereas Chapter 6 provides the answer to problem (ii) and problem (iii).

1.3 Research Objectives

Based on the research questions in Section 1.2, this study embarks on the following objectives:

(i) To derive a stochastic Taylor expansion of SDDE. It is a key feature to the development of higher–order methods for solving SDDE numerically.

(ii) To generalize a convergence proof of numerical methods for SDDEs when the drift and diffusion coefficients are Taylor approximations.

(iii) To develop a Stochastic Runge–Kutta of order 1.5 for SDDE by modifying SRK for SDE and RK for DDE.

(iv) To analyze the stability of SRK for SDDE.

(v) To apply the SRK method of 1.5 in simulating the strong solution of SDDE for batch fermentation process.

1.4 Scope of the Study

This study was undertaken to generalize the convergence proof of numerical methods for SDDEs when the drift and diffusion are Taylor expansion as well as to propose a derivative–free method, i.e. SRK up to order of 1.5 for solving SDDEs. To achieve this goal, the following scopes will be covered;

(i) The derivation of Stratonovich Taylor series expansion for both actual and numerical solutions.

(ii) The convergence proof of numerical methods from Taylor expansion has been generalized. The Euler–Maruyama, Milstein scheme and Taylor method having the order of convergence of 0.5, 1.0 and 1.5 respectively have been proposed.

(iii) The derivation of SRK4 for solving SDDEs with 1.5 order of convergence.

(iv) Stability analysis of Euler–Maruyama (EM), Milstein scheme and 4–stage SRK (SRK4) for solving SDDEs are measured via MS–stability. The algebraic computation is performed using Maple 15.

(v) Model the two phases of fermentation namely the growth phase of C. *acetobutylicum* P262 and the production of Acetone and Butanol via SDDEs. The strong solution of the corresponding mathematical model is simulated via newly developed SRK4.

1.5 Significance of the Findings

The influence of noise and delay in many fields of applications such as engineering, physics and biology contributes to an accelerating interest in the development of stochastic models with time delay. As a result, numerical methods for solving SDDEs are required, and work in this area is far less advanced. The recent work of numerical methods for SDDEs were based on the truncating of stochastic Taylor expansions. Moreover, the stochastic Taylor expansion as expounded in the literature currently is derived to develop the approximation method up to 1.0 order of convergence. In order to achieve high order of convergence, it is necessary to derive stochastic Taylor expansion of high order. The convergence proof of numerical methods of SDDEs when the drift and diffusion functions are Taylor expansion has been generalized in this research. Currently, there is no derivative–free method to approximate the strong solution of SDDEs and this research is aimed to develop SRK4 of order 1.5. By the end of this research, it is hoped that the newly developed SRK methods of SDDEs will benefit the mathematicians and scientists by providing the derivative–free tool for solving SDDEs in various fields. It can also be shown in this research, the SRK methods are easy to implement compare to the approximation methods obtained from the truncating stochastic Taylor expansion. In this way the computation of high–order partial derivatives can be avoided. Moreover, the generalization of convergence proof when the drift and diffusion functions are Taylor expansion is hoped can facilitate mathematicians to explore this area more widely.

1.6 Thesis Organization

A brief description of the chapters contained in the thesis is now presented.

Chapter 1: This chapter provides an introduction to the whole thesis. It introduces the concept of stochastic differential equations and stochastic delay differential equations. It also presents some numerical methods used to simulate the mathematical models of SDEs and SDDEs.

Chapter 2: Contains the review of literature for numerical methods in SDEs, DDEs and SDDEs.

Chapter 3: This chapter contains various theories and results from probability theory as well as stochastic calculus that are required in later chapters.

Chapter 4: In this chapter, the stochastic Taylor expansion for autonomous SDDEs with a constant time lag is derived. The derivation of three numerical schemes up to order 1.5 are presented and the convergence proof stated our fundamental result. Numerical examples are performed to assure the validity of the numerical methods.

Chapter 5: This chapter consists of our main result. A new class of SRK for solving SDDEs is formulated. The local truncation error and stability analysis for SRK are presented. Numerical algorithm is developed to perform a numerical example so that the efficiency of the newly develop numerical schemes of SRK4 can be assured.

Chapter 6: It is well–known that many of the natural systems in biology have the property of an after–effects and subject to the stochasticity. Thus, this chapter discusses the possibility of modeling a real phenomenon in batch fermentation via SDDEs. With no doubt that the exact solutions of these models are hard to be found, hence the newly developed SRK4 is used to simulate the approximation solutions of SDDEs.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

The purpose of this chapter is to survey the recent works of numerical methods for SDEs, DDEs and SDDEs. The survey is divided into three sections by focusing on those kinds of differential equations and numerical methods used to approximate them.

2.2 Stochastic Differential Equations, SDEs

SDEs arise when the random effect is incorporated into their deterministic counterpart. The necessity of this inclusion is due to the fact that almost every natural phenomenon in this world is influenced by environmental noise. Indeed, it is an inherent property of many physical systems in biology, epidemiology, finance and chemical reactions. In the last few years, there has been an accelerating interest in the study of SDEs. The inclusion of the noise term in differential equations may lead to a fundamentally different methods of analysis. Certainly, a reasonable mathematical interpretation of the noise term is a white noise, $W(t)$ i.e. frequently known as Wiener process. In SDEs, it is formally interpreted as a derivative of a Wiener process, $\dot{W}(t)$. This process possess the property of nowhere differentiable and unbounded variation, hence its integral cannot be defined in an ordinary way. In such a case, it is necessary to study the stochastic nature of the Wiener process, which then laid to a very important fundamental theory in stochastic area, i.e. Itô stochastic integral. Let consider the following SDE

$$dx = ax(t)dt + bdW(t) \tag{2.1}$$

where a and b are constants and process $W(t)$ is interpreted as an irregular stochastic process such as white noise. It is a Gaussian process which shall be treated in details in the next chapter. The white noise is closely linked to the theory of Markov processes, hence it provides a convenient tool for the investigation of such systems. For further details, we refer readers to a book by Has'minskii [17]. In integral form, Eq. (2.1) is written as

$$x(t) = x(t_0) + \int_{t_0}^{t} ax(s)ds + b\int_{t_0}^{t} dW(s) \tag{2.2}$$

where the second integral cannot be interpreted as a Riemann–Stieltjes integral. Conversely, the integral with respect to Wiener process can be interpreted either as Itô stochastic integral or Stratonovich integral.

As mentioned–above, the white noise process $W(t)$ is nowhere differentiable and it is not bounded variation on any bounded interval. Moreover, the consequences of unbounded variation property make this integral cannot even be interpreted as the Riemann–Stieltjes integral for each sample path. Obviously, a significant different between Itô and Riemann–Stieltjes integral is the corresponding integrand is evaluated at the left end point of the interval $t \in [t_{i-1}, t_i]$. However, Stratonovich integral follows the same rule with Riemann–Stieltjes integral as it is obtained as the mean–square limit of the Riemann–Stieltjes sums, that is evaluated at the middle points of the intervals $t \in [t_{i-1}, t_i]$. Evidently, deterministic calculus is much more robust to approximation than stochastic calculus because the integrand function in Riemann integral can be evaluated at an arbitrary point of the discretization sub–interval. Meanwhile, the integrand of stochastic integral needs to be evaluated at a specific point in the sub–interval, Kloeden and Platen [18].