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High order numerical integrators for single integrand Stratonovich 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 $\lfloor p_d/2 \rfloor$. 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.

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1. Introduction

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

$$\mathrm{d}X(t) = f(X(t))\,(\lambda\,\mathrm{d}t + \sigma \circ \mathrm{d}W(t)) = f(X(t)) \circ \mathrm{d}\mu(t), \qquad X(t_0) = x_0, \tag{1}$$

see, e.g. [1,3,8,9,14,17,22–27,37] 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:

Example 1 *(Fatigue cracking [34]).*

$$\mathrm{d}X(t) = aX^p(t)\,\mathrm{d}t + bX^p(t) \circ \mathrm{d}W(t), \qquad p > 1, a, b \in \mathbb{R}.$$

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Example 2 *(Stochastic Hamiltonian systems [25,35]).*

$$\mathrm{d}X(t) = J^{-1}\nabla H(X(t))\,(\,\mathrm{d}t + c\circ \mathrm{d}W(t))\,, \qquad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, c \in \mathbb{R}.$$

Example 3 *(Stochastic perturbations of Poisson systems [9]).*

$$\mathrm{d}X(t) = B(X(t))\nabla H(X(t))\,(\,\mathrm{d}t + c\circ \mathrm{d}W(t))\,, \qquad B = -B^{\top}, c \in \mathbb{R}.$$

In the present communication, we generalize the main results in [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). We recall that the notation $\lfloor x \rfloor$ denotes the floor function of a real number x.

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 3 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 [7,29], 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 [32,33] for strong converge in the Itô as well as the Stratonovich case, in [20] and [21] to study weak convergence in the Stratonovich case and in [30,31] 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 κ, 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

$$F(\tau)(x) = f^{(\kappa)}(x)\big(F(\tau_1)(x), F(\tau_2)(x), \ldots, F(\tau_\kappa)(x)\big)$$

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

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

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

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

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 τ.

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

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

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

$$\varphi_t(\tau)(h) = \frac{\mu_t(h)^{\rho(\tau)}}{\gamma(\tau)} \qquad \text{for } \tau \in T \tag{2}$$

where

$$\mu_t(s) := \mu(t+s) - \mu(t) = \lambda s + \sigma(W(t+s) - W(t)). \tag{3}$$

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 $\mu_t(h)$ 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 $\mathrm{d}X(t) = f(X(t))\,\mathrm{d}t$. Such methods can be written as [15]

$$Y(t+h) = B(\Phi_t, x; h) \tag{4}$$

with $\Phi_t(\tau)(h) = h^{\rho(\tau)} \cdot \hat{\Phi}(\tau)$ where $\hat{\Phi} : T \to \mathbb{R}$ fulfilling $\hat{\Phi}(\emptyset) = 1$. Replacing h by $\Delta_{t,t+h}\mu = \mu_t(h)$ 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 $\mathrm{d}X(t) = f(X(t))\,\mathrm{d}t$, the corresponding ODE-B-series method for (1) is given by

$$Y(t+h) = B(\Phi_t^\mu, x; h), \tag{5}$$

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 $C_P^l(\mathbb{R}^d, \mathbb{R}^{\hat{d}})$ denote the space of all $g \in C^l(\mathbb{R}^d, \mathbb{R}^{\hat{d}})$ 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 $\tilde{h} \to 0$ if for each $g \in C_P^{2(p+1)}(\mathbb{R}^d, \mathbb{R})$ there exist a constant C_g and a finite $\delta_0 > 0$ such that

$$|\,\mathrm{E}(g(Y(t))) - \mathrm{E}(g(X(t)))| \le C_g \tilde{h}^p$$

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. In this article, next to weak convergence, we will consider mean-square instead of strong convergence.

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 $\tilde{h} \to 0$ if there exist a constant C and a finite $\delta_0 > 0$ such that

$$\sqrt{\mathrm{E}(\|Y(t) - X(t)\|^2)} \leq C\,\tilde{h}^p$$

holds for each $\tilde{h} \in]0, \delta_0[$.

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 $p_\mu = \lfloor p_d/2 \rfloor$. Further, let $f \in C^{2p_\mu+1}(\mathbb{R}^d, \mathbb{R}^d)$ and f and $f'f$ 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 $f \in C_P^{2p_\mu+1}(\mathbb{R}^d, \mathbb{R}^d)$.*

Then this very same B-series method is of mean-square as well as weak order p_μ 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 $\mathcal{O}(h^{p_\mu+1})$.

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 fulfil the properties summarized in Definition 4. One can then directly extend the proof to the present situation of B-series methods. □

3. Applications to geometric numerical integration of single integrand SDEs

Geometric properties of numerical schemes for single integrand SDEs (1) are closely related to those of numerical schemes for their corresponding ODEs. This relation, which holds for B-series as well as non B-series (e.g. volume preserving) methods, can be specified furthermore: In principle, when applying any deterministic geometric numerical integrators to single integrand SDEs (1) with random step size $\Delta_{t,t+h}\mu$, one then obtains the same geometric property as by the corresponding deterministic numerical scheme. This is because the random perturbation in some sense respects the geometric structure of the phase space. Hence, proofs of conservation properties in the deterministic setting can be adapted to single integrand Stratonovich SDEs (1). 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 below and e.g. [18].
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 below 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. [25,27,35].
5. Deterministic (symmetric) projection methods can be directly applied to single integrand SDEs with constraints, e.g. [36].
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 $f(x) = B(x)\nabla H(x)$, where $B(x)$ represents a Poisson bracket, then it is also a Poisson integrator for single integrand SDEs.

4. Application to stochastic perturbations of Poisson systems

As application of Theorem 2 and the principles of the previous section, 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:

$$\begin{pmatrix} \mathrm{d}X_{[1]} \\ \mathrm{d}X_{[2]} \\ \mathrm{d}X_{[3]} \end{pmatrix} = \begin{pmatrix} 0 & -X_{[3]} & X_{[2]} \\ X_{[3]} & 0 & -X_{[1]} \\ -X_{[2]} & X_{[1]} & 0 \end{pmatrix} \begin{pmatrix} X_{[1]}/I_1 \\ X_{[2]}/I_2 \\ X_{[3]}/I_3 \end{pmatrix} \big(\mathrm{d}t + c \circ \mathrm{d}W\big), \tag{6}$$

with some initial value $X(0) \in \mathbb{R}^3$ at $t_0 = 0$, where $X = (X_{[1]}, X_{[2]}, X_{[3]})^\top$ and $I = (I_1, I_2, I_3)$ are the moments of inertia. The Hamiltonian

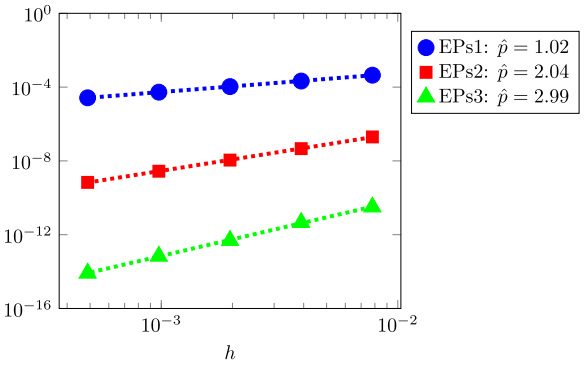

Fig. 1. Mean-square orders of convergence of the numerical schemes EPs1 to EPs3 for the stochastic rigid body (6). Used step sizes: $h = 2^{-7}$ to $h = 2^{-11}$.

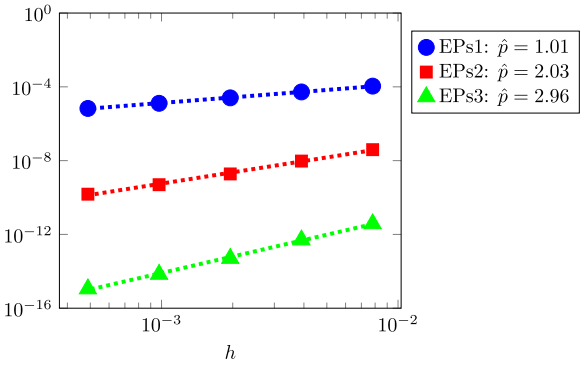

Fig. 2. Weak orders of convergence of the numerical schemes EPs1 to EPs3 for the second moments of approximations of solutions to the stochastic rigid body (6). Used step sizes: $h = 2^{-7}$ to $h = 2^{-11}$.

$$H(X) = \frac{1}{2}\left(X_{[1]}^2/I_1 + X_{[2]}^2/I_2 + X_{[3]}^2/I_3\right)$$

is thus a conserved quantity as well as the quadratic Casimir

$$C(X) = \|X\|_2^2 = X_{[1]}^2 + X_{[2]}^2 + X_{[3]}^2.$$

Note that the right hand side f of (6) is not globally Lipschitz continuous and does thus a priori not fulfill the conditions of Theorem 2. However, for methods that conserve the Casimir, we can replace f by a function being zero outside a suitable ball and fulfilling the conditions of Theorem 2, e.g. 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

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

Note that $\tilde{f}(X) = f(X)$ for all $\|X\|_2 \leq \sqrt{2}\|X(0)\|$ and $\tilde{f}(X) = 0$ for all $\|X\|_2 \geq 2\|X(0)\|$ (see e.g. [28]), and all derivatives of $\tilde{f}$ remain bounded. A similar modification can be made for numerical methods that preserve the Hamiltonian of the deterministic rigid body.

As a starting deterministic method, we choose the linear energy-preserving integrators of orders 2, 4 and 6 from [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 Figs. 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: $T_{end} = 0.5, c = 0.5, I = (0.345, 0.653, 1), X(0) = (0.8, 0.6, 0)$, and 200 samples are used to approximate the expectations. We have checked that 200 samples are sufficient for these numerical experiments. The reference solution is calculated with $h_{ref} = 2^{-14}$ and EPs3.

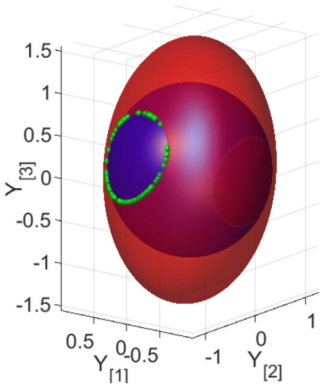

Fig. 3. Numerical simulation with the third order method (one path) for the stochastic rigid body problem (green points) and the two invariants $H(Y) = H(Y(0))$ (blue) and $C(Y) = C(Y(0))$ (red), with $T_{end} = 5$, $h = 2^{-4}$, other parameters as before. (For the black and white copy of this article, the green points correspond to light gray points on the inner circle, the blue area corresponds to the black area within this circle and the red area corresponds to the surface of the ellipsoid outside the circle, see also the coloured web version of this article.)

Furthermore, as it can be seen in Fig. 3, for the example of the third order method, these numerical schemes not only preserve the energy but also the quadratic Casimir $C(X)$. This follows from the discussion in Section 3, as the numerical integrators from [10] are known to preserve quadratic Casimirs.

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