A new weak approximation scheme of stochastic differential equations and the Runge–Kutta method

Mariko Ninomiya · Syoiti Ninomiya

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Abstract The authors report on the construction of a new algorithm for the weak approximation of stochastic differential equations. In this algorithm, an ODE-valued random variable whose average approximates the given stochastic differential equation is constructed by using the notion of free Lie algebra. It is proved that the classical Runge–Kutta method for ODEs is directly applicable to the drawn ODE from the random variable. In a numerical experiment, this is applied to the problem of pricing Asian options under the Heston stochastic volatility model. Compared with some other methods, this algorithm gives significantly faster calculation times.

Keywords stochastic differential equations · weak approximation · free Lie algebra · mathematical finance · Runge–Kutta method

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Mariko Ninomiya
Graduate School of Mathematical Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro-ku, Tokyo 153-8914, Japan
E-mail: mariko.nnmy@gmail.com

Syoiti Ninomiya
Center for Research in Advanced Financial Technology, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8552 Japan
E-mail: ninomiya@craft.titech.ac.jp
1 Introduction

1.1 The problem and background

1.1.1 The problem
Let \((\Omega, \mathcal{F}, P)\) be a probability space, \(B^0(t) = t\), and \((B^1(t), \ldots, B^d(t))\) be a \(d\)-dimensional standard Brownian motion. \(C^\infty_b(\mathbb{R}^N; \mathbb{R}^N)\) denotes the set of \(\mathbb{R}^N\)-valued infinitely differentiable functions defined in \(\mathbb{R}^N\) whose derivatives are all bounded. Our interest is in weak approximation, that is to say, approximation of \((P_t f)(x) = \mathbb{E}[f(X(t,x))]\) where \(f \in C^\infty_b(\mathbb{R}^N; \mathbb{R})\) and \(X(t,x)\) is a solution to the stochastic differential equation written in the Stratonovich form:

\[
X(t, x) = x + \sum_{i=0}^{d} \int_0^t V_i(X(s, x)) \circ dB^i(s),
\]

where \(V_i \in C^\infty_b(\mathbb{R}^N; \mathbb{R}^N)\) for \(i = 0, 1, \ldots, d\). Here, \(V_i \in C^\infty_b(\mathbb{R}^N; \mathbb{R}^N)\) is considered to be a vector field in the following way:

\[
V_i f(x) = \sum_{j=1}^{N} V^j_i(x) \frac{\partial f}{\partial x_j}(x), \quad \text{for } f \in C^\infty_b(\mathbb{R}^N; \mathbb{R}).
\]

It is well-known (e. g. [13]) that \(\mathbb{E}[f(X(T,x))]\) is equal to \(u(1,x)\) where \(u\) is the solution to the following partial differential equation for \(L = V_0 + (1/2) \sum_{i=1}^{d} V_i^2:\)

\[
\frac{\partial u}{\partial t}(t, x) = Lu, \quad u(0,x) = f(x).
\]

1.1.2 Background
A number of studies on numerical calculations of this problem have been conducted as there is a great demand for it in various fields. One often encounters this type of calculation particularly in mathematical finance. For example, the price of a financial derivative written on the diffusion \(X(t, x)\) is obtained by the calculation of \(\mathbb{E}[f(X(T,x))]\).

There are two approaches to the problem: PDE approach and simulation. The former one involves solving the partial differential equation (1.2) numerically. This method works only when \(L\) is elliptic and the dimension is relatively small. We do not go into details on the subject here but refer to [19]. These conditions are not necessarily satisfied in many practical problems so we are forced to take the other approach which is called the probabilistic method or simulation. In this paper, we focus on this approach.

Usually, the Euler–Maruyama scheme is used to discretize \(X(t,x)\) during simulations to weakly approximate \(X(t, x)\). It is shown in [18], [23], [24], and [28] that the new higher-order scheme introduced by Kusuoka in [15] calculates some finance problems much faster than the Euler–Maruyama scheme. Lyons and Victoir extensively developed the scheme in [21] using the notion of free Lie algebra. Recent developments can be found in [2] and [10].

We will discuss the reason why higher order schemes greatly improve the speed of numerical weak approximation in the later part of this paper (Section 6).
1.1.3 Our results

In this paper, we describe how successfully we constructed in Theorem 1.3 and Corollary 1.4 a new higher order weak approximation scheme for a broad class of
stochastic differential equations. This scheme owes a great deal to the scheme shown in [15] and to the cubature method on Wiener space introduced in [21].

An intuitive explanation of the scheme is as follows. We construct the ODE (ordinary differential equation)-valued random variable whose average approximates the given stochastic differential equation. From this random variable, an ODE itself is able to be drawn at one time.

This scheme has a remarkable advantage that once an ODE is drawn, the conventional Runge–Kutta method can be applied so as to approximate the ODE. The approximating random variable is constructed using Theorem 1.3 and Theorem 1.6 and can be approximated by the Runge–Kutta method for ODEs via Theorem 4.15.

We should note that another higher-order weak approximation method is introduced in [25]. Although the algorithm in [25] and the new method presented in this paper are based on the same scheme ([15] [21]) and have many common features, algorithms themselves differ significantly.

1.2 Notation

Let \( A = \{v_0, v_1, \ldots, v_d\} \) be an alphabet where \( d \in \mathbb{Z}_{\geq 1} \) and \( A' \) denote the set of all words consisting of the elements of \( A \). The empty word 1 is the identity of \( A' \). For \( u = v_{i_1} \cdots v_{i_n} \in A' \), \(|u|\) and \(||u|||\) are defined by \(|u| = n\) and \(||u|| = |u| + |\text{card} \{k | i_k = 0\}\}\) where \( \text{card}(S) \) denotes the cardinality of a set \( S \). Here, \( ||\cdot|| \) is related to the scaling property of the Brownian motion. \( A_{\leq m} \) and \( A_{\leq m} \) denote \( \{w \in A' | |w| = m\} \) and \( \{w \in A' | |w| \leq m\} \), respectively. Let \( \mathbb{R}(A) \) be the \( \mathbb{R} \)-coefficient free algebra with basis \( A' \) and \( \mathbb{R}(\langle A \rangle) \) be the set of all \( \mathbb{R} \)-coefficient formal series with basis \( A' \). Then, \( \mathbb{R}(A) \) is a sub-\( \mathbb{R} \)-algebra of \( \mathbb{R}(\langle A \rangle) \). We call an element of \( \mathbb{R}(A) \) a non-commutative polynomial. \( P \in \mathbb{R}(\langle A \rangle) \) is written as

\[
P = \sum_{w \in A'} (P, w) w \quad \text{or} \quad \sum_{w \in A'} a_w w,
\]

where \((P, w) = a_w \in \mathbb{R}\) denotes the coefficient of \( w \). Let

\[
\mathbb{R}(A)_m = \{P \in \mathbb{R}(A) | (P, w) = 0, \text{ if } ||w|| \neq m\}.
\]

The algebra structure is defined as usual, i.e.

\[
\left( \sum_{w \in A'} a_w w \right) \left( \sum_{w \in A'} b_w w \right) = \sum_{w \in A'} a_w b_w w.
\]

The Lie bracket is defined as \([x, y] = xy - yx\) for \( x, y \in \mathbb{R}(\langle A \rangle) \). For \( w = v_{i_1} \cdots v_{i_k} \in A' \), \( \mathfrak{r}(w) \) denotes \( [v_{i_1}, [v_{i_2}, \ldots, [v_{i_{k-1}}, v_{i_k}] \ldots]] \). We define \( L_\mathbb{R}(A) \) as the set of Lie polynomials in \( \mathbb{R}(A) \) and \( L_\mathbb{R}(\langle A \rangle) \) as the set of Lie series. This means that \( L_\mathbb{R}(A) \) is the smallest sub-\( \mathbb{R} \)-module of \( \mathbb{R}(A) \) including \( A \) and is closed under the Lie bracket, and that \( L_\mathbb{R}(\langle A \rangle) \) is the set of elements of \( \mathbb{R}(\langle A \rangle) \) whose homogeneous components
belong to $\mathcal{L}_R(A)$. We note that Lie polynomials correspond to vector fields while
general polynomials do not necessarily. For $m \in \mathbb{Z}_{\geq 0}$, let $j_m$ be a map defined by

$$j_m \left( \sum_{\nu \in \Lambda^A} a_{\nu} \bar{w} \right) = \sum_{||\nu|| \leq m} a_{\nu} \bar{w}.$$ 

For arbitrary $P, Q \in \mathbb{R}(A)$, the inner product $\langle P, Q \rangle$ is defined by

$$\langle P, Q \rangle = \sum_{\nu \in \Lambda^A} \langle P, w \rangle \langle Q, w \rangle.$$ 

Moreover we let $\|P\|_2 = (\langle P, P \rangle)^{1/2}$ for $P \in \mathbb{R}(A)$. For $P \in \mathbb{R}(\langle A \rangle)$ with $(P, 1) = 0$, we can define $\exp(P)$ as $1 + \sum_{k=1}^{\infty} P^k/k!$. In addition, $\log(Q)$ can be defined as $\sum_{k=1}^{\infty} (-1)^{k-1}(Q - 1)^k/k$ for $Q \in \mathbb{R}(\langle A \rangle)$ with $(Q, 1) = 1$. Then the following relations hold:

$$\log(\exp(P)) = P \quad \text{and} \quad \exp(\log(Q)) = Q.$$ 

By the natural identification $\mathbb{R}(\langle A \rangle) \simeq \mathbb{R}^\infty$, we can induce the direct product topology into $\mathbb{R}(\langle A \rangle)$. Then, $\mathbb{R}(\langle A \rangle)$ becomes a Polish space by the topology. We can also consider its Borel $\sigma$-algebra $\mathcal{B}(\mathbb{R}(\langle A \rangle))$, $\mathbb{R}(\langle A \rangle)$-valued random variables, their expectations, and other notions as usual.

Let $\Phi$ be the homomorphism between $\mathbb{R}(A)$ and the $\mathbb{R}$-algebra consisting of smooth differential operators over $\mathbb{R}^N$ such that

$$\Phi(1) = \text{Id},$$

$$\Phi(v_1 \cdots v_n) = V_{i_1} \cdots V_{i_n} \quad \text{for } i_1, \ldots, i_n \in \{0, 1, \ldots, d\}. \quad (1.3)$$

Considering the scaling property of the Brownian motion, we define the rescaling operator $\psi_s$ depending on $||\cdot||$. For $s \in \mathbb{R}_{>0}$, $\psi_s : \mathbb{R}(\langle A \rangle) \rightarrow \mathbb{R}(\langle A \rangle)$ is defined as follows:

$$\psi_s \left( \sum_{m=0}^{\infty} P_m \right) = \sum_{m=0}^{\infty} s^{m/2} P_m \quad \text{where } P_m \in \mathbb{R}(A)_m.$$ 

For a smooth vector field $V$, i.e. an element of $C^\infty_v(\mathbb{R}^N; \mathbb{R}^N)$, $\exp(V)(x)$ denotes the solution at time 1 of the ordinary differential equation

$$\frac{dz_t}{dt} = V(z_t), \quad z_0 = x.$$ 

We also define $||V||_{C^\infty}$ for $V \in C^\infty_v(\mathbb{R}^N; \mathbb{R}^N)$ as follows:

$$||V|| = \sup \left\{ |V(x)|; \ x \in \mathbb{R}^N \right\},$$

$$||V^{(n)}|| = \sup \left\{ |V^{(n)}(U_1, U_2, \ldots, U_n)|; \ x \in \mathbb{R}^N \text{ and } |U_i| = 1, \text{ for } i = 1, \ldots, n \right\},$$

$$||V||_{C^\infty} = \sum_{i=0}^{n} ||V^{(i)}||.$$ 

Here $V^{(i)}$ denotes the $i$th order total differential of $V$, i.e.

$$V^{(n)}(U_1, U_2, \ldots, U_n) = \sum_{i=1}^{N} \sum_{j_1=1}^{N} \cdots \sum_{j_n=1}^{N} \frac{\partial^n V}{\partial x_{j_1} \cdots \partial x_{j_n}}(x) U_1^{j_1} \cdots U_n^{j_n} e_i,$$

where each $e_i$ denotes an $N$-dimensional unit vector, $\{e_1, \ldots, e_N\}$ forms an orthonormal basis of $\mathbb{R}^N$, and $U_k^{j_k}$ is the $j_k$th component of $U_k \in \mathbb{R}^N$. 
1.3 Main results

Since in this paper we deal with the operators that are not necessarily linear with respect to time \( t \), we introduce the following definition:

**Definition 1.1** A map \( g \) from \( C_0^\infty (\mathbb{R}^N; \mathbb{R}^N) \) to the set of all maps from \( \mathbb{R}^N \) to \( \mathbb{R}^N \) is called an integration scheme of order \( m \) if there exists a positive constant \( C_m \) such that

\[
\sup_{x \in \mathbb{R}^N} |g(W)(x) - \exp (W)(x)| \leq C_m ||W||_C^{m+1},
\]

for all \( W \in C_0^\infty (\mathbb{R}^N; \mathbb{R}^N) \). Let \( IS(m) \) be the set of all integration schemes of order \( m \).

This definition is a generalization of the usual order of approximation.

**Definition 1.2** For \( z_1, z_2 \in L_{\mathbb{R}}((A)) \), we define \( z_2 \circ z_1 \) as \( \log (\exp (z_2) \exp (z_1)) \). Then from the definition, for \( z_1, z_2, z_3 \in L_{\mathbb{R}}((A)) \),

\[
(z_1 \circ z_2) \circ z_3 = \log (\exp (z_1) \exp (z_2) \exp (z_3)) = z_1 \circ (z_2 \circ z_3),
\]

and so we can write for \( z_1, \ldots, z_n \in L_{\mathbb{R}}((A)) \)

\[
z_1 \circ z_2 \circ \cdots \circ z_n = \log (\exp (z_1) \cdots \exp (z_n)).
\]

We notice that \( z_2 \circ z_1 \in L_{\mathbb{R}}((A)) \) if \( z_1, z_2 \in L_{\mathbb{R}}((A)) \) from the Baker–Campbell–Hausdorff formula(1).

The following are the main results.

**Theorem 1.3** Let \( m \geq 1, N \geq 2, \) and \( Z_1, \ldots, Z_M \) be \( L_{\mathbb{R}}((A)) \)-valued random variables. Assume that \( Z_1, \ldots, Z_M \) satisfy the followings:

\[
Z_i = j_m Z_i \quad \text{for } i = 1, \ldots, M, \quad \text{(1.6)}
\]

\[
E \left[ \left\| \sum_{j=1}^{M} \Phi \left( \Psi_j (Z_j) \right) \right\|_{l^{m-1}} \right] < \infty \quad \text{for } i = 1, \ldots, M, \quad \text{(1.7)}
\]

\[
E \left[ \exp \left( a \sum_{j=1}^{M} \left\| \Phi \left( \Psi_j (Z_j) \right) \right\|_{l^{m-1}} \right) \right] < \infty \quad \text{for any } a > 0. \quad \text{(1.8)}
\]

Then for \( p \in [1, \infty) \) and arbitrary \( g_1, \ldots, g_M \in IS(m) \), there exists a positive constant \( C_{m,M} \) such that

\[
\sup_{x \in \mathbb{R}^N} \left| \left| \Phi \left( \Psi_s (Z_1) \right) \circ \cdots \circ g_M \left( \Phi \left( \Psi_s (Z_M) \right) \right) (x) \right| - \exp \left( \Phi \left( \Psi_s (j_m (Z_M \circ \cdots \circ Z_1)) \right) \right) \right|_{L^p} \leq C_{m,M} s^{(m+1)/2} \quad \text{(1.9)}
\]

for \( s \in (0, 1] \) where \( C_{m,M} \) depends only on \( m \) and \( M \). Here for functions \( f \) and \( g \), \( f \circ g(x) \) denotes \( f (g(x)) \) as usual.
For \( i = 1, \ldots, d, \) and \( j = 1, \ldots, M, \) let \( S_j^i \) be \( \mathbb{R} \)-valued Gaussian random variables and for \( j, j' = 1, \ldots, M, \) let \( c_j \) and \( R_{jj'} \) be real numbers such that

\[
\sum_{j=1}^{M} c_j = 1, \quad E[S_j^i] = 0, \quad \text{and} \quad E[S_j^i S_j'^i] = R_{jj'} \delta_{ij}
\]  \hspace{1cm} (1.10)

for \( i, i' = 1, \ldots, d. \) We let \( S_j^0 = c_j \) for convenience. Taking (1.2) into account, we let \( Z_1, \ldots, Z_M \) be random variables such that \( Z_j = c_j v_0 + \sum_{i=1}^{d} S_j^i v_i \) for \( j = 1, \ldots, M \) and that

\[
E[j_m(\exp(Z_1) \cdots \exp(Z_M))] = j_m\left( v_0 + \frac{1}{2} \sum_{i=1}^{d} v_i^2 \right).
\]  \hspace{1cm} (1.11)

In usual ODE cases, this type of approximation technique is known as a splitting method (\cite{12}). The stochastic versions of this technique are considered in \cite{21} and \cite{25}.

**Corollary 1.4** Suppose that the following UFG condition is satisfied:

\textbf{(UFG)} There exist an integer \( l \) and \( \varphi_{u,u'} \in C_0^l(\mathbb{R}^N; \mathbb{R}) \) which satisfy

\[
\Phi(t) = \sum_{u' \in A' \backslash \{1,v_0\}} \varphi_{u,u'} \Phi(t(u'))
\]  \hspace{1cm} (1.12)

for any \( u \in A' \backslash \{1, v_0\}. \)

For \( j = 1, \ldots, M \) let \( Z_j \) be \( \mathcal{L}(A) \)-valued random variables constructed as above and define linear operators \( Q_{(s)} \) for \( s \in (0, 1] \) by

\[
\left( Q_{(s)} f \right) (x) = E[f(g(\Phi(\mathcal{L}_{s}(Z_1))) \cdots g(\Phi(\mathcal{L}_{s}(Z_M))))(x)]
\]  \hspace{1cm} (1.13)

where \( f \in C_0^l(\mathbb{R}^N; \mathbb{R}) \) and \( g \in I_{S}(m) \). Then

\[
\left\| P_s f - Q_{(s)} f \right\|_{\infty} \leq C s^{(m+1)/2} \left\| \text{grad}(f) \right\|_{\infty}
\]  \hspace{1cm} (1.14)

where \( C \) is a positive constant.

**Remark 1.5** In \cite{17}, it is shown that for the operator \( Q_{(s)} \) defined above, there exists a constant \( C \) and

\[
\left( P_s f \right) (x) - \left( Q_{(s)} f \right) (x) = C s^{(m+1)/2} + O(s^{(m+3)/2})
\]

holds. This means that the Romberg extrapolation can be applied to our new algorithm.

The intuitive understanding is that once we find the random variables \( Z_1, \ldots, Z_M \), repeatedly for each \( i \) as seen in \cite{19} in Theorem \cite{13}. Therefore, our primary interest is in finding \( Z_1, \ldots, Z_M. \)

**Theorem 1.6** Let \( m = 5 \) and \( M = 2. \) Then (1.11) holds if and only if

\[
c_1 = \pm \frac{\sqrt{2(2u-1)}}{2}, \quad c_2 = 1 \pm \frac{\sqrt{2(2u-1)}}{2}, \quad R_{11} = u \quad (1.15)
\]

\[
R_{22} = 1 + u \pm \frac{\sqrt{2(2u-1)}}{2}, \quad R_{12} = -u \pm \frac{\sqrt{2(2u-1)}}{2}
\]

for some \( u \geq 1/2. \)
Remark 1.7 We can show that in the case where \( m = 7 \) and \( M = 3 \) there is no solution to (1.11).

Now that we have obtained the random variables satisfying (1.11), we need a practical way of approximating these integration schemes (1.11). We can show that in the case where \( m \) is a positive integer, we can express the solution of the stochastic differential equation \( dX_t = f(X_t) \, dt + g(X_t) \, dB_t \) in the form of the \( m \)-th order Runge–Kutta method to ODEs to find that it belongs to \( IS(m) \).

Let \( A = (a_{ij})_{i,j=1,...,K} \) with \( a_{ij} \in \mathbb{R} \) and \( b = (b_1,\ldots,b_K) \in \mathbb{R}^K \). If \((A,b)\) satisfies the \( m \)-th-order conditions defined as (4.8) in Section 4, the \( K \)-stage Runge–Kutta method of order \( m \) in the sense of \( IS(m) \) can be written as follows:

\[
Y_i(W,s) = y_0 + s \sum_{j=1}^K a_{ij} W(Y_j(W,s)), \tag{1.16}
\]

\[
Y(y_0;W,s) = y_0 + s \sum_{j=1}^K b_j W(Y_j(W,s))
\]

for \( W \in C_b^\infty(\mathbb{R}^N, \mathbb{R}^N) \) and \( y_0 \in \mathbb{R}^N \). Let \( g(W)(y_0) \) be \( Y(y_0;W,1) \). We show that \( g \) belongs to \( IS(m) \) in Theorem 4.15.

Remark 1.8 Our scheme is fundamentally different from the class of numerical methods sometimes referred to as stochastic Runge–Kutta methods (5) (26) (27).

2 Proof of Theorem 1.3

We split the left-hand side of (1.9) as

\[
\left\| \sup_{x \in \mathbb{R}^N} \left| g_1(\Phi_s(Z_1)) \circ \cdots \circ g_M(\Phi_s(Z_M))(x) \right| \right\|_{L^p} \\
\leq \left\| \sup_{x \in \mathbb{R}^N} \left| \exp(\Phi_s(Z_1)) \circ \cdots \circ \exp(\Phi_s(Z_M))(x) \right| \right\|_{L^p} \\
+ \left\| \sup_{x \in \mathbb{R}^N} \left| g_1(\Phi_s(Z_1)) \circ \cdots \circ g_M(\Phi_s(Z_M))(x) \right| \right\|_{L^p} \\
- \left\| \sup_{x \in \mathbb{R}^N} \left| \exp(\Phi_s(Z_1)) \circ \cdots \circ \exp(\Phi_s(Z_M))(x) \right| \right\|_{L^p}.
\tag{2.1}
\]

Evaluation of each term of the right-hand side of (2.1) will be given by Lemma 2.6 or (2.14) in this section.

Proposition 2.1

(1) For any \( V \in C_b^\infty(\mathbb{R}^N, \mathbb{R}^N) \), \( f \in C_b^\infty(\mathbb{R}^N, \mathbb{R}) \), \( x \in \mathbb{R}^N \) and \( n \geq 1 \),

\[
f(\exp(tV)(x)) = \sum_{k=0}^n \frac{t^k}{k!} (V^k f)(x) + \int_0^t \frac{(t-s)^n}{n!} (V^{n+1} f)(\exp(sV)(x)) \, ds. \tag{2.2}
\]
(2) For all \( z \in \mathbb{R}((A)) \) and \( n, m \geq 1 \),
\[
\sup_{x \in \mathbb{R}^N} \left| f \left( \exp (\Phi(j_m z)) (x) \right) - \sum_{k=0}^{n} \frac{1}{k!} \left( \Phi \left( (j_m z)^k \right) f \right) (x) \right| \leq \frac{1}{(n+1)!} \left\| \Phi \left( (j_m z)^{n+1} \right) f \right\|_\infty. \tag{2.3}
\]

Proof Since we have
\[
\frac{d}{dt} f \left( \exp(tV)(x) \right) = (Vf) \left( \exp(tV)(x) \right),
\]
from the Taylor expansion, we obtain \eqref{2.2} by integration by parts and \eqref{2.3} can be derived from \eqref{2.2}. \( \square \)

**Lemma 2.2** For all \( n \geq 1 \), there exists a constant \( C_n > 0 \) such that
\[
\left\| \Phi(j_n z)f \right\|_\infty \leq C_n \left\| j_n z \right\|_2 \left\| \text{grad}(f) \right\|_{C^{1-}}, \tag{2.4}
\]
for all \( z \in \mathbb{R}((A)) \) and \( f \in C^\infty(\mathbb{R}^N; \mathbb{R}). \)

Proof Let \( p_m \) be a map such that
\[
p_m : \sum_{|a|=0}^{\infty} a_n D^a \mapsto \sum_{|a|=m} a_n D^a,
\]
where \( \alpha \) is a multi-index, \( a_\alpha \in C^\infty(\mathbb{R}^N; \mathbb{R}) \), and \( D^x = \frac{\partial |_x \cdots \partial |_x}{\partial x_1 \cdots \partial x_n} \). Then we have
\[
\Phi(w) = \sum_{i=1}^{\left| \alpha \right|} p_i(\Phi(w)),
\]
for \( w \in A^\star \setminus \{1\} \). Since there exists a constant \( C_{w,j} > 0 \) such that
\[
\left\| p_i(\Phi(w))f \right\|_\infty \leq C_{w,j} \sup_{a \in (\mathbb{Z}_o)^N \atop |a| \leq j} \left\| D^a(\text{grad}(f)) \right\|_\infty,
\]
we see that there exists a constant \( C'_n > 0 \) such that
\[
\left\| \Phi(j_n z)f \right\|_\infty \leq \sum_{|w| \leq n} \left( \Phi(\Phi(w))f \right)_{\infty} |(z, w)| \leq \sum_{1 \leq |w| \leq n} |C_{w,j} (z, w)| \sup_{a \in (\mathbb{Z}_o)^N \atop |a| \leq j} \left\| D^a(\text{grad}(f)) \right\|_\infty \leq C'_n \left\| j_n z \right\|_2 \sup_{a \in (\mathbb{Z}_o)^N \atop |a| \leq 1} \left\| D^a(\text{grad}(f)) \right\|_\infty \leq C_n \left\| j_n z \right\|_2 \left\| \text{grad}(f) \right\|_{C^{1-}},
\]
where \( C_n = \text{card} \left( \{w \in A^\star \setminus \{1\} \leq \left\| w \right\| \leq n\} \right) \sup_{1 \leq |w| \leq n} (\sum_{i=1}^{\left| \alpha \right|} C_{w,j}) \). \( \square \)
Lemma 2.3 (1) There exists a constant $C_{m,1} > 0$ such that
\[
\sup_{x \in \mathbb{R}^n} \left| f(\exp(\Phi_s(j_mz))(x)) - (\Phi_s(j_m \exp(j_mz)) f)(x) \right| 
\leq C_{m,1}^{(m+1)/2} \left( 1 + \|j_mz\|_2 \right)^{m+1} \|\text{grad}(f)\|_{C^{(m+1)-1}} \tag{2.5}
\]
for $z \in \mathcal{L}_R(A)$.

(2) There exists a constant $C_{m,M} > 0$ where $M \in \mathcal{Z}_{\geq 2}$ such that
\[
\sup_{x \in \mathbb{R}^n} \left| f(\exp(\Phi_s(j_m ((j_mz_M) \cdot \cdots \cdot (j_mz_1))))(x)) 
- (\Phi_s(j_m \exp((j_mz_M) \cdot \cdots \cdot (j_mz_1))) f)(x) \right| 
\leq C_{m,M}^{(m+1)/2} \left( 1 + \sum_{i=1}^M \|j_mz_i\|_2 \right)^{m+1} \|\text{grad}(f)\|_{C^{(m+1)-1}} \tag{2.6}
\]
for $z_1, \ldots, z_M \in \mathcal{L}_R(A)$.

Proof From the fact that for $z \in \mathcal{L}_R(A)$
\[
j_m(\exp(j_mz)) = \sum_{k=0}^m \frac{1}{k!} (j_mz)^k - \sum_{k=2}^m \frac{1}{k!} (j_m(j_mz)^{k-1}) - j_m \left( \left( (j_mz)^k \right) \right)
\]
and from (2.3) in Proposition 2.1 we see that
\[
\left| f(\exp(\Phi(j_mz))(x)) - (\Phi(j_m \exp(j_mz)) f)(x) \right| 
\leq \frac{1}{(m+1)!} \left\| \Phi(j_mz)^{m+1} f \right\|_\infty + \left| \sum_{k=2}^m \frac{1}{k!} \Phi(j_m(j_mz)^k) f(x) \right| \tag{2.7}
\]
Since we have
\[
(j_mz)^{m+1} = (j_m(j_mz)^k) \cdot j_mz^{m+1},
\]
the followings can be derived by applying Lemma 2.2
\[
\left| f(\exp(\Phi(j_mz))(x)) - (\Phi(j_m \exp(j_mz)) f)(x) \right| 
\leq \sum_{k=2}^m \frac{1}{k!} \left\| \Phi(j_m(j_mz)^k) f \right\|_\infty \tag{2.8}
\leq C_m \sum_{k=2}^m \left\| (j_m(j_mz)^k) \right\|_2 \|\text{grad}(f)\|_{C^{(m+1)-1}}
\leq C_{m,1} \left( 1 + \|j_mz\|_2 \right)^{m+1} \|\text{grad}(f)\|_{C^{(m+1)-1}}
\]
where $C_m$ and $C_{m,1}$ are positive constants. Thus (2.5) is proved. Taking $(j_mz_M) \cdot \cdots \cdot (j_mz_1)$ as $z$ above and evaluating by
\[
\sum_{k=2}^m \left\| (j_m(j_mz_M) \cdot \cdots \cdot (j_mz_1)) \right\|_2 \leq C_{m,M} \left( 1 + \sum_{i=1}^M \|j_mz_i\|_2 \right)^{m+1}
\]
we obtain (2.6). □
Lemma 2.4 There exists a constant $C_{m,M} > 0$ such that

$$\sup_{x \in \mathbb{R}^N} |f(\exp(\Phi_s(j_m z_1)) \circ \cdots \circ \exp(\Phi_s(j_M z_M))(x)) - (\Phi_s(j_m \exp(j_m ((j_M z_M) \circ \cdots \circ (j_2 z_2) \circ (j_1 z_1))) \circ \cdots \circ \exp(\Phi_s(j_M z_M))))(x)| \leq C_{m,M} s^{(m+1)/2} \sum_{i=1}^{M} \left(1 + \left\|j_m z_i\right\|_{L}^{m+1}\right) \left\|\text{grad}(f)\right\|_{C^{m(M+1)-1}}$$

for $z_1, \ldots, z_M \in \mathcal{L}_R(A)$. Here $C_{m,M}$ depends on $m$ and $M$.

Proof We prove the lemma by induction on $M$. When $M = 1$, (2.5) and (2.9) are equivalent. Assume that (2.9) holds for $M$. Splitting the left-hand side of (2.9) for $M + 1$ as

$$\sup_{x \in \mathbb{R}^N} |f(\exp(\Phi_s(j_m z_1)) \circ \cdots \circ \exp(\Phi_s(j_M z_M+1)))\circ \cdots \circ \exp(\Phi_s(j_M z_M))))(x)) - (\Phi_s(j_m \exp(j_m ((j_M z_M) \circ \cdots \circ (j_2 z_2) \circ (j_1 z_1))) \circ \cdots \circ \exp(\Phi_s(j_M z_M)))\circ \cdots \circ \exp(\Phi_s(j_M z_M+1))))(x)| \leq C_{1,s}^{(m+1)/2} \sum_{i=1}^{M} \left(1 + \left\|j_m z_i\right\|_{L}^{m+1}\right) \left\|\text{grad}(f)\right\|_{C^{m(M+1)-1}},$$

where $C_1 > 0$ is a constant depending on $m$ and $M$. Hence, (2.9) is proved. \hfill \Box

From Lemma 2.3 and 2.4 we have the following result.

Lemma 2.5 For all $m \geq 1$, there exists a constant $C_{m,M} > 0$ such that

$$\sup_{x \in \mathbb{R}^N} |f(\exp(\Phi_s(j_m z_1)) \circ \cdots \circ \exp(\Phi_s(j_M z_M))(x)) - f(\exp(\Phi_s(j_m ((j_M z_M) \circ \cdots \circ (j_2 z_2) \circ (j_1 z_1))) \circ \cdots \circ \exp(\Phi_s(j_M z_M)))\circ \cdots \circ \exp(\Phi_s(j_M z_M))))(x)| \leq C_{m,M} s^{(m+1)/2} \sum_{i=1}^{M} \left(1 + \left\|j_m z_i\right\|_{L}^{m+1}\right) \left\|\text{grad}(f)\right\|_{C^{m(M+1)-1}}$$

for all $s \in (0,1]$, $z_1, \ldots, z_M \in \mathcal{L}_R(A)$, and $f \in C^\infty(\mathbb{R}^N; \mathbb{R})$. 
Lemma 2.6 Let \( Z_1, \ldots, Z_M \) be \( L_\mathbb{R}(\mathcal{A}) \)-valued random variables such that for \( m \geq 1 \),
\[
\mathbb{E} \left[ \|z_i\|^2 \right] < \infty \text{ for } i = 1, \ldots, M. \text{ Then, for } p \in [1, \infty) \text{ there exists a constant } C_{m,M} > 0 \text{ such that }
\left\| \sup_{x \in \mathbb{R}^N} \exp \left( \Phi_s \left( j_m Z_1 \right) \right) \cdots \exp \left( \Phi_s \left( j_m Z_M \right) \right) (x) \right\|_{L^p} \leq C_{m,M} s^{(m+1)/2} \quad (2.11)
\]
for any \( s \in (0, 1] \).

Proof If for \( i \in \{1, \ldots, N\} \), \( f((x^1, \ldots, x^N)) = x^i \), then \( \| \text{grad}(f) \|_{C^{m+1}} = 1 \) for all \( m \geq 1 \),
therefore, applying Lemma 2.3 for this \( f \), we obtain (2.11). \( \square \)

We note that in [29] a similar result to this Lemma is obtained.

We now start discussion about the latter term of the right-hand side of (2.1).

Proposition 2.7 There exists a constant \( C > 0 \) such that
\[
\left| g(W)(x) - g(W)(y) \right| \leq C \|W\|_{C^{m+1}}^{m+1} + |x - y| \exp \left( \|W\|_{C^1} \right) \quad (2.12)
\]
for \( g \in IS(m) \) and \( W \in C^m_c(\mathbb{R}^N, \mathbb{R}^N) \).

Proof Since Gronwall’s inequality gives
\[
\left| \exp (W)(x) - \exp (W)(y) \right| \leq |x - y| \exp \left( \|W\|_{C^1} \right),
\]
(2.12) can be derived. \( \square \)

Since \( g_i \in IS(m) \) and each \( Z_i \) satisfies (1.8), we see that for some \( C_1 > 0 \),
\[
\left\| \sup_{x \in \mathbb{R}^N} \left[ g_M (\Phi_s (Z_M)) (x) - \exp (\Phi_s (Z_M)) (x) \right] \right\|_{L^p} \leq \left\| C_m \|\Phi_s (Z_M)\|_{C^{m+1}}^{m+1} \right\|_{L^p} \leq C_1 s^{(m+1)/2}. \quad (2.13)
\]
From this fact and Proposition 2.7, there exists a constant \( C_4 > 0 \) such that
\[
\left\| \sup_{x \in \mathbb{R}^N} \left[ g_{M-1} (\Phi_s (Z_{M-1})) \circ g_M (\Phi_s (Z_M)) (x) - \exp (\Phi_s (Z_{M-1})) \circ \exp (\Phi_s (Z_M)) (x) \right] \right\|_{L^p} \leq \left\| \sup_{x \in \mathbb{R}^N} \left[ g_{M-1} (\Phi_s (Z_{M-1})) \circ g_M (\Phi_s (Z_M)) (x) - \exp (\Phi_s (Z_{M-1})) \circ \exp (\Phi_s (Z_M)) (x) \right] \right\|_{L^p} \leq C_2 s^{(m+1)/2}
\]
\[
+ \left\| C_3 \|\Phi_s (Z_{M-1})\|_{C^{m+1}}^{m+1} + \sup_{x \in \mathbb{R}^N} \left[ g_M (\Phi_s (Z_M)) (x) - \exp (\Phi_s (Z_M)) (x) \right] \exp \left( \|\Phi_s (Z_{M-1})\|_{C^1} \right) \right\|_{L^p} \leq C_4 s^{(m+1)/2}
\]
where \( C_2 \) and \( C_3 \) are positive constants. Inductively,

\[
\left\| \sup_{x \in \mathbb{R}^d} [g_1 (\Phi_1 (Z_1)) \circ \cdots \circ g_M (\Phi_M (Z_M)) (x) \\
- \exp (\Phi_1 (Z_1)) \circ \cdots \circ \exp (\Phi_M (Z_M)) (x)] \right\|_F \leq C_5 s^{(m+1)/2} \tag{2.14}
\]

where \( C_5 > 0 \).

Lemma 2.6 and (2.14) complete the proof.

3 Construction of the \( L_\mathbb{R}((A)) \)-valued random variables \( Z_1, \ldots, Z_M \)

**Lemma 3.1** For \( i = 1, \ldots, M \), let \( Y_i \) be Gaussian random variables such that

\[
E [Y_i] = 0 \quad \text{and} \quad E [Y_i Y_j] = R(i, j), \quad \text{for } i, j = 1, \ldots, M
\]

where \( R(i, j) \in \mathbb{R} \). Moreover, for \( i = 1, \ldots, M \) let \( m_i \in \mathbb{Z}_{\geq 0} \) be such that \( \sum_{i=1}^M m_i \) is even. Then we have

\[
E \left[ Y_1^{m_1} \cdots Y_M^{m_M} \right] = \sum_{\{d_{ij}\}_{1 \leq i, j \leq M} \in e(m_1, \ldots, m_M)} 2^{-\sum_{i=1}^M d_{ii}} \prod_{1 \leq i < j \leq M} (d_{ij})! \prod_{1 \leq i \leq M} R(i, j)^{d_{ii}} \tag{3.1}
\]

where \( e(m_1, \ldots, m_M) \) is a set of \( \{d_{ij}\}_{1 \leq i, j \leq M} \) satisfying that \( d_{ij} \in \mathbb{Z}_{\geq 0} \) and that

\[
\sum_{1 \leq j < i} d_{ij} + 2d_{ii} + \sum_{i, j \leq M} d_{ij} = m_i
\]

for \( i = 1, \ldots, M \).

**Proof** Let \( l = \sum_{i=1}^M m_i \). We have

\[
E \left[ Y_1^{m_1} \cdots Y_M^{m_M} \right] = E \left[ \frac{\partial^l}{\partial z_1^{m_1} \cdots \partial z_M^{m_M}} \exp \left( \sum_{i=1}^M z_i Y_i \right) \right]_{z=0}
\]

\[
= \frac{\partial^l}{\partial z_1^{m_1} \cdots \partial z_M^{m_M}} \left( \exp \left( \frac{1}{2} \sum_{1 \leq i, j \leq M} R(i, j) z_i z_j \right) \right)_{z=0} \tag{3.2}
\]

\[
= \frac{1}{2^{l/2} (l/2)!} \frac{\partial^l}{\partial z_1^{m_1} \cdots \partial z_M^{m_M}} \left( \sum_{1 \leq i, j \leq M} R(i, j) z_i z_j \right)^{l/2} \Bigr|_{z=0}
\]

where \( z = (z_1, \ldots, z_M) \in \mathbb{R}^M \).

Let

\[
e_l = \left\{ \{d_{ij}\}_{1 \leq i, j \leq M} \mid d_{ij} \in \mathbb{Z}_{\geq 0} \text{ and } \sum_{1 \leq i < j \leq M} d_{ij} = \frac{l}{2} \right\} \tag{3.3}
\]
Then
\[
\left( \sum_{1 \leq i, j \leq M} R(i, j) |z_i z_j| \right)^{1/2} = \left( \sum_{i=1}^{M} R(i, i) z_i^2 + 2 \sum_{1 \leq i < j \leq M} R(i, j) z_i z_j \right)^{1/2}
\]
\[
= \sum_{\{d_{ij}\}_{1 \leq i, j \leq M} \in \mathcal{E}_0} (l/2)! \prod_{i=1}^{M} \left( R(i, i) z_i \right)^{d_{ii}} \prod_{1 \leq i < j \leq M} \left( 2 R(i, j) z_i z_j \right)^{d_{ij}}
\]
\[
= \sum_{\{d_{ij}\}_{1 \leq i, j \leq M} \in \mathcal{E}_0} (l/2)! \prod_{i=1}^{M} \left( \prod_{1 \leq i \leq M} R(i, j)^{d_{ij}} \right) \left( \prod_{1 \leq i \leq M} z_i^{(\sum_{1 \leq j \leq M} 2 d_{ij} + \sum_{1 \leq j < l} d_{ij})} \right)
\]
(3.4)

Hence
\[
\frac{\partial^l}{\partial z_1^{m_1} \cdots \partial z_M^{m_M}} \left( \sum_{1 \leq i, j \leq M} R(i, j) z_i z_j \right)^{1/2} \bigg|_{z=0} = (m_1! \cdots m_M)! \left( \frac{1}{2} \right)! \sum_{\{d_{ij}\}_{1 \leq i, j \leq M} \in \mathcal{E}(m_1, \ldots, m_M)} \prod_{i=1}^{M} \left( \prod_{1 \leq i \leq M} R(i, j)^{d_{ij}} \right) \prod_{1 \leq i \leq M} z_i^{(\sum_{1 \leq j \leq M} 2 d_{ij} + \sum_{1 \leq j < l} d_{ij})}.
\]
(3.5)

Since we have from the definition of \( e(m_1, \ldots, M) \) that
\[
\sum_{1 \leq i \leq M} d_{ii} = \frac{1}{2} \sum_{i=1}^{M} d_{ii}
\]
for \( \{d_{ij}\} \in e(m_1, \ldots, M) \), (3.1) is derived from (3.2) and (3.5).

We need a simple representation of the coefficient of each \( v_{i_1} v_{i_2} \cdots v_{i_t} \) in \( \exp(Z_1) \cdots \exp(Z_M) \) where \( (i_1, \ldots, i_t) \in \{0, 1, \ldots, d\}^t \) and \( Z_1, \ldots, Z_M \) are \( \mathcal{L}(\mathcal{A}) \)-valued random variables constructed with Gaussian random variables satisfying (1.10).

For \( \ell, M \in \mathbb{Z}_{>0} \), let \( \mathcal{K}(M) = \{ k = (k_1, \ldots, k_M) \in (\mathbb{Z}_{\geq 0})^M \mid k_1 + \cdots + k_M = \ell \} \). For \( w = v_{i_1} \cdots v_{i_t} \in A^* \), let \( N^w : \{0, 1, \ldots, d\} \times \{1, \ldots, M\} \times \mathcal{K}(M) \rightarrow \mathbb{Z}_{\geq 0} \) be a function such that
\[
N^w(i, j, k) = \text{card} \left( \left\{ r \mid i_r = i \quad \text{for} \quad k_1 + \cdots + k_{r-1} + 1 \leq r \leq k_1 + \cdots + k_t \right\} \right).
\]

**Theorem 3.2** Let \( w = v_{i_1} v_{i_2} \cdots v_{i_t} \in A^* \) and \( n^w(i) = \text{card} \left( \{ j \in \{1, \ldots, \ell \} \mid i_j = i \} \right) \) for \( i = 1, \ldots, d \). Then the coefficient of \( w, C(w) \), in \( \exp(Z_1) \cdots \exp(Z_M) \) becomes as follows:

If \( n^w(i) \) is odd for some \( i \in \{1, \ldots, d\} \), then
\[
C(w) = 0.
\]
(3.6)

If \( n^w(i) \) is even for every \( i \in \{1, \ldots, d\} \), then
\[
C(w) = \sum_{k = (k_1, \ldots, k_M) \in \mathcal{K}(M)} \frac{1}{k_1! \cdots k_M!} \prod_{j=1}^{M} (c_j)^{N^w(0, k)}
\]
\[
\times \prod_{j=1}^{d} \left( \sum_{\{d_{ij}\}_{1 \leq i, j \leq M} \in (N^w(i, 1, k), \ldots, N^w(i, M, k))} 2^{-\sum_{1 \leq j \leq M} d_{ij}} \prod_{1 \leq i \leq M} R_{ij}^{d_{ij}} \right)
\]
(3.7)
where $c_j$ and $R_{ij}$ are real numbers defined in (1.10).

**Proof** In the case where $n^w(i)$ is odd for some $i \in \{1, \ldots, d\}$, (3.6) is directly derived from (1.10).

We therefore consider the other case. By the Taylor expansion of $\exp (Z_1) \cdots \exp (Z_M)$, we have

$$E[\exp (Z_1) \cdots \exp (Z_M)] = \sum_{k_1 \ldots k_M = 0}^{\infty} \frac{1}{k_1! \cdots k_M!} E \left[ \left( c_1 v_0 + \sum_{i=1}^{d} S_i^j v_i \right) \cdots \left( c_M v_0 + \sum_{i=1}^{d} S_M^j v_i \right)^{k_1 \cdots k_M} \right].$$

Hence

$$C(w) = \langle E[\exp (Z_1) \cdots \exp (Z_M)], w \rangle$$

$$= \sum_{k=(k_1 \ldots k_M) \in K(M)} \frac{1}{k_1! \cdots k_M!} E \left[ S_1^{i_1} \cdots S_M^{i_M} \right]$$

$$= \sum_{k=(k_1 \ldots k_M) \in K(M)} \frac{1}{k_1! \cdots k_M!} E \left[ (c_1)^{N^w(0,1,k)} \cdots (c_M)^{N^w(0,M,k)} (S_j)^{N^w(1,1,k)} \cdots (S_M)^{N^w(1,M,k)} \right].$$

(3.8)

From the definition of $S_j^i$, $C(w) = \sum_{k=(k_1 \ldots k_M) \in K(M)} \frac{1}{k_1! \cdots k_M!} \prod_{j=1}^{M} \left( c_1 \right)^{N^w(0,j,k)} \prod_{p=1}^{d} E \left[ (S_j^p)^{N^w(p,1,k)} \cdots (S_M^p)^{N^w(p,M,k)} \right].$

Applying (3.1) from Lemma 3.1, we obtain (3.7).

On the other hand, the value of the coefficient of each $v_i \cdots v_i$ in $j_w \left( \exp (v_0 + 1/2 \sum_{i=1}^{d} v_i^2) \right)$ can be obtained by the following proposition.

**Proposition 3.3** Let $A^w = \{ v_0, v_1, v_2, \ldots, v_d \} \subset A^w$. Then

$$\exp \left( v_0 + \frac{1}{2} \sum_{i=1}^{d} v_i^2 \right) = \sum_{w \in \mathbb{B}^d \leq m} \frac{1}{2^{||w||!}} w.$$  

(3.9)

Therefore, taking $\{ S_j^i \}_{i=1, \ldots, d, j=1, \ldots, M}$ to equate (3.6) or (3.7) with (3.9) for $w = v_1, v_2, \ldots, v_d$ with $||w|| \leq m$, we can construct $Z_1, \ldots, Z_M$.

For $m = 5$, we take $M = 2$ to obtain solvable simultaneous equations which in fact become the following five:

$$c_1 + c_2 = 1, \quad \frac{1}{2} (c_1 R_{11} + c_2 R_{22}) + R_{12} = 1/2,$$

$$\frac{1}{6} (c_1 R_{11} + c_2 R_{22}) + \frac{1}{2} c_1 (R_{12} + R_{22}) = 1/4,$$

$$\frac{1}{6} (c_1 R_{11} + c_2 R_{22}) + \frac{1}{2} c_2 (R_{11} + R_{22}) = 1/4,$$

$$\frac{1}{24} (R_{11}^2 + R_{22}^2) + \frac{1}{6} R_{12} (R_{11} + R_{22}) + \frac{1}{4} R_{11} R_{22} = 1/8.$$  

(3.10)
The solution is (1.15). Since we let \( \{S'_i\}_{i=1,...,d,j=1,...,M} \) be the Gaussian system, such random variables can be constructed.

**Remark 3.4** If we let \( m = 5 \), then \( M \) must be at least two.

### 4 The Runge–Kutta method

We begin by briefly introducing the tree theory following [3], [6], and [7]. For details of the Runge–Kutta method, see [6], [7], and [26].

All trees introduced here are called directed or rooted trees in the literature listed above.

**Definition 4.1** A labelled tree \( t \) is a pair of finite sets \( (V(t), E(t)) \) that satisfies the following conditions:

1. \( V(t) \subset \mathbb{Z}, \ V(t) \neq \emptyset, \) and \( E(t) \subset \{(x, y) \in V(t) \times V(t) : x < y\} \).
2. For each \( x \in V(t) \), if \( (x, y) \in E(t) \) and \( (x', y) \in E(t) \), then \( x = x' \).
3. For two distinct elements \( x, y \in V(t) \), one of the followings holds:
   (i) There exists a path from \( x \) to \( y \).
   (ii) There exists a path from \( y \) to \( x \).
   (iii) For some \( z \in V(t) \setminus \{x, y\} \), there exist paths \( z \) to \( x \) and \( z \) to \( y \).

Here a path from \( p_1 \) to \( p_2 \) is a sequence \( (p_1, \ell_1), (\ell_1, \ell_2), \ldots, (\ell_{l-1}, p_2) \) of elements of \( E(t) \).

An element of \( V(t) \) is called a vertex of \( t \) and that of \( E(t) \) is called an edge of \( t \).

A particular labelled tree \( \tau_r \) is that with \( \text{card} (V(\tau_r)) = 1 \) and \( E(\tau_r) = \emptyset \).

For a labelled tree \( t = (V(t), E(t)) \), let \( r(t) \) be \( \text{card} (V(t)) \). We define \( T \) as the set of all labelled trees.

**Proposition 4.2** For each \( t = (V(t), E(t)) \), there exists a unique vertex \( r \in V(t) \) such that for any \( x \in V(t) \setminus \{r\} \), there is a path from \( r \) to \( x \).

Such a vertex \( r \) is called the root of \( t \). Here, \( \tau_r \) consists of only the root.

**Definition 4.3** For \( i = 1, \ldots, n \), let \( t_i = (V(t_i), E(t_i)) \in T \) be such that \( V(t_i) \cap V(t_j) = \emptyset \) if \( i \neq j \). Then \( [t_1 \cdots t_n] \) is defined as \( t = (V(t), E(t)) \in T \) such that

\[
V(t) = \{r\} \cup V(t_1) \cup \cdots \cup V(t_n)
\]

\[
E(t) = \{(r, r_1), \ldots, (r, r_n)\} \cup E(t_1) \cup \cdots \cup E(t_n)
\]

where each \( r_i \) denotes the root of \( t_i \) and \( r = \min\{r_1, \ldots, r_n\} - 1 \).

**Remark 4.4** For \( t_1, \ldots, t_n \in T \), we have that

\[
[t_1 \cdots t_n] = [t_{\omega(1)} \cdots t_{\omega(n)}]
\]

for any permutation \( \omega \in \mathfrak{S}_n \).

**Definition 4.5** Let \( t_i = (V(t_i), E(t_i)) \in T \) for \( i = 1, 2 \). We say that \( t_1 \) and \( t_2 \) are isomorphic, written as \( t_1 \sim t_2 \), if there exists a bijection \( \omega : V(t_1) \rightarrow V(t_2) \) such that \( (x, y) \in E(t_1) \) if and only if \( (\omega(x), \omega(y)) \in E(t_2) \).

In particular, when \( t_1 \sim t_2 \) and \( V(t_1) = V(t_2) \), that is, \( \omega \) is a permutation, we say that \( t_1 \) and \( t_2 \) are equivalent and write \( t_1 \sim t_2 \).
Proposition 4.6 Both \( \simeq \) and \( \sim \) are equivalence relations.

Proposition 4.7 Let \( t_i = (V(t_i), E(t_i)) \in \mathcal{T} \) and \( u_i = (V(u_i), E(u_i)) \in \mathcal{T} \) for \( i = 1, \ldots, n \). Suppose that \( t_i \sim u_i \) for \( i = 1, \ldots, n \) and that
\[
V(t_i) \cap V(t_j) = \emptyset \quad \text{and} \quad V(u_i) \cap V(u_j) = \emptyset
\]
if \( i \neq j \). Then
\[
[t_1 \cdots t_n] \simeq [u_1 \cdots u_n].
\]

Definition 4.8 We define \( T = \mathcal{T}/\simeq \). An element \( t \in T \) is called a non-labelled tree. For a labelled tree \( t \in \mathcal{T} \), \( |t| \) denotes the corresponding non-labelled tree \( t \in T \).

Then, from Proposition 4.7 the following result can be derived.

Proposition 4.9 Under the same condition as Proposition 4.7
\[
|[t_1 \cdots t_n]| = |[u_1 \cdots u_n]|
\]
holds.

By virtue of Proposition 4.9 we can define a non-labelled tree \( t = [t_1 \cdots t_n] \) for \( t_1, \ldots, t_n \in T \) as \( [t_1 \cdots t_n] \) where \( t_1 \in T \) is a representative labelled tree such that \( |t_1| = t_1 \). In particular, we let \( \tau = |\tau| \).

Proposition 4.10 For any \( t \in T \setminus \{\tau\} \), there exist \( t_1, \ldots, t_n \in T \) such that \( t = [t_1 \cdots t_n] \).

Moreover
\[
[t_1 \cdots t_n] = [t_{\omega(1)} \cdots t_{\omega(n)}]
\]
for any permutation \( \omega \in S_n \).

Here, \( [t_1^{m_1} \cdots t_n^{m_n}] \) denotes \( [t_1 \cdots t_n] \) where \( t_i \in T \) for \( i = 1, \ldots, n \).

Definition 4.11 (1) For \( t = (V(t), E(t)) \in \mathcal{T} \), we define \( \alpha : T \rightarrow \mathbb{Z}_{\geq 1}, \beta : T \rightarrow \mathbb{Z}_{\geq 1}, \text{ and } \sigma : T \rightarrow \mathbb{Z}_{\geq 1} \) by
\[
\alpha(t) = \text{card} \left( \left\{ u \in T \mid u \sim t \text{ where } t \in T \right\} \right)
\]
\[
\beta(t) = \text{card} \left( V(t) \right)
\]
\[
\sigma(t) = \begin{cases} 1 & \text{if } t = \tau \\ \prod_{i=1}^l m_i! \sigma (t_i)^{m_i} & \text{if } t = [t_1^{m_1} \cdots t_n^{m_n}], l \geq 1 \end{cases}
\]
where \( A = (a_{ij})_{i,j=1,\ldots,K} \). We notice that \( \alpha \) is well-defined because \( \alpha \) denotes the number of ways a tree may be labelled.

(2) Let \( \mathcal{A} \) be the set of \( K \times K \) real matrices. We inductively define derivative weights \( \zeta : T \times \mathcal{A} \rightarrow \mathbb{R} \) for \( i = 1, \ldots, K \) by
\[
\zeta_i(t; A) = \begin{cases} \sum_{j=1}^K a_{ij} & \text{if } t = \tau \\ \sum_{j=1}^K \prod_{i=1}^l \zeta_j(t_i; A) & \text{if } t = [t_1 \cdots t_l], l \geq 1. \end{cases}
\]

In addition, we define the elementary differentials \( D : C^\infty_b (\mathbb{R}^N; \mathbb{R}^N) \times T \rightarrow C^\infty_b (\mathbb{R}^N; \mathbb{R}^N) \) as follows:
\[
D(W,t)(x) = \begin{cases} W(x) & \text{if } t = \tau, \\
W^{(l)}(x) (D(W,t_1)(x), D(W,t_2)(x), \ldots, D(W,t_l)(x)) & \text{if } t = [t_1 \cdots t_l], l \geq 1. \end{cases}
\] (4.1)
Let $y(W,s)$ be a solution to an ODE
\[
\frac{d}{ds}y(W,s) = W(y(W,s)), \quad y(W,0) = y_0
\] (4.2)
where $W \in C^\infty_b(\mathbb{R}^N, \mathbb{R}^N)$ and $y_0 \in \mathbb{R}^N$. Then we have the following lemmas essentially proved in [21], pp. 139–145.

**Lemma 4.12** For $m \in \mathbb{Z}_{\geq 1}$,
\[
y^{(m)}(W,s) = \sum_{t \in T_m} D(W,t)(y(W,s)).
\] (4.3)

Let $T_m = \{ t \in T : r(t) = m \}$ and $T_{cm} = \bigsqcup_{m=0}^\infty T_m$ for $m \geq 0$ with $T_0 = \emptyset$.

Let $A_m \in A$ denote $A$ in (1.16) for the explicit Runge–Kutta method. Then $Y_t(W,s)$ is definitely determined by $A_m$ with $a_{ij} = 0$ if $i \neq j$ and so $Y_t(y_0;W,s)$ can be constructed with $b$ and $Y_t(W,s)$ as both seen in (1.16).

**Lemma 4.13** Let $m \geq 1$. If there exists a constant $C_m > 0$ such that
\[
\left| Y_t(W,s) - \left( y_0 + \sum_{t \in T_{cm}} \frac{g^{(l)}(t)}{\sigma}(W,t)(y_0) \right) \right| \leq C_m s^m ||W||_{cm}^m
\] (4.4)
for $i = 1, \ldots, K$, then there exists a constant $C_{m+1}$
\[
\left| sW \left( Y_t(W,s) \right) - \sum_{l=1}^{m+1} \frac{g^{(l)}(t)}{\sigma}(W,t)(y_0) \right| \leq C_{m+1} s^{m+1} ||W||_{cm+1}^{m+1}.
\] (4.5)

Applying these lemmas to evaluations of the solution to (4.2) and the Runge–Kutta method (1.16), we obtain the following result.

**Theorem 4.14** For $y$ satisfying (1.2), there exists a constant $C_{m+1}$
\[
\left| \exp(sW)(y_0) - \left( y_0 + \sum_{t \in T_{cm}} \frac{g^{(l)}(t)}{\sigma}(W,t)(y_0) \right) \right| \leq C_{m+1} s^m ||W||_{cm+1}^m.
\] (4.6)

On the other hand, for the Runge–Kutta method (1.16) there exists a constant $C_{m+1}$ such that
\[
\left| Y_t(y_0;W,s) - \left( y_0 + \sum_{l=1}^{m+1} \frac{g^{(l)}(t)}{\sigma}(W,t)(y_0) \right) \right| \leq C_{m+1} s^{m+1} ||W||_{cm+1}^{m+1}.
\] (4.7)

We say that $(A,b)$ satisfies $m$-th-order conditions if
\[
\frac{\alpha(t)}{r(t)!} = \sum_{l=1}^{m+1} b_l \prod_{k=1}^l \zeta(t_k;A) \frac{g^{(l)}(t)}{\sigma}(W,t)(y_0)
\] (4.8)
for all $t = [t_1 \cdots t_l] \in T_{cm}$.

From Theorem 4.14 the following result can be directly derived.

**Theorem 4.15** Suppose that $(A,b)$ satisfies the $m$th-order conditions (4.8). Let $g(W)(y_0) = Y_t(y_0;W,1)$ where $Y_t(y_0;W,1)$ is the Runge–Kutta method defined in (1.16). Then
\[
g \in IS(m).
\] (4.9)
The new simulation scheme and Corollary 1.4

Corollary 1.4 indicates the new implementation method of the new higher-order scheme proposed by Kusuoka in [15] and [16].

This implementation method seems to be distinct mainly because it has two advantages. One is that the approximation operator can be obtained by numerical calculations if the Runge–Kutta method is applied to the calculation of each \( \exp(Z_j) \) whereas the tediousness in symbolical calculations of the operator might be an obstacle for practical application, which can be observed in [18], [24], and [28]. The other advantage is that the partial sampling problem discussed in [18] and [24] can be resolved by using quasi-Monte Carlo methods. More precisely, the following two points make an effective use of the Low-Discrepancy sequences, which are essential to quasi-Monte Carlo methods ([22]):

- In this implementation, \( S_j \) can be taken to be a continuous random variable.
- The scheme itself is characterized by the need for a much less number discretization time steps, which leads to a reduction in the number of dimensions of the numerical integration.

6 Application

In this section we present a numerical example in order to illustrate the implementation method proposed in Corollary 1.4 and compare it with some existing schemes.

6.1 Simulation

Let \( X(t, x) \) be a diffusion process defined by (1.1). The most popular scheme of first order is the Euler–Maruyama scheme, which is shown in [14] and [32], for an arbitrary \( C^4 \) function \( f \)

\[
\left\| E \left[ f \left( X^{(EM)}(1), n \right) \right] \right\| - E \left[ f \left( X(1, x) \right) \right] \leq C f \frac{1}{n}
\]

(6.1)

where \( X^{(EM)}(1) \) denotes the Euler–Maruyama scheme approximating \( X(t, x) \). We note that this inequality holds for measurable \( f \) if \( \{V_i\}_{i=1, \ldots, d} \) satisfies some more conditions ([11]).

The construction of a higher-order scheme is based on the higher order stochastic Taylor formula ([8] [14]). When the vector fields \( \{V_i\}_{i=0}^d \) commute, higher-order schemes can be simplified to a direct product of one-dimensional problem as seen in [14]. In contrast, for non-commutative \( \{V_i\}_{i=0}^d \), the acquisition of all iterated integrals of Brownian motion is required, which is very demanding. This is done in [15], [20], [30], [31] and [18] and generalized as the cubature method on Wiener space ([21]).

Once a \( p \)th-order scheme \( \{X^{(ord,p)}(k), n\}_{k=0, \ldots, n} \) is obtained and expanded with some constant \( K_f \) as

\[
E \left[ f \left( X^{(ord,p)}(1), n \right) \right] - E \left[ f \left( X(1, x) \right) \right] = K_f \frac{1}{n^p} + O \left( \frac{1}{n^{p+r}} \right)
\]

(6.2)
the \((p + 1)\)th-order scheme can be derived as
\[
\frac{2^p}{2^p - 1} E\left[f\left(X_{(\text{ord } p) + 1}\right)\right] - \frac{1}{2^p - 1} E\left[f\left(X_{(\text{ord } p), 1}\right)\right].
\] (6.3)

This boosting method is called Romberg extrapolation and is shown to be applicable to the Euler–Maruyama scheme under certain conditions (32).

The simulation approach must be followed by the numerical calculation of \(E\left[f\left(X_{(\text{ord } p), 1}\right)\right]\). However, when \(n \times d\) is large, it is practically impossible to proceed with the integration by using the trapezoidal formula and so we fall back on the Monte Carlo or quasi-Monte Carlo method (22). Here we make only a few remarks on each method. For a more detailed analysis, see (25).

**Remark 6.1** As long as we use the Monte Carlo method for numerical approximation of \(E[f(X(1, x))]\), the number of sample points needed to attain a given accuracy is independent of the number of the dimensions of integration, namely both the number \(n\) of partitions and the order \(p\) of the approximation scheme.

**Remark 6.2** In contrast to the Monte Carlo case, the number of sample points needed for the quasi-Monte Carlo method for numerical approximation of \(E[f(X(1, x))]\) heavily depends on the number of the dimensions of integration. The fewer the dimensions, the fewer the samples that are needed.

### 6.2 The algorithm and competitors

#### 6.2.1 The algorithm of the new method

We take the algorithm which is proposed in Theorem 1.6 and Corollary 1.4 with \(u = \frac{3}{4}\). From Corollary 1.4, we can implement the second-order algorithm with a numerical approximation of \(\exp(Z_i)\) of at least fifth-order Runge–Kutta method because the order \(m\) for an integration scheme attained by \(Z_1\) and \(Z_2\) is five and so the order of the new implementation method becomes two. As a result of the same argument it can be shown that at least seventh-order explicit Runge–Kutta method has to be applied to the approximation of \(\exp(Z_i)\) when we boost the new method to the third order by Romberg extrapolation. Details of these Runge–Kutta algorithms used here are given in the Appendix.

#### 6.2.2 Competitive schemes

There there are numerous studies on the acceleration of Monte Carlo methods (11). We choose for the following reasons only the crude Euler–Maruyama scheme and the algorithm introduced in [25], which we will refer to in the remainder of this paper as N–V method, both with and without Romberg extrapolation, as competitors:

(i) Only these two schemes can be recognized as being comparable to the new method, since they are model-independent.
(ii) Almost all variance reduction techniques and dimension reduction techniques applicable to the Euler–Maruyama scheme are also applicable to the new method.
6.3 Numerical results

We provide an example on financial option pricing in the following part of this paper.

6.3.1 Asian option under the Heston model

We consider an Asian call option written on an asset whose price process follows the Heston stochastic volatility model. Comparison with the N-V method will also be given as well from the result shown in [25].

The non-commutativity of this example should be noted here.

Let \( Y_1 \) be the price process of an asset following the Heston model:
\[
Y_1(t, x) = x_1 + \int_0^t \mu Y_1(s, x) \, ds + \int_0^t \sqrt{Y_2(s, x)} \, dB^1(s),
\]
\[
Y_2(t, x) = x_2 + \int_0^t \alpha (\theta - Y_2(s, x)) \, ds + \int_0^t \beta \sqrt{Y_2(s, x)} \left( \rho \, dB^1(s) + \sqrt{1 - \rho^2} \, dB^2(s) \right),
\]
(6.4)

where \( x = (x_1, x_2) \in (\mathbb{R}_+, 0)^2 \), \((B^1(t), B^2(t))\) is a two-dimensional standard Brownian motion, \(-1 \leq \rho \leq 1\), and \(\alpha, \theta, \mu\) are some positive coefficients such that \(2\alpha \theta - \beta^2 > 0\) to ensure the existence and uniqueness of a solution to the stochastic differential equation (6.4). Then the payoff of Asian call option on this asset with maturity \(T\) and strike \(K\) is:
\[
Y_3(t, x) = \max \left( \frac{Y_3(T, x)}{T} - K, 0 \right)
\]
(6.5)

Hence, the price of this option becomes \( D \times E \left[ \max \left( \frac{Y_3(T, x)}{T} - K, 0 \right) \right] \) where \(D\) is an appropriate discount factor that we do not focus on here. We set \(T = 1\), \(K = 1.05\), \(\mu = 0.05\), \(\alpha = 2.0\), \(\beta = 0.1\), \(\theta = 0.09\), \(\rho = 0\), and \((x_1, x_2) = (1.0, 0.09)\) and take
\[
E \left[ \max \left( \frac{Y_3(T, x)}{T} - K, 0 \right) \right] = 6.0473534496 \times 10^{-2}
\]

that is obtained by the new method with Romberg extrapolation and the quasi-Monte Carlo with \(n = 96 + 48\), and \(M = 8 \times 10^8\) where \(M\) denotes the number of sample points.

Let \(Y(t, x) = (Y_1(t, x), Y_2(t, x), Y_3(t, x))\). Transformation of the stochastic differential equations (6.4) and (6.5) gives the following Stratonovich-form stochastic differential equations:
\[
Y(t, x) = \sum_{i=0}^2 \int_0^t V_i(Y(s, x)) \circ dB^i(s),
\]
(6.6)
Table 1: # of dimensions involved in each method.

| Method       | Number of dimensions |
|--------------|----------------------|
| Euler–Maruyama | $dn$                |
| N-V          | $n + dn$ ($n$-Bernoulli and $(d \times n)$-Gaussian) |
| New Method   | $2dn$                |

where

$$
V_0(t(y_1, y_2, y_3)) = t\left( y_1 \left( \mu - \frac{y_2}{2} - \frac{\rho \beta}{4} \right), \alpha(\theta - y_2) - \frac{\beta^2}{4}, y_1 \right)
$$

$$
V_1(t(y_1, y_2, y_3)) = t\left( y_1 \sqrt{\gamma^2}, \rho \beta \sqrt{\gamma^2}, 0 \right)
$$

$$
V_2(t(y_1, y_2, y_3)) = t\left( 0, \beta \sqrt{(1 - \rho^2)} y_2, 0 \right).
$$

(6.7)

6.3.2 Dimensions of integrations

As mentioned in Remarks 6.1 and 6.2, the dimensions of integrations in these methods affect the quasi-Monte Carlo method. The relation among $d$: the number of factors, $n$: the number of partitions, and the dimensions of integration of each method can be summarized as in Table 1.

6.3.3 Discretization Error

The relation between discretization error and the number of partitions of each algorithm is plotted in Figure 1. We can observe from this figure that for $10^{-4}$ accuracy the new method with Romberg extrapolation takes the minimum number of partitions as $n = 1 + 2$ whereas $n = 16$ for the Euler–Maruyama scheme with the extrapolation. Even without the extrapolation, the new method attains that accuracy with $n = 10$ while the Euler–Maruyama scheme takes $n = 2000$. Moreover, it may be said that the N-V method shows slightly worse performance than the new method.

6.3.4 Integration Error

Looking at Figure 2 we can compare convergence errors of respective methods for each number of sample points, $M$. For the Monte Carlo case, $2\sigma$ of 10 batches is taken as convergence error while for the quasi-Monte Carlo method, absolute difference from the value to be convergent is considered. For $10^{-4}$ accuracy with 95% confidence level ($2\sigma$), $M = 10^6$ is taken for the Monte Carlo method. On the other hand, if we apply instead the quasi-Monte Carlo method, the new method and the N-V method require $M = 2 \times 10^7$ sample points, though $M = 5 \times 10^6$ has to be taken for the Euler–Maruyama scheme.
Fig. 1 Error coming from the discretization

Fig. 2 Convergence Error from quasi-Monte Carlo and Monte Carlo
Table 2 #Partitions, #Samples, Dimension, and CPU time required for an accuracy of $10^{-4}$.

| Method          | #Part. | Dim. | #Samples | CPU time (sec) |
|-----------------|--------|------|----------|----------------|
| E-M + MC        | 2000   | 4000 | $10^8$   | $1.72 \times 10^5$ |
| E-M + Romb. + QMC | 16 + 8 | 48   | $5 \times 10^6$ | $1.27 \times 10^2$ |
| N-V + QMC       | 16     | 32 + 16 | 2 \times 10^5 | 4.38 |
| N-V + Romb. + QMC | 4 + 2  | 12 + 6 | 2 \times 10^5 | 1.76 |
| New Method + QMC | 10     | 40   | $2 \times 10^5$ | 3.4 |
| New Method + Romb. + QMC | 2 + 1  | 12   | $2 \times 10^5$ | 1.2 |

6.3.5 Overall performance comparison

The number of partitions, the number of samples, and the amount of computation time required for $10^{-4}$ accuracy for each method are summarized in Table 2. CPU used in this experiment is Athlon 64 3800+ by AMD.

Since the amount of time required to carry out the calculation for each sample point is proportional to the number of partitions, the total time spent on calculations is proportional both to the number of partitions and to the number of samples. We can see from the Table 2 that the speed of the new method is approximately 100 times faster than that of the Euler–Maruyama scheme when Romberg extrapolation and quasi-Monte Carlo are applied to each. Even when the extrapolation is not applied, the new method enables calculations some 37 times faster than the Euler–Maruyama scheme with Romberg extrapolation and quasi-Monte Carlo method. This fact shows that the reduction in the number of partitions sufficiently compensate for the slowness of one step of the new method at least in the present study.

Lastly, Remarks 6.1 and 6.2 should be emphasized to reiterate that the advantage of the new method is that it is deeply related to the properties of the quasi-Monte Carlo method.

Appendix: The fifth-order and the seventh-order Runge–Kutta algorithms

We present here the concrete algorithms of the explicit fifth- and seventh-order Runge–Kutta methods applied in Subsection 6.2. The fifth-order method is taken from [6] as follows:

\[
\begin{align*}
    a_{21} &= \frac{2}{5}, & a_{31} &= \frac{11}{64}, & a_{32} &= \frac{5}{64}, & a_{43} &= \frac{1}{2}, & a_{51} &= \frac{3}{64}, & a_{52} &= \frac{15}{64}, \\
    a_{53} &= \frac{3}{8}, & a_{54} &= \frac{9}{16}, & a_{62} &= \frac{5}{7}, & a_{63} &= \frac{6}{7}, & a_{64} &= -\frac{12}{7}, & a_{65} &= \frac{8}{7}, \\
    a_{ij} &= 0 \text{ otherwise}, \\
    b &= \begin{pmatrix} 7 & 32 & 12 & 32 & 7 \\ 90 & 90 & 90 & 90 & 90 \end{pmatrix}.
\end{align*}
\]
The seventh-order method is taken from [7] as follows:

\[
\begin{align*}
a_{21} &= \frac{1}{5}, & a_{32} &= \frac{1}{5}, & a_{41} &= \frac{1}{5}, & a_{43} &= \frac{3}{8}, & a_{51} &= \frac{148}{1331}, & a_{53} &= \frac{150}{1331}, & a_{54} &= -\frac{56}{1331}, \\
a_{61} &= -\frac{404}{243}, & a_{63} &= -\frac{170}{27}, & a_{64} &= \frac{4024}{1701}, & a_{65} &= \frac{10648}{1701}, & a_{71} &= \frac{2466}{2401}, & a_{73} &= \frac{1242}{343}, \\
a_{74} &= \frac{19176}{16807}, & a_{75} &= \frac{51909}{16807}, & a_{76} &= \frac{1053}{2401}, & a_{81} &= \frac{5}{154}, & a_{84} &= \frac{96}{539}, & a_{85} &= -\frac{1815}{20384}, \\
a_{86} &= \frac{405}{2464}, & a_{87} &= \frac{49}{1144}, & a_{91} &= \frac{113}{32}, & a_{93} &= -\frac{195}{22}, & a_{94} &= \frac{32}{7}, & a_{95} &= \frac{29403}{3584}, \\
b &= \begin{pmatrix} 0 & 0 & 32 & 1771561 & 243 & 16807 & 77 & 11 \\ 0 & 0 & 105 & 6289920 & 1560 & 74880 & 1440 & 70 \end{pmatrix}.
\end{align*}
\]

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