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Performance of stochastic Runge-Kutta Methods in approximating the solution of stochastic model in biological system

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Abstract. Recently, modelling the biological systems by using stochastic differential equations (SDEs) are becoming an interest among researchers. In SDEs the random fluctuations are taking into account, which resulting to the complexity of finding the exact solution of SDEs and contribute to the increasing number of research focusing in finding the best numerical approach to solve the systems of SDEs. This paper will examine the performance of 4-stage stochastic Runge-Kutta (SRK4) and specific stochastic Runge-Kutta (SRKS) methods with order 1.5 in approximating the solution of stochastic model in biological system. A comparative study of SRK4 and SRKS method will be presented in this paper. The non-linear biological model will be used to examine the performance of both methods and the result of numerical experiment will be discussed.

1. Introduction

Mathematical models have been widely used to describe the important characteristics of the physical and biological systems. Mathematical model is the simplified mathematical representation of a complex reality. All this while, ordinary differential equations (ODEs) is the most frequently used model to explain the behaviour of the physical and biological systems. However, ODEs cannot represent the behaviour of the systems whose subject to the environmental noise. In such case, stochastic differential equations (SDEs) is the most suitable model to describe the system incorporated with the environmental noise and disturbances.

Ito in 1951 doing a pioneering work in SDEs field by formulating SDEs as a differential equations of ODEs for the deterministic part and incorporated the Wiener process for the stochastic part [2]. Wiener process is a continuous time stochastic process named in honor of Robert Wiener. This process often called Brownian motion due to its connection with the physical process of Brownian movement. Brownian motion is perturbed into ODEs which then yield the SDEs. This motion will represents noise of the corresponding system. The fact that SDEs have been perturbed randomly by unpredictable movement of noise then contributes to the difficulty in finding the analytical solutions for SDEs. The presence of stochastic part in SDEs contribute to the complexity of finding the analytical solution of stochastic model. Therefore, most of the researchers are now focusing on the development of an efficient numerical integrator



for SDEs. In 1950, Maruyama introduces the most simplest numerical scheme of SDEs called Euler-Maruyama method. This method is developed by truncating the stochastic Taylor series expansion at second terms and it has 0.5 order of convergence [2]. Then, [10] increased the efficiency of the method by proposing a Milstein scheme with 1.0 order of convergence. The later method also being developed from the stochastic Taylor series expansion.

As in ODE, Runge-Kutta method becoming an efficient method for solving ODEs, Burrage in 1999 develop a new class of stochastic Runge-Kutta method for SDEs by applying rooted-tree theory [1]. In [5], SRK4 method with strong order 1.5 have been developed. As order of accuracy increase, the complexity to derive SRK method as well increase. This is due to the increasing number of equations to be solved in order to perform the order condition analysis. Subsequently, [7] proposed the improvement of SRK method known as specific SRK method (SRKS) with different internal stages. By applying the independent internal stages to the SRK method, the complexity of higher order SRK method for SDEs can be minimized and will reduce the computation time. Heretofore, number of researchers who discussing on numerical methods for SDEs increasing rapidly and can be seen in [3],[4],[5],[6],[7] and [8].

This paper will examine the performance of SRK4 and SRKS in approximating the solution of stochastic model in biological system. This paper is organized as follows: the next section will present the SRK4 and SRKS methods that will be used in this study. Next, the stochastic model in biological system shall be considered. Numerical experiment is then performed in Section 4. Section 5 devotes to the result discussion and concluding remarks.

2. Stochastic Runge-Kutta(SRK) methods for Stochastic Differential Equations(SDEs)

2.1. 4-stage Stochastic Runge-Kutta with high strong order 1.5

According to [4], the general form of SRK4 method can be written as

$$\begin{aligned}
 Y_i(t) &= Y_n(t_0) + \Delta \sum_{j=1}^{i-1} a_{ij} f(y_j(t)) + \sum_{j=1}^{i-1} (b_{ij}^{(1)} J_1 + b_{ij}^{(2)} \frac{J_{10}}{h}) g(y_j(t)) \\
 y_{n+1}(t) &= y_n + \Delta \sum_{j=1}^s \alpha_j f(y_j(t)) + \sum_{j=1}^s (\gamma_j^{(1)} J_1 + \gamma_j^{(2)} \frac{J_{10}}{h}) g(y_j(t))
 \end{aligned} \tag{1}$$

for $i = 1, \dots, s$ represent the stage of SRK method. SRK4 method with 1.5 order of convergence was developed based on the formulation (1) by [2] and the scheme is given by

$$\begin{aligned}
 y_{n+1}(t) &= y_n(t_0) + \Delta \alpha_1 f(Y_1) + \Delta \alpha_2 f(Y_2) + \Delta \alpha_3 f(Y_3) + \Delta \alpha_4 f(Y_4) \\
 &+ (\gamma_1^{(1)} J_1 + \gamma_1^{(2)} \frac{J_{10}}{\Delta}) g(Y_1) + (\gamma_2^{(1)} J_1 + \gamma_2^{(2)} \frac{J_{10}}{\Delta}) g(Y_2) \\
 &+ (\gamma_3^{(1)} J_1 + \gamma_3^{(2)} \frac{J_{10}}{\Delta}) g(Y_3) + (\gamma_4^{(1)} J_1 + \gamma_4^{(2)} \frac{J_{10}}{\Delta}) g(Y_4)
 \end{aligned} \tag{2}$$

where

$$\begin{aligned}
 Y_1 &= Y_0^{(n)} \\
 Y_2 &= Y_0^{(n)} + \Delta a_{21} f(Y_0^{(n)}) + \left(b_{21}^{(1)} J_1 + b_{21}^{(2)} \frac{J_{10}}{\Delta} \right) g(Y_0^{(n)}) \\
 Y_3 &= Y_0^{(n)} + \Delta a_{31} f(Y_1^{(n)}) + \Delta a_{32} f(Y_2^{(n)}) \\
 &\quad + \left(b_{31}^{(1)} J_1 + b_{31}^{(2)} \frac{J_{10}}{\Delta} \right) g(Y_1^{(n)}) + \left(b_{32}^{(1)} J_1 + b_{32}^{(2)} \frac{J_{10}}{\Delta} \right) g(Y_2^{(n)}) \\
 Y_4 &= Y_0^{(n)} + \Delta a_{41} f(Y_1^{(n)}) + \Delta a_{42} f(Y_2^{(n)}) + \Delta a_{43} f(Y_3^{(n)}) \\
 &\quad + \left(b_{41}^{(1)} J_1 + b_{41}^{(2)} \frac{J_{10}}{\Delta} \right) g(Y_1^{(n)}) + \left(b_{42}^{(1)} J_1 + b_{42}^{(2)} \frac{J_{10}}{\Delta} \right) g(Y_2^{(n)}) \\
 &\quad + \left(b_{43}^{(1)} J_1 + b_{43}^{(2)} \frac{J_{10}}{\Delta} \right) g(Y_3^{(n)})
 \end{aligned}$$

The numerical scheme of SRK4 method can be written in Butcher's tableau as below

$$\begin{array}{c|ccc}
 A & \frac{1}{2} & & \\
 & 0 & \frac{1}{2} & \\
 & 0 & 0 & 1 \\
 \hline
 \alpha & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
 \end{array}
 \quad
 \begin{array}{c|ccc}
 B^{(1)} & \frac{1}{2} & & \\
 & 0 & \frac{1}{2} & \\
 & 0 & 0 & 1 \\
 \hline
 \gamma^{(1)} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
 \end{array}
 \quad
 \begin{array}{c|ccc}
 B^{(2)} & \frac{1}{2} & & \\
 & 0 & \frac{1}{2} & \\
 & 0 & 0 & 1 \\
 \hline
 \gamma^{(2)} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
 \end{array}$$

2.2. Specific Explicit Stochastic Runge-Kutta method with order 1.5(SRKST2)

SRK method (1) suffer from the complexity of constructing the order conditions due to the large numbers of equations to be solved. Aiguo & Xia [7] overcome that difficulty by introducing a new explicit of SRK method with several groups of independent internal stages. The new specific SRK schemes with 1.5 order of convergence (SRKS 1.5) has been presented. The general form of independent s -stage specific SRK method is given by

$$\begin{aligned}
 Y_{i_0}^0(t) &= Y_n(t_0) + \Delta \sum_{j=1}^{s_0} a_{i_0 j}^{(0)} f(y_j^{(0)}(t)) + J_1 \sum_{j=1}^{s_0} b_{i_0 j}^{(0)} g(y_j^{(0)}(t)) \quad i_0 = 1, 2, \dots, s_0 \\
 Y_{i_1}^1(t) &= Y_n(t_0) + \Delta \sum_{j=1}^{s_1} a_{i_1 j}^{(1)} f(y_j^{(1)}(t)) + \frac{J_{10}}{\Delta} \sum_{j=1}^{s_1} b_{i_1 j}^{(1)} g(y_j^{(1)}(t)) \quad i_1 = 1, 2, \dots, s_1 \\
 y_{n+1}(t) &= y_n + \Delta \sum_{i_0=1}^{s_0} \alpha_{i_0}^{(0)} f(y_{i_0}^{(0)}(t)) + J_1 \sum_{i_0=1}^{s_0} \gamma_{i_0}^{(0)} g(y_{i_0}^{(0)}(t)) \\
 &\quad + \Delta \sum_{i_1=1}^{s_1} \alpha_{i_1}^{(1)} f(y_{i_1}^{(1)}(t)) + \frac{J_{10}}{\Delta} \sum_{i_1=1}^{s_1} \gamma_{i_1}^{(1)} g(y_{i_1}^{(1)}(t))
 \end{aligned} \tag{3}$$

Note that s_0 and s_1 represent the different internal stages of SRKS method. It was introduced for the purpose of reducing the number of equations to be solved. SRKS 1.5 method was developed by letting $s_0 = 4$ and $s_1 = 3$. This yield

$$\begin{aligned}
 y_{n+1}(t) = & y_n + \Delta(\alpha_1^{(0)} f(y_1^{(0)}(t)) + \alpha_2^{(0)} f(y_2^{(0)}(t)) + \alpha_3^{(0)} f(y_3^{(0)}(t)) + \alpha_4^{(0)} f(y_4^{(0)}(t))) \\
 & + J_1(\gamma_1^{(0)} g(y_1^{(0)}(t)) + \gamma_2^{(0)} g(y_2^{(0)}(t)) + \gamma_3^{(0)} g(y_3^{(0)}(t)) + \gamma_4^{(0)} g(y_4^{(0)}(t))) \\
 & + \Delta(\alpha_1^{(1)} f(y_1^{(1)}(t)) + \alpha_2^{(1)} f(y_2^{(1)}(t)) + \alpha_3^{(1)} f(y_3^{(1)}(t))) \\
 & + \frac{J_{10}}{\Delta}(\gamma_1^{(1)} g(y_1^{(1)}(t)) + \gamma_2^{(1)} g(y_2^{(1)}(t)) + \gamma_3^{(1)} g(y_3^{(1)}(t)))
 \end{aligned} \tag{4}$$

with

$$\begin{aligned}
 Y_1^0(t) &= Y_n(t_0) \\
 Y_2^0(t) &= Y_n(t_0) + \Delta a_{21}^{(0)} f(y_1^{(0)}(t)) + J_1 b_{21}^{(0)} g(y_1^{(0)}(t)) \\
 Y_3^0(t) &= Y_n(t_0) + \Delta(a_{31}^{(0)} f(y_1^{(0)}(t)) + a_{32}^{(0)} f(y_2^{(0)}(t))) + J_1(b_{31}^{(0)} g(y_1^{(0)}(t)) + b_{32}^{(0)} g(y_2^{(0)}(t))) \\
 Y_4^0(t) &= Y_n(t_0) + \Delta(a_{41}^{(0)} f(y_1^{(0)}(t)) + a_{42}^{(0)} f(y_2^{(0)}(t)) + a_{43}^{(0)} f(y_3^{(0)}(t))) \\
 & \quad + J_1(b_{41}^{(0)} g(y_1^{(0)}(t)) + b_{42}^{(0)} g(y_2^{(0)}(t)) + b_{43}^{(0)} g(y_3^{(0)}(t))) \\
 Y_1^1(t) &= Y_n(t_1) \\
 Y_2^1(t) &= Y_n(t_1) + \Delta a_{21}^{(1)} f(y_1^{(1)}(t)) + J_1 b_{21}^{(1)} g(y_1^{(1)}(t)) \\
 Y_3^1(t) &= Y_n(t_1) + \Delta(a_{31}^{(1)} f(y_1^{(1)}(t)) + a_{32}^{(1)} f(y_2^{(1)}(t))) + J_1(b_{31}^{(1)} g(y_1^{(1)}(t)) + b_{32}^{(1)} g(y_2^{(1)}(t)))
 \end{aligned}$$

SRKS 1.5 can be presented in tableau form as follow

$$\begin{array}{c|ccc}
 A^{(0)} & \frac{1}{2} & & \\
 & 1 & 0 & \\
 & 3 & 0 & 0 \\
 \hline
 \alpha^{(0)} & -1 & -1 & 0 & 0
 \end{array}
 \quad
 \begin{array}{c|ccc}
 B^{(0)} & \frac{1}{2} & & \\
 & 0 & \frac{1}{2} & \\
 & 0 & 0 & 1 \\
 \hline
 \gamma^{(0)} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
 \end{array}
 \quad
 \begin{array}{c|ccc}
 A^{(1)} & 0 & & \\
 & 1 & 0 & \\
 & -\frac{2}{3} & \frac{2}{3} & 0 \\
 \hline
 \alpha^{(1)} & & & &
 \end{array}
 \quad
 \begin{array}{c|ccc}
 B^{(1)} & \frac{3}{2} & & \\
 & \frac{3}{2} & 0 & \\
 & 0 & 1 & -1 \\
 \hline
 \gamma^{(1)} & & & &
 \end{array}$$

Moreover a general form of SRKS for the SDEs whose drift and diffusion terms are commutative, SRKST2 can be written as

$$\begin{aligned}
 Y_i(t) &= Y_n(t_0) + \Delta \sum_{j=1}^s a_{ij} f(y_j(t)) + J_1 \sum_{j=1}^{i-1} b_{ij} g(y_j(t)) \\
 y_{n+1}(t) &= y_n + \Delta \sum_{j=1}^s \alpha_j f(y_j(t)) + J_1 \sum_{j=1}^s \gamma_j^{(1)} g(y_j(t))
 \end{aligned} \tag{5}$$

for $j = 1, \dots, s$, where s is the stage of SRK method. SRKST2 method can be developed based on (5) and the method is written as

$$\begin{aligned}
 y_{n+1}(t) = & y_n + \Delta(\alpha_1 f(Y_1) + \alpha_2 f(Y_2) + \alpha_3 f(Y_3) + \alpha_4 f(Y_4) + \alpha_5 f(Y_5)) \\
 & + J_1(\gamma_1 g(Y_1) + \gamma_2 g(Y_2) + \gamma_3 g(Y_3) + \gamma_4 g(Y_4) + \gamma_5 g(Y_5))
 \end{aligned} \tag{6}$$

where

$$\begin{aligned}
 Y_1 &= Y_n \\
 Y_2 &= Y_n + \Delta a_{21}f(Y_1) + J_1 b_{21}g(Y_1) \\
 Y_3 &= Y_n + \Delta(a_{31}f(Y_1) + a_{32}f(Y_2)) + J_1(b_{31}g(Y_1) + b_{32}g(Y_2)) \\
 Y_4 &= Y_n + \Delta(a_{41}f(Y_1) + a_{42}f(Y_2) + a_{43}f(Y_3)) \\
 &\quad + J_1(b_{41}g(Y_1) + b_{42}g(Y_2) + b_{43}g(Y_3)) \\
 Y_5 &= Y_n + \Delta(a_{51}f(Y_1) + a_{52}f(Y_2) + a_{53}f(Y_3) + a_{54}f(Y_4)) \\
 &\quad + J_1(b_{51}g(Y_1) + b_{52}g(Y_2) + b_{53}g(Y_3) + b_{54}g(Y_4))
 \end{aligned}$$

In tableau form, SRKST2 (6) is

$$\begin{array}{c|cccc}
 A & 1 & & & \\
 & \frac{2}{3} & -\frac{1}{6} & & \\
 & -\frac{1}{3} & \frac{1}{3} & 0 & \\
 & \frac{2}{3} & 0 & 0 & 0 \\
 \hline
 \alpha & -\frac{1}{4} & 0 & 0 & \frac{3}{4}
 \end{array}
 \qquad
 \begin{array}{c|cccc}
 B & \frac{1}{2} & & & \\
 & 0 & \frac{1}{2} & & \\
 & 0 & 0 & 1 & \\
 & 0 & 0 & 0 & 0 \\
 \hline
 \gamma & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & 0
 \end{array}$$

3. Numerical Experiment

Prior to the implementation of the performance of the methods to SDE in biological system, we perform the numerical experiment to the linear SDE taken from [10]. Consider the form of linear SDE as

$$dX(t) = aX(t)dt + bX(t)dW(t) \qquad t \in [0, T] \tag{7}$$

The exact solution of (10) given as

$$X(t) = \Phi_{t,t_0}(X_0) \tag{8}$$

where $\Phi_{t,t_0} = \exp((a)(t - t_0) + b(W(t) - W(t_0)))$. Note that we compute this numerical experiment by setting the coefficients as $a = -2.0$, $b = 0.5$, $T = 2.0$, $X(0) = 1.0$ and $\Delta = 0.01$. 200 sample paths of strong solutions for SDEs via SRK4, SRKS1.5 and SRKST2 have been simulate and the results are presented in Figure 1 and Table 1. Figure 1 and Table 1 shows the mean square error (MSE) for the three method by comparing the simulated results of SRK4, SRK 1.5 and SRK 2.0 with the exact solution of the linear SDE (7).

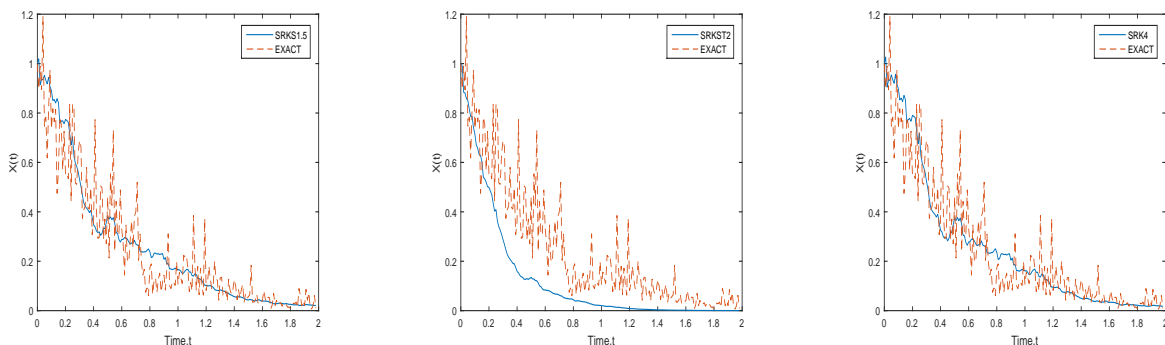


Figure 1. Exact solution versus numerical solution of (7) via three different methods.

Table 1. MSE for SRK4, SRKS1.5 and SRKST2.

Numerical Method	SRK4	SRKS1.5	SRKST2
MSE	0.011736	0.011098	0.031381

Consider the deterministic model of *C. acetobutylicum* P262 cell growth as below

$$\begin{aligned} dx(t) &= \mu_{\max} \left(1 - \frac{x(t)}{x_{\max}}\right) x(t) dt \\ x(t_0) &= x(0) \quad t \in [0, T] \end{aligned} \quad (9)$$

where x is a cell concentration, μ_{\max} is a growth coefficient and also x_{\max} is a maximum value of cell growth. The white noise is perturbed to ODE [7] such that

$$b \rightarrow b + \sigma \frac{dW}{dt}$$

where $b = -\frac{\mu_{\max}}{x_{\max}}$, σ is a diffusion coefficient and $W(t)$ is a Wiener process. The deterministic model with the addition of stochastic process can be written as

$$dx(t) = \mu_{\max} \left(1 - \frac{x(t)}{x_{\max}}\right) x(t) dt + \sigma x^2(t) dW(t) \quad (10)$$

Then, stochastic model (10), have been solved by using the same methods. We consider the stratonovich form of *C. acetobutylicum* P262 cell growth model with $t = 288$, $\mu_{\max} = 0.2576$, $x_{\max} = 4.565$, $\sigma = 0.0069$ and with initial condition $y(0) = 0.0025$. Cell growth of *C. acetobutylicum* P262 have been simulated in C++ and the result obtained as in Figure 2 and Table 2.

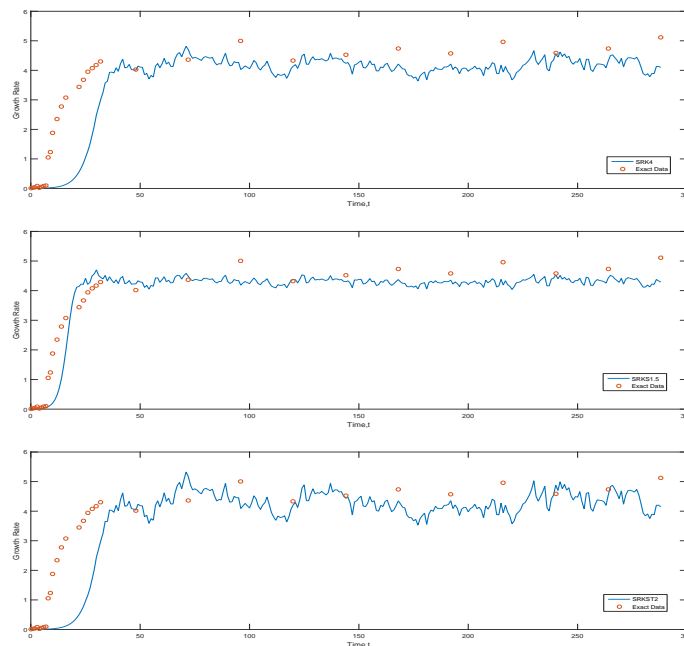


Figure 2. Experimental data versus numerical solution of (10) via three different methods.

Table 2. MSE for SRK4, SRKS1.5 and SRKST2.

Numerical Method	SRK4	SRKS1.5	SRKST2
MSE	2.68	0.51	2.80

Clearly seen that the SRKS method with strong order 1.5 proposed in [7] gives closest result as compared to the exact solution and the real data. The independence internal stages proposed give advantages since the computation become more cheaper but the stochastic process involved in the model still being considered. Compared to SRKST2, eventhough the method is simpler than SRKS1.5 but because of SRKST2 only evaluate the stochastic integral J_1 and ignore the stochastic integrals $\frac{J_{10}}{\Delta}$, hence the SRKS gives less efficient result compared to SRKS1.5 method.

4. Conclusion

As the complexity of the system increased when stochastic process considered, three different numerical methods have been used to approximate the numerical solution to the stochastic model. In conclusion, the new proposed method SRKS1.5 gives better solution compared to SRK4 and SRKST2. This method do not need to simulate the multiple stratonovich stochastic integrals which result in less complexity to solve the stochastic differential equations.

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