High order numerical integrators for single integrand SDEs

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Abstract

We show that applying any deterministic B-series method of order $p_d$ with a random step size to single integrand SDEs gives a numerical method converging in the mean-square and weak sense with order $\lfloor \frac{p_d}{2} \rfloor$. As an application, we derive high order energy-preserving methods for stochastic Poisson systems as well as further geometric numerical schemes for this wide class of Stratonovich SDEs.

1 Introduction

The last years have seen a great interest in the numerical analysis of single integrand Stratonovich stochastic differential equations

\[ dX(t) = f(X(t)) (\lambda dt + \sigma \circ dW(t)) = f(X(t)) \circ d\mu(t), \quad X(t_0) = x_0, \]  

(1)

see, e.g. \cite{1,3,8,9,14,18,22–27,36} as well as to the text below. Here, $t \geq t_0 \geq 0, x_0 \in \mathbb{R}^d, f: \mathbb{R}^d \to \mathbb{R}^d, (W(t))_{t \geq 0}$ is a standard one-dimensional Wiener process, $\lambda \in \{0,1\}$ and $\sigma \in \mathbb{R}$ are given constants, and $\mu(s) := \lambda s + \sigma W(s)$ for $s \geq 0$.

Stochastic differential equations (SDEs) of this form arise, e.g., when the right-hand side of an ordinary differential equation (ODE) model is randomly perturbed. Interesting applications are:

\textbf{Example 1} (Fatigue cracking \cite{33}).

\[ dX(t) = aX^p(t) \, dt + bX^p(t) \circ dW(t), \quad p > 1, a, b \in \mathbb{R}. \]
Example 2 (Stochastic Hamiltonian systems \[25,34\]).
\[
dX(t) = J^{-1} \nabla H(X(t)) \left( dt + c \circ dW(t) \right), \quad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, c \in \mathbb{R}.
\]

Example 3 (Stochastic perturbations of Poisson systems \[9\]).
\[
dX(t) = B(X(t)) \nabla H(X(t)) \left( dt + c \circ dW(t) \right), \quad B = -B^\top, c \in \mathbb{R}.
\]

In the present communication, we generalize the main results from \[14\] from Runge–Kutta methods to B-series methods. In particular, this permits to show that when applying any (deterministic) B-series numerical integrators of order \(p_d\) to (1) by replacing the deterministic step size \(h\) in the numerical scheme by \(\lambda h + \sigma(W(t + h) - W(t))\) when calculating one step of the approximation on the time interval \([t, t + h]\) respectively, one then automatically obtains a time integrator with step size \(h\) of mean-square as well as weak order \(\lfloor p_d/2 \rfloor\) for the SDE (1). On top of that, it can easily be observed that, in general, when a (deterministic) numerical integrator possesses some geometric properties, then the same geometric properties hold for the time integrator applied to single integrand SDEs \[1\]. This observation thus allows to carry forward various results already obtained in the literature as well as new ones, see for instance Section 4 below.

B-series methods encompass any reasonable one-step time integrators for ODEs: Besides Runge–Kutta methods \[15, 16\], other one-step methods can be represented as B-series, e. g. Taylor methods \[2, 12, 13\], averaged vector field methods \[7, 28\], and \(q\)-derivative Runge–Kutta methods \[16\].

2 Convergence of B-series methods applied to single integrand SDEs

B-series for solutions to SDEs and their numerical solution by stochastic Runge–Kutta methods have been developed in \[4, 5\] to study strong convergence in the Stratonovich case, in \[31, 32\] for strong converge in the Itô as well as the Stratonovich case, in \[21\] and \[20\] to study weak convergence in the Stratonovich case and in \[29, 30\] to study weak convergence in both the Itô and the Stratonovich case. A uniform and self-contained theory for the construction of stochastic B-series for the exact solution of SDEs and its numerical approximation by stochastic Runge–Kutta methods is given in \[11\]. Based on the notation used there, in \[14\] the B-series for the exact solution and Runge–Kutta approximations of single-integrand SDEs were derived. For convenience, we summarize the results we will need in the following. Due to the single integrand we do, similar to the ODE case \[6\], only need non-colored trees in the expansion of the solution.

**Definition 1 (Trees).** The set of rooted trees \(T\) related to single-integrand SDEs is recursively defined as follows:

a) The empty tree \(\emptyset\) and the graph \(\bullet = [\emptyset]\) with only one vertex belong to \(T\).
For a positive integer $\kappa$, let $\tau = [\tau_1, \tau_2, \ldots, \tau_\kappa]$ be the tree formed by joining the subtrees $\tau_1, \tau_2, \ldots, \tau_\kappa$ each by a single branch to a common root.

b) If $\tau_1, \tau_2, \ldots, \tau_\kappa \in T$ then $\tau = [\tau_1, \tau_2, \ldots, \tau_\kappa] \in T$.

**Definition 2** (Elementary differentials). For a tree $\tau \in T$ the elementary differential is a mapping $F(\tau) : \mathbb{R}^d \to \mathbb{R}^d$ defined recursively by

a) $F(\emptyset)(x) = x$,

b) $F(\bullet)(x) = f(x)$,

c) If $\tau = [\tau_1, \tau_2, \ldots, \tau_\kappa] \in T \setminus \{\emptyset\}$ then

$$F(\tau)(x) = f(\kappa)(x)(F(\tau_1)(x), F(\tau_2)(x), \ldots, F(\tau_\kappa)(x))$$

where $x \in \mathbb{R}^d$.

**Definition 3** (B-series). Consider for each $\tau \in T$ a stochastic process $(\phi(\tau)(h))_{h \geq 0}$ satisfying

$$\phi(\emptyset) \equiv 1 \quad \text{and} \quad \phi(\tau)(0) = 0, \quad \text{for} \quad \tau \in T \setminus \{\emptyset\}.$$ 

Let $x \in \mathbb{R}^d$ and $h \in \mathbb{R}$. A (stochastic) B-series is then a formal series of the form

$$B(\phi, x; h) = \sum_{\tau \in T} \alpha(\tau) \cdot \phi(\tau)(h) \cdot F(\tau)(x),$$

where $\alpha : T \to \mathbb{Q}$ is given by

$$\alpha(\emptyset) = 1, \quad \alpha(\bullet) = 1, \quad \alpha(\tau = [\tau_1, \ldots, \tau_\kappa]) = \frac{1}{r_1!r_2! \cdots r_q!} \prod_{j=1}^{\kappa} \alpha(\tau_j),$$

where $r_1, r_2, \ldots, r_q$ count equal trees among $\tau_1, \tau_2, \ldots, \tau_\kappa$.

We are now able to state the B-series of the exact solution to the SDE (1), see also [11,32]. In the following, $\rho(\tau)$ denotes the number of nodes in a tree $\tau$.

**Theorem 1** ([14]). Let $\gamma : T \to \mathbb{N}$ be given by

$$\gamma(\emptyset) = 1, \quad \gamma(\bullet) = 1,$$

$$\gamma([\tau_1, \ldots, \tau_\kappa]) = \rho([\tau_1, \ldots, \tau_\kappa]) \prod_{j=1}^{\kappa} \gamma(\tau_j).$$

Then the solution $X(t+h)$ of (1) starting at the point $(t, x)$ can be written as a B-series $B(\varphi_t, x; h)$ with

$$\varphi_t(\tau)(h) = \frac{\mu_t(h)^{\rho(\tau)}}{\gamma(\tau)} \quad \text{for} \quad \tau \in T$$

where

$$\mu_t(s) := \mu(t+s) - \mu(t) = \lambda s + \sigma(W(t+s) - W(t)).$$

(2)
That is, the B-series of the exact solution of (1) coincides with the one of the exact solution of an ODE (i.e. when \( \lambda = 1, \sigma = 0 \)) when replacing \( \mu(t) \) with \( h \).

Next, we derive the B-series for the numerical solution of the single integrand SDE (1). To do this, we consider B-series methods for the ODE \( dX(t) = f(X(t)) \, dt \). Such methods can be written as

\[
Y(t + h) = B(\Phi_t, x; h)
\]

with \( \Phi_t(\tau)(h) = h^{\rho(\tau)} \cdot \hat{\Phi}(\tau) \) where \( \hat{\Phi} : T \rightarrow \mathbb{R} \) fulfilling \( \hat{\Phi}(0) = 1 \). Replacing \( h \) by \( \Delta_{t,t+h,\mu} = \mu(t) \) defined in (3) we consider therefore the following B-series method for solving (1):

**Definition 4.** Given an ODE-B-series method (4) for the ODE \( dX(t) = f(X(t)) \, dt \), the corresponding ODE-B-series method for (1) is given by

\[
Y(t + h) = B(\Phi_t^\mu, x; h)
\]

where \( \Phi_t^\mu(\tau)(h) = (\Delta_{t,t+h,\mu})^{\rho(\tau)} \hat{\Phi}(\tau) \).

Now we give the definitions of both weak and strong convergence used in this note.

Let \( C^{l}_{P}(\mathbb{R}^d, \mathbb{R}^d) \) denote the space of all \( g \in C^l(\mathbb{R}^d, \mathbb{R}^d) \) fulfilling a polynomial growth condition [19] and \( I^{\tilde{h}} \) be the discretized time interval on which the numerical approximations are calculated.

**Definition 5.** A time discrete approximation \( Y = (Y(t))_{t \in I^{\tilde{h}}} \) converges weakly with order \( p \) to \( X \) at time \( t \in I^{\tilde{h}} \) as the maximum step size \( \tilde{h} \rightarrow 0 \) if for each \( g \in C^{2(p+1)}_{P}(\mathbb{R}^d, \mathbb{R}) \) there exist a constant \( C_g \) and a finite \( \delta_0 > 0 \) such that

\[
|\mathbb{E}(g(Y(t))) - \mathbb{E}(g(X(t)))| \leq C_g \tilde{h}^p
\]

holds for each \( \tilde{h} \in [0, \delta_0[ \).

Whereas weak approximation methods are used to estimate the expectation of functionals of the solution, strong approximation methods approach the solution path-wise.

**Definition 6.** A time discrete approximation \( Y = (Y(t))_{t \in I^{\tilde{h}}} \) converges in the mean square sense with order \( p \) to \( X \) at time \( t \in I^{\tilde{h}} \) as the maximum step size \( \tilde{h} \rightarrow 0 \) if there exist a constant \( C \) and a finite \( \delta_0 > 0 \) such that

\[
\sqrt{\mathbb{E}(|Y(t) - X(t)|^2)} \leq C \tilde{h}^p
\]

holds for each \( \tilde{h} \in [0, \delta_0[ \).

In this article we will consider convergence in the mean square sense. Observe that, by Jensen’s inequality, mean square convergence implies strong convergence of the same order.

We are now in position to state the main result of the present publication.
Theorem 2. Assume that the B-series method \( (5) \) is of deterministic order \( p_d \) and let \( p = \lfloor p_d / 2 \rfloor \). Further, let \( f \in C^{2p\mu+1}(\mathbb{R}^d, \mathbb{R}^d) \) and \( f \) and \( f' \) fulfill a Lipschitz condition. Finally, assume

- for mean-square convergence, that all elementary differentials \( F_\tau \) fulfill a linear growth condition,
- respectively for weak convergence, that \( f \in C^{2p\mu+1}(\mathbb{R}^d, \mathbb{R}^d) \). \( f \) and \( f' \) fulfill a Lipschitz condition.

Then this very same B-series method is of mean square as well as weak order \( p\mu \) when applied to the single integrand SDE \( (1) \) with step size \( \Delta_{t,t+h\mu} \). For weak convergence, it suffices that \( \Delta_{t,t+h\mu} \) is chosen such that at least the first \( 2p\mu + 1 \) moments coincide with those of \( \mu_t(h) \), and all the others are in \( O(h^{p\mu+1}) \).

Proof. To prove this result, one first observes that the corresponding Theorem for Runge–Kutta methods [14, Theorem 1.1] only uses that the B-series of the exact and numerical solutions fulfill the properties summarized in Definition 4. One can then directly extended the proof to the present situation of B-series methods. \( \square \)

3 Application to stochastic perturbations of Poisson systems

As application of the above theorem, we propose a high order energy-preserving and Casimir-preserving scheme for the stochastic rigid body [9]. The equations of motion of this stochastic rigid body are a Lie-Poisson system:

\[
\begin{pmatrix}
\frac{dX_1}{dt} \\
\frac{dX_2}{dt} \\
\frac{dX_3}{dt}
\end{pmatrix} =
\begin{pmatrix}
0 & -X_3 & X_2 \\
X_3 & 0 & -X_1 \\
-X_2 & X_1 & 0
\end{pmatrix}
\begin{pmatrix}
X_1/I_1 \\
X_2/I_2 \\
X_3/I_3
\end{pmatrix}
\left(dt + c \circ dW\right), \tag{6}
\]

where \( X = (X_1, X_2, X_3)^T \) and \( I = (I_1, I_2, I_3) \) are the moments of inertia. The Hamiltonian

\[
H(X) = \frac{1}{2}(X_1^2/I_1 + X_2^2/I_2 + X_3^2/I_3),
\]

is thus a conserved quantity as well as the quadratic Casimir

\[
C(X) = \|X\|^2 = X_1^2 + X_2^2 + X_3^2.
\]

Note that the right hand side \( f \) of \( (6) \) a priori does not fulfill the conditions of Theorem 2. However, for methods that conserve as well the Hamiltonian or the Casimir, we can replace \( f \) by a function being zero outside a suitable ball and fulfilling the conditions of Theorem 2, e.g. when the Casimir being conserved replacing \( f \) by

\[
\tilde{f}(X) = f(X) \frac{\varphi(4C(X(0)) - C(X))}{\varphi(C(X) - 2C(X(0))) + \varphi(4C(X(0)) - C(X))}
\]
where

\[ \varphi(r) = \begin{cases} 
0 & \text{for } r \leq 0 \\
e^{-1/r} & \text{for } r > 0.
\end{cases} \]

As a starting deterministic method, we choose the linear energy-preserving integrators of orders 2, 4 and 6 from \cite{10}. By Theorem 2, we thus expect a first, resp. second, resp. third strong and weak order energy-preserving numerical integrator for the stochastic rigid body (6), denoted by EPs1, EPs2, EPs3. Recall that these novel numerical methods are simply given by replacing the step size \( h \) by \( \lambda h + \sigma \Delta W_n \) in the deterministic scheme. The orders of convergence can be seen in Figures 1 and 2, where the numerically determined orders of convergence \( \hat{p} \) correspond to the slopes of the dashed regression lines. The parameters for these numerical experiments are: \( T_{\text{end}} = 0.5, c = 0.5, I = (0.345, 0.653, 1), X(0) = (0.8, 0.6, 0) \) and 200 samples are used to approximate the expectations. We have checked that 200 samples are enough for these numerical experiments. The reference solution is calculated with \( h_{\text{ref}} = 2^{-14} \) and EPs3.

Furthermore, as it can be seen in Figure 3 for the example of the third order method, these numerical schemes not only preserve the energy but also the quadratic Casimir, see also the next section.

4 Applications to geometric numerical integration of single integrand SDEs

As seen in the previous sections, properties of numerical schemes for single integrand SDEs \cite{1} are closely related to those of numerical schemes for their corresponding ODEs.
**Figure 2:** Weak orders of convergence of the proposed numerical schemes for the second moments.

**Figure 3:** Numerical simulation with the third order method (one path) for the stochastic rigid body problem (green points) and the two invariants $H(Y) = H(Y(0))$ (blue) and $C(Y) = C(Y(0))$ (red), with $T_{end} = 5$, $h = 2^{-4}$, other parameters as before.
This relation can be specified furthermore: In principle, when applying any determinis-
tic geometric numerical integrators to single integrand SDEs (1) with random step size
$\Delta_{t,t+h}$, one then obtains the same geometric property as by the corresponding deter-
ministic numerical scheme. This is because, the random perturbation in some sense
respects the geometric structure of the phase space. With the main idea used in this
paper, one easily derives several results already obtained in the literature as well as new
ones for geometric numerical integrators of single integrand SDEs (1):

1. If the deterministic numerical method preserves linear or quadratic invariants, so
does it for single integrand SDEs. See the example above and e.g. [17].

2. If the deterministic scheme is energy or invariant-preserving, then it is also energy
or invariant-preserving for single integrand SDEs. See the example above and e.g.
[9,22,23,26].

3. If the deterministic numerical method is symmetric, then it is also symmetric for
the SDE (1).

4. If the deterministic time integrator is symplectic and $f(x) = J^{-1}\nabla H(x)$, then it
is symplectic for single integrand SDEs, e.g. [25,27,34].

5. Deterministic (symmetric) projection methods can be directly applied to single
integrand SDEs with constraints, e.g. [35].

6. If the deterministic numerical method is volume preserving, then it is also volume
preserving for single integrand SDEs.

7. If the deterministic numerical scheme is a Poisson integrator and it holds
$f(x) = B(x)\nabla H(x)$, where $B(x)$ represents a Poisson bracket, then it is also a Poisson
integrator for single integrand SDEs.

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