Order conditions for stochastic Runge–Kutta methods preserving quadratic invariants of Stratonovich SDEs.

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Abstract

In this paper we prove that for a stochastic Runge–Kutta method, the conditions for preserving quadratic invariants work as simplifying assumptions. For such methods, the method coefficients only have to satisfy one condition for each unrooted tree. This is a generalization of the result obtained for deterministic Runge–Kutta methods by Sanz-Serna and Abia in 1991.

Keywords: Stratonovich SDEs, stochastic Runge–Kutta methods, quadratic invariants, stochastic B–series, order conditions

1. Introduction

Over the last 25 years, numerical solution of stochastic differential equations (SDEs) has been a quite active field of research. Results and theories known from the literature on deterministic ordinary differential equations (ODEs) have been adapted to the stochastic setting. Recently, there has been a growing interest for stochastic methods preserving symplecticity, see e.g. [1, 2, 3, 4, 5]. In this paper, we will show that a quite elegant result by Sanz-Serna and Abia [6] for symplectic Runge–Kutta methods for ODEs also applies to SDEs. An s-stage Runge–Kutta method with coefficients $\{a_{ij}\}_{i,j=1}^{s}$ and weights $\{b_i\}_{i=1}^{s}$ is symplectic, and thus preserves quadratic invariants, if $b_i a_{ij} + b_j a_{ji} = b_i b_j$ for all $1 \le i, j \le s$. As proved in [6], this condition also serves as a simplifying assumption; when satisfied, only one order condition per unrooted tree remains to be satisfied. In this paper, we prove that this result can be extended to stochastic Runge–Kutta methods.

Consider the Stratonovich SDE

$$X(t) = x_0 + \sum_{l=0}^{m} \int_{t_0}^{t} g_l(X(s)) \circ dW_l(s), \tag{1}$$

where $W_0(t) = t$ and $W_l(t)$, $l = 1, \dots, m$ are independent Wiener processes. We assume that the coefficients $g_l : \mathbb{R}^d \to \mathbb{R}^d$ are sufficiently smooth and that g_l and $g_l' g_l$ satisfy a linear growth condition. The SDE is then guaranteed to have a unique solution. A differentiable function $I : \mathbb{R}^d \to \mathbb{R}$ is called an invariant of (1) if it satisfies

$$\nabla I(x)^T g_l(x) = 0, \qquad \text{for } l = 0, 1, \dots, m$$

for all x. In this paper, we are only interested in methods preserving quadratic invariants, that is $I(x) = x^T C x$ where C is a symmetric, constant $d \times d$ matrix.

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For the numerical solution of the SDE (1) we consider a stochastic Runge–Kutta (SRK) method defined by

$$H_i = Y_n + \sum_{l=0}^{m} \sum_{j=1}^{s} Z_{ij}^{(l)} g_l(H_j), \tag{2a}$$

$$Y_{n+1} = Y_n + \sum_{l=0}^{m} \sum_{i=1}^{s} \gamma_i^{(l)} g_l(H_i) \tag{2b}$$

where the coefficients $Z_{ij}^{(l)}$ and $\gamma_i^{(l)}$ include random variables which depend on the stepsize h.

The set of conditions for preserving quadratic invariants (or symplectic structure) of SRKs has been derived by Milstein et al. [1] for SDEs with additive noise and by Ma et al. [2] for problems with multiplicative scalar noise. The full problem was discussed by Hong et al. in [3], in which the following result has been proved:

Theorem 1. *If an SRK-method (2) satisfies*

$$\gamma_i^{(l)} Z_{ij}^{(k)} + \gamma_j^{(k)} Z_{ji}^{(l)} = \gamma_i^{(l)} \gamma_j^{(k)} \qquad \text{for all } i, j = 1, \ldots, s \text{ and } k, l = 0, \ldots, m, \tag{3}$$

then it conserves invariants of the form $I(x) = x^T C x + b^T x + c$ where C is a symmetric, constant $d \times d$ matrix, b is a constant vector of dimension d and c is a constant.

Condition (3) is what we will use as our simplifying assumption. The necessary background on order theory for SRKs in terms of B–series and rooted trees is given in Section 2. The main result is derived in Section 3. Section 4 is devoted to a numerical experiment, in which the stochastic rigid body problem is solved by a stochastic Gauss method.

2. Order conditions for SRKs

Order conditions for the method (2) by use of multicolored rooted trees have been developed by Burrage and Burrage [7, 8, 9] to study strong convergence and by Komori [10] and Rößler [11, 12] for weak convergence. A unified theory, covering both Itô and Stratonovich SDEs, and weak and strong convergence was developed in [13], and we will use this approach in the following.

In [13] a stochastic B–series for (1) is defined as a formal series:

$$B(\phi, x_0; h) = \sum_{\tau \in T} \alpha(\tau) \cdot \phi(\tau)(h) \cdot F(\tau)(x_0), \tag{4}$$

where T is the set of $m+1$-colored rooted trees $T = \{\emptyset\} \cup T_0 \cup T_1 \cup \cdots \cup T_m$ defined recursively as follows:

a) The graph $\bullet_l = [\emptyset]_l$ with only one vertex of color l belongs to T_l.

Let $\tau = [\tau_1, \tau_2, \ldots, \tau_\kappa]_l$ be the tree formed by joining the subtrees $\tau_1, \tau_2, \ldots, \tau_\kappa$ each by a single branch to a common root of color l.

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

Thus, T_l is the set of trees with an l-colored root, and T is the union of these sets. For a tree $\tau \in T$ the *elementary differential* $F(\tau)(x_0)$ is defined by

$$\begin{aligned} F(\emptyset)(x_0) &= x_0, \\ F(\bullet_l)(x_0) &= g_l(x_0), \\ F(\tau = [\tau_1, \ldots, \tau_\kappa]_l)(x_0) &= g_l^{(\kappa)}(x_0)\big(F(\tau_1)(x_0), \ldots, F(\tau_\kappa)(x_0)\big), \end{aligned} \tag{5}$$

and α is given by

$$\alpha(\emptyset) = 1, \qquad \alpha(\bullet_l) = 1, \qquad \alpha(\tau = [\tau_1, \dots, \tau_\kappa]_l) = \frac{1}{r_1! \dots r_q!} \prod_{k=1}^{\kappa} \alpha(\tau_k),$$

where $r_1, \dots, r_q$ count equal trees among $\tau_1, \dots, \tau_\kappa$. The elementary weight functions φ are stochastic integrals or random variables that depend on the stepsize h. Following [9] the order of a tree is given by

$$\rho(\emptyset) = 0, \qquad \rho(\tau = [\tau_1, \dots, \tau_\kappa]_l) = \sum_{k=1}^{\kappa} \rho(\tau_k) + \begin{cases} 1 & \text{for } l = 0, \\ \frac{1}{2} & \text{otherwise.} \end{cases}$$

The number of nodes in a tree is denoted $|\tau|$. The following theorem was proved in [13]:

Theorem 2. *The exact solution $X(t_0 + h)$ of (1) as well as the numerical solution Y_1 and the stage values H_i, $i = 1, \dots, s$ from (2) can be written as stochastic B–series,*

$$X(t_0 + h) = B(\varphi, x_0; h), \qquad H_i = B(\Phi_i, x_0; h) \quad \textit{and} \quad Y_1 = B(\Phi, x_0; h)$$

with

$$\varphi(\emptyset)(h) = 1, \qquad \varphi(\bullet_l)(h) = W_l(h), \qquad \varphi(\tau)(h) = \int_0^h \left(\prod_{k=1}^{\kappa} \varphi(\tau_k)(s) \right) \circ dW_l(s), \tag{6a}$$

$$\Phi_i(\emptyset)(h) = 1, \qquad \Phi_i(\bullet_l)(h) = \sum_{j=1}^{s} Z_{ij}^{(l)}, \qquad \Phi_i(\tau)(h) = \sum_{j=1}^{s} Z_{ij}^{(l)} \prod_{k=1}^{\kappa} \Phi_j(\tau_k)(h), \qquad i = 1, \dots, s \tag{6b}$$

$$\Phi(\emptyset)(h) = 1, \qquad \Phi(\bullet_l)(h) = \sum_{i=1}^{s} \gamma_i^{(l)}, \qquad \Phi(\tau)(h) = \sum_{i=1}^{s} \gamma_i^{(l)} \prod_{k=1}^{\kappa} \Phi_i(\tau_k)(h), \tag{6c}$$

where $\tau = [\tau_1, \dots, \tau_\kappa]_l$.

Remark 1. By replacing Stratonovich integrals with Itô integrals, this theorem holds for Itô SDEs as well.

Example 1. Given the tree $\tau = [[\bullet_1, \bullet_1]_0, [\bullet_2]_2]_1 \in T$. Let ● $\in T_0$ (deterministic), ● $\in T_1$ and ● $\in T_2$ (stochastic). Then the graphical representation of τ is given to the left, and its corresponding terms to the right.

$\tau =$

$$F(\tau) = g_1''\big(g_0''(g_1, g_1), g_2' g_2\big),$$

$$\alpha(\tau) = 1/2, \qquad \rho(\tau) = 7/2, \qquad |\tau| = 6,$$

$$\varphi(\tau)(h) = \int_0^h \left(\int_0^s W_1^2(u)\, du \cdot \int_0^s W_2(u) \circ dW_2(u) \right) \circ dW_1(s),$$

$$\Phi(\tau)(h) = \sum_{i,j,l,m,n,o=1}^{s} \gamma_i^{(1)} Z_{ij}^{(0)} Z_{jl}^{(1)} Z_{jm}^{(1)} Z_{in}^{(2)} Z_{no}^{(2)}.$$

The local order of an SRK can now be decided by comparing the B–series of the exact and the numerical solution. The global order is given by the following theorem:

Theorem 3. *The method has mean square global order p if*

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

$$E\Phi(\tau)(h) = E\varphi(\tau)(h) + \mathcal{O}(h^{p+1}), \qquad \forall \tau \in T \textit{ with } \rho(\tau) \le p + \frac{1}{2} \tag{7b}$$

and weak consistency of order p if and only if

$$E \prod_{j=1}^{\kappa} \Phi(\tau_j)(h) = E \prod_{j=1}^{\kappa} \varphi(\tau_j)(h) + \mathcal{O}(h^{p+1}) \quad \textit{whenever} \quad \sum_{j=1}^{\kappa} \rho(\tau_j) \le p + \frac{1}{2}. \tag{8}$$

$u = [u_1]_{l_1}$	$v = [v_1, v_2]_{l_2}$	$u \circ v$	$v \circ u$
$\varphi(u)$	$\varphi(v)$	$\varphi(u \circ v)$	$\varphi(v \circ u)$
$\shortparallel$	$\shortparallel$	$\shortparallel$	$\shortparallel$
$\int_0^h \varphi(u_1) dW_{l_1}$	$\int_0^h \varphi(v_1)\varphi(v_2) dW_{l_2}$	$\int_0^h \varphi(u_1)\varphi(v) dW_{l_1}$	$\int_0^h \varphi(u)\varphi(v_1)\varphi(v_2) dW_{l_2}$

Figure 1: The Butcher product of two trees u and v and their elementary weight functions.

We assume that the method (2) is constructed such that $\Phi(\tau)(h) = \mathcal{O}(h^{\rho(\tau)})\ \forall \tau \in T$, where the $\mathcal{O}(\cdot)$-notation refers to the $L^2(\Omega)$-norm and $h \to 0$. The result (7) was first proved in [8], the second is a consequence of a result of Milstein [14], see [13] for details.

3. Simplifying assumptions and unrooted trees

In this section, we present the main result of this paper: When the condition of Theorem 1 is satisfied, the method coefficients have to satisfy no more than one condition for each unrooted tree to satisfy (7a). The key ingredient in this is the Butcher product of two trees $u, v \in T \setminus \emptyset$. If

$$u = [u_1, \ldots, u_{\kappa_1}]_{l_1},$$

then the Butcher product is defined as

$$u \circ v = [u_1, \ldots, u_{\kappa_1}, v]_{l_1},$$

the tree obtained by adding v as a branch to the root of u. This is illustrated in Figure 1, which also illustrates the first part of the following lemma:

Lemma 4. *For all $u \in T_{l_1} \setminus \emptyset$ and $v \in T_{l_2} \setminus \emptyset$, $l_1, l_2 = 0, \ldots, m$, we have*

$$\varphi(u)(h) \cdot \varphi(v)(h) = \varphi(u \circ v)(h) + \varphi(v \circ u)(h). \tag{9a}$$

If the SRK preserves quadratic invariants by satisfying (3) *then*

$$\Phi(u)(h) \cdot \Phi(v)(h) = \Phi(u \circ v)(h) + \Phi(v \circ u)(h). \tag{9b}$$

Proof. Let $u = [u_1, \ldots, u_{\kappa_1}]_{l_1} \in T_{l_1} \setminus \emptyset$ and $v = [v_1, \ldots, v_{\kappa_2}]_{l_2} \in T_{l_2} \setminus \emptyset$ for $l_1, l_2 = 0, \ldots, m$. The first statement (9a) is a direct consequence of the integration by parts rule valid for Stratonovich integrals together with the definition of φ from Theorem 2:

$$\varphi(u)(h) \cdot \varphi(v)(h) = \int_0^h \varphi(v)(s) \circ d\big(\varphi(u)(s)\big) + \int_0^h \varphi(u)(h) \circ d\big(\varphi(v)(s)\big)$$

with $d\big(\varphi(u)(s)\big) = \prod_{k=1}^{\kappa_1} \varphi(u_k)(s) \circ dW_{l_1}(s)$ and $d\big(\varphi(v)(s)\big) = \prod_{k=1}^{\kappa_2} \varphi(v_k)(s) \circ dW_{l_2}(s)$. For the second part, (9b), use (6b), (6c) together with (3) to obtain

$$\begin{aligned}
\Phi(u)(h) \cdot \Phi(v)(h) &= \sum_{i=1}^{s} \gamma_i^{(l_1)} \prod_{k_1=1}^{\kappa_1} \Phi_i(u_{k_1})(h) \cdot \sum_{j=1}^{s} \gamma_j^{(l_2)} \prod_{k_2=1}^{\kappa_2} \Phi_j(v_{k_2})(h) \\
&= \sum_{i=1}^{s} \sum_{j=1}^{s} (\gamma_i^{(l_1)} Z_{ij}^{(l_2)} + \gamma_j^{(l_2)} Z_{ji}^{(l_1)}) \prod_{k_1=1}^{\kappa_1} \Phi_i(u_{k_1})(h) \prod_{k_2=1}^{\kappa_2} \Phi_j(v_{k_2})(h) \\
&= \sum_{i=1}^{s} \gamma_i^{(l_1)} \Phi_i(v)(h) \prod_{k_1=1}^{\kappa_1} \Phi_i(u_{k_1})(h) + \sum_{j=1}^{s} \gamma_j^{(l_2)} \Phi_j(u)(h) \prod_{k_2=1}^{\kappa_2} \Phi_j(v_{k_2})(h) \\
&= \Phi(u \circ v)(h) + \Phi(v \circ u)(h),
\end{aligned}$$

which proves the lemma.

We are now ready to present the main result of this paper. Given a $\tau \in T$, let $\hat{\tau}$ be the corresponding unrooted tree, and let $\hat{T}(\hat{\tau}) \subset T$ be the set of trees obtained from $\hat{\tau}$ by assigning one of the nodes as the root, see Figure 2 for an illustration. We can now state the following theorem:

Theorem 5. *Assume that* (3) *is satisfied. Let $\hat{\tau} \in \hat{T}$ be an unrooted tree of order $q \leq p$. If $\varphi(\tau)(h) = \Phi(\tau)(h) + \mathcal{O}(h^{p+\frac{1}{2}})$ for one rooted tree $\tau \in \hat{T}(\hat{\tau})$ and all rooted trees of order less than q, then it holds that $\varphi(\tau)(h) = \Phi(\tau)(h) + \mathcal{O}(h^{p+\frac{1}{2}})$ for all $\tau \in \hat{T}(\hat{\tau})$.*

Proof. For trees with one node the theorem is trivially true. Let $\hat{\tau}$ be an unrooted tree of order q and two or more nodes, and let τ be a corresponding rooted tree $\tau \in \hat{T}(\hat{\tau})$. Pick one branch v from the root of τ and let the remaining part of τ be u, so that $\tau = u \circ v$. Clearly, the orders of u and v are less than the order of τ, and by Lemma 4 and the assumptions of the Theorem we then have

$$\varphi(v \circ u)(h) = \Phi(v \circ u)(h) + \mathcal{O}(h^{p+\frac{1}{2}})$$

Because the choice of branch v was arbitrary, this means that this condition is satisfied for all trees with the same graph as τ, but with a root shifted to one of its neighbouring nodes. A repeated use of this argument proves the result. The process is illustrated in Figure 2.

Table 1 shows the number of rooted and unrooted trees of order 2.5 and less in the case of one stochastic process.

$\rho(\tau)$	Rooted	Unrooted
0.5	1	1
1.0	2	2
1.5	4	2
2.0	10	5
2.5	27	9

Table 1: For one stochastic process, $m = 1$, the second and third column show the number of different rooted and unrooted trees, respectively, that have order $\rho(\tau) \leq 2.5$.

4. Numerical experiment

Although application of Theorem 5 reduces the number of order conditions significantly, the conditions of Theorem 1 are hard to fulfill. In the case of scalar noise, methods of strong order 1 can be found in e.g. [2, 3, 4] and a weak order 2 method is given in [3]. And as an experiment, we will see how the extension of

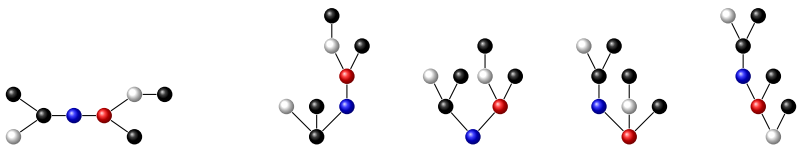


Figure 2: An unrooted tree $\hat{\tau}$ to the left, and some of the trees in $\hat{T}(\hat{\tau})$. The figure also illustrates the process described in the proof of Theorem 5.

the Gauss methods performs when solving a stochastic rigid body problem [15]. The problem with scalar noise is given by:

$$dX = A(X)Xdt + g_1(X) \circ dW \tag{10}$$

with

$$A(X) = \begin{pmatrix} 0 & X_3/I_3 & -X_2/I_2 \\ -X_3/I_3 & 0 & X_1/I_1 \\ X_2/I_2 & -X_1/I_1 & 0 \end{pmatrix}.$$

With $g_1 = 0$ this is the deterministic rigid body problem described in [16], and we will here use the same parameters: $I_1 = 2$, $I_2 = 1$ and $I_3 = 2/3$, and as initial values $X(0) = (\cos(1.1), 0, \sin(1.1))^T$. In the stochastic case, we consider two different diffusion processes:

$$P1: \qquad g_1(X) = A(X)X, \tag{11a}$$

$$P2: \qquad g_1(X) = (X_2, -X_1, 0). \tag{11b}$$

Problem P1 conserves the Hamiltonian

$$H(X) = \frac{1}{2}\left(\frac{X_1^2}{I_1} + \frac{X_2^2}{I_2} + \frac{X_3^2}{I_3}\right), \tag{12}$$

and both problems preserve the Casimir

$$C(X) = X_1^2 + X_2^2 + X_3^2. \tag{13}$$

The problems are solved by the straightforward generalization of the Gauss method

$$s = 1: \qquad Z^{(l)} = \tfrac{1}{2} J_l, \qquad \gamma^{(l)} = J_l \tag{14a}$$

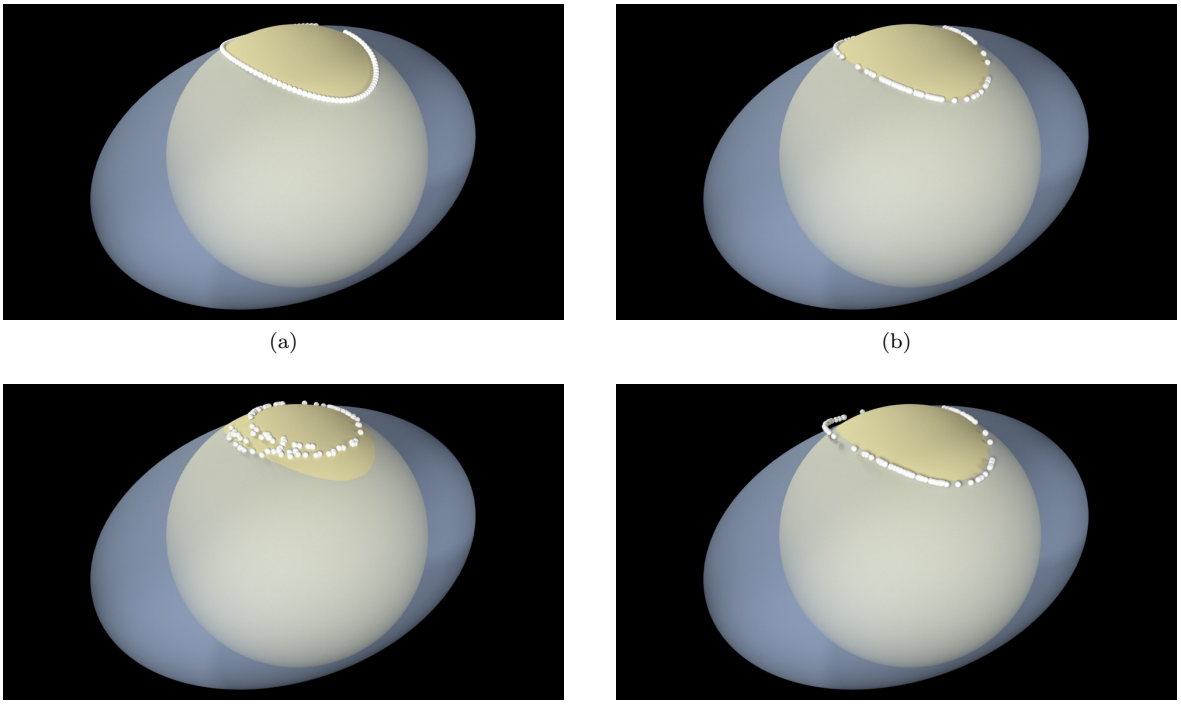
$$s = 2: \qquad Z^{(l)} = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \end{pmatrix} J_l, \qquad \gamma^{(l)} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} J_l \tag{14b}$$

for $l = 0, 1$. The methods are referred to as Gauss(s), with $s = 1, 2$. By Theorem 1 they both preserve quadratic invariants. And due to the lack of a J_{01} term, they are both only of mean square order 1. For comparison, we have also included Platen's method [7]:

$$Z^{(l)} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} J_l, \quad l = 0, 1, \qquad \gamma^{(0)} = \begin{pmatrix} 1 & 0 \end{pmatrix} J_0, \qquad \gamma^{(1)} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} J_1. \tag{15}$$

This method is also of mean square order 1, but does not preserve quadratic invariants.

The Gauss method with $s = 2$ was used to solve the deterministic rigid body problem, as well as the two stochastic cases $P1$ and $P2$. The result of one path is given in Figure 3, (a)-(c). Here, we clearly can see that for P1 as well as in the deterministic case, the solution stays on the intersection between the two manifolds given by H and C, while for $P2$, it will only stay at the second one. When Platen's method (15) is applied to P1, none of the invariants are preserved, as shown in (d).



(a) (b) (c) (d)

Figure 3: Numerical simulation of the stochastic rigid body problem and the two invariants H (blue) and C (gold). The pictures show the result of Gauss(2) applied to (a) the deterministic problem, (b) P1 and (c) P2. In (d) Platen's method is applied to P1. All simulations are run for 100 steps with the stepsize $h = 0.1$.

Figure 4 shows the convergence plots for the Gauss methods as well as Platen's method applied to the two stochastic rigid body problems. Here, the interval of integration is $[0, T]$ with $T = 0.1$. The reference solution is computed by the Gauss(2) method using the stepsize $h = 2^{-11} \cdot T$, and $M = 1000$ independent simulations are used for the expectation. A mean-square order 1 is observed in all cases but one. When Gauss(2) is applied to P1, the observed order is 2. This problem is a single integrand problem, in the sense that $g_1 = \sigma g_0$ for some constant σ. In this case the elementary differentials $F(\tau)$ are the same for all trees τ with the same graph and the same number of deterministic and stochastic nodes. To obtain order 2 it is then sufficient that the sum of the elementary weight functions over such trees are the same for the exact and the numerical solutions. This fact is explored by Debrabant et al. [17], where it is proved that all stochastic Gauss methods of the form (14) are of mean square global order s for single integrand problems.

The Gauss methods are implicit. For the convergence plots, the underlying nonlinear algebraic equations were solved by a modified Newton method. Even without truncation of the random variables [1], the iterations converged for stepsizes $h \leq 0.0125$. For the simulations in Figure 3 in which case $h = 0.1$, the nonlinear equations were solved by MATLABs `fsolve`, which managed to find the solutions of each step.

5. Concluding remarks

In this paper we have proved that for stochastic Runge–Kutta methods fulfilling condition (3) it is sufficient to consider the order conditions (7a) related to unrooted trees. This does lead to a significant reduction of order conditions. However, the conditions (3) are very restrictive, and we have so far not been able to construct methods of mean square order higher than 1, even in the case of scalar noise. The numerical example indicates however that the situation is more optimistic for single integrand problems, this is further explored in [17].

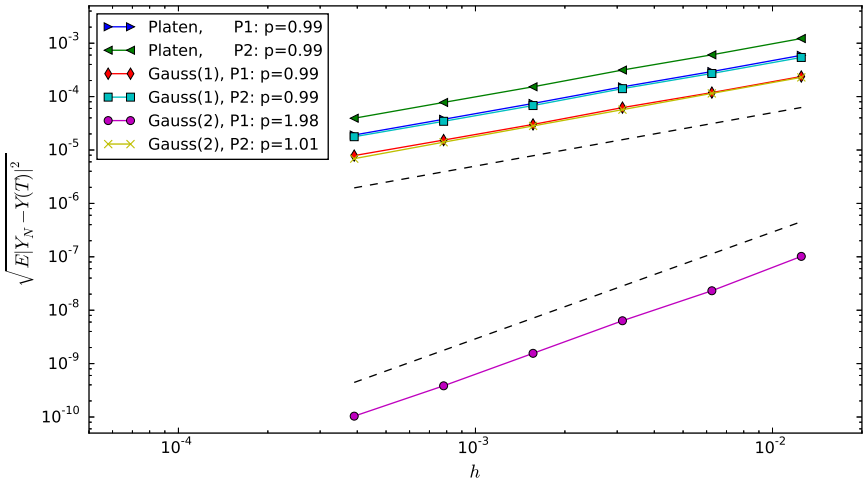


Figure 4: Mean-square error of Platen's method as well as the two Gauss methods applied to the two rigid body problems. The dashed lines are reference lines with slopes 1 and 2.

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