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 Runge–Kutta integrators. Representing the exact and approximate solutions using B-series and rooted trees, we derive the order conditions for stochastic exponential Runge–Kutta 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

$$\mathrm{d}X(t) = \Big(AX(t)+g_0\big(X(t)\big)\Big)\mathrm{d}t+\sum_{m=1}^{M} g_m(X(t))\star\mathrm{d}W_m(t), \quad X(0)=x_0, \tag{1}$$

or in integral form

$$X(t) = \mathrm{e}^{tA}x_0 + \int_0^t \mathrm{e}^{(t-s)A}g_0(X(s))\mathrm{d}s + \sum_{m=1}^{M}\int_0^t \mathrm{e}^{(t-s)A}g_m(X(s))\star\mathrm{d}W_m(s), \tag{2}$$

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 Runge–Kutta integrators, see e.g. [1,5,10] 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 $g_m : \mathbb{R}^d \to \mathbb{R}^d$ are assumed to be sufficiently differentiable and to satisfy a Lipschitz and a linear growth condition. For Stratonovich SDEs, we require in addition that the coefficients 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 $\mathrm{d}t = \mathrm{d}W_0(t)$.

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

$$H_i = \mathrm{e}^{c_i hA} Y_n + \sum_{m=0}^{M} \sum_{j=1}^{\nu} Z_{ij}^{(m)}(A) \cdot g_m(H_j), \qquad i = 1, \ldots, \nu, \tag{3a}$$

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

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, and c_i are real coefficients, $i = 1, \ldots, \nu$. For vanishing A the method (3) reduces to a standard stochastic Runge–Kutta method. For an example of a 2-stage stochastic exponential Runge–Kutta method, see Example 11 below.

Although convergence and order results of specific stochastic exponential methods proposed in the literature are given, see for instance [1,5,10], there is to our knowledge up to now no general order and convergence theory for stochastic exponential Runge–Kutta methods. In this paper, such a theory is provided. The theory is derived based on a combination of the ideas of stochastic B-series and rooted trees developed in [6], and the similar ideas for deterministic exponential Runge–Kutta methods, as derived in [2,8].

2 Some notation, definitions and preliminary results on stochastic B-series

In Section 3 we will develop B-series for the exact solution of the stochastic differential equation (1) and stochastic exponential Runge–Kutta integrators of the form (3). For this, we will use the following definitions of the trees associated to (1), their corresponding elementary differentials and associated B-series.

Definition 1 (trees). The set of $M+2$-colored, rooted trees

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

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 $\tau = [\tau_1, \tau_2, \ldots, \tau_\kappa]_m$ be the tree formed by joining the subtrees $\tau_1, \tau_2, \ldots, \tau_\kappa$ 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 $\tau_1, \tau_2, \ldots, \tau_\kappa \in T \setminus \{\emptyset\}$, then $\tau = [\tau_1, \tau_2, \ldots, \tau_\kappa]_m \in T_m$ and $[\tau_1]_A \in T_A$,

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

Definition 2 (elementary differential). For a tree $\tau \in T$ the elementary differential is a mapping $F(\tau) : \mathbb{R}^d \to \mathbb{R}^d$ 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 $\tau_1, \tau_2, \ldots, \tau_\kappa \in T \setminus \{\emptyset\}$, then $F([\tau_1]_A)(x_0) = AF(\tau_1)(x_0)$ and

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

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

Now we give the definition of B-series.

Definition 3 (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 $\alpha : T \to \mathbb{Q}$ is given by

$$\alpha(\emptyset) = 1, \qquad \alpha(\bullet_m) = 1, \qquad \alpha(\bullet_A) = 1,$$
$$\alpha([\tau_1, \ldots, \tau_\kappa]_m) = \frac{1}{r_1! r_2! \cdots r_l!} \prod_{k=1}^{\kappa} \alpha(\tau_k), \quad \alpha([\tau_1]_A) = \alpha(\tau_1),$$

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

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

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

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

(i) $[\emptyset]_f \in U$, *and* $u = [\tau_1, \tau_2, \ldots, \tau_\kappa]_f \in U_f$,
(ii) $G([\emptyset]_f)(x_0) = f(x_0)$ *and*

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

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

for all $\tau_1, \tau_2, \dots, \tau_\kappa \in T \setminus \{\emptyset\}$ *and* $\kappa = 1, 2, \dots$.

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

Applying Lemma 4 to the functions g_m on the right hand side of (1) gives

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

where

$$\phi'_m(\tau)(h) = \begin{cases} 1 & \text{if } \tau = \bullet_m, \\ \prod_{k=1}^{\kappa} \phi(\tau_k)(h) & \text{if } \tau = [\tau_1, \dots, \tau_\kappa]_m \in T_m. \end{cases} \tag{6}$$

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

Definition 5 (order). The order $\rho(\tau)$ of a tree $\tau \in T$ is defined by

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

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

Assuming we have derived B-series representations for the exact solution of the stochastic differential equation (1) and stochastic exponential Runge–Kutta integrators of the form (3), we can now apply the following B-series criterion for the convergence of one–step methods, see [9,3,6], to determine the order of convergence of a given one-step approximation:

Theorem 6. *Assume that the exact solution of* (1) *has B-series representation* $X(h) = B(\varphi, x_0; h)$ *and a numerical approximation of it by a one-step method has B-series representation* $Y_{n+1} = B(\Phi, Y_n; h)$. *Then the method has mean square global order* p *if*

$$\Phi(\tau)(h) = \varphi(\tau)(h) + \mathcal{O}(h^{p+\frac{1}{2}}) \text{ for all } \tau \in T \text{ with } \rho(\tau) \le p, \tag{7a}$$

$$\mathbb{E}\Phi(\tau)(h) = \mathbb{E}\varphi(\tau)(h) + \mathcal{O}(h^{p+1}) \text{ for all } \tau \in T \text{ with } \rho(\tau) \le p + \frac{1}{2}. \tag{7b}$$

Here, the $\mathcal{O}(\cdot)$-notation refers to $h \to 0$ and, especially in (7a), to the L^2-norm.

3 Main results

In this section we will develop B-series for the exact solution of the stochastic differential equation (1) and of the stochastic exponential Runge–Kutta integrators of the form (3) such that Theorem (6) can be applied.

Theorem 7. *The solution $X(h)$ of the SDE* (1) *can be written as a B-series $B(\varphi, x_0; h)$ with $\varphi(\emptyset)(h) = 1$, $\varphi([\emptyset]_A^q)(h) = \frac{h^q}{q!}$,*

$$\varphi([[\tau_1, \dots, \tau_\kappa]_m]_A^q)(h) = \int_0^h \frac{(h-s)^q}{q!} \prod_{k=1}^{\kappa} \varphi(\tau_k)(s) \star \mathrm{d}W_m(s),$$

for $\tau_1, \dots, \tau_\kappa \in T$, $\kappa = 1, 2, \dots$, $q = 0, 1, \dots$ and $m = 0, \dots, M$, where $\tau_i \neq \emptyset$ for $i = 1, \dots, \kappa$ if $\kappa > 1$ and $[\hat{\tau}]_A^q = [\dots[[\hat{\tau}\overbrace{]_A]_A \dots]_A}^{q\text{-times}}$ for $\hat{\tau} \in T \setminus T_A$.

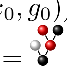
Proof. Write the exact solution $X(h)$ of (1) at $t = h$ as a B-series $B(\varphi, x_0; h)$. Substituting $X(h) = B(\varphi, x_0; h)$ in (2) and using (5) gives

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

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

$$B(\varphi, x_0; h) = x_0 + \sum_{q=1}^{\infty} \frac{h^q}{q!} A^q x_0$$
$$+ \sum_{m=0}^{M} \sum_{\hat{\tau} \in T_m} \alpha(\hat{\tau}) \sum_{q=0}^{\infty} \left(\int_0^h \frac{(h-s)^q}{q!} \varphi'_m(\hat{\tau})(s) \star \mathrm{d}W_m(s) \cdot A^q F(\hat{\tau})(x_0) \right). \quad (8)$$

Note that any tree $\tau \in T$ can be rewritten as $\tau = [\hat{\tau}]_A^q$ 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 $F([\hat{\tau}]_A^q) = A^q F(\hat{\tau})$ and $\alpha([\hat{\tau}]_A^q) = \alpha(\hat{\tau})$. Especially, for $\tau = [\emptyset]_A^q$ it holds that $\alpha(\tau) = 1$ and $F(\tau)(x_0) = A^q F(\emptyset) = A^q x_0$. Using (6) and the linear independence of the elementary differentials finishes the proof. □

Example 8. Let $\tau =$ , where the colors black, white and red correspond to the deterministic function g_0, the stochastic function g_1 and an application of the matrix A, respectively. Then $\alpha(\tau) = 1$, $F(\tau)(x_0) = g_0''(g_1, g_1''(Ax_0, g_0))(x_0)$ and $\varphi(\tau)(h) = \int_0^h \left(W_1(s) \int_0^s s_1^2 \star \mathrm{d}W_1(s_1)\right) \mathrm{d}s$. Note also that e.g. $\tau =$  $\notin T$ since it is impossible for node to have more than one branch.

Next we derive the B-series representation for one step of the stochastic exponential Runge–Kutta integrator (3).

Theorem 9. *Assume that the coefficients $Z_{ij}^{(m)}(A)$ and $z_i^{(m)}(A)$ can be expressed as power series of the form*

$$Z_{ij}^{(m)}(A) = \sum_{q=0}^{\infty} Z_{ij}^{(m,q)} A^q \qquad \text{and} \qquad z_i^{(m)}(A) = \sum_{q=0}^{\infty} z_i^{(m,q)} A^q, \tag{9}$$

for $i,j = 1,\dots,\nu$, and $m = 0,\dots,M$. Then the stage values H_i and the numerical solution Y_{n+1} defined by (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 $\Phi(\tau)(h)$,

$$\Phi_i(\emptyset) = \Phi(\emptyset) \equiv 1, \quad \Phi_i([\emptyset]_A^q)(h) = \frac{(c_i h)^q}{q!}, \quad \Phi([\emptyset]_A^q)(h) = \frac{h^q}{q!},$$

$$\Phi_i([[\tau_1,\dots,\tau_\kappa]_m]_A^q)(h) = \sum_{j=1}^{\nu} Z_{ij}^{(m,q)} \prod_{k=1}^{\kappa} \Phi_j(\tau_k)(h),$$

$$\Phi([[\tau_1,\dots,\tau_\kappa]_m]_A^q)(h) = \sum_{i=1}^{\nu} z_i^{(m,q)} \prod_{k=1}^{\kappa} \Phi_i(\tau_k)(h),$$

for $\tau_1,\dots,\tau_\kappa \in T$, $\kappa = 1,2,\dots$, $q = 0,1,\dots$ and $m = 0,\dots,M$, where $\tau_j \neq \emptyset$ for $j = 1,\dots,\kappa$ if $\kappa > 1$.

Proof. Write the stage values H_i and the approximation Y_{n+1} to the exact solution as B-series:

$$H_i = B(\Phi_i, Y_n; h), \qquad i = 1,\dots,\nu \qquad \text{and} \qquad Y_{n+1} = B(\Phi, Y_n; h). \tag{10}$$

Substituting (5) into (3) and using (9) 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 (10) and the linear independence of the elementary differentials yields the assertion. □

Remark 10. When A vanishes, all elementary differentials corresponding to trees in T_A are zero, and the above B-series theory agrees with the B-series theory developed in [6]. In the deterministic case, with $g_m = 0$ for $m \geq 1$, the elementary differentials corresponding to trees in T_m, $m \geq 1$, vanish, and our results agree with those given in [2,8].

We conclude this article with an example on how to apply the theorems of this section to decide the order of a given stochastic exponential integrator.

Example 11. We will apply Theorems 6, 7 and 9 to the 2-stage stochastic exponential time-differencing Runge–Kutta (SETDRK) method for $M = 1$ given by

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

where $t_{n+1} = t_n + h$. Using the expansion (for the manipulation of stochastic integrals, see e. g. [7])

$$
\begin{aligned}
\int_0^h \mathrm{e}^{(h-s)A} \star \mathrm{d}W_1(s) &= \int_0^h 1 \star \mathrm{d}W_1(s) A^0 + \int_0^h (h-s) \star \mathrm{d}W_1(s) A^1\\
&+ \int_0^h \frac{(h-s)^2}{2} \star \mathrm{d}W_1(s) A^2 + \dots\\
&= I^*_{(1)} A^0 + I^*_{(10)} A^1 + I^*_{(100)} A^2 + \dots
\end{aligned}
$$

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

$$
\begin{aligned}
z_1^{(0)} &= \int_0^h \mathrm{e}^{(h-s)A} \mathrm{d}s = hA^0 + \frac{h^2}{2} A^1 + \frac{h^3}{6} A^2 + \dots,\\
z_1^{(1)} &= \int_0^h \mathrm{e}^{(h-s)A} \left(1 - \frac{W_1(s)}{\sqrt{h}}\right) \star \mathrm{d}W_1(s)\\
&= \left(I_1^* - \frac{I^*_{(11)}}{\sqrt{h}}\right) A^0 + \left(I^*_{(10)} - \frac{I^*_{(110)}}{\sqrt{h}}\right) A^1 + \dots,\\
z_2^{(1)} &= \int_0^h \mathrm{e}^{(h-s)A} \frac{W_1(s)}{\sqrt{h}} \star \mathrm{d}W_1(s) = \frac{I^*_{(11)}}{\sqrt{h}} A^0 + \frac{I^*_{(110)}}{\sqrt{h}} A^1 + \dots.
\end{aligned}
$$

We also have (with colors as in Example 8) $z_2^{(0)} = 0$, $\Phi_1(\bullet) = \Phi_2(\bullet) = \Phi_1(\bullet) = \Phi_2(\bullet) = \Phi_1(\circ) = \Phi_1(\circ\circ\circ) = \Phi_2(\circ\circ\circ) = 0$ and $\Phi_2(\circ) = \sqrt{h}$, resulting in the weight functions given in Table **??**. While the weight functions for the exact solution and the numerical approximation of the order 1.5 trees do not coincide, their expectation values coincide in case of Itô integrals but not for Stratonovich integrals (when $\tau = \circ\circ\circ$). Thus, by Theorem 7 the above method has mean square order 1 in the Itô case but only 0.5 in the Stratonovich case.

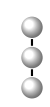
τ	$\rho(\tau)$	$\varphi(\tau)(h)$	$\Phi(\tau)(h)$
	0.5	$I^*_{(1)}$	$z_1^{(1,0)} + z_2^{(1,0)} = I^*_{(1)}$
	1	h	$z_1^{(0,0)} + z_2^{(0,0)} = h$
		h	h
		$I^*_{(11)}$	$z_1^{(1,0)}\Phi_1($$) + z_2^{(1,0)}\Phi_2($$) = I^*_{(11)}$
	1.5	$I^*_{(10)}$	$z_1^{(0,0)}\Phi_1($$) + z_2^{(0,0)}\Phi_2($$) = 0$
		$hI^*_{(1)} - I^*_{(01)}$	$z_1^{(1,1)}\Phi_1(\emptyset) + z_2^{(1,1)}\Phi_2(\emptyset) = I^*_{(10)}$
		$I^*_{(01)}$	$z_1^{(1,0)}\Phi_1($$) + z_2^{(1,0)}\Phi_2($$) = 0$
		$I^*_{(01)}$	$z_1^{(1,0)}\Phi_1($$) + z_2^{(1,0)}\Phi_2($$) = 0$
		$\int_0^h W_1^2(s) \star \mathrm{d}W_1(s)$	$z_1^{(1,0)}\Phi_1^2($$) + z_2^{(1,0)}\Phi_2^2($$) = \sqrt{h}I^*_{(11)}$
		$I^*_{(111)}$	$z_1^{(1,0)}\Phi_1($$) + z_2^{(1,0)}\Phi_2($$) = 0$

Table 1. Trees, corresponding order and weight functions for Example 11.

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