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A class of orthogonal integrators for stochastic differential equations☆

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Abstract

The purpose of this paper is to construct a class of orthogonal integrators for stochastic differential equations (SDEs). The family of SDEs with orthogonal solutions is univocally characterized. For this, a class of orthogonal integrators is introduced by imposing constraints to Runge–Kutta (RK) matrices and weights of the standard stochastic RK schemes.The performance of the method is illustrated by means of numerical simulations.

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1. Introduction

During the last few years there has been a growing interest in the use of geometric integrators for the numerical integration of ordinary differential equations (ODEs) (see [15,6,3] and references therein). These types of integrators are those that preserve some relevant geometric structure of the original solution (symplecticness, orthogonality, isospectrality, energy-conservation, etc.), which ensure that, in most cases, the approximate solutions have smaller long-term qualitative error than other standard integrators. They have found a number of applications for the study of Hamiltonian systems [16] and the computation of the Lyapunov exponents (LEs) [7], for instance.

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Accordingly, interest in the geometric-preserving structure in the numerical integration of stochastic differential equations (SDEs) has also increased. Examples are the symplectic and energy-preserving integrators proposed in [10–14]. However, orthogonal stochastic integrators have not been studied so far. This orthogonality-preserving property of the numerical integrators becomes essential in the *QR* decomposition of the fundamental solution of certain multidimensional linear equations that arise in the characterization of the Lyapunov spectrum [5] and more recently in the construction of the continuous *QR* methods of computing the Lyapunov exponents of SDEs [4]. Therefore, the need for developing orthogonal integrators for SDEs is in order.

The goal of this paper is the construction of orthogonal integrators for SDEs. First, the class of SDEs that produce orthogonal solutions is univocally characterized. Then, for this type of equations, a class of Runge–Kutta (RK) integrators is obtained by imposing orthogonality restrictions to the RK matrices and weights.

The plan of the paper is as follows: In Section 2, the concepts of orthogonal stochastic solutions and skew-symmetric SDEs are introduced, and a necessary and sufficient condition that characterizes the orthogonality of the solutions is given. In Section 3, a sufficient condition for the orthogonality of the RK schemes is provided. Then, in Section 4, a particular class of the orthogonal RK schemes is considered. Some details about the numerical implementation of these automatic orthogonal schemes are presented in Section 5 and finally, two numerical test examples are presented in Section 6.

2. Orthogonal solutions and skew-symmetric equations

Let $(\Omega, \mathscr{F}, P)$ be an underlying complete probability space and $\{\mathscr{F}_t,\ t \geqslant 0\}$ be an increasing right continuous family of complete sub σ-algebras of $\mathscr{F}$. Consider the following Stratanovich SDE:

$$\mathrm{d}\mathbf{X}_t = \sum_{j=0}^{m} \mathbf{F}_j(t, \mathbf{X}_t) \circ \mathrm{d}\mathbf{w}_t^j, \quad \mathbf{X}_{t_0} = \mathbf{X}_0 \in \mathbb{R}^{d\times d}, \tag{1}$$

where $\mathbf{F}_j$ are nonlinear matrix functions, $\mathbf{w} = (\mathbf{w}^1, \ldots, \mathbf{w}^m)$ is an m-dimensional $\mathscr{F}_t$-adapted standard Wiener process, and the convention $\mathrm{d}\mathbf{w}_t^0 = \mathrm{d}t$. Suppose further that the conditions for the existence and uniqueness of the solution are satisfied.

The following definition is a straightforward extension to the SDEs case of the concept of orthogonal solution.

Definition 1. Eq. (1) with the condition $\mathbf{X}_0^\top \mathbf{X}_0 = \mathbf{I}_d$ is said to generate an orthogonal solution if $\mathbf{X}_t$ is an orthogonal matrix for every $t \geqslant t_0$, w.p.1.

The family of SDEs that generate orthogonal solutions is univocally characterized by the following theorem.

Theorem 2. *Eq.* (1) *with the condition* $\mathbf{X}_0^\top \mathbf{X}_0 = \mathbf{I}_d$ *generates an orthogonal solution if and only if for each* $j = 0, \ldots, m$

$$\mathbf{F}_j(t, \mathbf{X}_t) = \mathbf{G}_j(t, \mathbf{X}_t)\mathbf{X}_t,$$

where the functions $\mathbf{G}_j$ *satisfy*

$$\mathbf{G}_j(t,\mathbf{X}_t)^{\top} = -\mathbf{G}_j(t,\mathbf{X}_t).$$

Proof. First suppose that for each $j = 0, \ldots, m$

$$\mathbf{F}_j(t,\mathbf{X}_t) = \mathbf{G}_j(t,\mathbf{X}_t)\mathbf{X}_t \quad \text{with } \mathbf{G}_j(t,\mathbf{X}_t)^{\top} = -\mathbf{G}_j(t,\mathbf{X}_t).$$

Then, by considering the following differentials in Stratanovich's sense it is obtained that

$$\begin{aligned}
\mathrm{d}(\mathbf{X}_t^{\top}\mathbf{X}_t) &= (\mathrm{d}\mathbf{X}_t^{\top})\mathbf{X}_t + \mathbf{X}_t^{\top}(\mathrm{d}\mathbf{X}_t)\\
&= \sum_{j=0}^{m} (\mathbf{X}_t^{\top}\mathbf{G}_j(t,\mathbf{X}_t)^{\top}\mathbf{X}_t + \mathbf{X}_t^{\top}\mathbf{G}_j(t,\mathbf{X}_t)\mathbf{X}_t) \circ \mathrm{d}\mathbf{w}_t^j\\
&= \sum_{j=0}^{m} \mathbf{X}_t^{\top}(\mathbf{G}_j(t,\mathbf{X}_t)^{\top} + \mathbf{G}_j(t,\mathbf{X}_t))\mathbf{X}_t \circ \mathrm{d}\mathbf{w}_t^j\\
&= 0.
\end{aligned}$$

Therefore, $\mathbf{X}_t^{\top}\mathbf{X}_t = \mathbf{X}_0^{\top}\mathbf{X}_0 = \mathbf{I}_d$, which implies the orthogonality of the solution.

Now suppose that the solution is orthogonal. That is,

$$\mathbf{X}_t^{\top}\mathbf{X}_t = \mathbf{I}_d \quad \forall t \geqslant t_0.$$

Taking differential in the sense of Stratanovich it is obtained that

$$\begin{aligned}
0 &= \mathrm{d}(\mathbf{X}_t^{\top}\mathbf{X}_t)\\
&= (\mathrm{d}\mathbf{X}_t^{\top})\mathbf{X}_t + \mathbf{X}_t^{\top}(\mathrm{d}\mathbf{X}_t)\\
&= \sum_{j=0}^{m} (\mathbf{F}_j(t,\mathbf{X}_t)^{\top}\mathbf{X}_t + \mathbf{X}_t^{\top}\mathbf{F}_j(t,\mathbf{X}_t)) \circ \mathrm{d}\mathbf{w}_t^j\\
&= \sum_{j=0}^{m} \mathbf{X}_t^{\top}(\mathbf{G}_j(t,\mathbf{X}_t)^{\top} + \mathbf{G}_j(t,\mathbf{X}_t))\mathbf{X}_t \circ \mathrm{d}\mathbf{w}_t^j,
\end{aligned}$$

where $\mathbf{G}_j(t,\mathbf{X}_t)$ is defined by $\mathbf{G}_j(t,\mathbf{X}_t) = \mathbf{F}_j(t,\mathbf{X}_t)\mathbf{X}_t^{\top}$, for each $j = 0, \ldots, m$. Hence, from the last equality it is obtained that $\mathbf{G}_j(t,\mathbf{X}_t)^{\top} + \mathbf{G}_j(t,\mathbf{X}_t) = 0$. This concludes the proof. □

The above theorem motivates us to consider the following type of SDEs, which trivially generate orthogonal solutions.

Definition 3. The equations of the type

$$\mathrm{d}\mathbf{X}_t = \sum_{j=0}^{m} \mathbf{G}_j(t,\mathbf{X}_t)\mathbf{X}_t \circ \mathrm{d}\mathbf{w}_t^j, \quad \mathbf{X}_{t_0} = \mathbf{X}_0, \quad \mathbf{X}_0^{\top}\mathbf{X}_0 = \mathbf{I}_d, \tag{2}$$

where $\mathbf{G}_j(t,\mathbf{X})$ are skew-symmetric matrix functions (i.e. $\mathbf{G}_j(t,\mathbf{X})^{\top} = -\mathbf{G}_j(t,\mathbf{X})$ for all $t \in \mathbb{R}$, $\mathbf{X} \in \mathbb{R}^{d\times d}$) are called skew-symmetric SDEs.

3. A sufficient condition for the orthogonality of the RK methods

Consider the skew-symmetric SDE

$$\mathrm{d}\mathbf{X}_t = \mathbf{G}_0(t,\mathbf{X}_t)\mathbf{X}_t\,\mathrm{d}t + \mathbf{G}_1(t,\mathbf{X}_t)\mathbf{X}_t \circ \mathrm{d}w_t,$$

$$\mathbf{X}_{t_0} = \mathbf{X}_0, \quad \mathbf{X}_0^\top \mathbf{X}_0 = \mathbf{I}_d, \tag{3}$$

where $\mathbf{G}_0$ and $\mathbf{G}_1$ are differentiable matrix functions. Consider further the time discretization $(t)_h = \{t_n = t_0 + nh : n = 0, 1, 2, \ldots\}$ with step size $h \in (0, 1)$ and the class of s-stage order 1 stochastic RK integrators [8,1] defined by

$$\mathbf{\Phi}_i = \mathbf{Y}_n + h\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{G}_0(t_n+\mathbf{c}_j h, \mathbf{\Phi}_j)\mathbf{\Phi}_j + J_1\sum_{j=1}^{s}\mathbf{B}_{ij}\mathbf{G}_1(t_n+\mathbf{c}_j h, \mathbf{\Phi}_j)\mathbf{\Phi}_j, \quad i = 1, \ldots, s, \tag{4}$$

$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + h\sum_{j=1}^{s}\boldsymbol{\alpha}_j\mathbf{G}_0(t_n+\mathbf{c}_j h, \mathbf{\Phi}_j)\mathbf{\Phi}_j + J_1\sum_{j=1}^{s}\gamma_j\mathbf{G}_1(t_n+\mathbf{c}_j h, \mathbf{\Phi}_j)\mathbf{\Phi}_j, \quad n = 0, 1, \ldots, \tag{5}$$

where $\mathbf{A} = (\mathbf{A}_{ij})$, $\mathbf{B} = (\mathbf{B}_{ij})$ are the $s \times s$ RK matrices, $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_s)$, $\gamma = (\gamma_1, \ldots, \gamma_s)$ are the s-dimensional RK weights, $\mathbf{c} = (\mathbf{c}_1, \ldots, \mathbf{c}_s)$ is the s-dimensional RK node and J_1 denotes Stratanovich's integral $\int_0^h \circ\,\mathrm{d}w$.

Definition 4. The numerical scheme (4–5) is said to be orthogonal if $\mathbf{Y}_n^\top \mathbf{Y}_n = \mathbf{I}_d$, for each n, w.p.1.

A sufficient condition for the orthogonality of the above numerical scheme is given by the following theorem.

Theorem 5. *Let* $\mathbf{M}^1, \mathbf{M}^2, \mathbf{M}^3$ *be the* $s \times s$ *matrices defined by*

$$(\mathbf{M}^1_{lj}) = \boldsymbol{\alpha}_l\boldsymbol{\alpha}_j - \boldsymbol{\alpha}_l\mathbf{A}_{lj} - \boldsymbol{\alpha}_j\mathbf{A}_{jl},$$

$$(\mathbf{M}^2_{lj}) = \boldsymbol{\alpha}_l\gamma_j - \gamma_j\mathbf{A}_{jl} - \boldsymbol{\alpha}_l\mathbf{B}_{lj},$$

$$(\mathbf{M}^3_{lj}) = \gamma_l\gamma_j - \gamma_l\mathbf{B}_{lj} - \gamma_j\mathbf{B}_{jl}.$$

If

$$\mathbf{M}^1 = \mathbf{M}^2 = \mathbf{M}^3 = \mathbf{0}, \tag{6}$$

then (4–5) *is an orthogonal scheme.*

Proof. For each $j = 1, \ldots, s$ denote

$$\mathbf{U}_{0j} = \mathbf{G}_0(t_n + \mathbf{c}_j h, \mathbf{\Phi}_j)\mathbf{\Phi}_j \quad \text{and} \quad \mathbf{U}_{1j} = \mathbf{G}_1(t_n + \mathbf{c}_j h, \mathbf{\Phi}_j)\mathbf{\Phi}_j.$$

From (5) it follows that

$$
\begin{aligned}
\mathbf{Y}_{n+1}^{\top}\mathbf{Y}_{n+1} = \mathbf{Y}_n^{\top}\mathbf{Y}_n + h\Bigg[&\mathbf{Y}_n^{\top}\sum_{j=1}^{s}\boldsymbol{\alpha}_j\mathbf{U}_{0j} + \sum_{j=1}^{s}\boldsymbol{\alpha}_j\mathbf{U}_{0j}^{\top}\mathbf{Y}_n + h\sum_{l=1}^{s}\sum_{j=1}^{s}\boldsymbol{\alpha}_l\boldsymbol{\alpha}_j\mathbf{U}_{0l}^{\top}\mathbf{U}_{0j}\\
&+ J_1\sum_{l=1}^{s}\sum_{j=1}^{s}\boldsymbol{\alpha}_j\gamma_l\mathbf{U}_{1l}^{\top}\mathbf{U}_{0j}\Bigg] + J_1\Bigg[\mathbf{Y}_n^{\top}\sum_{j=1}^{s}\gamma_j\mathbf{U}_{1j} + \sum_{j=1}^{s}\gamma_j\mathbf{U}_{1j}^{\top}\mathbf{Y}_n\\
&+ h\sum_{l=1}^{s}\sum_{j=1}^{s}\boldsymbol{\alpha}_l\gamma_j\mathbf{U}_{0l}^{\top}\mathbf{U}_{1j} + J_1\sum_{l=1}^{s}\sum_{j=1}^{s}\gamma_l\gamma_j\mathbf{U}_{1l}^{\top}\mathbf{U}_{1j}\Bigg]. \qquad (7)
\end{aligned}
$$

Now, from (4) and a suitable exchange of the summation indices it is obtained that

$$
\mathbf{Y}_n^{\top}\sum_{l=1}^{s}\boldsymbol{\alpha}_l\mathbf{U}_{0l} = \sum_{l=1}^{s}\boldsymbol{\alpha}_l\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{0l} - h\sum_{l=1}^{s}\sum_{j=1}^{s}\boldsymbol{\alpha}_j\mathbf{A}_{jl}\mathbf{U}_{0l}^{\top}\mathbf{U}_{0j} - J_1\sum_{l=1}^{s}\sum_{j=1}^{s}\boldsymbol{\alpha}_j\mathbf{B}_{jl}\mathbf{U}_{1l}^{\top}\mathbf{U}_{0j},
$$

$$
\sum_{l=1}^{s}\boldsymbol{\alpha}_l\mathbf{U}_{0l}^{\top}\mathbf{Y}_n = \sum_{l=1}^{s}\boldsymbol{\alpha}_l\mathbf{U}_{0l}^{\top}\boldsymbol{\Phi}_l - h\sum_{l=1}^{s}\sum_{j=1}^{s}\boldsymbol{\alpha}_l\mathbf{A}_{lj}\mathbf{U}_{0l}^{\top}\mathbf{U}_{0j} - J_1\sum_{l=1}^{s}\sum_{j=1}^{s}\boldsymbol{\alpha}_l\mathbf{B}_{lj}\mathbf{U}_{0l}^{\top}\mathbf{U}_{1j},
$$

$$
\mathbf{Y}_n^{\top}\sum_{l=1}^{s}\gamma_l\mathbf{U}_{1l} = \sum_{l=1}^{s}\gamma_l\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{1l} - h\sum_{l=1}^{s}\sum_{j=1}^{s}\gamma_j\mathbf{A}_{jl}\mathbf{U}_{0l}^{\top}\mathbf{U}_{1j} - J_1\sum_{l=1}^{s}\sum_{j=1}^{s}\gamma_j\mathbf{B}_{jl}\mathbf{U}_{1l}^{\top}\mathbf{U}_{1j},
$$

$$
\sum_{l=1}^{s}\gamma_l\mathbf{U}_{1l}^{\top}\mathbf{Y}_n = \sum_{l=1}^{s}\gamma_l\mathbf{U}_{1l}^{\top}\boldsymbol{\Phi}_l - h\sum_{l=1}^{s}\sum_{j=1}^{s}\gamma_l\mathbf{A}_{lj}\mathbf{U}_{1l}^{\top}\mathbf{U}_{0j} - J_1\sum_{l=1}^{s}\sum_{j=1}^{s}\gamma_l\mathbf{B}_{lj}\mathbf{U}_{1l}^{\top}\mathbf{U}_{1j},
$$

which, when substituted into (7), gives

$$
\begin{aligned}
\mathbf{Y}_{n+1}^{\top}\mathbf{Y}_{n+1} = \mathbf{Y}_n^{\top}\mathbf{Y}_n &+ h\sum_{l=1}^{s}\boldsymbol{\alpha}_l(\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{0l} + \mathbf{U}_{0l}^{\top}\boldsymbol{\Phi}_l) + J_1\sum_{l=1}^{s}\gamma_l(\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{1l} + \mathbf{U}_{1l}^{\top}\boldsymbol{\Phi}_l)\\
&+ h^2\sum_{l=1}^{s}\sum_{j=1}^{s}(\boldsymbol{\alpha}_l\boldsymbol{\alpha}_j - \boldsymbol{\alpha}_l\mathbf{A}_{lj} - \boldsymbol{\alpha}_j\mathbf{A}_{jl})\mathbf{U}_{0l}^{\top}\mathbf{U}_{0j}\\
&+ hJ_1\sum_{l=1}^{s}\sum_{j=1}^{s}(\boldsymbol{\alpha}_j\gamma_l - \boldsymbol{\alpha}_j\mathbf{B}_{jl} - \gamma_l\mathbf{A}_{lj})\mathbf{U}_{1l}^{\top}\mathbf{U}_{0j}\\
&+ hJ_1\sum_{l=1}^{s}\sum_{j=1}^{s}(\boldsymbol{\alpha}_l\gamma_j - \gamma_j\mathbf{A}_{jl} - \boldsymbol{\alpha}_l\mathbf{B}_{lj})\mathbf{U}_{0l}^{\top}\mathbf{U}_{1j}\\
&+ J_1^2\sum_{l=1}^{s}\sum_{j=1}^{s}(\gamma_l\gamma_j - \gamma_l\mathbf{B}_{lj} - \gamma_j\mathbf{B}_{jl})\mathbf{U}_{1l}^{\top}\mathbf{U}_{1j}.
\end{aligned}
$$

Since

$$\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{0l}+\mathbf{U}_{0l}^{\top}\boldsymbol{\Phi}_l=\boldsymbol{\Phi}_l^{\top}(\mathbf{G}_0(t_n+\mathbf{c}_l h,\boldsymbol{\Phi}_l)+\mathbf{G}_0(t_n+\mathbf{c}_l h,\boldsymbol{\Phi}_l)^{\top})\boldsymbol{\Phi}_l,$$

$$\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{1l}+\mathbf{U}_{1l}^{\top}\boldsymbol{\Phi}_l=\boldsymbol{\Phi}_l^{\top}(\mathbf{G}_1(t_n+\mathbf{c}_l h,\boldsymbol{\Phi}_l)+\mathbf{G}_1(t_n+\mathbf{c}_l h,\boldsymbol{\Phi}_l)^{\top})\boldsymbol{\Phi}_l$$

and $\mathbf{G}_0$, $\mathbf{G}_1$ are skew-symmetric matrix functions then

$$\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{0l}+\mathbf{U}_{0l}^{\top}\boldsymbol{\Phi}_l=\mathbf{0},$$

$$\boldsymbol{\Phi}_l^{\top}\mathbf{U}_{1l}+\mathbf{U}_{1l}^{\top}\boldsymbol{\Phi}_l=\mathbf{0}.$$

From this and the definition of the matrices $\mathbf{M}^i$, $i=1,\ldots,3$ it is obtained that

$$\begin{aligned}\mathbf{Y}_{n+1}^{\top}\mathbf{Y}_{n+1}=\mathbf{Y}_n^{\top}\mathbf{Y}_n&+h^2\sum_{l=1}^{s}\sum_{j=1}^{s}\mathbf{M}_{lj}^1\mathbf{U}_{0l}^{\top}\mathbf{U}_{0j}+hJ_1\sum_{l=1}^{s}\sum_{j=1}^{s}\mathbf{M}_{jl}^2\mathbf{U}_{1l}^{\top}\mathbf{U}_{0j}\\&+hJ_1\sum_{l=1}^{s}\sum_{j=1}^{s}\mathbf{M}_{lj}^2\mathbf{U}_{0l}^{\top}\mathbf{U}_{1j}+J_1^2\sum_{l=1}^{s}\sum_{j=1}^{s}\mathbf{M}_{lj}^3\mathbf{U}_{1l}^{\top}\mathbf{U}_{1j},\end{aligned}$$

which by condition (6) gives $\mathbf{Y}_{n+1}^{\top}\mathbf{Y}_{n+1}=\mathbf{Y}_n^{\top}\mathbf{Y}_n$. □

The following corollary follows straightforwardly from the proof of the above theorem.

Corollary 6. *Let $\mathbf{G}_0$, $\mathbf{G}_1$ be commutative matrix functions. Scheme* (4–5) *is orthogonal if $\mathbf{M}^1=\mathbf{M}^3=\mathbf{0}$ and $\mathbf{M}^2$ is a skew-symmetric matrix.*

Remark 7. It is not difficult to see that the last theorem reduces to Theorem 2 in [9] for the particular case of ODEs. On the other hand, Theorem 5 could be directly extended to a more general class of stochastic Runge–Kutta integrators for SDEs with 1-dimensional Wiener process, namely, those defined by

$$\boldsymbol{\Phi}_i=\mathbf{Y}_n+h\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{G}_0(t_n+\mathbf{c}_j h,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j+\sum_{k=1}^{p}\left(\sum_{j=1}^{s}\mathbf{B}_{ij}^k\mathbf{G}_1(t_n+\mathbf{c}_j h,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j\right)\theta_k,$$
$$i=1,\ldots,s,$$

$$\mathbf{Y}_{n+1}=\mathbf{Y}_n+h\sum_{j=1}^{s}\boldsymbol{\alpha}_j\mathbf{G}_0(t_n+\mathbf{c}_j h,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j+\sum_{k=1}^{p}\left(\sum_{j=1}^{s}\boldsymbol{\gamma}_j^k\mathbf{G}_1(t_n+\mathbf{c}_j h,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j\right)\theta_k,$$
$$n=0,1,\ldots$$

with the Butcher tableau

$\mathbf{c}$	$\mathbf{A}$	$\mathbf{B}^1$	$\cdots$	$\mathbf{B}^p$
	$\boldsymbol{\alpha}$	$\boldsymbol{\gamma}^1$	$\cdots$	$\boldsymbol{\gamma}^p$

where θ_i, $i=1,\ldots,p$ are different random variables [1]. In a similar way, the Runge–Kutta integrators for the general case of skew-symmetric SDE (2) could also be considered with *m*-dimensional Wiener process, which are given by

$$\boldsymbol{\Phi}_i = \mathbf{Y}_n + h\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{G}_0(t_n+\mathbf{c}_jh,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j + \sum_{k=1}^{m}\left(\sum_{j=1}^{s}\mathbf{B}_{ij}^{k}\mathbf{G}_k(t_n+\mathbf{c}_jh,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j\right)\theta_k,$$
$$i=1,\ldots,s,$$

$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + h\sum_{j=1}^{s}\boldsymbol{\alpha}_j\mathbf{G}_0(t_n+\mathbf{c}_jh,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j + \sum_{k=1}^{m}\left(\sum_{j=1}^{s}\boldsymbol{\gamma}_j^{k}\mathbf{G}_k(t_n+\mathbf{c}_jh,\boldsymbol{\Phi}_j)\boldsymbol{\Phi}_j\right)\theta_k,$$
$$n=0,1,\ldots,$$

with $\theta_k = \int_0^h \circ\,\mathrm{d}\mathbf{w}^k$.

4. A class of orthogonal stochastic RK schemes

In this section a class of order 1 orthogonal RK schemes is presented. Specifically, it is defined by the expression (4)–(5) with RK matrices $\mathbf{A}$, $\mathbf{B}$ and RK weights $\boldsymbol{\alpha}$, $\boldsymbol{\gamma}$ satisfying the orthogonality conditions (6) and the strong global order 1 conditions

$$\boldsymbol{\alpha}\mathbf{e}_s = 1,\quad \boldsymbol{\gamma}\mathbf{e}_s = 1,\quad \boldsymbol{\alpha}\mathbf{B}\mathbf{e}_s = \tfrac{1}{2},$$
$$\mathbf{e}_s = (1,\ldots,1)^{\mathsf{T}}\quad \text{(vector of } s \text{ ones)}$$

stated in [2].

It is not hard to see that the above conditions are fulfilled by setting $\mathbf{B}=\mathbf{A}$ and $\boldsymbol{\gamma}=\boldsymbol{\alpha}$, with $\mathbf{A}$ and $\boldsymbol{\alpha}$ defined by

$$\mathbf{A}_{ij} = \int_0^{c_i}\frac{\rho_j(t)}{\rho_j(\mathbf{c}_j)}\,\mathrm{d}t,\quad \boldsymbol{\alpha}_i = \int_0^{1}\frac{\rho_i(t)}{\rho_i(\mathbf{c}_i)}\,\mathrm{d}t,\quad i,j=1,\ldots,s, \tag{8}$$

where $\rho(t)=\prod_{i=1}^{s}(t-\mathbf{c}_i)$, $\rho_i(t)=\rho(t)/(t-\mathbf{c}_i)$ and the RK nodes $\mathbf{c}_i\in[0,1]$, $i=1,\ldots,s$ are the zeros of the Legendre polynomial P_s, linearly translated to [0, 1]. For instance,

$$\text{for } s=1:\ \mathbf{A}=\mathbf{B}=\left(\frac{1}{2}\right),\quad \boldsymbol{\alpha}=\boldsymbol{\gamma}=(1),\quad \mathbf{c}=\left(\frac{1}{2}\right), \tag{9}$$

$$\text{for } s=2:\ \mathbf{A}=\mathbf{B}=\begin{pmatrix}\frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6}\\ \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4}\end{pmatrix},\quad \boldsymbol{\alpha}=\boldsymbol{\gamma}=\left(\frac{1}{2},\frac{1}{2}\right),$$
$$\mathbf{c}=\left(\frac{1}{2}-\frac{\sqrt{3}}{6},\frac{1}{2}+\frac{\sqrt{3}}{6}\right) \tag{10}$$

and so on.

At this point, it is opportune to remark that for ODEs the above scheme reduces to the well-known Gauss–Legendre–RK schemes [6]. Therefore, the schemes constructed in this section could be called stochastic Gauss–Legendre–RK schemes.

5. Computational aspects

Note that condition (6) in Theorem 5 implies that the orthogonal stochastic RK integrators (4–5) are implicit schemes. Thus, a matrix equation must be solved at each step. In this section, two explicit expressions for the stochastic Gauss–Legendre–RK schemes are obtained by considering either the exact or approximate solution of the above-mentioned matrix equation.

For the skew-symmetric linear SDE

$$\begin{aligned} &\mathrm{d}\mathbf{X}_t = \mathbf{G}_0(t)\mathbf{X}_t\,\mathrm{d}t + \mathbf{G}_1(t)\mathbf{X}_t \circ \mathrm{d}w_t, \\ &\mathbf{X}_{t_0} = \mathbf{X}_0, \quad \mathbf{X}_0^{\top}\mathbf{X}_0 = \mathbf{I}_d, \end{aligned} \tag{11}$$

the numerical scheme (4–5) can be rewritten as

$$\mathbf{\Phi} = \mathbf{e}_s \otimes \mathbf{Y}_n + \mathbf{\Omega}(t_n)\mathbf{\Phi}, \tag{12}$$

$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + \boldsymbol{\omega}(t_n)\mathbf{\Phi}, \tag{13}$$

where $\mathbf{\Phi} = (\mathbf{\Phi}_1^{\top}, \dots, \mathbf{\Phi}_s^{\top})^{\top}$,

$$\mathbf{\Omega}(t) = h(\mathbf{A} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{01}(t), \dots, \mathbf{G}_{0s}(t)) + J_1(\mathbf{B} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{11}(t), \dots, \mathbf{G}_{1s}(t)),$$

$$\boldsymbol{\omega}(t) = h(\boldsymbol{\alpha} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{01}(t), \dots, \mathbf{G}_{0s}(t)) + J_1(\boldsymbol{\gamma} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{11}(t), \dots, \mathbf{G}_{1s}(t)),$$

$$\mathbf{G}_{0j}(t) = \mathbf{G}_0(t + \mathbf{c}_j h), \quad \mathbf{G}_{1j}(t) = \mathbf{G}_1(t + \mathbf{c}_j h), \qquad j = 1, \dots, s,$$

the symbol $\otimes$ denotes the Kronecker product and for any square matrices $\mathbf{A}_1, \dots, \mathbf{A}_s$,

$$\operatorname{diag}(\mathbf{A}_1, \dots, \mathbf{A}_s) = \begin{pmatrix} \mathbf{A}_1 & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \cdots & \mathbf{A}_s \end{pmatrix}.$$

Solving explicitly the linear equation (12), the following numerical scheme is obtained:

$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + \boldsymbol{\omega}(t_n)(\mathbf{I}_{ds} - \mathbf{\Omega}(t_n))^{-1}(\mathbf{e}_s \otimes \mathbf{Y}_n), \tag{14}$$

which could be easily implemented.

In the case of nonlinear skew-symmetric SDE like (3) the numerical scheme (4–5) can be rewritten as

$$\mathbf{\Phi} = \mathbf{e}_s \otimes \mathbf{Y}_n + \mathbf{\Omega}(t_n, \mathbf{\Phi})\mathbf{\Phi}, \tag{15}$$

$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + \boldsymbol{\omega}(t_n, \mathbf{\Phi})\mathbf{\Phi}, \tag{16}$$

where

$$\begin{aligned} \mathbf{\Omega}(t, \mathbf{\Phi}) = {} & h(\mathbf{A} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{01}(t, \mathbf{\Phi}), \dots, \mathbf{G}_{0s}(t, \mathbf{\Phi})) \\ & + J_1(\mathbf{B} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{11}(t, \mathbf{\Phi}), \dots, \mathbf{G}_{1s}(t, \mathbf{\Phi})), \end{aligned}$$

$$\begin{aligned} \boldsymbol{\omega}(t, \mathbf{\Phi}) = {} & h(\boldsymbol{\alpha} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{01}(t, \mathbf{\Phi}), \dots, \mathbf{G}_{0s}(t, \mathbf{\Phi})) \\ & + J_1(\boldsymbol{\gamma} \otimes \mathbf{I}_d)\operatorname{diag}(\mathbf{G}_{11}(t, \mathbf{\Phi}), \dots, \mathbf{G}_{1s}(t, \mathbf{\Phi})), \end{aligned}$$

$$\mathbf{G}_{0j}(t, \mathbf{\Phi}) = \mathbf{G}_0(t + \mathbf{c}_j h, \mathbf{\Phi}_j), \quad \mathbf{G}_{1j}(t, \mathbf{\Phi}) = \mathbf{G}_1(t + \mathbf{c}_j h, \mathbf{\Phi}_j).$$

As in the deterministic case, the nonlinear equation (15) must be solved numerically by some kind of iterative process. The natural choice to do this is the well-known Newton's method. However, as it was pointed out in [6], a large number of iterations should be performed in order to retain the orthogonality property of the solution. So, the use of the Newton's method seems to be a quite expensive choice. Alternatively, by following the approach introduced in [6], let us consider the implicit iteration

$$\mathbf{\Phi}^{(k+1)} = \mathbf{e}_s \otimes \mathbf{Y}_n + \mathbf{\Omega}(t_n, \mathbf{\Phi}^{(k)})\mathbf{\Phi}^{(k+1)},$$

$$\mathbf{Y}_{n+1}^{(k+1)} = \mathbf{Y}_n + \boldsymbol{\omega}(t_n, \mathbf{\Phi}^{(k)})\mathbf{\Phi}^{(k+1)}, \quad k = 0, 1, 2, \ldots$$

with initial value $\mathbf{\Phi}^{(0)} = \mathbf{e}_s \otimes \mathbf{Y}_n$, which corresponds to the RK discretization of a linear SDE of the type (11). Therefore,

$$\mathbf{\Phi}^{(k+1)} = (\mathbf{I}_{ds} - \mathbf{\Omega}(t_n, \mathbf{\Phi}^{(k)}))^{-1}(\mathbf{e}_s \otimes \mathbf{Y}_n) \tag{17}$$

and so the following explicit scheme is obtained:

$$\mathbf{Y}_{n+1}^{(k+1)} = \mathbf{Y}_n + \boldsymbol{\omega}(t_n, \mathbf{\Phi}^{(k)})(\mathbf{I}_{ds} - \mathbf{\Omega}(t_n, \mathbf{\Phi}^{(k)}))^{-1}(\mathbf{e}_s \otimes \mathbf{Y}_n), \tag{18}$$

which could be easily implemented. The iteration stops when

$$\|\mathbf{\Phi}^{(k)} - \mathbf{e}_s \otimes \mathbf{Y}_n - \mathbf{\Omega}(t_n, \mathbf{\Phi}^{(k)})\mathbf{\Phi}^{(k)}\|_\infty < \varepsilon, \tag{19}$$

for a given $\varepsilon > 0$.

Remark 8. At this point it is worth noting that the iteration $\mathbf{Y}_n^{(k)}$ converges to $\mathbf{Y}_n$ w.p.1, for all fixed n. To see this one should realize that (17) is just an usual fixed-point iteration corresponding to the problem $\mathbf{\Phi} = \mathbf{F}(\mathbf{\Phi})$, where

$$\mathbf{F}(\mathbf{\Phi}) = (\mathbf{I}_{ds} - \mathbf{\Omega}(t_n, \mathbf{\Phi}))^{-1}(\mathbf{e}_s \otimes \mathbf{Y}_n).$$

It is well-known that $\|\frac{\mathrm{d}\mathbf{F}}{\mathrm{d}\mathbf{\Phi}}(\mathbf{\Phi})\| \leqslant 1$ is a sufficient condition to assure the contractivity property for $\mathbf{F}$ and so, the convergence of the iteration (17). Since

$$\left\|\frac{\mathrm{d}\mathbf{F}}{\mathrm{d}\mathbf{\Phi}}(\mathbf{\Phi})\right\| \leqslant \frac{\left\|\frac{\mathrm{d}\mathbf{\Omega}}{\mathrm{d}\mathbf{\Phi}}(t_n, \mathbf{\Phi})\right\|}{\|\mathbf{I}_{ds} - \mathbf{\Omega}(t_n, \mathbf{\Phi})\|^2} < 1,$$

for sufficiently small h then the convergence follows. Therefore, for h and ε small enough the theoretical order 1 of the RK schemes is guaranteed.

6. Numerical experiments

In this section, the performance of the orthogonal stochastic integrators is illustrated with two examples. With this purpose, both the orthogonality preservation and integration errors are analyzed. Specifically, for the time discretization $(t)_h = \{t_n = t_0 + nh : n = 0, 1, 2, \ldots, N\}$, the uniform mean orthogonality error

$$\mathrm{Oe}(h) = E\left(\max_{0 \leqslant n \leqslant N} \|\mathbf{Y}_n^{\mathsf{T}}\mathbf{Y}_n - \mathbf{I}_d\|\right)$$

Table 1
Values of the mean convergence error and the uniform mean orthogonality error for the linear test example

h	Stages $=1$		Stages $=2$	
	Se	Oe($\times 10^{-14}$)	Se($\times 10^{-4}$)	Oe($\times 10^{-14}$)
2^{-8}	0.1805	0.1365	0.9043	0.1359
2^{-9}	0.0888	0.1422	0.4456	0.1433
2^{-10}	0.0451	0.1477	0.2217	0.1489
2^{-11}	0.0227	0.1532	0.1238	0.1517

and the mean convergence error at $t = t_N$

$$\mathrm{Se}(h) = E(\|\mathbf{X}_{t_N} - \mathbf{Y}_N\|),$$

are computed. Here, $E(.)$ denotes the mathematical expectation.

6.1. Example 1 (Linear case)

Consider the following skew-symmetric linear equation:

$$\mathrm{d}\mathbf{X}_t = \mathbf{G}_0\mathbf{X}_t\,\mathrm{d}t + \mathbf{G}_1\mathbf{X}_t \circ \mathrm{d}w_t, \quad 0 \leqslant t \leqslant 10,$$

$$\mathbf{X}_0 = \mathbf{I}_3,$$

with the skew-symmetric matrices

$$\mathbf{G}_0 = \begin{pmatrix} 0 & 3 & -1 \\ -3 & 0 & -2 \\ 1 & 2 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{G}_1 = \begin{pmatrix} 0 & -\frac{3}{2} & \frac{1}{2} \\ \frac{3}{2} & 0 & 1 \\ -\frac{1}{2} & -1 & 0 \end{pmatrix}.$$

By Theorem 2, the above equation has an orthogonal solution, which due to the commutativity of $\mathbf{G}_0$ and $\mathbf{G}_1$ is given by $\mathbf{X}_t = \mathrm{e}^{\mathbf{G}_0 t + \mathbf{G}_1 w_t}$.

For each $h = 2^{-8}, 2^{-9}, 2^{-10}, 2^{-11}$ this equation was solved numerically by using the scheme (14) for the stages $s = 1, 2$, whose RK matrices, RK weights and RK nodes are given by (9) and (10), respectively. For each s and h, 1000 simulations were carried out for estimating the errors $\mathrm{Oe}(h)$ and $\mathrm{Se}(h)$. Table 1 shows these estimated values. Note that, in contrast to the mean convergence errors, the uniform mean orthogonality errors are very similar in both cases.

6.2. Example 2 (Nonlinear case)

The deterministic version of skew-symmetric SDEs (i.e. no stochastic component) has arisen in a number of applications (see [6] and references therein). The stability analysis of nonlinear dynamical systems via the computation of the Lyapunov exponents [7] is perhaps one of the most interesting of such applications. In fact, the skew-symmetric systems constitute the main component of the continuous *QR* method for computing the Lyapunov exponents of ODEs. More recently a continuous *QR* method for computing the Lyapunov exponents of SDEs was proposed in [4]. It holds that, as in the deterministic

Table 2
Values of the mean convergence error and the uniform mean orthogonality error for the nonlinear test example

h	Stages $=1$		Stages $=2$	
	Se	Oe($\times 10^{-15}$)	Se($\times 10^{-5}$)	Oe($\times 10^{-15}$)
2^{-8}	0.0171	0.8693	0.1922	0.8594
2^{-9}	0.0084	0.8958	0.0798	0.8971
2^{-10}	0.0042	0.9169	0.0431	0.9061
2^{-11}	0.0021	0.9312	0.0202	0.9211

case, the numerical integration of skew-symmetric SDEs becomes a crucial element for such stochastic continuous QR method. Thus, the following skew-symmetric cubic SDE is a very interesting example from that application point of view.

$$\begin{aligned} \mathrm{d}\mathbf{X}_t &= \mathbf{G}_0(\mathbf{X}_t)\mathbf{X}_t\,\mathrm{d}t + \mathbf{G}_1(\mathbf{X}_t)\mathbf{X}_t \circ \mathrm{d}w_t, \quad 0 \leqslant t \leqslant 10, \\ \mathbf{X}_0 &= \mathbf{I}_2, \end{aligned} \tag{20}$$

where

$$\mathbf{G}_0(\mathbf{X}) = \begin{pmatrix} 0 & -(\mathbf{X}^\top\mathbf{C}\mathbf{X})_{21} \\ (\mathbf{X}^\top\mathbf{C}\mathbf{X})_{21} & 0 \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}$$

and

$$\mathbf{G}_1(\mathbf{X}) = \begin{pmatrix} 0 & -(\mathbf{X}^\top\mathbf{D}\mathbf{X})_{21} \\ (\mathbf{X}^\top\mathbf{D}\mathbf{X})_{21} & 0 \end{pmatrix}, \quad \mathbf{D} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

As in Example 1, 1000 simulations were carried out for each $h = 2^{-8}, 2^{-9}, 2^{-10}, 2^{-11}$ and $s = 1, 2$ by means of the scheme (18) with RK matrices, RK weights and RK nodes given by (9) and (10), respectively, and the stop condition (19) with $\varepsilon = 10^{-6}$. These approximated solutions were compared with the exact solution of Eq. (20), namely, the factor Q in the QR decomposition of $\mathrm{e}^{\mathbf{C}t+\mathbf{D}w_t}$ (see details in [4]). The values of the mean convergence errors and the uniform mean orthogonality errors are shown in Table 2. Note that, in this nonlinear example, the orthogonal integrator on consideration also performs well.

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