Derivation of optimal stochastic Runge-Kutta methods with exotic and decorated Butcher series for the weak integration of stochastic dynamics

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Abstract

The design of numerical integrators for solving stochastic dynamics with high weak order relies on tedious calculations and is subject to a high number of order conditions. The original approaches from the literature consider strong approximations and adapt them for the weak approximation by replacing the iterated stochastic integrals by appropriate random variables. The methods obtained this way are sub-optimal in their number of function evaluations and the analysis of order conditions is unnecessarily complicated. We provide in this paper a novel approach, relying on well-chosen sets of random Runge-Kutta coefficients, that greatly reduce the number of order conditions. The approach is successfully applied to the creation of a collection of new stochastic Runge-Kutta methods of second weak order with an optimal number of function evaluations and a smaller number of random variables. The efficiency of the new methods is confirmed with numerical experiments and a modern algebraic approach using Hopf algebras is provided for the derivation and the study of the order conditions.

Keywords: stochastic differential equations, stochastic Runge-Kutta methods, order conditions, Butcher series, exotic forests, exotic series, decorated forests, Hopf algebra.

AMS subject classification (2020): 60H35, 65L06, 41A58, 16T05.

1 Introduction

We present new approaches for the high order numerical integration in the weak sense of general Itô stochastic differential equations of the form

$$dX(t) = f^0(X(t))dt + \sum_{p=1}^{m} f^p(X(t))dW^p(t), \quad X(0) = X_0, \tag{1.1}$$

and SDEs with Stratonovich noise

$$dX(t) = f^0(X(t))dt + \sum_{p=1}^{m} f^p(X(t)) \circ dW^p(t), \quad X(0) = X_0, \tag{1.2}$$

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where the f^p are smooth Lipschitz vector fields and the W^p are standard independent Brownian motions defined on a probability space fulfilling the standard assumptions.

The first approaches for the numerical approximation with high weak order of (1.1) and (1.2) were derived from strong methods, that are, pathwise approximations. This resulted in unnecessarily complicated methods and tedious order conditions and analysis. The first stochastic Runge-Kutta methods of second weak order had a number of function evaluations in the order of m^2 (see [70, 43, 80, 46, 29]), where one could theoretically expect the optimal number of $2m+2$ function evaluations (at least in the Itô case). The methods were simplified using a B-series approach in [74, 75] to obtain a number of function evaluations that is affine in m. The methods were further simplified in [79] in the Itô case, without reaching the optimal number of function evaluations. In the present paper, we focus on deriving weak approximations without relying on any intermediate strong approximation, and we provide new methods with the optimal number of function evaluations for general Itô and Stratonovich SDEs (1.1)-(1.2). We consider the following general class of stochastic Runge-Kutta methods, in the spirit of the methods introduced in [73]:

$$\begin{aligned} H_i^p &= X_n + h\sum_{j=1}^{s} Z_{i,j}^{p,0} f^0(H_j^0) + \sqrt{h}\sum_{j=1}^{s}\sum_{q=1}^{m} Z_{i,j}^{p,q} f^q(H_j^q), \quad i=1,\dots,s,\\ X_{n+1} &= X_n + h\sum_{i=1}^{s} z_i^0 f^0(H_i^0) + \sqrt{h}\sum_{i=1}^{s}\sum_{p=1}^{m} z_i^p f^p(H_i^p), \end{aligned} \tag{1.3}$$

with the Runge-Kutta coefficients $z^p \in \mathbb{R}^s$ and $Z^{p,q} \in \mathbb{R}^{s,s}$ being random variables and the dependency in n of the H_i^p being omitted for simplicity. We follow the standard approach for the design of high weak order methods with the Milstein methodology [63], which uses local estimates. Under standard bounded moments properties, one typically obtains global weak order (see, for instance, the textbooks [43, 64, 65] and references therein). The focus in this paper is on the design of new high-order methods for the weak error, with the minimal number of function evaluations, and on the development of the algebraic foundations underlying stochastic numerics of general SDEs.

The calculation of order conditions is tedious and requires the use of Butcher series techniques. In the last decades, several works extended the standard Butcher-series [18, 36] (see also the textbooks [35, 19, 20] and the review [62]) to the stochastic context. Burrage and Burrage [13, 14] and Komori, Mitsui and Sugiura [48] introduced stochastic B-series in the context of strong convergence. The analysis was later extended to stochastic Runge-Kutta methods by Rößler [71, 72, 73, 76, 77], Komori [45, 46, 47] and Debrabant and Kværnø [26, 25, 27, 28, 4] for the creation of high order weak and strong integrators. We take inspiration from the previous tree formalisms and use decorated forests, where we enforce the forests to be independent of the dimension of the problem and the number of noises, so that one order condition corresponds to one forest only. The decorated forests formalism allows to represent the Taylor expansion of the numerical methods and we shall see that a smaller formalism of exotic forests is sufficient to write the Taylor expansion of the exact flow. In the context of additive noise, the formalism of exotic series was introduced by Bronasco, Laurent, and Vilmart in [55, 51, 9] for the creation of integrators for solving stochastic dynamics with high order in the weak sense and for the invariant measure (see also, for instance, [8, 57, 1, 2, 58]). This formalism, combined with the aromatic B-series [22, 41, 6, 53, 52] and the LB-series [40], was extended in [56, 11] for the extrinsic and intrinsic numerical integration of SDEs on manifolds, and analogous algebraic formalisms are now used in a variety of different fields [3, 31, 7]. The fundamental geometric and algebraic properties of the exotic formalism of trees were later studied in [10, 54] (see also [21, 61, 66, 5] in the deterministic setting). The exotic and decorated series formalism conveniently unifies the previous forests formalisms for the study of Euclidean SDEs with multiplicative noise and proves to be a crucial tool for simplifying the tedious calculation. We adapt the expansions of the exact and numerical flows in exotic and decorated series, uncover the combinatorial links between the two types of expansions, and use a modern combinatorial approach to study the order conditions and the algebraic properties of the Taylor expansions of flows.

The article is organised as follows. We derive in Section 2 the general order conditions of stochastic Runge-Kutta methods and present a new set of random Runge-Kutta coefficients that reduces considerably the number of order conditions. A collection of new methods with optimal number of stages and function evaluations is presented in Section 3. We propose numerical illustrations to confirm our theoretical findings in Section 4. The calculation of order conditions and their algebraic study with exotic and decorated forests is then detailed in Section 5. We discuss outlooks and future works in Section 6.

2 Reduced order conditions for stochastic Runge-Kutta methods

In order to construct methods whose coefficients have to fulfill comparatively few order conditions for weak order two, we will first derive general order conditions and then consider a well chosen ansatz for the coefficients that splits the role of the Runge-Kutta coefficients and the random variables. This will then allow us to obtain a collection of new stochastic Runge-Kutta integrators with minimal number of function evaluations.

2.1 General order conditions for weak order two

Let $\mathcal{C}_P^\infty(\mathbb{R}^d)$ be the space of smooth functions ϕ that satisfy polynomial estimates of the form

$$|\phi^{(k)}(x)| \leqslant C(1+|x|^K), \quad k=0,1,\dots.$$

Similarly, let $\mathfrak{X}_P(\mathbb{R}^d)$ be the space of globally Lipschitz vector fields whose components lie in $\mathcal{C}_P^\infty(\mathbb{R}^d)$. In all that follows, we assume for simplicity that $f^p \in \mathfrak{X}_P(\mathbb{R}^d)$ and we use the following notation for the i-th component of the partial derivatives of f^p:

$$f^{p,i}_{j_1\dots j_k}(x) := \frac{\partial f^{p,i}}{\partial x_{j_1}\dots \partial x_{j_k}}(x).$$

As our approach focuses on the high order analysis of numerical integrators, we use smooth maps for simplicity and refer to [65] for weaker assumptions.

A one-step numerical integrator $X_{n+1} = \psi_h(X_n)$ for solving (1.1)/(1.2) is of local weak order p if for $h \leqslant h_0$ small enough and all $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d)$, the following estimate is satisfied

$$|\mathbb{E}[\phi(X(h))|X(0)=x] - \mathbb{E}[\phi(X_1)|X_0=x]| \leqslant C(1+|x|^K)h^{p+1}.$$

For a test function $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d)$, a weak approximation focuses on approaching $u(x,t) = \mathbb{E}[\phi(X(t))|X(0)=x]$. A classical tool for the study of equations (1.1)/(1.2) is the backward Kolmogorov equation (see, for instance, [37, 65, 33, 1, 49, 50, 51]). It states that $u(x,t)$ solves the following deterministic parabolic PDE in $\mathbb{R}^d$,

$$\frac{\partial u}{\partial t} = \mathcal{L}u, \quad u(x,0)=\phi(x), \quad x\in\mathbb{R}^d, \quad t>0, \tag{2.1}$$

where the generator $\mathcal{L}$ is given for the Itô SDE (1.1) by

$$\mathcal{L}_{\text{Itô}}\phi = \sum_{i=1}^{d} \phi_i f^{0,i} + \frac{1}{2} \sum_{i,j=1}^{d} \sum_{p=1}^{m} \phi_{ij}(f^{p,i}, f^{p,j}),$$

and for the Stratonovich SDE (1.2) by

$$\mathcal{L}_{\text{Strato}}\phi = \sum_{i=1}^{d} \phi_i f^{0,i} + \frac{1}{2} \sum_{i,j=1}^{d} \sum_{p=1}^{m} \phi_{ij}(f^{p,i}, f^{p,j}) + \frac{1}{2} \sum_{i,j=1}^{d} \sum_{p=1}^{m} \phi_i f_j^{p,i} f^{p,j}.$$

Using (2.1), the weak quantity $u(x,h)$ thus has the following expansion for all p:

$$u(x,h) = \phi(x) + h\mathcal{L}\phi(x) + \cdots + \frac{h^p}{p!}\mathcal{L}^p\phi(x) + h^{p+1}R_p\phi(x), \quad |R_p\phi(x)| \leqslant C(1+|x|^K). \quad (2.2)$$

Let us now consider the Taylor expansion of $\mathbb{E}[\phi(X_1)|X_0 = x]$. We assume the following natural assumption on the Runge-Kutta coefficients, which ensures that the method (1.3) has bounded moments of all order and that non-integer powers in their Taylor expansion vanish.

Assumption 2.1. *For any bijection $\sigma\colon \{0,\dots,m\} \to \{0,\dots,m\}$ with $\sigma(0) = 0$, the coefficients of the numerical method* (1.3) *satisfy for $\alpha, \beta \in \mathbb{N}$, $p_{l_1}, q_{l_2}, r_{l_2} \in \{0,1,\dots,m\}$ and $i_{l_1}, j_{l_2}, k_{l_2} \in \{1,\dots,s\}$ for $l_1 \in \{1,\dots,\alpha\}$, $l_2 \in \{1,\dots,\beta\}$*

$$\mathbb{E}[z_{i_1}^{\sigma(p_1)} \dots z_{i_\alpha}^{\sigma(p_\alpha)} Z_{j_1,k_1}^{\sigma(q_1),\sigma(r_1)} \dots Z_{j_\beta,k_\beta}^{\sigma(q_\beta),\sigma(r_\beta)}] = \mathbb{E}[z_{i_1}^{p_1} \dots z_{i_\alpha}^{p_\alpha} Z_{j_1,k_1}^{q_1,r_1} \dots Z_{j_\beta,k_\beta}^{q_\beta,r_\beta}] < \infty,$$

and the following moments vanish:

$$\mathbb{E}[z_{i_1}^{p_1} \dots z_{i_\alpha}^{p_\alpha} Z_{j_1,k_1}^{q_1,r_1} \dots Z_{j_\beta,k_\beta}^{q_\beta,r_\beta}] = 0 \text{ if } |\{p_i \neq 0\}| + |\{r_i \neq 0\}| \text{ is odd.}$$

Under Assumption 2.1, the stochastic Runge-Kutta methods satisfy a similar expansion to (2.2) [63]:

$$\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{A}_1\phi(x) + \cdots + h^p\mathcal{A}_p\phi(x) + h^{p+1}R_p\phi(x), \quad (2.3)$$

where the remainder satisfies $|R_p\phi(x)| \leqslant C(1+|x|^K)$ and the $\mathcal{A}_i$ are linear differential operators with coefficients depending smoothly on the f^p and their partial derivatives (that is, the coefficients are polynomials in the coordinates of the infinite jet space over the f^p [44, 66]). If the expansions (2.2) and (2.3) match up to order p, we obtain a method of (at least) local weak order p. Sufficient conditions for global weak order p are given by the following result.

Proposition 2.2 ([63, 65])**.** *Consider a one-step integrator that has a Taylor expansion* (2.3) *that satisfies*

$$\mathcal{A}_j = \frac{\mathcal{L}^j}{j!}, \quad j = 1,\dots,p. \quad (2.4)$$

Assume further that the integrator has bounded moments of any order,

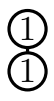
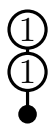
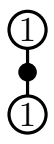
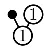
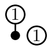
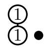
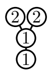
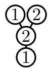
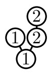
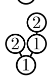
$$\sup_{n \geqslant 0} \mathbb{E}[|X_n|^{2k}] < \infty.$$

Then, the method has global weak order p, that is, for $T > 0$, for all $h \leqslant h_0$ small enough with $Nh = T$, for all test functions $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d)$ and initial conditions X_0, there exists $C > 0$ such that

$$|\mathbb{E}[\phi(X_N)] - \mathbb{E}[\phi(X(T))]| \leqslant Ch^p.$$

The derivation of order conditions is straightforward thanks to Proposition 2.2. However, it relies on the explicit knowledge of the operators $\mathcal{A}_j$ and $\mathcal{L}^j$. As the calculations get tedious, we use algebraic objects to derive the explicit combinatorics.

Theorem 2.3. *Consider a stochastic Runge-Kutta method of the form* (1.3) *with coefficients that satisfy Assumption 2.1. Assume further that the exotic and Isserlis order conditions given in Tables 1 and 2 are satisfied for* $p_1, p_2 \in \{1, \dots, m\}$*, that is, for each forest, the Runge-Kutta coefficient is equal to the Itô (respectively Stratonovich) coefficient. Then, the method is of global weak order two for solving* (1.1) *(respectively* (1.2)*).*

Ex. forest	Differential	RK coefficient ($p_1 \neq p_2$)	Itô	Str.
	$\phi_i f^{0,i}$	$\mathbb{E}[z_i^0]$	1	1
	$\phi_{ij} f^{p_1,i} f^{p_1,j}$	$\mathbb{E}[z_i^{p_1} z_j^{p_1}]$	1	1
	$\phi_i f_{i_1}^{p_1,i} f^{p_1,i_1}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1}]$	0	$\frac{1}{2}$
	$\phi_i f_{i_1}^{0,i} f^{0,i_1}$	$\mathbb{E}[z_i^0 Z_{i,i_1}^{0,0}]$	$\frac{1}{2}$	$\frac{1}{2}$
	$\phi_{ij} f^{0,i} f^{0,j}$	$\mathbb{E}[z_i^0 z_j^0]$	1	1
	$\phi_i f_{i_1}^{0,i} f_{i_2}^{p_1,i_1} f^{p_1,i_2}$	$\mathbb{E}[z_i^0 Z_{i,i_1}^{0,p_1} Z_{i_1,i_2}^{p_1,p_1}]$	0	$\frac{1}{4}$
	$\phi_i f_{i_1}^{p_1,i} f_{i_2}^{0,i_1} f^{p_1,i_2}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,0} Z_{i_1,i_2}^{0,p_1}]$	0	0
	$\phi_i f_{i_1}^{p_1,i} f_{i_2}^{p_1,i_1} f^{0,i_2}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i_1,i_2}^{p_1,0}]$	0	$\frac{1}{4}$
	$\phi_i f_{i_1 i_2}^{0,i} f^{p_1,i_1} f^{p_1,i_2}$	$\mathbb{E}[z_i^0 Z_{i,i_1}^{0,p_1} Z_{i,i_2}^{0,p_1}]$	$\frac{1}{2}$	$\frac{1}{2}$
	$\phi_i f_{i_1 i_2}^{p_1,i} f^{0,i_1} f^{p_1,i_2}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,0} Z_{i,i_2}^{p_1,p_1}]$	0	$\frac{1}{4}$
	$\phi_{ij} f_{i_1}^{0,i} f^{p_1,i_1} f^{p_1,j}$	$\mathbb{E}[z_i^0 Z_{i,i_1}^{0,p_1} z_j^{p_1}]$	$\frac{1}{2}$	$\frac{1}{2}$
	$\phi_{ij} f_{i_1}^{p_1,i} f^{0,i_1} f^{p_1,j}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,0} z_j^{p_1}]$	$\frac{1}{2}$	$\frac{1}{2}$
	$\phi_{ij} f_{i_1}^{p_1,i} f^{p_1,i_1} f^{0,j}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} z_j^0]$	0	$\frac{1}{2}$
	$\phi_{ijk} f^{0,i} f^{p_1,j} f^{p_1,k}$	$\mathbb{E}[z_i^0 z_j^{p_1} z_k^{p_1}]$	1	1
	$\phi_i f_{i_1}^{p_1,i} f_{i_2}^{p_1,i_1} f_{i_3}^{p_2,i_2} f^{p_2,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i_1,i_2}^{p_1,p_2} Z_{i_2,i_3}^{p_2,p_2}]$	0	$\frac{1}{8}$
	$\phi_i f_{i_1}^{p_1,i} f_{i_2}^{p_2,i_1} f_{i_3}^{p_1,i_2} f^{p_2,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} Z_{i_1,i_2}^{p_2,p_1} Z_{i_2,i_3}^{p_1,p_2}]$	0	0
	$\phi_i f_{i_1}^{p_1,i} f_{i_2}^{p_2,i_1} f_{i_3}^{p_2,i_2} f^{p_1,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} Z_{i_1,i_2}^{p_2,p_2} Z_{i_2,i_3}^{p_2,p_1}]$	0	0
	$\phi_i f_{i_1}^{p_1,i} f_{i_2 i_3}^{p_1,i_1} f^{p_2,i_2} f^{p_2,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i_1,i_2}^{p_1,p_2} Z_{i_1,i_3}^{p_1,p_2}]$	0	$\frac{1}{4}$
	$\phi_i f_{i_1}^{p_1,i} f_{i_2 i_3}^{p_2,i_1} f^{p_1,i_2} f^{p_2,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} Z_{i_1,i_2}^{p_2,p_1} Z_{i_1,i_3}^{p_2,p_2}]$	0	0
	$\phi_i f_{i_1 i_2}^{p_1,i} f^{p_1,i_1} f_{i_3}^{p_2,i_2} f^{p_2,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i,i_2}^{p_1,p_2} Z_{i_2,i_3}^{p_2,p_2}]$	0	$\frac{1}{8}$
	$\phi_i f_{i_1 i_2}^{p_1,i} f^{p_2,i_1} f_{i_3}^{p_1,i_2} f^{p_2,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} Z_{i,i_2}^{p_1,p_1} Z_{i_2,i_3}^{p_1,p_2}]$	0	$\frac{1}{4}$

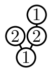
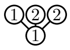
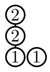
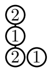
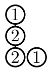
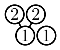
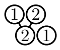
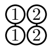
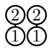
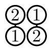
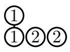
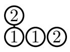
	$\phi_i f^{p_1,i}_{i_1 i_2} f^{p_2,i_1} f^{p_2,i_2}_{i_3} f^{p_1,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} Z_{i,i_2}^{p_1,p_2} Z_{i_2,i_3}^{p_2,p_1}]$	0	0
	$\phi_i f^{p_1,i}_{i_1 i_2 i_3} f^{p_1,i_1} f^{p_2,i_2} f^{p_2,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i,i_2}^{p_1,p_2} Z_{i,i_3}^{p_1,p_2}]$	0	$\frac{1}{4}$
	$\phi_{ij} f^{p_1,i}_{i_1} f^{p_2,i_1}_{i_2} f^{p_2,i_2} f^{p_1,j}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} Z_{i_1,i_2}^{p_2,p_2} z_j^{p_1}]$	0	$\frac{1}{4}$
	$\phi_{ij} f^{p_2,i}_{i_1} f^{p_1,i_1}_{i_2} f^{p_2,i_2} f^{p_1,j}$	$\mathbb{E}[z_i^{p_2} Z_{i,i_1}^{p_2,p_1} Z_{i_1,i_2}^{p_1,p_2} z_j^{p_1}]$	0	0
	$\phi_{ij} f^{p_2,i}_{i_1} f^{p_2,i_1}_{i_2} f^{p_1,i_2} f^{p_1,j}$	$\mathbb{E}[z_i^{p_2} Z_{i,i_1}^{p_2,p_2} Z_{i_1,i_2}^{p_2,p_1} z_j^{p_1}]$	0	$\frac{1}{4}$
	$\phi_{ij} f^{p_1,i}_{i_1 i_2} f^{p_2,i_1} f^{p_2,i_2} f^{p_1,j}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} Z_{i,i_2}^{p_1,p_2} z_j^{p_1}]$	$\frac{1}{2}$	$\frac{1}{2}$
	$\phi_{ij} f^{p_2,i}_{i_1 i_2} f^{p_1,i_1} f^{p_2,i_2} f^{p_1,j}$	$\mathbb{E}[z_i^{p_2} Z_{i,i_1}^{p_2,p_1} Z_{i,i_2}^{p_2,p_2} z_j^{p_1}]$	0	$\frac{1}{4}$
	$\phi_{ij} f^{p_1,i}_{i_1} f^{p_1,i_1} f^{p_2,j}_{j_1} f^{p_2,j_1}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} z_j^{p_2} Z_{j,j_1}^{p_2,p_2}]$	0	$\frac{1}{4}$
	$\phi_{ij} f^{p_1,i}_{i_1} f^{p_2,i_1} f^{p_1,j}_{j_1} f^{p_2,j_1}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} z_j^{p_1} Z_{j,j_1}^{p_1,p_2}]$	$\frac{1}{2}$	$\frac{1}{2}$
	$\phi_{ij} f^{p_1,i}_{i_1} f^{p_2,i_1} f^{p_2,j}_{j_1} f^{p_1,j_1}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} z_j^{p_2} Z_{j,j_1}^{p_2,p_1}]$	0	0
	$\phi_{ijk} f^{p_1,i}_{i_1} f^{p_1,i_1} f^{p_2,j} f^{p_2,k}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} z_j^{p_2} z_k^{p_2}]$	0	$\frac{1}{2}$
	$\phi_{ijk} f^{p_1,i}_{i_1} f^{p_2,i_1} f^{p_1,j} f^{p_2,k}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_2} z_j^{p_1} z_k^{p_2}]$	$\frac{1}{2}$	$\frac{1}{2}$
	$\phi_{ijkl} f^{p_1,i} f^{p_1,j} f^{p_2,k} f^{p_2,l}$	$\mathbb{E}[z_i^{p_1} z_j^{p_1} z_k^{p_2} z_l^{p_2}]$	1	1

Table 1: Exotic order conditions of stochastic Runge-Kutta method of the form (1.3) up to weak order 2. The order conditions do not depend on the dimension of the problem and on the number of noise terms. The sums on all involved indices except p_1, p_2 are omitted for conciseness.

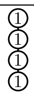
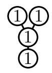
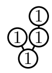
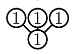
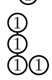
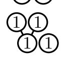
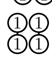
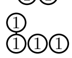
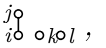
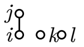
Dec. forest	Differential	RK coefficient	Itô	Str.
	$\phi_i f^{p_1,i}_{i_1} f^{p_1,i_1}_{i_2} f^{p_1,i_2}_{i_3} f^{p_1,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i_1,i_2}^{p_1,p_1} Z_{i_2,i_3}^{p_1,p_1}]$	0	$\frac{1}{8}$
	$\phi_i f^{p_1,i}_{i_1} f^{p_1,i_1}_{i_2 i_3} f^{p_1,i_2} f^{p_1,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i_1,i_2}^{p_1,p_1} Z_{i_1,i_3}^{p_1,p_1}]$	0	$\frac{1}{4}$
	$\phi_i f^{p_1,i}_{i_1 i_2} f^{p_1,i_1} f^{p_1,i_2}_{i_3} f^{p_1,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i,i_2}^{p_1,p_1} Z_{i_2,i_3}^{p_1,p_1}]$	0	$\frac{3}{8}$
	$\phi_i f^{p_1,i}_{i_1 i_2 i_3} f^{p_1,i_1} f^{p_1,i_2} f^{p_1,i_3}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i,i_2}^{p_1,p_1} Z_{i,i_3}^{p_1,p_1}]$	0	$\frac{3}{4}$
	$\phi_{ij} f^{p_1,i}_{i_1} f^{p_1,i_1}_{i_2} f^{p_1,i_2} f^{p_1,j}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i_1,i_2}^{p_1,p_1} z_j^{p_1}]$	0	$\frac{1}{2}$
	$\phi_{ij} f^{p_1,i}_{i_1 i_2} f^{p_1,i_1} f^{p_1,i_2} f^{p_1,j}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} Z_{i,i_2}^{p_1,p_1} z_j^{p_1}]$	$\frac{1}{2}$	1
	$\phi_{ij} f^{p_1,i}_{i_1} f^{p_1,i_1} f^{p_1,j}_{j_1} f^{p_1,j_1}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} z_j^{p_1} Z_{j,j_1}^{p_1,p_1}]$	$\frac{1}{2}$	$\frac{3}{4}$
	$\phi_{ijk} f^{p_1,i}_{i_1} f^{p_1,i_1} f^{p_1,j} f^{p_1,k}$	$\mathbb{E}[z_i^{p_1} Z_{i,i_1}^{p_1,p_1} z_j^{p_1} z_k^{p_1}]$	1	$\frac{3}{2}$
	$\phi_{ijkl} f^{p_1,i} f^{p_1,j} f^{p_1,k} f^{p_1,l}$	$\mathbb{E}[z_i^{p_1} z_j^{p_1} z_k^{p_1} z_l^{p_1}]$	3	3

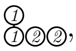
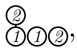
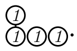
Table 2: Isserlis order conditions of stochastic Runge-Kutta method of the form (1.3) for weak order 2. The order conditions do not depend on the dimension of the problem and on the number of noise terms. The sums on all involved indices except p_1 are omitted for conciseness.

The weak order conditions are traditionally derived by use of Butcher series as explained in [72, 73, 26]. The order conditions presented in Tables 1 and 2 are based on the more recent formalism of exotic forests [55]. This formalism reduces the complexity in the sense that all redundant order conditions are removed, and terms for which the pair of colors (representing the different Brownian motions) appears several times are given as separate forests. Thus each forest represents exactly one unique order condition. Note that the invariance in law of the moments of the Runge-Kutta coefficients when applying permutations, as prescribed in Assumption 2.1, is key to the representation of flows with tree structures. We emphasize that the algebraic and combinatorial details underlying the computation of the order conditions can be skipped by the reader interested only in the creation of numerical methods of high weak order. The proof of Theorem 2.3 and the study of the algebraic structures underlying stochastic numerics are postponed to Section 5.

Remark 2.4. *The previous stochastic B-series formalisms [72] typically rely on forests of the form*  *, where i, j, k, l range from 1 to m. The random variable corresponding to this forest will satisfy*

$$\frac{1}{h^2}\mathbb{E}[\int_0^h W^j \star dW^i \int_0^h dW^k \int_0^h dW^l] = \begin{cases} \textit{Itô/Strat.} & \\ 0 \;/\; \frac{1}{2} & \textit{if } i=j,\ k=l \textit{ and } i \neq l, \\ \frac{1}{2} \;/\; \frac{1}{2} & \textit{if } i=l,\ j=k \textit{ and } i \neq k, \\ 1 \;/\; \frac{3}{2} & \textit{if } i=j=k=l, \\ 0 \;/\; 0 & \textit{otherwise.} \end{cases}$$

Thus, the m^4 forests of the form  *generate three non-trivial order conditions under Assumption 2.1. Using the exotic forests formalism, these will appear as three different decorated forests, given by*

$\pi_{d_1} =$ , $\quad \pi_{d_2} =$ , $\quad \pi_{d_3} =$ .

The weak order condition corresponding to π_{d_1} is then

$$\mathbb{E}[\sum_{i,j,k,l} z_i^{p_1} Z_{i,j}^{p_1,p_1} z_k^{p_2} z_l^{p_2}] = \begin{cases} 0 & \textit{Itô} \\ \frac{1}{2} & \textit{Stratonovich} \end{cases}$$

The other two conditions can be found in Tables 1 and 2.

We say that order conditions of the form $\sum \mathbb{E}[\dots] = 0$ are *potentially superfluous* as they can potentially be satisfied automatically with a particular choice of random coefficients. Note that there is a relatively high number of these order conditions in the Itô case. In the next section, we propose a carefully chosen ansatz for the Runge-Kutta coefficients so that most potentially superfluous order conditions are satisfied automatically.

2.2 Reduced order conditions for Itô SDEs

We consider coefficients of the form

$$\begin{aligned} z^0 &= \alpha\theta_0, & z^p &= \beta\theta_p, \\ Z^{0,0} &= A^0\Theta_{0,0}, & Z^{0,q} &= B^0\Theta_{0,q}, \\ Z^{p,0} &= A^1\Theta_{p,0}, & Z^{p,q} &= B^1\Theta_{p,q}. \end{aligned} \tag{2.5}$$

where $\alpha \in \mathbb{R}^{s_1}$, $\beta \in \mathbb{R}^{s_2}$, $A^0 \in \mathbb{R}^{s_1,s_1}$, $A^1 \in \mathbb{R}^{s_2,s_1}$, $B^0 \in \mathbb{R}^{s_1,s_2}$, $B^1 \in \mathbb{R}^{s_2,s_2}$ and (s_1, s_2) is the number of stages for the deterministic and stochastic parts of the method. This choice of coefficients fits in the class of methods (1.3) by choosing $s = \max(s_1, s_2)$ and filling the missing entries of the Runge-Kutta coefficients by zeros. The standard methodology mimicking strong expansions and using weak approximations of iterated stochastic integrals is tedious and yields unnecessarily complicated methods. We simplify this approach by instead choosing random variables such that most potentially superfluous order conditions are satisfied automatically. Let η_p, $p = 0, \ldots, m$, and θ_p, $p = 1, \ldots, m$, be discrete independent random variables satisfying

$$\mathbb{P}(\eta_p = \pm 1) = \frac{1}{2}, \quad \mathbb{P}(\theta_p = \pm\sqrt{2+\sqrt{3}}) = \frac{3-\sqrt{3}}{12}, \quad \mathbb{P}(\theta_p = \pm\sqrt{2-\sqrt{3}}) = \frac{3+\sqrt{3}}{12}.$$

Define for $c \in (0, \frac{1}{2})$

$$\begin{aligned} &\theta_0 = 1, && \Theta_{0,p} = \theta_p + \eta_p\sqrt{\tfrac{1}{2c} - 1}, && \Theta_{p,q} = \theta_q(1+\eta_0), \quad q > p \geqslant 1, \\ &\Theta_{0,0} = 1, && \Theta_{p,0} = 1 - \eta_p\theta_p\sqrt{\tfrac{2c}{1-2c}}, && \Theta_{p,q} = \theta_q(1-\eta_0), \quad 1 \leqslant q < p, \\ &\Theta_{p,p} = -3\theta_p + \theta_p^3. \end{aligned} \tag{2.6}$$

These random variables do, for c not too close to $\{0, \frac{1}{2}\}$, not impact stability more than using Gaussians or iterated stochastic integrals as their moments are of similar (if not smaller) amplitude.

Using the ansatz (2.5) and the random variables (2.6) in Theorem 2.3, Assumption 2.1 is automatically satisfied and we obtain the following result, where most potentially superfluous order conditions vanish, leaving us with 9 reduced order conditions for weak order two. By choosing carefully the random variables, we got rid of most of the 59 order conditions of [30] and improved further on the 15 order conditions of [79].

Theorem 2.5. *The reduced order conditions for weak order one for solving the Itô SDE* (1.1) *by method* (1.3) *with method coefficients* (2.5)*, random variables* (2.6) *and* $c \in (0, \frac{1}{2})$ *are:*

1. $\alpha^\top \mathbb{1} = 1$, *2.* $\beta^\top \mathbb{1} = 1$,

and the additional conditions for weak order two are:

3. $\alpha^\top A^0 \mathbb{1} = \frac{1}{2}$,
4. $\alpha^\top B^0 \mathbb{1} = \frac{1}{2}$,
5. $\alpha^\top (B^0 \mathbb{1})^{\odot 2} = c$,
6. $\beta^\top A^1 \mathbb{1} = \frac{1}{2}$,
7. $\beta^\top B^1 \mathbb{1} = \frac{1}{2}$,
8. $\beta^\top (B^1 \mathbb{1})^{\odot 2} = \frac{1}{4}$,
9. $\beta^\top B^1 B^1 \mathbb{1} = 0$,

where we use the Hadamard product on vectors in $\mathbb{R}^s$*:*

$$y^1 \odot \ldots \odot y^n = \left(\prod_{k=1}^n y_i^k \right)_{i=1,\ldots,s}.$$

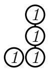
It is also possible to choose $c = \frac{1}{2}$ *when adapting* (2.6) *by* $\Theta_{0,p} = \theta_p$, $\Theta_{p,0} = 1$, *in which case also the following additional order condition needs to be fulfilled for weak order two:*

10. $\beta^\top A^1 B^0 \mathbb{1} = 0$.

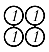
Note that condition 9 and, in case $c = \frac{1}{2}$, also condition 10, in Theorem (2.5), are still derived from potentially superfluous conditions. Note also that for $c < \frac{1}{2}$, we always can choose $A^0 = B^0$ and $A^1 = B^1$, and that the parameters α, A^0 and B^0 on the one hand and β, A^1 and B^1 are independent of each other. A natural choice for c is $c = \frac{1}{4}$, which ensures that conditions 1 and 3 to 5 and conditions 2 and 6 to 8 are congruent and we thus can choose $B^0 = B^1$ and $\alpha = \beta$. Another natural choice would be $c = \frac{1}{3}$, which allows for a method with $A^0 = B^0$ already fulfilling one of the deterministic order three conditions. Choosing $c = \frac{1}{2}$ on the other hand reduces the number of random variables needed per step from $2m + 1$ to $m + 1$.

Remark 2.6. *The coefficients* (2.5) *do not allow for weak order three methods, as the following second and third order conditions are contradictive:*

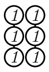
$$(\beta^\top \mathbb{1})^2 \mathbb{E}[\theta_p^2] = 1 \quad \Rightarrow \quad \beta^\top \mathbb{1} \neq 0 \text{ and } \mathbb{E}[\theta_p^2] \neq 0,$$



$$(\beta^\top \mathbb{1})(\beta^\top B^1 B^1 \mathbb{1}) \mathbb{E}[\theta_p^2 \Theta_{pp}^2] = 0 \quad \Rightarrow \quad \beta^\top \mathbb{1} = 0 \text{ or } \beta^\top B^1 B^1 \mathbb{1} = 0 \text{ or } \mathbb{E}[\theta_p^2 \Theta_{pp}^2] = 0,$$



$$(\beta^\top B^1 \mathbb{1})^2 \mathbb{E}[\theta_p^2 \Theta_{pp}^2] = \frac{1}{2} \quad \Rightarrow \quad \beta^\top B^1 \mathbb{1} \neq 0 \text{ and } \mathbb{E}[\theta_p^2 \Theta_{pp}^2] \neq 0,$$



$$(\beta^\top B^1 B^1 \mathbb{1})^2 \mathbb{E}[\theta_p^2 \Theta_{pp}^4] = \frac{1}{6} \quad \Rightarrow \quad \beta^\top B^1 B^1 \mathbb{1} \neq 0 \text{ and } \mathbb{E}[\theta_p^2 \Theta_{pp}^4] \neq 0.$$

Hence a more general ansatz for third order Runge-Kutta coefficients is needed.

2.3 Reduced order conditions for Stratonovich SDEs

There are fewer potentially superfluous order conditions in the Stratonovich case, which prevents us from removing most of the conditions with a certain choice of random variables. We still present a substantial reduction of order conditions compared to the literature. We consider coefficients of the form

$$\begin{aligned} z^0 &= \alpha\theta_0, & z^p &= \beta\theta_p, \\ Z^{0,0} &= A^0\Theta_{0,0}, & Z^{0,q} &= B^0\Theta_{0,q}, \\ Z^{p,0} &= A^1\Theta_{p,0}, & Z^{p,q} &= B^1\Theta_{p,q}\mathbb{1}_{p\neq q} + \hat{B}^1\Theta_{p,p}\mathbb{1}_{p=q}. \end{aligned} \tag{2.7}$$

Let η_p, $p = 0, \ldots, m$, and θ_p, $p = 1, \ldots, m$, be discrete independent random variables satisfying

$$\mathbb{P}(\eta_p = \pm 1) = \frac{1}{2}, \quad \mathbb{P}(\theta_p = \pm\sqrt{3}) = \frac{1}{6}, \quad \mathbb{P}(\theta_p = 0) = \frac{2}{3}.$$

Define

$$\begin{aligned} &\theta_0 = 1, && \Theta_{0,p} = \theta_p + \eta_p\sqrt{\tfrac{1}{2c} - 1}, && \Theta_{p,q} = \theta_q(1+\eta_0), \quad q > p \geqslant 1, \\ &\Theta_{0,0} = 1, && \Theta_{p,0} = 1 - \eta_p\theta_p\sqrt{\tfrac{2c}{1-2c}}, && \Theta_{p,q} = \theta_q(1-\eta_0), \quad 1 \leqslant q < p. \\ &\Theta_{p,p} = \theta_p, \end{aligned} \tag{2.8}$$

Using the ansatz (2.7) and the random variables (2.8) in Theorem 2.3, Assumption 2.1 is automatically satisfied and we obtain the following 26 reduced order conditions. These conditions improve significantly on the 55 order conditions in [74].

Theorem 2.7. *The reduced order conditions for weak order one for solving the Stratonovich SDE* (1.2) *by method* (1.3) *with method coefficients* (2.7)*, random variables* (2.8) *and* $c \in (0, \frac{1}{2})$ *are:*

1. $\alpha^\top \mathbb{1} = 1$, *2.* $\beta^\top \mathbb{1} = 1$, *3.* $\beta^\top \hat{B}^1 \mathbb{1} = \frac{1}{2}$,

and the additional conditions for weak order two are:

4. $\alpha^\top A^0 \mathbb{1} = \frac{1}{2}$,

5. $\alpha^\top B^0 \mathbb{1} = \frac{1}{2}$,

6. $\alpha^\top (B^0 \mathbb{1})^{\odot 2} = c$,

7. $\alpha^\top B^0 \hat{B}^1 \mathbb{1} = \frac{1}{4}$,

8. $\beta^\top A^1 \mathbb{1} = \frac{1}{2}$,

9. $\beta^\top (\hat{B}^1 \mathbb{1} \odot A^1 \mathbb{1}) = \frac{1}{4}$,

10. $\beta^\top \hat{B}^1 A^1 \mathbb{1} = \frac{1}{4}$,

11. $\beta^\top B^1 \mathbb{1} = \frac{1}{2}$,

12. $\beta^\top (B^1 \mathbb{1})^{\odot 2} = \frac{1}{4}$,

13. $\beta^\top \hat{B}^1 B^1 \hat{B}^1 \mathbb{1} = \frac{1}{8}$,

14. $\beta^\top (\hat{B}^1 \mathbb{1} \odot B^1 \hat{B}^1 \mathbb{1}) = \frac{1}{8}$,

15. $\beta^\top (\hat{B}^1 \mathbb{1} \odot (B^1 \mathbb{1})^{\odot 2}) = \frac{1}{8}$,

16. $\beta^\top (B^1 \mathbb{1} \odot \hat{B}^1 B^1 \mathbb{1}) = \frac{1}{8}$,

17. $\beta^\top \hat{B}^1 (B^1 \mathbb{1})^{\odot 2} = \frac{1}{8}$,

18. $\beta^\top (B^1 \mathbb{1} \odot \hat{B}^1 \mathbb{1}) = \frac{1}{4}$,

19. $\beta^\top \hat{B}^1 B^1 \mathbb{1} = \frac{1}{4}$,

20. $\beta^\top B^1 \hat{B}^1 \mathbb{1} = \frac{1}{4}$,

21. $\beta^\top (\hat{B}^1 \mathbb{1} \odot \hat{B}^1 \hat{B}^1 \mathbb{1}) = \frac{1}{8}$,

22. $\beta^\top \hat{B}^1 (\hat{B}^1 \mathbb{1})^{\odot 2} = \frac{1}{12}$,

23. $\beta^\top \hat{B}^1 \hat{B}^1 \hat{B}^1 \mathbb{1} = \frac{1}{24}$,

24. $\beta^\top (\hat{B}^1 \mathbb{1})^{\odot 3} = \frac{1}{4}$,

25. $\beta^\top (\hat{B}^1 \mathbb{1})^{\odot 2} = \frac{1}{3}$,

26. $\beta^\top \hat{B}^1 \hat{B}^1 \mathbb{1} = \frac{1}{6}$.

It is also possible to choose $c = \frac{1}{2}$ *when adapting* (2.8) *by* $\Theta_{0,p} = \theta_p$, $\Theta_{p,0} = 1$, *in which case also the following additional order condition needs to be fulfilled for weak order two:*

27. $\beta^\top A^1 B^0 \mathbb{1} = 0$.

Analogously to the Itô case, one can reduce the number of stochastic variables needed per step from $2m + 1$ to $m + 1$ by adding condition 27.

3 New second order stochastic Runge-Kutta methods

We use the reduced order conditions of Section 2 to propose a handful of new stochastic methods with the minimal number of function evaluations for solving (1.1)-(1.2) with second weak order. We focus on explicit methods and methods with high deterministic order. Further IMEX methods are presented in Appendix A.

3.1 Optimal stochastic Runge-Kutta methods

Thanks to the reduced order conditions, we propose a variety of new simple stochastic Runge-Kutta methods of weak order two. We emphasize that, similarly to the deterministic setting, an explicit method needs at least two evaluations of f^0 and two evaluations of each f^p per step. The Butcher tableaux are written in the following ways for Itô and Stratonovich.

$$\text{Itô:} \quad \begin{array}{c|c} A^0 & B^0 \\ \hline A^1 & B^1 \\ \hline \alpha^\top & \beta^\top \end{array}, \qquad \text{Stratonovich:} \quad \begin{array}{c|c|c} A^0 & B^0 & \\ \hline A^1 & B^1 & \hat{B}^1 \\ \hline \alpha^\top & \beta^\top & \end{array}$$

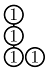
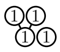
Itô explicit A $(2,2)$-stages method is the following mix of the Heun and explicit midpoint methods.

$$\begin{aligned} X_{n+1} &= X_n + \tfrac{h}{2} f^0(X_n) + \tfrac{h}{2} f^0\Big(X_n + hf^0(X_n) \\ &\quad + \sqrt{h}\textstyle\sum_{q=1}^m \theta_q f^q(X_n)\Big) \\ &\quad + \sqrt{h}\textstyle\sum_{p=1}^m \theta_p f^p\Big(X_n + \tfrac{h}{2} f^0(X_n) + \tfrac{\sqrt{h}}{2}\sum_{q=1}^m \Theta_{p,q} f^q(X_n)\Big) \end{aligned} \qquad \begin{array}{cc|cc} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \hline \frac{1}{2} & \frac{1}{2} & 0 & 1 \end{array}$$

This method, in the following denoted by BDK1, is an improvement of the methods presented both in [30] and [79], as it uses only $m+1$ random variables per step and attains order 2 for solving (1.1) (with $c = \frac{1}{2}$ in Theorem 2.5), with the optimal number of stages.

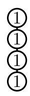
Itô implicit When constructing an $(1,2)$-stages method of order 2 for solving (1.1), we observe that condition 1 in Theorem 2.5 implies that $\alpha = 1$, which together with conditions 4 and 5 implies that we must choose $c = \frac{1}{4}$ in this case. A possible method is then the following:

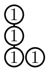
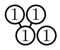
$$\begin{aligned} H_1^0 &= X_n + \tfrac{h}{2} f^0(H_1^0) + \tfrac{\sqrt{h}}{2}\textstyle\sum_{q=1}^m \Theta_{0,q} f^q(H_1^q) \\ H_1^p &= X_n + \sqrt{h}\textstyle\sum_{q=1}^m \Theta_{p,q} f^q(H_1^q) \\ H_2^p &= X_n + \tfrac{h}{2}\Theta_{p,0} f^0(H_1^0) + \sqrt{h}\textstyle\sum_{q=1}^m \Theta_{p,q}\Big(f^q(H_2^q) - \tfrac{1}{2} f^q(H_1^q)\Big) \\ X_{n+1} &= X_n + hf^0(H_1^0) + \sqrt{h}\textstyle\sum_{p=1}^m \theta_p f^p(H_2^p) \end{aligned} \qquad \begin{array}{c|cc} \frac{1}{2} & \frac{1}{2} & 0 \\ \hline 0 & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 \\ \hline 1 & 0 & 1 \end{array}$$

An order 2 method with one stage for the stochastic part is impossible in general as the order conditions of Theorem 2.3 for the forests  and  cannot be satisfied simultaneously. If the noise is additive, it is however straightforwardly achieved [25, 55].

Stratonovich explicit We propose the following $(2,4)$-stages explicit method with $c = \frac{1}{2}$ of weak order two for solving (1.2), which is a mild improvement on the methods in [74] as it uses fewer stages in the deterministic part, and only $m+1$ random variables per step instead of $2m-1$.

$$\begin{array}{cc|cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & & & & \\ 1 & 0 & 0 & 1 & 0 & 0 & & & & \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & -1 & \frac{3}{2} & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & -1 & \frac{3}{2} & 0 & 0 & -\frac{3}{2} & \frac{3}{2} & 1 & 0 \\ \hline \frac{1}{2} & \frac{1}{2} & 0 & \frac{2}{3} & \frac{1}{6} & \frac{1}{6} & & & & \end{array}$$

The number of stochastic stages is minimal thanks to the condition for  in Theorem 2.3.

Stratonovich implicit Analogously to the Itô case, it follows by conditions 1, 5 and 6 in Theorem 2.7 that a $(1,2)$-stage method for solving (1.2) with weak order two requires $c = \frac{1}{4}$. An example for such a method is given below. Observe that both A^0 and B^1 correspond to well-known Gauss–Legendre methods. A $(1,1)$-stages method cannot be achieved as the order conditions associated to  and  in Theorem 2.3 would bring a contradiction.

$$\begin{array}{c|cc|cc}
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & & \\
\hline
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\
\hline
1 & \frac{1}{2} & \frac{1}{2} & &
\end{array}$$

3.2 Stochastic Runge-Kutta methods with high deterministic order

Let us now present a handful of explicit methods with second weak order, optimal number of function evaluations, and third deterministic order, as these methods often display improved error constants and rates of convergence for stochastic perturbation of deterministic dynamics.

Itô explicit of deterministic order 3 We propose the following two methods BDK2 and BDK3 (respectively with $c = \frac{1}{2}$ and $c = \frac{1}{3}$) of order 2 and deterministic order 3. Note that the deterministic part of these methods coincides with Kutta's RK32 [19].

$$\begin{array}{ccc|cc}
0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & 0 & \frac{3}{5}-\frac{\sqrt{6}}{10} & 0 \\
-1 & 2 & 0 & \frac{3}{5}+\frac{2}{5}\sqrt{6} & 0 \\
\hline
0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\
\hline
\frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 & 1
\end{array}
\qquad
\begin{array}{ccc|cc}
0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\
-1 & 2 & 0 & 1 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\
\hline
\frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 & 1
\end{array}$$

Stratonovich explicit of deterministic order 3 ($c = \frac{1}{2}$)

$$\begin{array}{ccc|cccc|cccc}
0 & 0 & 0 & \frac{1}{2}-\frac{\sqrt{3}}{2} & 0 & 0 & 0 & & & & \\
\frac{1}{3} & 0 & 0 & \sqrt{3}-1 & 0 & 0 & 0 & & & & \\
0 & \frac{2}{3} & 0 & \frac{1}{6}+\frac{\sqrt{3}}{6} & 0 & 0 & \frac{1}{3} & & & & \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\
-\frac{1}{2} & 1 & 0 & -1 & \frac{3}{2} & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & 0 \\
\frac{1}{2} & 0 & 0 & -\frac{1}{2} & \frac{3}{2} & -\frac{1}{2} & 0 & -\frac{3}{2} & \frac{3}{2} & 1 & 0 \\
\hline
\frac{1}{4} & 0 & \frac{3}{4} & 0 & \frac{2}{3} & \frac{1}{6} & \frac{1}{6} & & & &
\end{array}$$

4 Numerical applications

In this section, in Examples 4.1 and 4.2 we first numerically confirm the theoretical findings on two test problems and conclude then with Example 4.3 illustrating an application to invariant measure sampling.

In Examples 4.1 and 4.2, we will compare the computational effort and accuracy of the newly derived methods BDK1, BDK2 and BDK3 with some integrators from the literature, namely DRI1 from [30], W2Ito1 from [79], RI5 and RI6 from [75]. Note that RI6 coincides for $m = 1$ with Platen's second order method [70]. The numbers N_d and N_s of evaluations of the integrands f^0 and f^p, $p = 1, \dots, m$, as well as the number N_r of random variables per step of the new methods are lower as presented in Table 3. In the numerical illustrations, the solution $\mathbb{E}[\phi(X(t))]$ will be approximated with step sizes $2^{-1}, \ldots, 2^{-5}$. We will define the computational effort per time step as $N_d + mN_s + N_r$ [30] and the numerically observed order of convergence $\hat{p}$ as slope of the regression line in the double–logarithmic plot of the approximated weak error vs. step size. The expectation in the error term $|\mathbb{E}[\phi(X_N) - \phi(X(T_N))]|$ will be approximated by Monte Carlo simulation $|\hat{\mathbb{E}}[\phi(X_N) - \phi(X(T_N))]|$, using 40000 batches of 25000 simulations.

Method	p_D	p_S	N_d	N_s	N_r if $m=1$	N_r for $m>1$
RI6	2	2	2	5	1	$2m-1$
BDK1	2	2	2	2	1	$m+1$
RI5,DRI1	3	2	3	5	1	$2m-1$
W2Ito1	3	2	3	3	2	$m+2$
BDK3	3	2	3	2	2	$2m+1$
BDK2	3	2	3	2	1	$m+1$

Table 3: Comparison of the considered explicit stochastic Runge-Kutta methods for solving (1.1) in terms of deterministic order p_D and stochastic order p_S, numbers N_d and N_s of function evaluations and number N_r of random variables.

Example 4.1. *As first example, we consider the non-linear SDE [43, 60, 30]*

$$dX(t) = \left(\tfrac{1}{2}X(t) + \sqrt{X(t)^2+1}\right) dt + \sqrt{X(t)^2+1}\, dW(t), \qquad X(0) = 0, \tag{4.1}$$

on the time interval $I = [0,2]$ with the solution $X(t) = \sinh(t + W(t))$. Choosing $\phi(x) = p(\operatorname{arsinh}(x))$, where $p(z) = z^3 - 6z^2 + 8z$, the expectation of the solution is given by

$$\mathbb{E}[\phi(X(t))] = t^3 - 3t^2 + 2t. \tag{4.2}$$

The simulation results at time $t = 2$, presented in Figures 1 and 2, show that with one noise term, the new methods behave similarly in terms of convergence to the ones from the literature, with a slightly reduced cost. The method BDK3 displays higher convergence rate than expected.

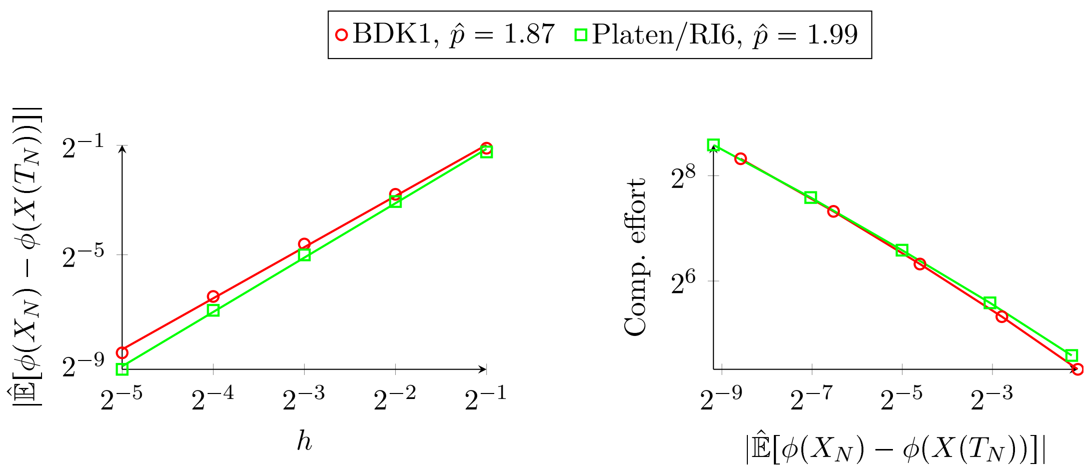


Figure 1: Numerical results for Example 4.1, methods of order (2,2)

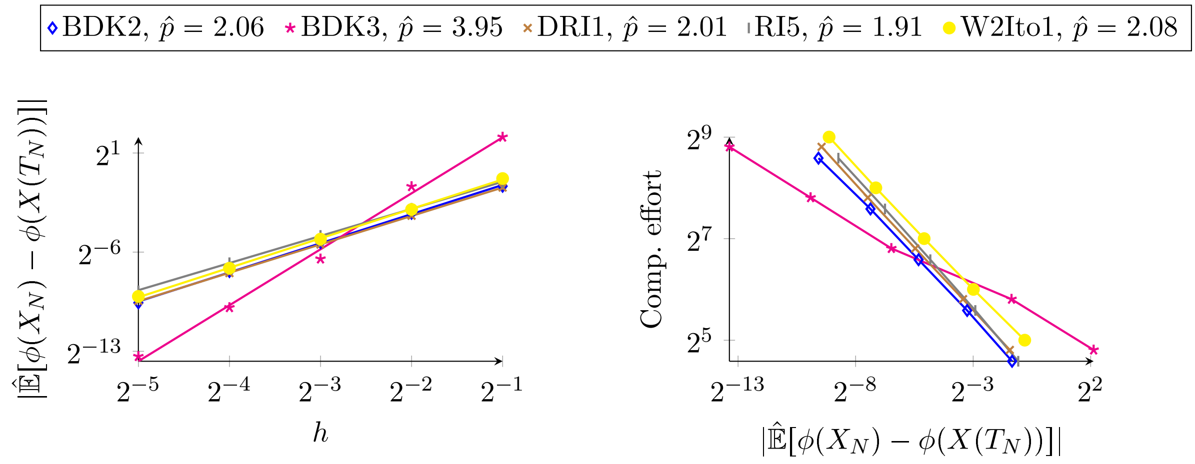


Figure 2: Numerical results for Example 4.1, methods of order (3,2)

Example 4.2. *As second example, we consider a nonlinear SDE with 10 Wiener processes [30, 79]*

$$\begin{aligned} dX(t) &= X(t)\,dt + \frac{1}{10}\sqrt{X(t)+\frac{1}{2}}\,dW_1(t) + \frac{1}{15}\sqrt{X(t)+\frac{1}{4}}\,dW_2(t) \\ &+ \frac{1}{20}\sqrt{X(t)+\frac{1}{5}}\,dW_3(t) + \frac{1}{25}\sqrt{X(t)+\frac{1}{10}}\,dW_4(t) + \frac{1}{40}\sqrt{X(t)+\frac{1}{20}}\,dW_5(t) \\ &+ \frac{1}{25}\sqrt{X(t)+\frac{1}{2}}\,dW_6(t) + \frac{1}{20}\sqrt{X(t)+\frac{1}{4}}\,dW_7(t) + \frac{1}{15}\sqrt{X(t)+\frac{1}{5}}\,dW_8(t) \\ &+ \frac{1}{20}\sqrt{X(t)+\frac{1}{10}}\,dW_9(t) + \frac{1}{25}\sqrt{X(t)+\frac{1}{20}}\,dW_{10}(t), \qquad X(0) = 1. \end{aligned} \tag{4.3}$$

We approximate the fourth moment, i. e., $\phi(x) = x^4$, with exact solution

$$\mathbb{E}[\phi(X(t))] = \frac{4625768169}{73570420483600} - \frac{2998776077847}{113706563209000} e^{\frac{731453}{360000}t} + \frac{80235120932849}{78178246418000} e^{\frac{251453}{60000}t} \tag{4.4}$$

on the time interval $I = [0,1]$. The simulation results at time $t = 1$ are shown in Figures 3 and 4. We observe that with multiple noise terms, the new methods have similar convergence to the standard methods, but with a significantly reduced cost. The method BDK3 displays an improved constant of convergence.

Example 4.3. *For our last example, we are interested in the sampling of the invariant measure of the following ergodic dynamics in a context of molecular dynamics:*

$$dX(t) = F(X(t))dt + \operatorname{div}(D^2(X(t)))dt + \sqrt{2}D(X(t))dW(t), \quad F(x) = -D^2(x)\nabla V(x) \tag{4.5}$$

where $V\colon \mathbb{R}^d \to \mathbb{R}$ is a smooth potential, W is a d-dimensional Brownian motion, and $D\colon \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is smooth. Choosing $D(x) = I_d$ yields the standard overdamped Langevin dynamics [59]. The dynamics of equation (4.5) is naturally ergodic under technical assumptions on V and D, that is, for all test function ϕ,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \phi(X(t))dt = \int_{\mathbb{R}^d} \phi(x)\rho_\infty(x)dx, \quad \rho_\infty(x) \propto \exp(-V(x)).$$

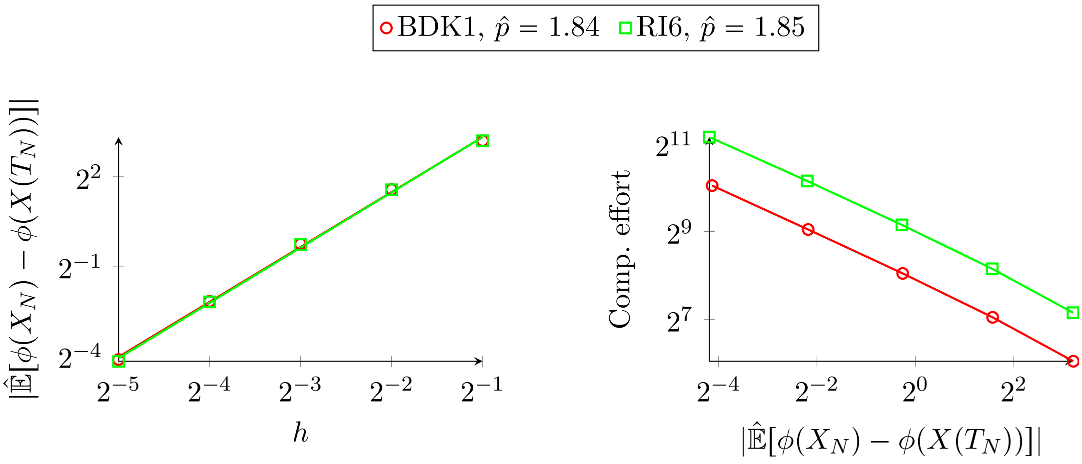


Figure 3: Numerical results for Example 4.2, methods of order (2,2)

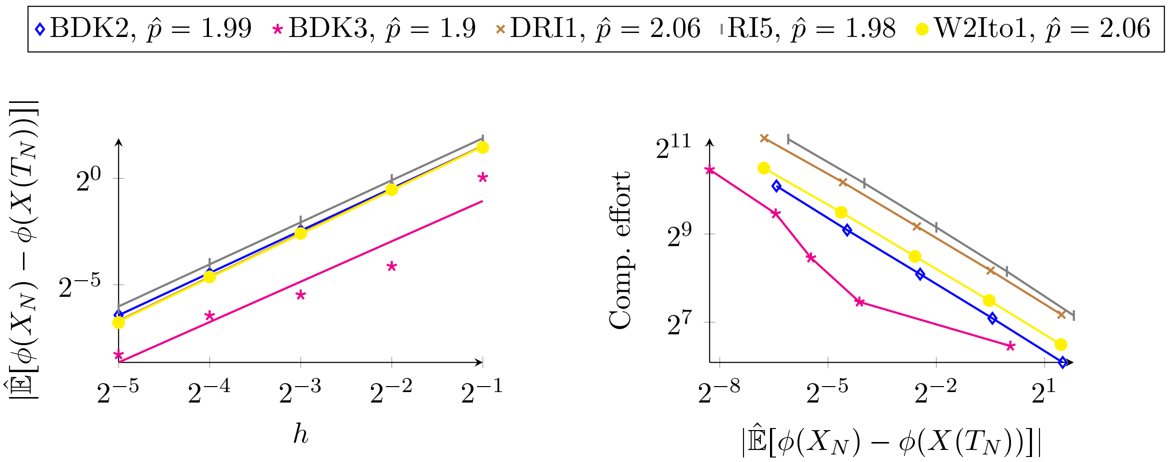


Figure 4: Numerical results for Example 4.2, methods of order (3,2)

The choice of a non-constant D map does not modify the sampled measure ρ_∞, but it can allow for more efficient sampling. In [12], a generalisation of the popular Leimkuhler-Matthews integrator [57] for sampling the invariant measure of (4.5) *with order two is proposed. It is a postprocessed integrator [81] and it relies on a non-detailed second order weak integrator for the Itô SDE:*

$$dX(t) = \sqrt{2}D(X(t))dW(t).$$

Using our analysis, we propose the following postprocessed method for sampling the invariant measure of (4.5),

$$\begin{aligned}
H_n &= X_n + \frac{h}{4}F(\overline{X}_{n-1}),\\
X_{n+1} &= X_n + hF(\overline{X}_n) + \sqrt{2h}\sum_p D_{:,p}(H_n + \sqrt{\frac{h}{2}}\sum_q D_{:,q}(H_n)\Theta^n_{p,q})\theta^n_p,\\
\overline{X}_n &= X_n + \sqrt{\frac{h}{2}}\sum_p D_{:,p}(H_n)\theta^n_p,
\end{aligned}$$

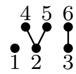
with the random variables defined in Section 2.2 and for any initial condition $\overline{X}_{-1} = X_0$*. Assuming ergodicity of the scheme, applying the analysis of [69] yields that* $(\overline{X}_n)$ *is an explicit method of first weak order and of second order for sampling the invariant measure of* (4.5)*. This method uses only one evaluation of* F *and two evaluations of* D *per step. It does not rely on a specific form of* D *as in [69].*

5 High order analysis with decorated and exotic series

We derive here the general order conditions for the weak approximation of stochastic dynamics. While the idea is not new [72, 73], we present a new approach with exotic forests that simplifies the analysis and reduces the number of forests, together with modern algebraic tools from Hopf algebra theory for the derivation of stochastic order conditions.

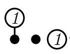
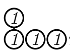
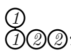
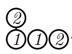
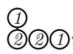
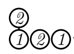
5.1 Decorated and exotic Butcher forests

We consider graphs $\pi = (V, E)$ where V is a finite set of nodes and $E \subset V \times V$ is a set of directed edges. If $e = (v, w) \in E$, the edge e is going from the node v to the node w, v is a predecessor of w, and w is a successor of v. We impose that each node has at most one outgoing edge. The nodes that do not have a successor are called roots and we impose that the connected components, called trees, have exactly one root. Such graphs are then called a forest. By convention, we draw the edges going from top to bottom and the roots as the bottommost nodes. For instance, the following graph has three roots:

$$V = \{1, 2, 3, 4, 5, 6\}, \quad E = \{(4, 2), (5, 2), (6, 3)\}, \quad \pi = (V, E) =$$  .

We attach specific decorations, also called colours in numerics, to the graphs. A decoration of a graph $\pi = (V, E)$ is a map $d\colon V \to \mathbb{N}$ such that for $n > 0$, $\left|d^{-1}(n)\right| \in 2\mathbb{N}$. A decorated graph is written π_d. Given two decorations d_1 and d_2 of a given graph π, we say that d_2 is finer than d_1, written $d_2 \leqslant d_1$, if there exists $\alpha\colon \mathbb{N} \to \mathbb{N}$ such that $d_1 = \alpha \circ d_2$ and $\alpha(n) = 0$ if and only if $n = 0$. The map α identifies colours. If $d_1 \leqslant d_2$ and $d_2 \leqslant d_1$, the decorations are equivalent. We write $d_1 < d_2$ if $d_1 \leqslant d_2$ and d_1 and d_2 are not equivalent. The nodes of decoration 0 are drawn in black.

Example 5.1. *A forest* π *can be decorated in different ways:*

$\pi_{d_1} =$ , $\pi_{d_2} =$ , $\pi_{d_3} =$ , $\pi_{d_4} =$ , $\pi_{d_5} =$ , $\pi_{d_6} =$ . (5.1)

In this example, the decorations d_3*,* d_4*,* d_5*,* d_6 *are finer than* d_2*.*

The numerical and the exact flow of stochastic differential equations rewrite naturally with decorated forests. However, let us introduce a simpler set of forests that is sufficient for expanding the exact flow, in the spirit of [55, 9].

Definition 5.2. *Two decorated graphs* $\pi^1_{d_1}$ *and* $\pi^2_{d_2}$ *are equivalent if there exists a bijection between their sets of nodes that preserves the oriented edges and sends the decoration* d_1 *to a decoration equivalent to* d_2*. We call decorated forests the equivalence classes of such graphs, where we also add the empty forest* ***1****.*

Analogously, we call exotic forests the equivalence classes of decorated forests π_d *such that for all* $n > 0$*,* $\left|d^{-1}(n)\right| \in \{0, 2\}$*. A pair of nodes with matching non-zero decoration is called a liana.*

We gather the decorated and exotic forests in the sets DF and EF and write $\mathcal{DF} = \mathrm{Span}_{\mathbb{R}}(DF)$, $\mathcal{EF} = \mathrm{Span}_{\mathbb{R}}(EF)$.

The order of a decorated forest is

$$|\pi_d| = \left|d^{-1}(0)\right| + \frac{1}{2}\sum_{n>0}\left|d^{-1}(n)\right|.$$

The number of automorphisms of a given decorated forest π_d is the symmetry coefficient $\sigma(\pi_d)$.

Example 5.3. *In Example 5.1, all forests are exotic, except π_{d_2} as the decoration 1 appears more than two times. The decorated forests of Example 5.1 have the order*

$$|\pi_{d_1}| = 3, \quad |\pi_{d_2}| = |\pi_{d_3}| = |\pi_{d_4}| = |\pi_{d_5}| = |\pi_{d_6}| = 2,$$

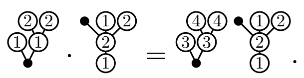
and the symmetry coefficients satisfy

$$\sigma(\pi_{d_1}) = \sigma(\pi_{d_4}) = \sigma(\pi_{d_5}) = \sigma(\pi_{d_6}) = 1, \quad \sigma(\pi_{d_2}) = \sigma(\pi_{d_3}) = 2.$$

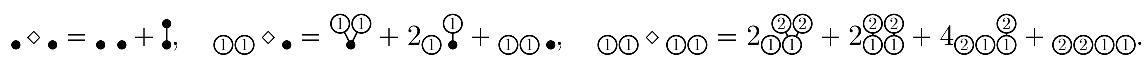
The list of all exotic and decorated forests of order one and two is presented in Tables 1 and 2.

Remark 5.4. *Note that two decorated forests can be equivalent, while having non-equivalent decorations. For instance in Example 5.1, the forests π_{d_4}, π_{d_5}, and π_{d_6} are equivalent, but only the decorations d_4 and d_5 are equivalent. Given two decorated forests π_{d_1}, π_{d_2} with $d_2 \leqslant d_1$, we write $m(\pi_{d_2}, \pi_{d_1})$ the number of different finer decorations of π_{d_1} that yield a decorated forest equivalent to π_{d_2}.*

Let us now equip $\mathcal{EF}$ with algebraic structures. On one hand, the concatenation product of two decorated forests, denoted $\pi_{d_1} \cdot \pi_{d_2}$, yields a decorated forest given by the union of the two graphs, with the decoration that preserves the nodes of same decoration in π_{d_1} and π_{d_2}, but does not use the same non-zero decoration for nodes in $\pi_{d_1} \cdot \pi_{d_2}$:



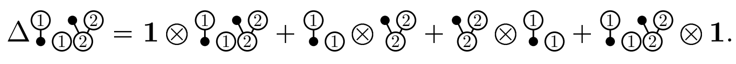
On the other hand, the Grossman-Larson product $\pi^1_{d_1} \diamond \pi^2_{d_2}$ concatenates and grafts the roots of $\pi^1_{d_1}$ on all nodes of $\pi^2_{d_2}$ in all possible ways (counting multiplicity), using different non-zero decorations for the nodes in d_1 and d_2. For instance, we find



Let the deshuffle coproduct $\Delta\colon \mathcal{EF} \to \mathcal{EF} \otimes \mathcal{EF}$:

$$\Delta\pi = \sum_{\pi_1,\pi_2\in EF, \pi_1\cdot\pi_2=\pi} \pi_1 \otimes \pi_2, \quad \Delta\mathbf{1} = \mathbf{1}\otimes\mathbf{1}.$$

For instance, we find (note that lianas cannot be split on different sides of the tensor product)



The exotic forests are naturally equipped with two structures of Hopf algebras. We refer to [9, 10] for similar structures in the simpler context of SDEs with additive noise.

Proposition 5.5. *The exotic forests equipped with the concatenation product and the Grossman-Larson product have a structure of Hopf algebras $(\mathcal{EF}, \cdot, \Delta)$ and $(\mathcal{EF}, \diamond, \Delta)$, graded by the order.*

Remark 5.6. *An exotic forest π_d is called primitive if*

$$\Delta\pi_d = \mathbf{1} \otimes \pi_d + \pi_d \otimes \mathbf{1}.$$

In contrast to the deterministic setting, primitive forests are not the exotic trees. For instance, ①① and ②②/①① are primitive as they cannot be written as a concatenation of exotic trees. In a variety of numerical contexts, the primitive elements exactly correspond to the order conditions of the numerical methods, so that the number of order conditions is given by the number of primitive elements [32, 10]. One of the major difficulties of stochastic numerics for general SDEs is that the coefficient maps of stochastic Runge-Kutta methods are not characters w.r.t. concatenation in general, so that one has to consider all decorated forests for the order conditions. Hence the high number of order conditions in Theorem 2.3.

5.2 Algebraic expansion of flows with decorated and exotic forests

The decorated and exotic forests represent elementary differentials via the use of the elementary differential map F^{dec}.

Definition 5.7. *Let a decorated forest $\pi_d = (V, E, d)$. Then, the decorated elementary differential map F^{dec} is the differential operator acting on test functions $\phi \in \mathcal{C}_P^\infty(\mathbb{R}^d)$ satisfying $F^{dec}(\mathbf{1})[\phi](x) = \phi(x)$ and*

$$F^{dec}(\pi_d)[\phi](x) = \sum_{\substack{i_w=1,\dots,d \\ w\in V}} \sum_{\substack{p_n=1,\dots,m,\ n\in \mathrm{Im}(d)\backslash 0 \\ p_0=0,\ p_{n_1}\neq p_{n_2}\ \text{if } n_1\neq n_2}} \phi_{I_R}(x) \prod_{v\in V} f_{I_{\Pi(v)}}^{p_{d(v)},i_v}(x),$$

where $R \subset V$ is the set of roots, $\Pi(v)$ denotes the set of predecessors of v, and $I_S = i_{w_1} \dots i_{w_n}$ for $S = \{w_1, \dots, w_n\}$. Analogously, the exotic elementary differential map on $\pi_d \in EF$ satisfies $F^{exo}(\mathbf{1})[\phi](x) = \phi(x)$ and

$$F^{exo}(\pi_d)[\phi](x) = \sum_{\substack{i_w=1,\dots,d \\ w\in V}} \sum_{\substack{p_n=1,\dots,m,\ n\in \mathrm{Im}(d)\backslash 0 \\ p_0=0}} \phi_{I_R}(x) \prod_{v\in V} f_{I_{\Pi(v)}}^{p_{d(v)},i_v}(x).$$

The two elementary differential maps F^{dec} and F^{exo} are very similar, the only difference lying in the additional summing restriction $p_{n_1} \neq p_{n_2}$ in the definition of F^{dec}. For instance, the forest π_{d_3} from Example 5.1 yields

$$F^{\text{dec}}(\pi_{d_3})[\phi] = \sum_{i,j,k,l=1}^{d} \sum_{\substack{p,q=1 \\ p\neq q}}^{m} \phi_{ijk} f_l^{p,i} f^{p,l} f^{q,j} f^{q,k},$$

$$F^{\text{exo}}(\pi_{d_3})[\phi] = \sum_{i,j,k,l=1}^{d} \sum_{p,q=1}^{m} \phi_{ijk} f_l^{p,i} f^{p,l} f^{q,j} f^{q,k}.$$

We observe in particular

$$F^{\text{exo}}(\pi_{d_3}) = F^{\text{dec}}(\pi_{d_3}) + F^{\text{dec}}(\pi_{d_2}).$$

We refer to Tables 1 and 2 for further examples. The exotic formalism is simpler as it does not require to work with different cases depending on the equal values in p_n, which quickly becomes tedious as the order of the method goes up.

The following result, in the spirit of [78], allows one to translate elementary differentials between the exotic and decorated formalisms.

Proposition 5.8. *Let $\pi_d \in EF$ be an exotic forest, then the exotic differential map satisfies*

$$F^{exo}(\pi_d) = \sum_{\substack{\pi_{d_0} \in DF \\ d \leqslant d_0}} F^{dec}(\pi_{d_0}),$$

and F^{exo} can thus be extended to $\mathcal{DF}$ with this identity. Then, the Moebius inversion formula holds for $\pi_d \in DF$,

$$F^{dec}(\pi_d) = \sum_{\substack{\pi_{d_0} \in DF \\ d \leqslant d_0}} \mu(\pi_d, \pi_{d_0}) F^{exo}(\pi_{d_0}),$$

where the Moebius function is

$$\mu(\pi_{d_1}, \pi_{d_1}) = 1, \quad \mu(\pi_{d_1}, \pi_{d_2}) = -\sum_{\substack{\pi_d \in DF \\ d_1 \leqslant d < d_2}} \mu(\pi_{d_1}, \pi_d).$$

The elementary differential translates the operations on forests to operations on differential operators.

Lemma 5.9. *The composition of differential operators is given by the Grossman-Larson product: for π_d, $\hat{\pi}_{\hat{d}} \in EF$, one has for all $\phi \in \mathcal{C}_P\infty(\mathbb{R}^d)$,*

$$(F^{exo}(\pi_d) \circ F^{exo}(\hat{\pi}_{\hat{d}}))[\phi] = F^{exo}(\pi_d)[F^{exo}(\hat{\pi}_{\hat{d}})[\phi]] = F^{exo}(\pi_d \diamond \hat{\pi}_{\hat{d}})[\phi].$$

The generators of the SDEs (1.1)/(1.2) are represented by exotic forests as

$$\mathcal{L}_{\text{Itô}} = F^{\text{exo}}(\bullet + \frac{1}{2}\textcircled{1}\textcircled{1}), \quad \mathcal{L}_{\text{Strato}} = F^{\text{exo}}(\bullet + \frac{1}{2}\textcircled{1}\textcircled{1} + \frac{1}{2}\genfrac{}{}{0pt}{}{\textcircled{1}}{\textcircled{1}}).$$

The expansion (2.2) rewrites in terms of exotic forests, using Lemma 5.9.

Proposition 5.10. *The Taylor expansion of the flow* (2.2) *is represented by the Grossman-Larson exponential* $\exp^\diamond(\tau) = \sum_{n=0}^{\infty} \frac{1}{n!}\tau^{\diamond n}$*, that is,*

$$u_{Itô}(x, h) = F^{exo}(\exp^\diamond(h\bullet + \frac{h}{2}\textcircled{1}\textcircled{1}))[\phi],$$
$$u_{Strato}(x, h) = F^{exo}(\exp^\diamond(h\bullet + \frac{h}{2}\textcircled{1}\textcircled{1} + \frac{h}{2}\genfrac{}{}{0pt}{}{\textcircled{1}}{\textcircled{1}}))[\phi].$$

5.3 Decorated and exotic S-series for stochastic numerics

The main tool for representing the Taylor expansions of our analysis are S-series, which generalise Butcher series [17, 18, 35] to represent differential operators.

Definition 5.11. *Given 1-forms, called coefficient maps, $a \in \mathcal{DF}^*$ and $b \in \mathcal{EF}^*$, the associated decorated and exotic S-series are the following formal power series*

$$S_h^{dec}(a)[\phi] = \sum_{\pi_d \in DF} h^{|\pi_d|} \frac{a(\pi_d)}{\sigma(\pi_d)} F^{dec}(\pi_d)[\phi],$$
$$S_h^{exo}(b)[\phi] = \sum_{\pi_d \in EF} h^{|\pi_d|} \frac{b(\pi_d)}{\sigma(\pi_d)} F^{exo}(\pi_d)[\phi].$$

We denote $S^{dec}(a) = S_1^{dec}(a)$ and $S^{exo}(a) = S_1^{exo}(a)$.

Remark 5.12. *Similar to the exotic S-series being formal sums indexed by exotic forests, the exotic B-series are formal series indexed by exotic trees, whose use is central in the numerical approximation for the invariant measure of ergodic stochastic dynamics [55, 56, 9, 10]. It is proven in [54] that the exotic B-series from the additive noise case are not just a combinatorial tool for the simplification of tedious calculations, but are a universal geometric object characterised by the properties of locality and orthogonal equivariance (see also [61, 66]). To the best of our knowledge, such geometric properties have not yet been studied for the exotic and decorated S-series presented in this work.*

The Taylor expansion (2.2) of the flow and the corresponding expansion (2.3) of the stochastic Runge-Kutta method (1.3) can typically be written in terms of decorated S-series, but unfortunately not by exotic S-series for the numerical flow in general, in opposition to the additive noise case. The previous works rely on a set of forests that is unnecessarily bigger than DF. The use of decorated forests allows us to avoid repeating the same condition multiple times and to take into account the symmetries of the conditions: one decorated forest stands for one order condition exactly.

Theorem 5.13. *The exact flow of* (1.1)/(1.2) *is given by an exotic S-series:*

$$\mathbb{E}[\phi(X(h))|X_0 = x] = S_h^{exo}(e)[\phi](x).$$

Consider a stochastic Runge-Kutta method of the form (1.3) *whose coefficients satisfy Assumption 2.1. Then, the expansion* (2.3) *of the integrator is well defined and is given by a decorated S-series:*

$$\mathbb{E}[\phi(X_1)|X_0 = x] = S_h^{dec}(a)[\phi](x).$$

The coefficient e can be computed by iteration of the Grossman-Larson product as in Proposition 5.10 and then multiplying by the symmetry coefficient (see also the expression in [71]). For instance, one finds in the Itô case (1.1):

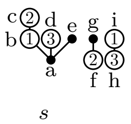
$$\exp^\diamond\Big(h\bullet + \frac{h}{2}\text{①①}\Big) = h\Big(\bullet + \frac{1}{2}\text{①①}\Big) + h^2\Big(\frac{1}{2}\overset{\bullet}{\bullet} + \frac{1}{2}\bullet\,\bullet + \dots\Big) + \dots,$$

so that e satisfies

$$\frac{e}{\sigma}(\bullet) = 1, \quad \frac{e}{\sigma}(\text{①①}) = \frac{1}{2}, \quad \frac{e}{\sigma}\Big(\overset{\text{①}}{\text{⑧}}\Big) = 0, \quad \frac{e}{\sigma}\Big(\overset{\bullet}{\bullet}\Big) = \frac{1}{2}, \quad \frac{e}{\sigma}(\bullet\,\bullet) = \frac{1}{2}, \dots$$

Alternatively, we provide in Proposition 5.18 and equation (5.2) an explicit expression of e using an extension of the Butcher-Connes-Kreimer Hopf algebra. The values of e for exotic forests of order up to two are presented in Table 1.

The coefficient map of stochastic Runge-Kutta methods (1.3) is deduced from the decorated graph, similarly to the deterministic literature [35, Chap. III]. One arbitrarily labels the nodes of the forest and writes $z_r^{p_d}$ if a root is labeled with r and decorated with the decoration d, with the convention $p_0 = 0$. Similarly, we write $Z_{v,w}^{p,q}$ if an edge goes from the node w with decoration q to the node v with decoration p. The coefficient a is then obtained by summing on every indices involved and taking the expectation. We provide an example and refer the reader to [9, Prop. 4.3] and [72, 26] for further details,

$\pi_d =$  ,

$$a(\pi_d) = \sum_{a,b,c,\dots=1}^{s} \sum_{p_1,p_2,p_3=1}^{m} \mathbb{E}[z_a^0 Z_{a,b}^{0,p_1} Z_{b,c}^{p_1,p_2} Z_{a,d}^{0,p_3} Z_{a,e}^{0,0} z_f^{p_2} Z_{f,g}^{p_2,0} z_h^{p_3} Z_{h,i}^{p_3,p_1}].$$

Remark 5.14. *A 1-form $a \in \mathcal{H}^*$ over an algebra $(\mathcal{H}, \cdot)$ is called a character if*

$$a(x \cdot y) = a(x)a(y), \quad x, y \in \mathcal{H}.$$

The coefficient map $e \in \mathcal{EF}^*$ of the exact flow naturally is a character. In most numerical contexts, the methods are represented by characters on some Hopf algebra. A major difficulty of stochastic numerics with multiplicative noise is that the coefficient map a of stochastic Runge-Kutta methods is not a character (as $\mathbb{E}[XY] \neq \mathbb{E}[X]\mathbb{E}[Y]$ in general).

For the approximation of SDEs with additive noise, it is sufficient to use only Gaussian random Runge-Kutta coefficients. In this context, the Isserlis theorem [42, 67] (also called the Wick formula) guarantees that the S-series of the numerical solution rewrites as an exotic series. Gaussian Runge-Kutta coefficients do not suffice for high order in the case of multiplicative noise. We thus rely on decorated forests and we split in Theorem 2.3 the order conditions into two sets, namely exotic and Isserlis order conditions. The Isserlis order conditions allow to write the Taylor expansion (2.3) as an exotic S-series up to the order studied and are computed using the following result.

Theorem 5.15. *Consider a numerical method whose expansion takes the form of a decorated S-series with coefficient map a. Then, the expansion writes as an exotic S-series if for all $\pi_d \in DF$, the following condition, that we call Isserlis condition, is satisfied,*

$$a(\pi_d) = \sum_{\substack{\pi_{d_0} \in EF \\ d_0 \leqslant d}} \frac{\sigma(\pi_d)}{\sigma(\pi_{d_0})} a(\pi_{d_0}) = \sum_{\substack{d_0 \leqslant d \\ \pi_{d_0} \in EF}} a(\pi_{d_0}).$$

Theorem 5.15 is a straightforward consequence of the identity $m(\pi_{d_0}, \pi_d) = \frac{\sigma(\pi_d)}{\sigma(\pi_{d_0})}$ and Proposition 5.8. We emphasize that the first sum in Theorem 5.15 is indexed by all the exotic forests with a finer decoration than d, while the second one is indexed by all the exotic decorations finer than d, so that it allows some repetition. For example, we have the following Isserlis condition of order two:

$$a(\overset{\textcircled{1}}{\textcircled{1}}\textcircled{1}\textcircled{1}) = a(\overset{\textcircled{2}}{\textcircled{1}}\textcircled{1}\textcircled{2}) + a(\overset{\textcircled{2}}{\textcircled{1}}\textcircled{2}\textcircled{1}) + a(\overset{\textcircled{1}}{\textcircled{1}}\textcircled{2}\textcircled{2}) = 2a(\overset{\textcircled{2}}{\textcircled{1}}\textcircled{1}\textcircled{2}) + a(\overset{\textcircled{1}}{\textcircled{1}}\textcircled{2}\textcircled{2}).$$

From the expansions in exotic and decorated S-series of the exact and numerical flow and the characterisation of Isserlis conditions, we derive the weak order conditions of Theorem 2.3.

Proof of Theorem 2.3. Thanks to Theorem 5.13, the exact and numerical flow write respectively as an exotic S-series $S_h^{\text{exo}}(e)$ and a decorated S-series $S_h^{\text{dec}}(a)$. The Isserlis order conditions from Theorem 5.15 impose that the numerical flow writes as the exotic S-series $S_h^{\text{exo}}(a)$. Then, the order conditions are obtained by identifying the coefficient maps on exotic forests: $a(\pi) = e(\pi)$ for $\pi \in EF$. Together with Assumption 2.1, they ensure that the prerequisites for Proposition 2.2 are satisfied. □

To complete our description of exotic S-series, let us describe the composition of differential operators represented by exotic S-series using the celebrated Butcher-Connes-Kreimer (BCK) Hopf algebra [23, 24].

Definition 5.16. *A cut c of $\pi \in EF$ is a (possibly empty) choice of edges of π. Removing these edges yields a forest $W_c(\pi)$, the component of $W_c(\pi)$ containing the roots of π is written $R_c(\pi)$ and the other components are gathered in the forest $P_c(\pi)$. A cut is admissible, written $c \in \operatorname{Adm}(\pi)$, if any path from a root to a leaf of π has at most one cut and if $R_c(\pi), P_c(\pi) \in \mathcal{EF}$.*

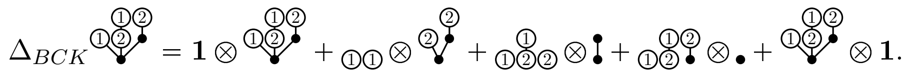
We define the exotic extension of the BCK Hopf algebra in the following result. The proof is analogous to the additive noise case [9, 10] and is thus omitted (see also [68, 38]).

Proposition 5.17. *Define the BCK coproduct on $\mathcal{EF}$ by*

$$\Delta_{BCK}\mathbf{1} = \mathbf{1} \otimes \mathbf{1}, \quad \Delta_{BCK}\pi = \pi \otimes \mathbf{1} + \sum_{c \in \mathrm{Adm}(\pi)} P_c(\pi) \otimes R_c(\pi).$$

Then, $(\mathcal{EF}, \cdot, \Delta_{BCK})$ is a graded connected commutative Hopf algebra and its graded dual is isomorphic (up to the symmetry coefficient) to the Grossman-Larson Hopf algebra $(\mathcal{EF}, \diamond, \Delta)$.

The main difference with the deterministic setting [21] and the standard Hopf algebra formalisms over decorated forests [34] is that the nodes sharing the same decoration cannot be split by the Butcher-Connes-Kreimer coproduct:



The composition of exotic S-series is described by the BCK coproduct (see also [27] for an analogous description of the composition without the Hopf algebra formalism).

Proposition 5.18. *Let $a, b \in \mathcal{EF}^*$, then the composition of exotic S-series satisfies*

$$S^{exo}(a) \circ S^{exo}(b) = S^{exo}(a * b), \quad a * b = \mu \circ (a \otimes b) \circ \Delta_{BCK},$$

where μ is the multiplication and $*$ is called the composition law.

Define the coefficient map of the Itô generator $l\colon \mathcal{EF} \to \mathbb{R}$ by $l = \delta_{\bullet} + \delta_{①①}$ (respectively $l = \delta_{\bullet} + \delta_{①①} + \frac{1}{2}\delta_{①-①}$ for Stratonovich), where $\delta_\tau(\hat{\tau}) = \mathbb{1}_{\tau=\hat{\tau}}$. The associated S-series yields the generator $S^{\mathrm{exo}}(l) = \mathcal{L}$. Then, the coefficient map e of the exact flow satisfies

$$u(x,h) = S^{\mathrm{exo}}(e)[\phi](x), \quad e = \exp^*(hl). \tag{5.2}$$

6 Conclusion

In this paper, we provided a novel approach based on specific choices of random Runge-Kutta coefficients that allows to greatly reduce the number of order conditions for stochastic Runge-Kutta methods of high weak order in the case of multiplicative noise. We provide a collection of new methods with similar accuracy and cheaper cost compared to the literature. The methods are optimal in the sense that they use the minimal number of function evaluations. The analysis of the order conditions relies on exotic and decorated S-series and the associated Hopf algebra structures. The algebraic approach allows to obtain a formalism where one forest exactly corresponds to one order condition, to emphasize the central role of exotic series in stochastic numerics, and to identify the major algebraic difficulties brought by multiplicative noise.

The present work raises several new questions, from both algebraic and numerical perspectives, in the design of efficient discretisations. First, it would greatly simplify the analysis to find a class of methods whose Taylor expansions write as exotic series directly. Moreover, the design of the random variables was done by hand, and a formalisation of the definition of random variables satisfying given moment identities would help in the challenging calculations for higher order. The simplifying approach and the new methods presented in the present paper could be extended to other contexts such as, for instance, the creation of invariant measure-preserving methods for ergodic dynamics [12], symplectic schemes for the study of stochastic Hamiltonian systems [39], or for stochastic integration on manifolds. For the latter, the exotic Butcher series formalism is extended to the study of stochastic Lie-group methods with additive noise in [11]. The extension of such methods for multiplicative noise, for sampling ergodic dynamics, and the study of the associated algebraic structures (in the spirit of [15, 16]) is exciting matter for future work.

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References

[1] A. Abdulle, G. Vilmart, and K. C. Zygalakis. High order numerical approximation of the invariant measure of ergodic SDEs. *SIAM J. Numer. Anal.*, 52(4):1600–1622, 2014.

[2] A. Abdulle, G. Vilmart, and K. C. Zygalakis. Long time accuracy of Lie-Trotter splitting methods for Langevin dynamics. *SIAM J. Numer. Anal.*, 53(1):1–16, 2015.

[3] Y. Alama Bronsard, Y. Bruned, and K. Schratz. Approximations of dispersive PDEs in the presence of low-regularity randomness. *Foundations of Computational Mathematics*, pages 1–51, 2024.

[4] S. Anmarkrud, K. Debrabant, and A. Kværnø. General order conditions for stochastic partitioned Runge-Kutta methods. *BIT*, 58(2):257–280, 2018.

[5] G. Bogfjellmo. Algebraic structure of aromatic B-series. *J. Comput. Dyn.*, 6(2):199–222, 2019.

[6] G. Bogfjellmo, E. Celledoni, R. I. McLachlan, B. Owren, and G. R. W. Quispel. Using aromas to search for preserved measures and integrals in Kahan's method. *Math. Comp.*, 93(348):1633–1653, 2024.

[7] A. Bonicelli. Exotic B-series representation of the Feller semigroup for Itô diffusions and the MSR path integral. *arXiv preprint arXiv:2510.23102*, 2025.

[8] N. Bou-Rabee and H. Owhadi. Long-run accuracy of variational integrators in the stochastic context. *SIAM J. Numer. Anal.*, 48(1):278–297, 2010.

[9] E. Bronasco. Exotic B-series and S-series: algebraic structures and order conditions for invariant measure sampling. *Found. Comput. Math.*, pages 1–31, 2024.

[10] E. Bronasco and A. Busnot Laurent. Hopf algebra structures for the backward error analysis of ergodic stochastic differential equations. *Numer. Math.*, pages 1–61, 2026.

[11] E. Bronasco, A. Busnot Laurent, and B. Huguet. High order integration of stochastic dynamics on Riemannian manifolds with frozen-flow methods. *arXiv:2503.21855*, 2025.

[12] E. Bronasco, B. Leimkuhler, D. Phillips, and G. Vilmart. Efficient Langevin sampling with position-dependent diffusion. *arXiv preprint arXiv:2501.02943*, 2025.

[13] K. Burrage and P. M. Burrage. High strong order explicit Runge-Kutta methods for stochastic ordinary differential equations. *Appl. Numer. Math.*, 22(1-3):81–101, 1996. Special issue celebrating the centenary of Runge-Kutta methods.

[14] K. Burrage and P. M. Burrage. Order conditions of stochastic Runge-Kutta methods by B-series. *SIAM J. Numer. Anal.*, 38(5):1626–1646, 2000.

[15] A. Busnot Laurent, Y. Li, and Y. Sheng. Post-Hopf algebroids, post-Lie-Rinehart algebras and geometric numerical integration. *arXiv:2512.21971*, 2025.

[16] A. Busnot Laurent, H. Munthe-Kaas, and G. S. Venkatesh. The free tracial post-Lie-Rinehart algebra of planar aromatic trees for the numerical preservation of volume forms by Lie-group methods. *Submitted*, 2026.

[17] J. C. Butcher. The effective order of Runge-Kutta methods. In *Conf. on Numerical Solution of Differential Equations (Dundee, 1969)*, pages 133–139. Springer, Berlin, 1969.

[18] J. C. Butcher. An algebraic theory of integration methods. *Math. Comp.*, 26:79–106, 1972.

[19] J. C. Butcher. *Numerical methods for ordinary differential equations*. John Wiley & Sons, Ltd., Chichester, third edition, 2016.

[20] J. C. Butcher. *B-series: algebraic analysis of numerical methods*. Springer, 2021.

[21] P. Chartier, E. Hairer, and G. Vilmart. Algebraic structures of B-series. *Found. Comput. Math.*, 10(4):407–427, 2010.

[22] P. Chartier and A. Murua. Preserving first integrals and volume forms of additively split systems. *IMA J. Numer. Anal.*, 27(2):381–405, 2007.

[23] A. Connes and D. Kreimer. Hopf algebras, renormalization and noncommutative geometry. *Comm. Math. Phys.*, 199(1):203–242, 1998.

[24] A. Connes and D. Kreimer. Lessons from quantum field theory: Hopf algebras and spacetime geometries. *Letters in Mathematical Physics*, 48(1):85–96, 1999.

[25] K. Debrabant. Runge-Kutta methods for third order weak approximation of SDEs with multidimensional additive noise. *BIT Numer. Math.*, 50(3):541–558, 2010.

[26] K. Debrabant and A. Kværnø. B-series analysis of stochastic Runge-Kutta methods that use an iterative scheme to compute their internal stage values. *SIAM J. Numer. Anal.*, 47(1):181–203, 2008/09.

[27] K. Debrabant and A. Kværnø. Composition of stochastic B-series with applications to implicit Taylor methods. *Appl. Numer. Math.*, 61(4):501–511, 2011.

[28] K. Debrabant and A. Kværnø. Cheap arbitrary high order methods for single integrand SDEs. *BIT*, 57(1):153–168, 2017.

[29] K. Debrabant and A. Rößler. Classification of stochastic Runge-Kutta methods for the weak approximation of stochastic differential equations. *Math. Comput. Simulation*, 77(4):408–420, 2008.

[30] K. Debrabant and A. Rößler. Families of efficient second order Runge-Kutta methods for the weak approximation of Itô stochastic differential equations. *Appl. Numer. Math.*, 59(3-4):582–594, 2009.

[31] Y. Deng and Z. Hani. Full derivation of the wave kinetic equation. *Inventiones mathematicae*, 233(2):543–724, 2023.

[32] K. Ebrahimi-Fard and L. Rahm. A survey on the Munthe-Kaas–Wright Hopf algebra. *Journal of Computational Dynamics*, 2024.

[33] E. Faou and T. Lelièvre. Conservative stochastic differential equations: mathematical and numerical analysis. *Math. Comp.*, 78(268):2047–2074, 2009.

[34] L. Foissy. Algebraic structures on typed decorated rooted trees. *SIGMA Symmetry Integrability Geom. Methods Appl.*, 17:Paper No. 086, 28, 2021.

[35] E. Hairer, C. Lubich, and G. Wanner. *Geometric numerical integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006. Structure-preserving algorithms for ordinary differential equations.

[36] E. Hairer and G. Wanner. On the Butcher group and general multi-value methods. *Computing (Arch. Elektron. Rechnen)*, 13(1):1–15, 1974.

[37] R. Z. Hasminskii. *Stochastic stability of differential equations*, volume 7 of *Monographs and Textbooks on Mechanics of Solids and Fluids: Mechanics and Analysis*. Sijthoff & Noordhoff, Alphen aan den Rijn—Germantown, Md., 1980. Translated from the Russian by D. Louvish.

[38] M. E. Hoffman. Combinatorics of rooted trees and Hopf algebras. *Trans. Amer. Math. Soc.*, 355(9):3795–3811, 2003.

[39] J. Hong and L. Sun. *Symplectic integration of stochastic Hamiltonian systems*, volume 2314 of *Lecture Notes in Mathematics*. Springer, Singapore, [2022] ©2022.

[40] A. Iserles, H. Z. Munthe-Kaas, S. P. Nørsett, and A. Zanna. Lie-group methods. In *Acta numerica, 2000*, volume 9 of *Acta Numer.*, pages 215–365. Cambridge Univ. Press, Cambridge, 2000.

[41] A. Iserles, G. R. W. Quispel, and P. S. P. Tse. B-series methods cannot be volume-preserving. *BIT Numer. Math.*, 47(2):351–378, 2007.

[42] L. Isserlis. On a formula for the product-moment coefficient of any order of a normal frequency distribution in any number of variables. *Biometrika*, 12, 11 1918.

[43] P. E. Kloeden and E. Platen. *Numerical solution of stochastic differential equations*, volume 23 of *Applications of Mathematics (New York)*. Springer-Verlag, Berlin, 1992.

[44] I. Kolář, P. W. Michor, and J. Slovák. *Natural operations in differential geometry*. Springer-Verlag, Berlin, 1993.

[45] Y. Komori. Multi-colored rooted tree analysis of the weak order conditions of a stochastic Runge-Kutta family. *Appl. Numer. Math.*, 57(2):147–165, 2007.

[46] Y. Komori. Weak second-order stochastic Runge–Kutta methods for non-commutative stochastic differential equations. *J. Comput. Appl. Math.*, 206(1):158–173, 2007.

[47] Y. Komori, D. Cohen, and K. Burrage. Weak second order explicit exponential Runge-Kutta methods for stochastic differential equations. *SIAM J. Sci. Comput.*, 39(6):A2857–A2878, 2017.

[48] Y. Komori, T. Mitsui, and H. Sugiura. Rooted tree analysis of the order conditions of ROW-type scheme for stochastic differential equations. *BIT Numer. Math.*, 37(1):43–66, 1997.

[49] M. Kopec. Weak backward error analysis for Langevin process. *BIT Numer. Math.*, 55(4):1057–1103, 2015.

[50] M. Kopec. Weak backward error analysis for overdamped Langevin processes. *IMA J. Numer. Anal.*, 35(2):583–614, 2015.

[51] A. Laurent. *Algebraic Tools and Multiscale Methods for the Numerical Integration of Stochastic Evolutionary Problems.* PhD thesis, University of Geneva, 2021.

[52] A. Laurent. The Lie derivative and Noether's theorem on the aromatic bicomplex for the study of volume-preserving numerical integrators. *J. Comput. Dyn.*, 11(1):10–22, 2024.

[53] A. Laurent, R. I. McLachlan, H. Z. Munthe-Kaas, and O. Verdier. The aromatic bicomplex for the description of divergence-free aromatic forms and volume-preserving integrators. *Forum Math. Sigma*, 11:Paper No. e69, 2023.

[54] A. Laurent and H. Munthe-Kaas. The universal equivariance properties of exotic aromatic B-series. *Foundations of Computational Mathematics*, 25(5):1595–1626, 2025.

[55] A. Laurent and G. Vilmart. Exotic aromatic B-series for the study of long time integrators for a class of ergodic SDEs. *Math. Comp.*, 89(321):169–202, 2020.

[56] A. Laurent and G. Vilmart. Order conditions for sampling the invariant measure of ergodic stochastic differential equations on manifolds. *Found. Comput. Math.*, 22(3):649–695, 2022.

[57] B. Leimkuhler and C. Matthews. Rational construction of stochastic numerical methods for molecular sampling. *Appl. Math. Res. Express. AMRX*, 2013(1):34–56, 2013.

[58] B. Leimkuhler, C. Matthews, and G. Stoltz. The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics. *IMA J. Numer. Anal.*, 36(1):13–79, 2016.

[59] T. Lelièvre, M. Rousset, and G. Stoltz. *Free energy computations.* Imperial College Press, London, 2010. A mathematical perspective.

[60] V. Mackevičius and J. Navikas. Second order weak Runge-Kutta type methods of Itô equations. *Math. Comput. Simulation*, 57(1-2):29–34, 2001.

[61] R. I. McLachlan, K. Modin, H. Munthe-Kaas, and O. Verdier. B-series methods are exactly the affine equivariant methods. *Numer. Math.*, 133(3):599–622, 2016.

[62] R. I. McLachlan, K. Modin, H. Munthe-Kaas, and O. Verdier. Butcher series: a story of rooted trees and numerical methods for evolution equations. *Asia Pac. Math. Newsl.*, 7(1):1–11, 2017.

[63] G. N. Milstein. Weak approximation of solutions of systems of stochastic differential equations. *Teor. Veroyatnost. i Primenen.*, 30(4):706–721, 1985.

[64] G. N. Milstein. *Numerical integration of stochastic differential equations*, volume 313 of *Mathematics and its Applications*. Kluwer Academic Publishers Group, Dordrecht, 1995. Translated and revised from the 1988 Russian original.

[65] G. N. Milstein and M. V. Tretyakov. *Stochastic numerics for mathematical physics*. Scientific Computation. Springer-Verlag, Berlin, 2004.

[66] H. Munthe-Kaas and O. Verdier. Aromatic Butcher series. *Found. Comput. Math.*, 16(1):183–215, 2016.

[67] H. Z. Munthe-Kaas, O. Verdier, and G. Vilmart. A short proof of Isserlis' theorem. *arXiv preprint arXiv:2503.01588*, 2025.

[68] F. Panaite. Relating the Connes–Kreimer and Grossman–Larson Hopf algebras built on rooted trees. *Letters in Mathematical Physics*, 51(3):211–219, 2000.

[69] D. Phillips, B. Leimkuhler, and C. Matthews. Numerics with coordinate transforms for efficient Brownian dynamics simulations. *Molecular Physics*, 123(7-8):e2347546, 2025.

[70] E. Platen. *Zur zeitdiskreten Approximation von Itoprozessen*. PhD thesis, Akad. der Wiss. Der DDR, 1984.

[71] A. Rößler. Stochastic Taylor expansions for the expectation of functionals of diffusion processes. *Stochastic Anal. Appl.*, 22(6):1553–1576, 2004.

[72] A. Rößler. Rooted tree analysis for order conditions of stochastic Runge-Kutta methods for the weak approximation of stochastic differential equations. *Stoch. Anal. Appl.*, 24(1):97–134, 2006.

[73] A. Rößler. Runge-Kutta methods for Itô stochastic differential equations with scalar noise. *BIT Numer. Math.*, 46(1):97–110, 2006.

[74] A. Rößler. Second order Runge-Kutta methods for Stratonovich stochastic differential equations. *BIT Numer. Math.*, 47(3):657–680, 2007.

[75] A. Rößler. Second order Runge-Kutta methods for Itô stochastic differential equations. *SIAM Journal on Numerical Analysis*, 47(3):1713–1738, 2009.

[76] A. Rößler. Stochastic Taylor expansions for functionals of diffusion processes. *Stoch. Anal. Appl.*, 28(3):415–429, 2010.

[77] A. Rößler. Strong and weak approximation methods for stochastic differential equations—some recent developments. In *Recent developments in applied probability and statistics*, pages 127–153. Physica, Heidelberg, 2010.

[78] G.-C. Rota. On the foundations of combinatorial theory: I. theory of Möbius functions. In *Classic Papers in Combinatorics*, pages 332–360. Springer, 1964.

[79] X. Tang and A. Xiao. Efficient weak second-order stochastic Runge-Kutta methods for Itô stochastic differential equations. *BIT Numer. Math.*, 57(1):241–260, 2017.

[80] Á. Tocino and J. Vigo-Aguiar. Weak second order conditions for stochastic Runge–Kutta methods. *SIAM J. Sci. Comput.*, 24(2):507–523 (electronic), 2002.

[81] G. Vilmart. Postprocessed integrators for the high order integration of ergodic SDEs. *SIAM J. Sci. Comput.*, 37(1):A201–A220, 2015.

Appendices

A Implicit-explicit stochastic Runge-Kutta methods

We present in this section a collection of new IMEX methods with optimal number of stages. Such methods could typically be used for solving multiscale stochastic systems.

Itô diagonally implicit-explicit ($c = \frac{1}{4}$)

$\frac{1}{2}$	$\frac{1}{2}$	0
0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0
1	0	1

Itô explicit-diagonally implicit ($c = \frac{1}{2}$)

0	0	0	0
1	0	1	0
0	0	1	0
$\frac{1}{2}$	0	$-\frac{1}{2}$	1
$\frac{1}{2}$	$\frac{1}{2}$	0	1

Stratonovich diagonally implicit-explicit ($c = \frac{1}{4}$)

$\frac{1}{2}$	0	$\frac{1}{2}$	0	0				
0	0	0	0	0	0	0	0	0
0	$\frac{1}{2}$	0	0	0	$\frac{1}{2}$	0	0	0
$\frac{3}{2}$	-1	$\frac{3}{2}$	0	0	$-\frac{1}{2}$	$\frac{1}{2}$	0	0
$\frac{3}{2}$	$-\frac{1}{2}$	$\frac{3}{2}$	$-\frac{1}{2}$	0	$-\frac{3}{2}$	$\frac{3}{2}$	1	0
1	0	$\frac{2}{3}$	$\frac{1}{6}$	$\frac{1}{6}$				

Stratonovich explicit-diagonally implicit ($c = \frac{1}{2}$)

0	0	0	0	0			
1	0	1	0	0			
0	0	0	0	0	$\frac{1}{2}$	0	0
$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	$\frac{3-2\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	0
$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	$\frac{-3+2\sqrt{3}}{6}$	$\frac{1}{2}$	$\frac{3-\sqrt{3}}{6}$
$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$			

Stratonovich diagonally implicit ($c = \frac{1}{4}$)

$\frac{1}{2}$	$\frac{1}{2}$	0	0			
0	0	0	0	$\frac{1}{2}$	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	$\frac{3-2\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	$\frac{-3+2\sqrt{3}}{6}$	$\frac{1}{2}$	$\frac{3-\sqrt{3}}{6}$
1	0	$\frac{1}{2}$	$\frac{1}{2}$			