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Stochastic B-series and order conditions for exponential integrators

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Abstract. We discuss stochastic differential equations with a stiff linear part and their approximation by stochastic exponential integrators. Representing the exact and approximate solutions using B-series and rooted trees, we derive the order conditions for stochastic exponential integrators. The resulting general order theory covers both Itô and Stratonovich integration.

1 Introduction

The idea of expressing the exact and numerical solutions of different blends of differential equations in terms of B-series and rooted trees has been an indispensable tool ever since John Butcher introduced the idea in 1963 [4]. Naturally then, such series have also been derived for stochastic differential equations (SDEs) by several authors, see e.g. [6] for an overview.

In this paper, the focus is on d -dimensional SDEs of the form

$$dX(t) = \left(AX(t) + g_0(X(t)) \right) dt + \sum_{m=1}^M g_m(X(t)) \star dW_m(t), \quad X(0) = x_0, \quad (1)$$

or in integral form

$$X(t) = e^{tA} x_0 + \int_0^t e^{(t-s)A} g_0(X(s)) ds + \sum_{m=1}^M \int_0^t e^{(t-s)A} g_m(X(s)) \star dW_m(s), \quad (2)$$

in which case the linear term $AX(t)$, $A \in \mathbb{R}^{d \times d}$ constant will be treated with particular care by the use of exponential integrators, see e.g. [1,5,9] and references therein. The integrals w. r. t. the components of the M -dimensional Wiener process $W(t)$ can be interpreted e.g. as an Itô or a Stratonovich integral. The coefficients $g_m : \mathbb{R}^d \rightarrow \mathbb{R}^d$ are sufficiently differentiable and satisfy a Lipschitz and a linear growth condition. For Stratonovich SDEs, we require in addition that g_m are differentiable and that also the $g'_m g_m$ satisfy a Lipschitz and a linear growth condition. In the following, we will denote $dt = dW_0(t)$.

For the numerical solution of (1) we consider a general class of ν -stage stochastic exponential integrators:

$$H_i = e^{c_i h A} Y_n + \sum_{m=0}^M \sum_{j=1}^{\nu} Z_{ij}^{(m)}(A) \cdot g_m(H_j), \quad i = 1, \dots, \nu, \quad (3a)$$

$$Y_{n+1} = e^{hA} Y_n + \sum_{m=0}^M \sum_{i=1}^{\nu} z_i^{(m)}(A) \cdot g_m(H_i), \quad (3b)$$

where typically the coefficients $Z_{ij}^{(m)}$ and $z_i^{(m)}$ are random variables depending on the stepsize h , the matrix A and the Wiener processes.

Example 1. A 2-stage stochastic exponential time-differencing Runge–Kutta method (SETDRK) for $M = 1$ is given by:

$$\begin{aligned} H_1 &= Y_n, \\ H_2 &= Y_n + \sqrt{h} g_1(H_1), \\ Y_{n+1} &= e^{hA} Y_n + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)A} ds \cdot g_0(H_1) \\ &\quad + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)A} \star dW_1(s) \cdot g_1(H_1) \\ &\quad + \frac{1}{\sqrt{h}} \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)A} W_1(s) \star dW_1(s) \cdot (-g_1(H_1) + g_1(H_2)), \end{aligned}$$

where $t_{n+1} = t_n + h$.

In the following, the ideas introduced in [6] will be used to derive a B-series representation of (2) and corresponding order conditions for the method (3). In the deterministic case, such analysis has been carried out in [2,8].

2 B-series and order conditions for exponential integrators

To develop B-series for the exact solution of (1) and one step numerical exponential integrators of the form (3), we use the following definitions of the trees associated to the stochastic differential equation (1) and their corresponding elementary differentials.

Definition 2 (trees). The set of $M + 2$ -colored, rooted trees

$$T = \{\emptyset\} \cup T_0 \cup T_1 \cup \dots \cup T_M \cup T_A$$

is recursively defined as follows:

1. The graph $\bullet_m = [\emptyset]_m$ with only one vertex of color m belongs to T_m , and $\bullet_A = [\emptyset]_A$ with only one vertex of color A belongs to T_A ,
2. Let $\tau = [\tau_1, \tau_2, \dots, \tau_\kappa]_m$ be the tree formed by joining the subtrees $\tau_1, \tau_2, \dots, \tau_\kappa$ each by a single branch to a common root of color m and $\tau = [\tau_1]_A$ be the tree formed by joining the subtree τ_1 to a root of color A . If $\tau_1, \tau_2, \dots, \tau_\kappa \in T$, then $\tau = [\tau_1, \tau_2, \dots, \tau_\kappa]_m \in T_m$ and $[\tau_1]_A \in T_A$,

for $m = 0, \dots, M$.

Definition 3 (elementary differential). For a tree $\tau \in T$ the elementary differential is a mapping $F(\tau) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ defined recursively by

1. $F(\emptyset)(x_0) = x_0$,
2. $F(\bullet_m)(x_0) = g_m(x_0)$, $F(\bullet_A)(x_0) = Ax_0$,
3. If $\tau_1, \tau_2, \dots, \tau_\kappa \in T$, then $F([\tau_1]_A)(x_0) = AF(\tau_1)(x_0)$ and

$$F([\tau_1, \tau_2, \dots, \tau_\kappa]_m)(x_0) = g_m^{(\kappa)}(x_0)(F(\tau_1)(x_0), \dots, F(\tau_\kappa)(x_0))$$

for $m = 0, \dots, M$.

Now we give the definition of B-series.

Definition 4 (B-series). A (stochastic) B-series is a formal series of the form

$$B(\phi, x_0; h) = \sum_{\tau \in T} \alpha(\tau) \cdot \phi(\tau)(h) \cdot F(\tau)(x_0),$$

where $\phi(\tau)(h)$ is a random variable satisfying $\phi(\emptyset) \equiv 1$ and $\phi(\tau)(0) = 0$ for all $\tau \in T \setminus \{\emptyset\}$, and $\alpha : T \rightarrow \mathbb{Q}$ is given by

$$\begin{aligned} \alpha(\emptyset) &= 1, & \alpha(\bullet_m) &= 1, & \alpha(\bullet_A) &= 1, \\ \alpha([\tau_1, \dots, \tau_\kappa]_m) &= \frac{1}{r_1! r_2! \dots r_\kappa!} \prod_{k=1}^{\kappa} \alpha(\tau_k), & \alpha([\tau_1]_A) &= \alpha(\tau_1), \end{aligned}$$

where r_1, r_2, \dots, r_l count equal trees among $\tau_1, \tau_2, \dots, \tau_\kappa$, and $m = 0, \dots, M$.

Next we give an important lemma to derive B-series for the exact and numerical solutions. It states that if $Y(h)$ can be expressed as a B-series, then $f(Y(h))$ can also be expressed as a B-series where the sum is taken over trees with a root of color f and subtrees in T .

Lemma 5. *If $Y(h) = B(\phi, x_0; h)$ is some B-series and $f \in C^\infty(\mathbb{R}^d, \mathbb{R}^d)$, then $f(Y(h))$ can be written as a formal series of the form*

$$f(Y(h)) = \sum_{u \in U_f} \beta(u) \cdot \psi_\phi(u)(h) \cdot G(u)(x_0) \quad (4)$$

where U_f is a set of trees derived from T , by

- (i) $[\emptyset]_f \in U$, and if $\tau_1, \tau_2, \dots, \tau_\kappa \in T$, then $u = [\tau_1, \tau_2, \dots, \tau_\kappa]_f \in U_f$.
(ii) $G([\emptyset]_f)(x_0) = f(x_0)$ and

$$G([\tau_1, \tau_2, \dots, \tau_\kappa]_f)(x_0) = f^{(\kappa)}(x_0)(F(\tau_1)(x_0), \dots, F(\tau_\kappa)(x_0)).$$

- (iii) $\beta([\emptyset]_f) = 1$ and $\beta([\tau_1, \dots, \tau_\kappa]_f) = \frac{1}{r_1!r_2!\dots r_\kappa!} \prod_{k=1}^{\kappa} \alpha(\tau_k)$, with $r_1, r_2, \dots, r_\kappa$ counting equal trees among $\tau_1, \tau_2, \dots, \tau_\kappa$.
(iv) $\psi_\phi([\emptyset]_f) \equiv 1$ and $\psi_\phi([\tau_1, \tau_2, \dots, \tau_\kappa]_f)(h) = \prod_{k=1}^{\kappa} \phi(\tau_k)(h)$.

Proof. The proof of this lemma is given in [6]. \square

Applying Lemma 5 to the functions g_m on the right hand side of (1) gives

$$g_m(B(\phi, x_0; h)) = \sum_{\tau \in T_m} \alpha(\tau) \cdot \phi'_m(\tau)(h) \cdot F(\tau)(x_0), \quad (5)$$

where

$$\phi'_m(\tau)(h) = \begin{cases} 1 & \text{if } \tau = \bullet_m, \\ \prod_{k=1}^{\kappa} \phi(\tau_k)(h) & \text{if } \tau = [\tau_1, \dots, \tau_\kappa]_m \in T_m. \end{cases}$$

Assume the exact solution $X(h)$ of (1) at $t = h$ can be written as a B-series $B(\varphi, x_0; h)$. Substituting $X(h) = B(\varphi, x_0; h)$ in (2) and using (5) gives

$$\begin{aligned} & B(\varphi, x_0; h) \\ &= e^{hA}x_0 + \sum_{m=0}^M \int_0^h e^{(h-s)A} \sum_{\hat{\tau} \in T_m} \alpha(\hat{\tau}) \cdot \varphi'_m(\hat{\tau})(s) \cdot F(\hat{\tau})(x_0) \star dW_m(s). \end{aligned}$$

Inserting the series representation $e^{hA}x_0 = \sum_{q=0}^{\infty} \frac{h^q A^q}{q!} x_0$ yields

$$\begin{aligned} B(\varphi, x_0; h) &= x_0 + \sum_{q=1}^{\infty} \frac{h^q}{q!} A^q x_0 \\ &+ \sum_{m=0}^M \sum_{\hat{\tau} \in T_m} \alpha(\hat{\tau}) \sum_{q=0}^{\infty} \left(\int_0^h \frac{(h-s)^q}{q!} \varphi'_m(\hat{\tau})(s) \star dW_m(s) \cdot A^q F(\hat{\tau})(x_0) \right). \quad (6) \end{aligned}$$

Note that any tree $\tau \in T$ can be rewritten as $\tau = [\dots \overbrace{[[\hat{\tau}]_A]_A \dots}]_A = [\hat{\tau}]_A^q$ for $q = 0, 1, \dots$, with $\hat{\tau} \in T \setminus T_A$, that means $\hat{\tau} = \emptyset$ or $\hat{\tau} = [\tau_1, \dots, \tau_\kappa]_m$ for an $m \in \{1, \dots, M\}$. It holds that $F([\hat{\tau}]_A^q) = A^q F(\hat{\tau})$, $\alpha([\hat{\tau}]_A^q) = \alpha(\hat{\tau})$. Especially, for $\tau = [\emptyset]_A^q$ it holds that $\alpha(\tau) = 1$ and $F(\tau)(x_0) = A^q F(\emptyset) = A^q x_0$. In conclusion (6) implies the following theorem:

Theorem 6. *The solution $X(h)$ of the SDE (1) can be written as a B-series $B(\varphi, x_0; h)$ with*

$$\begin{aligned}\varphi(\emptyset)(h) &= 1, & \varphi([\emptyset]_A^q)(h) &= \frac{h^q}{q!}, \\ \varphi([\tau_1, \dots, \tau_\kappa]_m^q)(h) &= \int_0^h \frac{(h-s)^q}{q!} \prod_{k=1}^{\kappa} \varphi(\tau_k)(s) \star dW_m(s),\end{aligned}$$

for $\tau_1, \dots, \tau_\kappa \in T$, $\kappa = 0, 1, \dots$, $q = 0, 1, \dots$ and $m = 0, \dots, M$, where $\tau_i \neq \emptyset$ for $i = 1, \dots, \kappa$ if $\kappa > 1$.

Example 7. Let $\tau = \begin{array}{c} \bullet \\ \swarrow \downarrow \searrow \\ \bullet \bullet \bullet \end{array}$, where the colors red, black and white correspond to the matrix A , deterministic function g_0 and stochastic function g_1 respectively. Then $\alpha(\tau) = 1$, $F(\tau)(x_0) = g_0''(g_1, g_1''(Ax_0, g_0))(x_0)$ and $\varphi(\tau)(h) = \int_0^h (W_1(s) \int_0^s s_1^2 \star dW_1(s_1)) ds$. Note also that e.g. the tree $\tau = \begin{array}{c} \bullet \\ \swarrow \downarrow \searrow \\ \bullet \bullet \bullet \end{array} \notin T$ since it is impossible for node \bullet to have more than one branch.

Now we derive the B-series representation for one step of the exponential stochastic integrator (3). Assume both the stage values H_i and the approximation Y_{n+1} to the exact solution can be written as B-series:

$$H_i = B(\Phi_i, Y_n; h), \quad i = 1, \dots, \nu \quad \text{and} \quad Y_{n+1} = B(\Phi, Y_n; h). \quad (7)$$

In addition we assume that the coefficients $Z_{ij}^{(m)}(A)$ and $z_i^{(m)}(A)$ can be expressed as power series of the form

$$Z_{ij}^{(m)}(A) = \sum_{q=0}^{\infty} Z_{ij}^{(m,q)} A^q \quad \text{and} \quad z_i^{(m)}(A) = \sum_{q=0}^{\infty} z_i^{(m,q)} A^q,$$

for $i, j = 1, \dots, \nu$, and $m = 0, \dots, M$. Substituting these formulas into (3) and using (5) we get

$$\begin{aligned}H_i &= \sum_{q=0}^{\infty} \frac{(c_i h)^q}{q!} A^q Y_n + \sum_{m=0}^M \sum_{j=1}^{\nu} Z_{ij}^{(m)}(A) \sum_{\tau \in T_m} \alpha(\tau) \cdot \Phi_j'(\tau)(h) \cdot F(\tau)(Y_n) \\ &= \sum_{q=0}^{\infty} \frac{(c_i h)^q}{q!} A^q Y_n + \sum_{m=0}^M \sum_{j=1}^{\nu} \sum_{\tau \in T_m} \alpha(\tau) \sum_{q=0}^{\infty} Z_{ij}^{(m,q)} \Phi_j'(\tau)(h) \cdot A^q F(\tau)(Y_n),\end{aligned}$$

and similarly

$$Y_{n+1} = \sum_{q=0}^{\infty} \frac{h^q}{q!} A^q Y_n + \sum_{m=0}^M \sum_{i=1}^{\nu} \sum_{\tau \in T_m} \alpha(\tau) \sum_{q=0}^{\infty} z_i^{(m,q)} \Phi_i'(\tau)(h) \cdot A^q F(\tau)(Y_n).$$

Now using (7) and the linear independence of the elementary differentials yields the following theorem.

Theorem 8. *The stage values H_i and the numerical solution Y_{n+1} of (3) can be written as B-series $H_i = B(\Phi_i, Y_n; h)$, $i = 1, \dots, \nu$, and $Y_{n+1} = B(\Phi, Y_n; h)$ with the following recurrence relations for the functions $\Phi_i(\tau)(h)$ and $\Phi(\tau)(h)$,*

$$\begin{aligned}\Phi_i(\emptyset) &= \Phi(\emptyset) \equiv 1, & \Phi_i([\emptyset]_A^q)(h) &= \frac{(c_i h)^q}{q!}, & \Phi([\emptyset]_A^q)(h) &= \frac{h^q}{q!}, \\ \Phi_i([\tau_1, \dots, \tau_\kappa]_m^q)(h) &= \sum_{j=1}^{\nu} Z_{ij}^{(m,q)} \prod_{k=1}^{\kappa} \Phi_j(\tau_k)(h), \\ \Phi([\tau_1, \dots, \tau_\kappa]_m^q)(h) &= \sum_{i=1}^{\nu} z_i^{(m,q)} \prod_{k=1}^{\kappa} \Phi_i(\tau_k)(h),\end{aligned}$$

for $\tau_1, \dots, \tau_\kappa \in T$, $\kappa = 0, 1, \dots$, $q = 0, 1, \dots$ and $m = 0, \dots, M$, where $\tau_i \neq \emptyset$ for $i = 1, \dots, \kappa$ if $\kappa > 1$.

To discuss the order of the method, we need the following definition.

Definition 9 (order). The order $\rho(\tau)$ of a tree $\tau \in T$ is defined by

$$\rho(\emptyset) = 0, \quad \rho([\tau_1]_A) = \rho(\tau_1) + 1$$

and

$$\rho([\tau_1, \dots, \tau_\kappa]_m) = \sum_{k=1}^{\kappa} \rho(\tau_k) + \begin{cases} 1 & \text{if } m = 0, \\ \frac{1}{2} & \text{otherwise,} \end{cases}$$

for $m = 0, 1, \dots, M$.

With Theorems 6 and 8 in place, we can now analyze the order of a given method:

Theorem 10. *The method has mean square global order p if*

$$\Phi(\tau)(h) = \varphi(\tau)(h) + \mathcal{O}(h^{p+\frac{1}{2}}) \text{ for all } \tau \in T \text{ with } \rho(\tau) \leq p, \quad (8a)$$

$$E\Phi(\tau)(h) = E\varphi(\tau)(h) + \mathcal{O}(h^{p+1}) \text{ for all } \tau \in T \text{ with } \rho(\tau) \leq p + \frac{1}{2}. \quad (8b)$$

Here, the $\mathcal{O}(\cdot)$ -notation refers to $h \rightarrow 0$ and, especially in (8a), to the L^2 -norm. The result (8) was first proved in [3].

We conclude this article with an example.

Example 11. We will apply Theorem 10 to the method given in Example 1. Using the expansion (for the manipulation of stochastic integrals, see e.g.

[7])

$$\begin{aligned} \int_0^h e^{(h-s)A} \star dW_1(s) &= \int_0^h 1 \star dW_1(s)A^0 + \int_0^h (h-s) \star dW_1(s)A^1 \\ &\quad + \int_0^h \frac{(h-s)^2}{2} \star dW_1(s)A^2 + \dots \\ &= I_{(1)}^*A^0 + I_{(10)}^*A^1 + I_{(100)}^*A^2 + \dots \end{aligned}$$

where $I_{(m_1 \dots m_n)}^* = \int_0^h \int_0^{s_1} \dots \int_0^{s_{n-1}} \star dW_{m_1}(s_n) \dots \star dW_{m_n}(s_1)$, and the similar expansion $\int_0^h e^{(h-s)A} W_1(s) \star dW_1(s) = I_{(11)}^*A^0 + I_{(110)}^*A^1 + \dots$ we obtain

$$\begin{aligned} z_1^{(0)} &= \int_0^h e^{(h-s)A} ds = hA^0 + \frac{h^2}{2}A^1 + \frac{h^3}{6}A^2 + \dots, \\ z_1^{(1)} &= \int_0^h e^{(h-s)A} \left(1 - \frac{W_1(s)}{\sqrt{h}}\right) \star dW_1(s) \\ &= \left(I_{(1)}^* - \frac{I_{(11)}^*}{\sqrt{h}}\right)A^0 + \left(I_{(10)}^* - \frac{I_{(110)}^*}{\sqrt{h}}\right)A^1 + \dots, \\ z_2^{(1)} &= \int_0^h e^{(h-s)A} \frac{W_1(s)}{\sqrt{h}} \star dW_1(s) = \frac{I_{(11)}^*}{\sqrt{h}}A^0 + \frac{I_{(110)}^*}{\sqrt{h}}A^1 + \dots \end{aligned}$$

We also have (with colors as in Example 7) $z_2^{(0)} = 0$, $\Phi_1(\bullet) = \Phi_2(\bullet) = \Phi_1(\circ) = \Phi_2(\circ) = \Phi_1(\circlearrowleft) = \Phi_2(\circlearrowleft) = 0$ and $\Phi_2(\circlearrowright) = \sqrt{h}$, resulting in the weight functions given in the following table:

τ	$\rho(\tau)$	$\varphi(\tau)(h)$	$\Phi(\tau)(h)$
	0.5	$I_{(1)}^*$	$z_1^{(1,0)} + z_2^{(1,0)} = I_{(1)}^*$
	1	h	$z_1^{(0,0)} + z_2^{(0,0)} = h$
		h	h
		$I_{(11)}^*$	$z_1^{(1,0)}\Phi_1(\circlearrowleft) + z_2^{(1,0)}\Phi_2(\circlearrowleft) = I_{(11)}^*$
	1.5	$I_{(10)}^*$	$z_1^{(0,0)}\Phi_1(\circlearrowright) + z_2^{(0,0)}\Phi_2(\circlearrowright) = 0$
		$hI_{(1)}^* - I_{(01)}^*$	$z_1^{(1,1)}\Phi_1(\emptyset) + z_2^{(1,1)}\Phi_2(\emptyset) = I_{(10)}^*$
		$I_{(01)}^*$	$z_1^{(1,0)}\Phi_1(\bullet) + z_2^{(1,0)}\Phi_2(\bullet) = 0$
		$I_{(01)}^*$	$z_1^{(1,0)}\Phi_1(\circ) + z_2^{(1,0)}\Phi_2(\circ) = 0$
		$I_{(01)}^*$	$z_1^{(1,0)}\Phi_1(\circlearrowleft) + z_2^{(1,0)}\Phi_2(\circlearrowleft) = 0$
		$\int_0^h W_1^2(s) \star dW_1(s)$	$z_1^{(1,0)}\Phi_1^2(\circlearrowright) + z_2^{(1,0)}\Phi_2^2(\circlearrowright) = \sqrt{h}I_{(11)}^*$
		$I_{(111)}^*$	$z_1^{(1,0)}\Phi_1(\circlearrowleft) + z_2^{(1,0)}\Phi_2(\circlearrowleft) = 0$

While the weight functions for the exact solution and numerical approximation of the order 1.5 trees do not coincide, their expectation values coincide for Itô integral but not for Stratonovich (when $\tau = \circlearrowleft$). Thus, the method given in Example 1 has mean square order 1 for the Itô case but 0.5 in the Stratonovich case.

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