The strong convergence of operator-splitting methods for the Langevin dynamics model

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Abstract

We study the strong convergence of some operator-splitting methods for the Langevin dynamics model with additive noise. It will be shown that a direct splitting of deterministic and random terms, including the symmetric splitting methods, only offers strong convergence of order 1. To improve the order of strong convergence, a new class of operator-splitting methods based on Kunita’s solution representation [1] are proposed. We present stochastic algorithms with strong orders up to 3. Both mathematical analysis and numerical evidence are provided to verify the desired order of accuracy.

Keywords: Langevin equation, Brownian motion, strong convergence, operator splitting methods, Itô Taylor approximation

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1. Introduction

The Langevin dynamics (LD) equation plays a fundamental role in the modeling of many complex dynamical systems subject to random noise. In its simplest form, it can be expressed as the Newton’s equations of motion with added frictional and random forces, which are usually posed to satisfy the fluctuation-dissipation theorem.

As a system of stochastic differential equations (SDE), there are various classical methods for approximating the solutions [2]. However, low order methods, such as the Euler-Maruyama method, often do not have sufficient accuracy. On the other hand, higher order methods that are constructed based on direct expansions of solutions (Itô-Taylor expansion) usually involve high order derivatives of the drift and diffusion coefficients, which makes the implementation rather difficult. For instance, for bio-molecular research supported by the National Science Foundation DMS-1522617 and DMS-1619661.
models [3], this implies that one has to compute the derivatives of the inter-molecular forces, which typically is not plausible. As a result, these methods have been largely neglected in the molecular simulation community. Instead, operator splitting methods have been more widely used. Such algorithms, especially with applications to molecular dynamics simulations, have been treated extensively in [4, 5], where many theoretical and practical aspects have been discussed. The idea is to separate out terms on the right hand side and form two or more SDEs that can be solved explicitly. This is denoted by an [ABO] notation in [4]. Many existing methods can be recast into this form, e.g., [6, 7, 8, 9, 10, 11]. One particular advantage of the splitting methods is that they are very easy to implement, since each substep can be carried out exactly. The splitting methods can also be designed to better sample the equilibrium averages. Another approach is based on solving the coordinate and momentum equations consecutively. For example, one can start by assuming the coordinates remain constant, and integrate out the momentum equation exactly. Then using this solution for the momentum, one can integrate the first equation and obtain an updated coordinate for the next step. A further correction can be made by assuming the force is linear in time, constructed using the coordinates at the current and next steps. This led to the stochastic velocity Verlet method (SVV) [12, 13, 14], which has been implemented in simulation packages, e.g., TINKER [15]. Other integration methods can also be found in the literature, e.g., [16, 17, 18, 10, 19].

Part of this paper is concerned with the numerical accuracy of the Langevin integrators. This fundamental issue has been discussed in [4] as well. In particular, the weak convergence of the numerical solution has been rigorously proved in [20]. Such analysis is crucial when the approximation methods are used to sample the corresponding equilibrium statistics. This is particularly useful when the averages of certain quantities are of interest. On the other hand, to the best of our knowledge, the strong convergence has not been fully studied. Strong convergence ensures the accuracy in terms of individual realizations and solutions at transient stages. Strong convergence usually implies weak convergence, but not vice versa. Typically, strong convergence can be examined by comparing to the Itô-Taylor expansion. Therefore, the fact that the splitting methods discussed in the literature often do not involve multiple Itô integrals of order 2 or higher is already an indication that those methods are only of strong order 1 or less. In general, each improvement of the strong convergence will only increase the order by 0.5 [2].

The purpose of this paper is to present some mathematical analysis of the strong convergence properties for some existing numerical algorithms for the Langevin dynamics model. In addition, we present a new formalism for constructing algorithms that are robust and easy to implement. Our starting point is the solution representation by Kunita [1]. Written formally as an operator exponential form, the differ-
ential operator is expressed in terms of the commutators involving the differential operators associated with the drift and diffusion coefficients, along with multiple Itô integrals. Intuitively, we can make truncations at various levels, to obtain approximation methods of increasing order. Such truncation schemes have been used in [21] as a starting point to construct robust algorithms for scalar SDEs with multiplicative noise. It was demonstrated that such algorithms can preserve the non-negativity of the solution. For the applications of these truncations to the Langevin dynamics, we provide the mathematical analysis of these approximations, and examine the strong order of the approximations. The strong convergence is in the $L^1$ sense following the notations in [2].

With the truncations of the solution operator, we obtain approximate solutions that can be written as solutions of ODEs, for which many efficient methods exist. We choose the well established operator-splitting methods. With the various truncation schemes, together with an appropriate operator splitting for the resulting ODEs, we found methods of higher strong order. More specifically, we present the explicit forms of the methods with strong order 2 and 3.

The rest of the paper is organized as follows. Section 2 presents the analysis of some existing numerical methods. In section 3, we introduce the new class of operator splitting methods based on the truncations of the Kunita's solution operator and examined the strong order of accuracy. Section 4 contains numerical tests that will demonstrate the expected order of convergence.

2. The basic theory

Let us start with the Langevin dynamics model with $n$ space dimension,

\[
\begin{cases}
    x' = v, \\
    v' = f(x) - \Gamma v + \sigma W'(t),
\end{cases}
\]

where $x = (x^1, \ldots, x^n)$, $v = (v^1, \ldots, v^n) \in \mathbb{R}^n$ can be interpreted as position and velocity components respectively, $W(t) = (W^1(t), \ldots, W^n(t)) \in \mathbb{R}^n$ is the standard $n$-dimensional Brownian motion and $0 \leq t \leq T$. Assume the function $f = f(x) : \mathbb{R}^n \to \mathbb{R}^n$, representing the conservative force (for example, the Morse potential), has bounded second derivatives. Here we will consider the case where $\sigma$ and $\Gamma$ are constant $n \times n$ matrices. In particular, the noise is additive, and as a consequence, (1) may be interpreted as either an Itô or Stratonovich SDE: in differential form, $\sigma dW_t = dW_t = W'(t)dt$. For particle dynamics, typically $n = 3N$, with $N$ being the total number of particles.
2.1. Itô-Taylor expansion of the solution.

For numerical solutions of the Langevin dynamics model \([1]\), the consistency is defined via a comparison with the Itô-Taylor expansion of the exact solution. Let us recall \([2\text{, eq. 5.5.3}]\) that in general, for a multi-dimensional SDE,

\[
\begin{align*}
    dX_t &= a(X_t)\,dt + b\,dW_t, \\
\end{align*}
\]

where \(a = a(x) : \mathbb{R}^d \rightarrow \mathbb{R}^d\), \(b \in \mathbb{R}^{d \times m}\) and \(W_t\) is the standard \(m\)-dimensional Brownian motion, the strong order \(\gamma \in \{0.5, 1, 1.5, 2, 2.5, 3, \ldots\}\) Itô-Taylor expansion is given by

\[
X_{k+1} = X_k + \sum_{\alpha \in A_\gamma} f_\alpha(X_k) I_\alpha + \sum_{\alpha \in B_\gamma} I_\alpha(f_\alpha(X_t))_{t_n, t_{n+1}},
\]

where we have denoted \(t_k = k\Delta t\), \(X(k\Delta t) = X_k\), with \(k\) being the time step with step size \(\Delta t\), and final time step \(n_f\) satisfying \(n_f \Delta t = T\). In addition, \(A_\gamma\) and \(B_\gamma\) are sets of multi-indices, \(f_\alpha = f_\alpha(x)\) are coefficient functions, and \(I_\alpha\) are multiple Itô integrals. This idea generalizes the Taylor expansion of a deterministic function. Specifically the set \(A_\gamma\) is defined as,

\[
A_\gamma = \{\alpha : l(\alpha) + n(\alpha) \leq 2\gamma \text{ or } l(\alpha) = n(\alpha) = \gamma + 0.5\},
\]

where \(l(\alpha) := l\) is the length of the multi-index \(\alpha = (j_1, j_2, \ldots, j_l)\), with entries \(j_k \in [0, 1, \ldots, m]\), \(n(\alpha)\) is the number of zero entries in \(\alpha\), and the remainder set \(B_\gamma\) is defined by

\[
B_\gamma = \{\alpha = (j_1, j_2, \ldots, j_l) \notin A_\gamma : (j_2, j_3, \ldots, j_l) \in A_\gamma\}.
\]

The coefficient functions \(f_\alpha\) are given by

\[
f_\alpha(x) = L^{j_1} \cdots L^{j_l-1} L^{j_l} x
\]

where the \(L^j\) are differential operators

\[
\begin{align*}
    L^0 &= a \cdot \nabla x + \frac{1}{2} (b \cdot \nabla x)^2, \\
    L^j &= b \cdot \nabla x = \sum_{k=1}^d b_k \frac{\partial}{\partial x_k} \quad \text{for } 1 \leq j \leq m
\end{align*}
\]

and \(\nabla x = \left( \frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_m} \right)\). Finally, the multiple Itô integrals \(I_\alpha = I_{a, ik, \ell_{k+1}}\) are given by

\[
I_{a, ik, \ell_{k+1}} = \int_{t_k}^{t_{k+1}} \int_{t_k}^{t_{k+1}} \cdots \int_{t_k}^{t_{k+1}} dW_{s_1}^{j_1} dW_{s_2}^{j_2} \cdots dW_{s_l}^{j_l},
\]
where by convention $dW_t^0 := dt$, and more generally,
\[
I_a[f_a(X_t)|I_{t_k}, I_{t_{k+1}} = \int_{t_k}^{t_{k+1}} \int_{t_k}^{t_{k+1}} \cdots \int_{t_k}^{t_{k+1}} f_a(X_{t_k}) dW_{s_1}^I \cdots dW_{s_m}^I.
\]  
(9)

This reduces to the usual Taylor expansion when $d = 1, a = 1$, and $b = 0$. We refer the readers to [2] for the detailed explanation of the notations.

One-step numerical schemes can be directly obtained from the Itô-Taylor expansion [3]. For example, to find the strong order $\gamma = 0.5$ Itô-Taylor approximation of $X_n$, first notice $\mathcal{A}_{0.5} = \{0,(j) : j = 1, \ldots, m\}$, then calculate $f_0 = a$ and $f_j = b_j^I$ ($j = 1, \ldots, m$). Next, calculate $I_0 = \Delta t, I_j = W_{2\Delta t}^j =: \Delta W^j$, so that
\[
Y_{n+1} = Y_n + a(Y_n)\Delta t + \sum_{j=1}^m b^I_j(Y_n)\Delta W^j.
\]
(10)

Here we have used $Y_n$ to denote the numerical solution at step $n$. This is the Euler-Maruyama method. In simulations, the increments $\Delta W^j \in N(0, \Delta t)$ are implemented as $\sqrt{\Delta t} \xi^j$ where $\xi^j \in N(0, 1)$ are standard normal random variables. The strong order $\gamma = 1$ Itô Taylor approximation can be found by simply adding more multi-indices $\alpha = (j_1, j_2)$, with $j_1, j_2 = 1, 2, \cdots, m$, and computing $f_{(j_1, j_2)} = bb'$, so that
\[
Y_{n+1} = Y_n + a(Y_n)\Delta t + \sum_{j=1}^m b^I_j(Y_n)\Delta W^j + \sum_{j_1, j_2 = 1}^l L^{j_1 j_2} b^{j_2} I_{(j_1, j_2)},
\]
(11)

also known as the Milstein method [2] eq. 10.3.3]

**Definition 1.** Let $\gamma \in \{0.5, 1, 1.5, 2, 2.5, 3, \ldots\}$. A discrete time approximation $Y$ of $X$ with uniform step size $\Delta t$ converges with strong order $\gamma$ at time $T$ [2] eq. 10.6.3] provided that there are constants $C$ and $\Delta > 0$ such that
\[
\mathbb{E}(|X(T) - Y(T)|) \leq C \Delta t^\gamma \quad \text{for all } 0 < \Delta t < \Delta.
\]
(12)

**Theorem 2.** [2 Thm. 11.5.1] The strong Itô-Taylor approximation [3] $X_t$ of order $\gamma$ converges strongly to the solution of [2] with order $\gamma$. Furthermore, any discrete approximation
\[
Y_{k+1} = Y_k + \sum_{a \in \mathcal{A}_\gamma} \mathbb{G}_{a,k} I_a + R_k \quad (k = 0, 1, 2, \ldots)
\]
(13)

with continuous functions $\mathbb{G}_{a,k}$ satisfying the following two conditions
\[
\mathbb{E} \left( \max_{0 \leq k \leq n_T} \left| \mathbb{G}_{a,k} - f_a(Y_k) \right|^2 \right) \leq K_1 \Delta t^{2\gamma - \phi(\alpha)} \quad (k = 0, 1, 2, \ldots)
\]
(14)

\[
\phi(\alpha) = \begin{cases} 
2l(\alpha) - 2 & \text{if } l(\alpha) = n(\alpha), \\
 l(\alpha) + n(\alpha) - 1 & \text{if } l(\alpha) \neq n(\alpha)
\end{cases}
\]

\[
\text{eq: conv1}
\]
and
\[ E \left( \max_{1 \leq l \leq n} \sum_{k=0}^{l-1} R_k \right)^2 \leq K_2 \Delta t^{2\gamma}, \] (15)

for some constants \( K_1, K_2 > 0 \), converges strongly to the exact solution \( X \) of (2) with order \( \gamma \). In this case we call \( Y \) a strong Itô scheme of order \( \gamma \).

Our main result in this paper is that we have developed strong Itô schemes of orders 1, 2 and 3 for the Langevin equation with additive noise. These schemes are stochastic operator splitting methods, which are natural generalizations of well-known operator splitting methods for ODEs. These methods will be presented in section 3. To analyze the strong order of accuracy, we first show the strong Itô-Taylor approximations of order 1, 2 and 3 for the Langevin equation. In particular, for the Langevin equation (1), we have \( X_t = (x(t), v(t)) \in \mathbb{R}^{2n} \) so that \( d = 2n \). In addition, the drift and diffusion coefficients are given by,
\[
    a = \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 0 \\ \sigma \end{pmatrix},
\] (16)
so that \( m = n \).

**Theorem 3.** The strong Itô-Taylor approximations of order 1, 2 and 3 for the Langevin equation with ad-
We will just verify the strong order 1 Itô-Taylor approximation here. The derivations of the higher
order 0.5, 1.5 and 2.5 Itô-Taylor approximations are the same as the strong order 1, 2 and 3 approximations,
\( \sigma \)
where

\[
\begin{align*}
L^0 &= \mathbf{a} \cdot \nabla \mathbf{x} = \begin{pmatrix} \mathbf{v} \\ f(x) - \Gamma \mathbf{v} \end{pmatrix} = \mathbf{v} \cdot \nabla \mathbf{x} + (f(x) - \Gamma \mathbf{v}) \cdot \nabla \mathbf{v}, \\
L^j &= \mathbf{b}^j \cdot \nabla \mathbf{x} = \begin{pmatrix} 0 \\ \sigma^j \end{pmatrix} = \sigma^j \cdot \nabla \mathbf{v}.
\end{align*}
\]

Next observe that the differential operators \( L^j \) are given by

\[
D f(x) v - \Gamma f(x) + \Gamma^2 v
\]

where \( \sigma^j = \sigma(\text{column } j) \), and \( D f(x) \) is the Jacobian of \( f \) at \( x \), \( (D f(x))_{ij} = \frac{\partial f(x)}{\partial x_i}. \) Furthermore, the strong order 0.5, 1.5 and 2.5 Itô-Taylor approximations are the same as the strong order 1, 2 and 3 approximations, respectively, due to the fact that the noise is additive.

**Proof.** We will just verify the strong order 1 Itô-Taylor approximation here. The derivations of the higher order approximations are very similar, yet more tedious (see \([84],[88],\) and \([92] \) in the appendix).

First observe that the multi-index set is

\[
A_1 = \{ \alpha : l(\alpha) + n(\alpha) \leq 2 \}
\]

\[
= \{(0), (j_1), (j_1, j_2) : j_1, j_2 = 1, 2, \cdots, n \}.
\]

Next observe that the differential operators \( L^j \) are given by

\[
L^0 = \mathbf{a} \cdot \nabla \mathbf{x} = \begin{pmatrix} \mathbf{v} \\ f(x) - \Gamma \mathbf{v} \end{pmatrix} = \mathbf{v} \cdot \nabla \mathbf{x} + (f(x) - \Gamma \mathbf{v}) \cdot \nabla \mathbf{v},
\]

\[
L^j = \mathbf{b}^j \cdot \nabla \mathbf{x} = \begin{pmatrix} 0 \\ \sigma^j \end{pmatrix} = \sigma^j \cdot \nabla \mathbf{v}.
\]
Then we can calculate the coefficient functions:

\[
\begin{align*}
 f_0(x) &= \begin{pmatrix} L^0 x \\ L^0 v \end{pmatrix} = \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \\
 f_{j_1}(x) &= \begin{pmatrix} L_{j_1} x \\ L_{j_1} v \end{pmatrix} = \begin{pmatrix} D_{j_1}(x) \sigma^j \\ D_{j_1}(v) \sigma^j \end{pmatrix} = \begin{pmatrix} 0_{n \times 1} \\ \sigma^j \end{pmatrix} \\
 f_{j_1,j_2}(x) &= \begin{pmatrix} L_{j_1} L_{j_2} x \\ L_{j_1} L_{j_2} v \end{pmatrix} = \begin{pmatrix} L_{j_1,0} n_{\times 1} \\ L_{j_1, \sigma^j_{j_2}} \end{pmatrix} = 0_{2n \times 1} 
\end{align*}
\]

(20)

We do not need to compute \( I_{j_1,j_2}(\Delta t) \) because the corresponding coefficient functions \( f_{j_1,j_2} \) above are identically zero. We just need to observe that

\[
\begin{align*}
 I_{0}(\Delta t) &= \int_0^{\Delta t} d t = \Delta t \\
 I_{j}(\Delta t) &= \int_0^{\Delta t} d W^j(t) = W^j(\Delta t) - W^j(0) =: \Delta W^j, 1 \leq j \leq n. 
\end{align*}
\]

(21)

Therefore, the strong order 1 Itô-Taylor approximation of (1) is

\[
\begin{pmatrix} x(\Delta t) \\ v(\Delta t) \end{pmatrix} = \begin{pmatrix} x \\ v \end{pmatrix} + \sum_{\alpha \in A_1} f_\alpha \begin{pmatrix} x \\ v \end{pmatrix} I_\alpha(\Delta t)
\]

(22)

\[
= \begin{pmatrix} x \\ v \end{pmatrix} + \frac{v}{f(x) - \Gamma v} \Delta t + \sum_{j=1}^{n} \begin{pmatrix} 0 \\ \sigma^j \end{pmatrix} \Delta W^j,
\]

as desired. To see why the strong order 0.5 approximation is the same, simply observe that the multi-index set \( A_{0.5} \) satisfies \( A_{0.5} = \{(0), (j_1) : j_1 = 1, 2, \cdots, n\} = A_1 - \{\alpha \in A_1 : f_\alpha = 0\} \).

2.2. Analysis of some existing methods

The Itô-Taylor approximations \( \ref{17} \) revealed the leading terms in the Itô-Taylor expansion, and they serve as an important reference to study the strong convergence, as indicated by Theorem 2. On the other hand, a direct implementation of these approximation may not be practical, especially because the formulas \( \ref{17} \) contains the derivatives of \( f(x) \) which are not easy to compute in practice. Here we consider some existing methods and examine their strong order of accuracy.

2.2.1. Direct operator splitting methods

A natural approximation of \( \ref{17} \) can be obtained by splitting the equation into several subproblems, each of which can be solved exactly. A wide variety of splitting methods have been discussed in \( \ref{4} \). For
example, we may consider to split the Langevin equation as follows,

\[
\begin{aligned}
    x' &= v \\
    v' &= 0,
\end{aligned} \tag{23}
\]

and

\[
\begin{aligned}
    x' &= 0 \\
    v' &= f(x) - \Gamma v + \sigma W'(t).
\end{aligned} \tag{24}
\]

Both of these equations have explicit solutions. The solution steps can be denoted by A and B, respectively, and approximations can be obtained by following the operations, e.g., \( AB, A^2 B A^2 \), etc [4].

**Theorem 4.** The splitting methods have strong order at most 1.

The proof will be postponed to the next section.

2.2.2. The stochastic velocity-Verlet’s method

Here we analyze another widely implemented scheme – the stochastic velocity-Verlet’s (SVV) method [14]. This method starts with an assumption that \( x(t) \) remains as a constant, and integrates the second equation in (1) exactly, giving rise to,

\[
    v(t) = e^{-\Gamma t} v(0) + \Gamma^{-1}(I - e^{-\Gamma t}) f(x(0)) + \int_0^t e^{-\Gamma(t-s)} \sigma dW_s, \tag{25}
\]

where \( I \) denotes the \( n \times n \) identity matrix.

With this approximation of \( v(t) \), one can now turn to the first equation, and integrate. This gives,

\[
    x(\Delta t) = x(0) + c_1 v(0) \Delta t + c_2 \Delta t^2 f(x(0)) + \int_0^{\Delta t} \int_0^t e^{-\Gamma(t-s)} \sigma dW_s d t. \tag{26}
\]

Here the coefficients are given by,

\[
    c_0 = e^{-\Gamma \Delta t}, c_1 = (\Gamma \Delta t)^{-1}(I - e^{-\Gamma \Delta t}), c_2 = \frac{1}{\Delta t^2} \int_0^{\Delta t} \Gamma^{-1}(I - e^{-\Gamma t}) d t. \tag{27}
\]

One might stop here and accept the position and velocity values. Or one can use the updated position value and approximate the function \( f \) by a linear function,

\[
    f(x(t)) \approx f(x(0)) + (f(x(\Delta t)) - f(x(0))) t. \tag{28}
\]

With this approximation, one can integrate the velocity equation again. One finds that,

\[
    v(\Delta t) = c_0 v(0) + c_1 f(x(0)) \Delta t + c_2 (f(x(\Delta t)) - f(x(0))) \Delta t + \int_0^{\Delta t} e^{-\Gamma(t-s)} \sigma dW_s. \tag{29}
\]

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Equations (26) and (29) form the basis for the SVV method. The formulas can be repeated, and at each step, the function $f$ is evaluated only once at each step, which is typically considered as an considerable advantage.

**Theorem 5.** The SVV algorithm has strong order 2.

**Proof.** The details are in the appendix. To sketch the proof, we compare SVV to the strong order $\gamma = 2$ Ito Taylor approximation, finding that the remainder term $R_k$, $k = 0, 1, \cdots, n_T - 1$ for the position after the $k$th step is a discrete martingale [2, pg. 195]

$$R_k = \sum_{j=1}^{n} \int_{(k+1)\Delta t}^{(k+1)\Delta t} \int_{k\Delta t}^{t} (e^{-\Gamma(t-s)} - 1) \sigma_j^j dW_j^j d t,$$

which satisfies convergence estimate [15] by using Doob’s lemma.

For the velocity components, the strategy is similar, with

$$R_k = \sum_{j=1}^{n} \int_{(k+1)\Delta t}^{(k+1)\Delta t} \int_{k\Delta t}^{t} (e^{-\Gamma(\Delta t-s)} - I + \Gamma(\Delta t - s)) \sigma_j^j dW_j^j, \quad k = 0, \ldots, n_T - 1. \quad (31)$$

\[ \Box \]

3. **New operator-splitting algorithm with higher order strong convergence**

Here we will present new splitting algorithms. Our starting point is the Kunita’s solution operator [1]. In particular, for the standard SDE (2) we define the differential operators,

$$X_0 = a \cdot \nabla_x, \quad X_j = b^j \cdot \nabla_x. \quad (32)$$

These are none other than the familiar operators $L^0$ and $L^j$. Then the exact solution of the SDE can be formally expressed as,

$$X_t = \exp(D_t)X_0, \quad (33)$$

where, by [21 eq. (2.5)],

$$D_{\Delta t} = \Delta t X_0 + \sum_{j=1}^{n} \Delta W^j X_j + \frac{1}{2} \sum_{j=1}^{n} [\Delta W^j, X_j] + \frac{1}{18} \sum_{j=1}^{n} [[\Delta W^j, X_j], X_j] + \cdots \quad (34)$$

and $[X_0, X_j]$ denotes the commutator bracket

$$X_0 X_j - X_j X_0, \quad (35)$$

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which is a differential operator, so that \([X_0, X_j] = [X_0, X_j] \circ X_0 - X_0 \circ [X_0, X_j]\). The terms \([\Delta t, \Delta W_j]\) are given by

\[
[\Delta t, \Delta W_j] := \int_0^{\Delta t} dW_t^j - \int_0^{\Delta t} W_t^j dt, \tag{36}
\]

In particular, we will use \(\exp(D_{\Delta t})\) to define our numerical solution.

3.1. First-order truncation

We first make a truncation and keep the first two terms \([21, eq. 3.18]\): \n
\[
D_I^{\Delta t} = \Delta t X_0 + \sum_{j=1}^{n} \Delta W_j X_j
\]

\[
= \Delta t v \cdot \nabla x + \left( \Delta t f(x) - \Gamma v + \sum_{j=1}^{n} \sigma^j \Delta W_j \right) \cdot \nabla v. \tag{37}
\]

Once the Brownian motion \(\Delta W\) has been sampled (and realized), the operator \(\exp(D_I^{\Delta t})\) corresponds to the solution operator of the following ODE system,

\[
\begin{align*}
x' &= \Delta t v \\
v' &= \Delta t (f(x) - \Gamma v) + \sum_{j=1}^{n} \sigma^j \Delta W_j.
\end{align*} \tag{38} \text{ eq: ODE-I}
\]

This approximation by the solution of the above ODE system will be referred to as truncation I.

At this point, we can prove the strong order convergence. While the first order truncation is incapable of competing with the SVV algorithm, it serves as an alternative to understand operator splitting methods surveyed in \([4, Sec. 7.3.1]\).

**Lemma 1.** By \([100]\) in the appendix,

\[
\exp(D_I^{\Delta t}) \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} x \\ v \end{pmatrix} + \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \Delta t + \begin{pmatrix} f(x) - \Gamma v \\ Df(x) v - \Gamma f(x) - \Gamma v \end{pmatrix} \frac{\Delta t^2}{2} + \sum_{j=1}^{n} \begin{pmatrix} 0 \\ \sigma^j \end{pmatrix} \Delta W_j
\]

\[
+ \sum_{j=1}^{n} \begin{pmatrix} \sigma^j \\ -\Gamma \sigma^j \end{pmatrix} (I_{(0,j)} + I_{(j,0)}) + \text{higher order terms}
\]

where the higher order terms do not involve \(I_{(j,0)}\).

**Theorem 6.** For the Langevin equation with additive noise, truncation I given by \(X_{\Delta t} = \exp(D_I^{\Delta t})(X_0)\) is precisely a strong order 1 approximation.
Proof. Use the lemma above and recall that the strong order 1.5 and 2 Itô Taylor method is
\[
\begin{pmatrix}
  x(\Delta t) \\
  v(\Delta t)
\end{pmatrix} =
\begin{pmatrix}
  x \\
  v
\end{pmatrix} + \begin{pmatrix}
  v \\
  f(x) - \Gamma v
\end{pmatrix} \Delta t + \begin{pmatrix}
  f(x) - \Gamma v \\
  Df(x) - \Gamma (f(x) - \Gamma v)
\end{pmatrix} \frac{\Delta t^2}{2} + \sum_{j=1}^{n} \begin{pmatrix}
  0 \\
  \sigma^j
\end{pmatrix} \Delta W^j + \sum_{j=1}^{n} \begin{pmatrix}
  -\Gamma \sigma^j
\end{pmatrix} I_{(j,0)}.
\]
(40)

We can match terms exactly for all \( \alpha \in A_2 \) (see (81)) except for the term \( \alpha = (0, j) \), and \( I_{(0,j)}(\Delta t) \in N(0, \Delta t^3/3) \).

Criterion (14) is satisfied for order \( \gamma = 1 \) and \( \gamma = 2 \), since \( g_{a} = f_{a} \) for all \( \alpha \in A_{1} \cap A_{2} \) except for \( \alpha = (0, j) \). For \( \alpha = (0, j) \) and \( \gamma = 2 \), we have \( 2\gamma - \phi(\alpha) = 2 \) and \( g_{a j} - f_{a j} = (\sigma^j, -\Gamma \sigma^j) I_{(a,j)} \in N(0, \Delta t^3) \). Thus, (14) is satisfied with powers 3 on the left hand side and 2 on the right hand side. As for criterion (15), the remainder term \( R_k \) after \( k \) steps \((k = 0, \ldots, n_T - 1)\) is
\[
R_k = \sum_{j=1}^{n} \begin{pmatrix}
  \sigma^j \\
  -\Gamma \sigma^j
\end{pmatrix} I_{(0,j)} \in N(0_{2n \times n}, O(\Delta t^3))
\]
(41)

and satisfies
\[
\mathbb{E} \left( \max_{1 \leq m \leq n_T} \left| \sum_{k=0}^{m-1} R_k \right|^2 \right) \leq 4 \mathbb{E} \left( \sum_{k=0}^{n_T-1} R_k^2 \right) \text{ by Doob's lemma}
\]
\[
\leq 4 \mathbb{E} \left( \sum_{k=0}^{n_T-1} R_k^2 \right) \text{ since } \mathbb{E}(R_k R_l) = \delta_{kl} \mathbb{E}(R_k^2)
\]
\[
= 4 \sum_{k=0}^{n_T-1} \mathbb{E}(R_k^2)
\]
\[
= 4 \sum_{k=0}^{n_T-1} O(\Delta t^3)
\]
\[
= 4n_T O(\Delta t^3) \text{ since } n_T \Delta t = T.
\]

Then, letting \( Y_{k+1} = Y_k + \sum_{a \in \mathcal{A}_f} f_a(X_n) I_a \) and \( Z_{k+1} = Z_k + \sum_{a \in \mathcal{A}_f} g_{a,k} I_a + R_k \) denote the strong order \( \gamma \in \{1,2\} \) Itô Taylor approximation and truncation 1 method, respectively, we have that
\[
\mathbb{E}(\|Y(n_T) - Z(n_T)\|) \leq \sqrt{\mathbb{E}(\|Y(n_T) - Z(n_T)\|^2)} \text{ by Jensen's inequality}
\]
\[
\leq \sqrt{\mathbb{E} \left( \max_{1 \leq m \leq n_T} |Y_m - Z_m|^2 \right)}
\]
\[
= \sqrt{\mathbb{E} \left( \max_{1 \leq m \leq n_T} \sum_{k=0}^{m-1} R_k^2 \right)}
\]
\[
\leq \sqrt{O(\Delta t^2)}
\]
\[
= O(\Delta t). \]
Then, since $Y$ has strong order $\gamma \in \{1, 2\}$, by the triangle inequality $Z$ converges strongly at time $T = nT\Delta t$ with order 1 to the exact solution, $X$:

$$
\mathbb{E}(|X(nT) - Z(nT)|) \leq \mathbb{E}(|X(nT) - Y(nT)|) + \mathbb{E}(|Z(nT) - Y(nT)|) = O(\Delta t^\gamma) + O(\Delta t) = O(\Delta t).
$$
(44)

For the symmetric and non-symmetric operator splitting methods, consider $D^I = A + B$ where

$$
A = v\Delta t \cdot \nabla_x \quad \text{and} \quad B = \left( (f(x) - \Gamma v)\Delta t + \sigma \Delta W \right) \nabla v.
$$
(45)

**Lemma 2.** We have

$$
\left(I + A + B + \frac{1}{2} [A, B] + \frac{1}{2} (A^2 + AB + BA + B^2)\right)\begin{pmatrix} x \vline \\
v \vline \end{pmatrix} = \begin{pmatrix} x(\Delta t) \\
v(\Delta t) \end{pmatrix} + \left(\begin{array}{c} 0_{n \times 1} \\
D_x f(x)v - (1/2)\Gamma f(x) + (1/2)\Gamma^2 v \vline \end{array}\right) \Delta t^2
+ \sum_{j=1}^n \left(0_{n \times 1} \vline -\Gamma \sigma^j \right) \frac{\Delta t \Delta W}{2},
$$
(46)

and

$$
\left(I + A + B + \frac{1}{2} (A^2 + AB + BA + B^2)\right)\begin{pmatrix} x \vline \\
v \vline \end{pmatrix} = \begin{pmatrix} x(\Delta t) \\
v(\Delta t) \end{pmatrix} + \left(\begin{array}{c} f(x) - \Gamma v \\
D_x f(x)v - \Gamma f(x) + \Gamma^2 v \vline \end{array}\right) \frac{\Delta t^2}{2}
+ \sum_{j=1}^n \left(\sigma^j \vline -\Gamma \sigma^j \right) \frac{\Delta t \Delta W}{2},
$$
(47)

where $(x(\Delta t), v(\Delta t))$ denotes the strong order $\gamma = 1$ Ito Taylor approximation.

**Proof.** See appendix.

**Theorem 7.** The non-symmetric splitting scheme

$$
\exp(D^I) \approx \exp(A) \exp(B)
$$
(48)

and symmetric splitting scheme

$$
\exp(D^I) \approx \exp(A/2) \exp(B) \exp(A/2)
$$
(49)

both yield approximations with strong order $\gamma = 1$. 

13
Proof. Use the previous lemma and the fact that
\[
\exp(A) \exp(B) \begin{pmatrix} x \\ v \end{pmatrix} \approx \begin{pmatrix} I + A + B + \frac{1}{2} [A, B] + \frac{1}{2} (A^2 + AB + BA + B^2) \end{pmatrix} \begin{pmatrix} x \\ v \end{pmatrix} \tag{50}
\]
and
\[
\exp(A/2) \exp(B) \exp(A/2) \begin{pmatrix} x \\ v \end{pmatrix} \approx \begin{pmatrix} I + A + B + \frac{1}{2} (A^2 + AB + BA + B^2) \end{pmatrix} \begin{pmatrix} x \\ v \end{pmatrix}. \tag{51}
\]

In our numerical tests (see Figures 1 and 2), we see that the (naive and symmetric) operator splitting methods applied to truncation \(D^I_{\Delta t} \) both converge with order 1.

3.2. Second-order truncation

Now we consider the truncation of \(D \) which includes the first order bracket \([21, \text{eq. 3.22}]:\)
\[
D^{II}_{\Delta t} = \Delta t \mathcal{X}_0 + \sum_{j=1}^{n} \Delta W^j \mathcal{X}_j + \frac{1}{2} \sum_{j=1}^{n} [\Delta t, \Delta W^j] [\mathcal{X}_0, \mathcal{X}_j]
\]
\[
= \left( \Delta t v - \frac{1}{2} \sum_{j=1}^{n} \sigma^j [\Delta t, \Delta W^j] \right) \cdot \nabla_x + \left( \Delta t (f(x) - \Gamma v) + \frac{1}{2} \sum_{j=1}^{n} \sigma^j [\Delta t, \Delta W^j] \right) \cdot \nabla_v \tag{52}
\]

Here, \([\Delta t, \Delta W^j] \) is given by \([21, \text{pg.169}]:\)
\[
[\Delta t, \Delta W^j] = I_{(0,j)} - I_{(j,0)} = \int_0^{\Delta t} t W^j_t \, dt - \int_0^{\Delta t} W^j_t \, dt = 2I_{(0,j)} - \Delta t \Delta W^j.
\]

In the computation, the integral \(I_{(0,j)} \) can be sampled as normal random variables. In \([2],\) the following variable was introduced,
\[
\hat{\gamma}^j = \frac{\sqrt{3}}{\Delta t^{3/2}} \left( 2I_{(0,j)} - \Delta t \Delta W^j \right).
\]

Using the fact that \(I_{(0,j)}^2 = \Delta t^3/3 \) and \(I_{(0,j)} \Delta W^j = \Delta t^2/2,\) one finds that \(\hat{\gamma}^j \sim N(0,1),\) for \(1 \leq j \leq n.\)

Here for the analysis we choose to define \(\Delta U = (\Delta U^1, \ldots, \Delta U^n),\) where

\[
\Delta U^j = \frac{1}{2} [\Delta t, \Delta W^j] = I_{(0,j)} - \frac{1}{2} \Delta t \Delta W^j, \quad j = 1, 2, \ldots, n. \tag{53}
\]

We now write our operator as follows, with \(\Delta W := (\Delta W^1, \ldots, \Delta W^n):\)
\[
D^{II}_{\Delta t} = (\Delta t v - \sigma \Delta U) \cdot \nabla_x + \left( \Delta t (f(x) - \Gamma v) + \sigma \Delta W + \Gamma \sigma \Delta U \right) \cdot \nabla_v \tag{54}
\]

Once \(\Delta W \) and \(\Delta U \) are realized, the solution corresponds to that of the following ODEs at time \(t = 1,\)
\[
\begin{cases}
x' = v \Delta t - \sigma \Delta U, \\
v' = f(x) \Delta t - \Gamma v \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U.
\end{cases}
\]
Lemma 3. We have

\[
\exp D^{II} \frac{x}{v} = \left( \frac{x}{v} \right) + \left( \frac{v}{f(x) - \Gamma v} \right) \Delta t + \left( \frac{f(x) - \Gamma v}{D_x f(x) - \Gamma f(x) + \Gamma^2 v} \right) \frac{\Delta t^2}{2} + \sum_{j=1}^{n} \left( \frac{0_n \times \sigma^j}{\sigma^j} \right) \Delta W^j + \sum_{j=1}^{n} \left( \frac{\Gamma \sigma^j}{-D_x f(x) \sigma^j - \Gamma^2 \sigma^j} \right) \frac{\Delta t \Delta U^j}{2} + \frac{1}{3!} (D^{II})^3 \frac{x}{v} + \text{higher order terms.}
\]

(55)

Proof. See appendix, (110).

Theorem 8. The operator \( \exp (D^{II}_{\Delta t}) \) generates a solution with strong order 2.

Proof. By the previous lemma, we see that

\[
\exp(D^{II}) \frac{x}{v} = \left( \frac{x(\Delta t)}{v(\Delta t)} \right) + \sum_{j=1}^{n} \left( \frac{\Gamma \sigma^j}{-D_x f(x) \sigma^j - \Gamma^2 \sigma^j} \right) \frac{\Delta t \Delta U^j}{2} + \frac{1}{3!} (D^{II})^3 \frac{x}{v} + \text{higher order terms},
\]

(56)

where \((x(\Delta t), v(\Delta t))\) denotes the strong order \( \gamma = 2 \) Itô Taylor approximation. With \( g_{\alpha,n} = f_{\alpha} \) for all \( \alpha \in \mathcal{A}_2 \) (see appendix for \( \mathcal{A}_2 \)), we observe that the convergence criterion (14) is trivially satisfied: \( E(\max_{1 \leq m \leq n} |g_{\alpha,m} - f_{\alpha}(X_m)|^2) = 0 \). The multi-index \( \alpha \) in the remainder set \( \mathcal{B}_2 \) whose corresponding multiple Itô integral \( I_\alpha \) has minimal variance is \( \alpha = (j,0,0) \) where \( j = 1,2,\cdots,n \), since \( \mathcal{B}_2 = \{ (j,0,0), (0,0,0) : j = 1,2,\cdots,n \} \) and \( I_{(j,0,0)} \in N(0,\Delta t^2) \) has lower order variance than \( I_{(0,0,0)} = \Delta t^3/6! \). Specifically, by [2, Lemma 5.7.3], \( I_{(j,0,0)}(\Delta t) \) has variance bound

\[
E(I_{(j,0,0)}^2(\Delta t)) \leq 4\Delta t^4 \int_{k\Delta t}^{(k+1)\Delta t} 1 \, dt = 4\Delta t^5.
\]

(57)

Observe that \( R_k = \sum_{j=1}^{n} c_j I_{(j,0,0)}(k\Delta t,(k+1)\Delta t) + O(\Delta t^3) \) for some constants \( c_j \), which are bounded be-
cause $f$ has bounded derivatives. Then

$$
E\left(\max_{1 \leq m \leq n_T} \left| \sum_{k=0}^{n_T-1} R_k \right|^2\right) \leq E\left(\sum_{k=0}^{n_T-1} R_k^2\right)
$$

by Doob’s lemma, since $R_k$ is a Martingale

$$
\leq \sum_{k=0}^{n_T-1} E\left(R_k^2\right) \quad \text{since } E(R_k R_l) = \delta_{kl} E(R_k^2)
$$

$$
\leq \sum_{k=0}^{n_T-1} \sum_{j=1}^n c_j^2 E(I_{j,0,0}^2) \quad \text{since } I_{j,0,0} \text{ are independent}
$$

$$
\leq \sum_{k=0}^{n_T-1} 4\Delta t^5 \cdot \sum_{j=1}^n c_j^2
$$

$$
= 4Kn_T \Delta t^5
$$

$$
= O(\Delta t^4) \quad \text{for } K := \sum_{j=1}^n c_j << n_T \text{ and } n_T \Delta t = T.
$$

(58)

Taking square roots and using Jensen's inequality, we get that the method converges with order $\gamma = 2$. \qed

For the numerical implementation, we use the follow splitting, $D_{\Delta t}^{ll} = A + B$, where,

$$
A = (\Delta t v + -\sigma \Delta U) \cdot \nabla x
$$

$$
B = (f(x) \Delta t - \Gamma \nu \Delta t + \sigma \Delta W + \sigma \Gamma \Delta U) \cdot \nabla \nu.
$$

(59)

**Theorem 9.** The naive splitting scheme

$$
\exp(D_{\Delta t}^{ll}) \approx \exp(A) \exp(B)
$$

yields an approximation with strong order 1. The symmetric splitting scheme,

$$
\exp(D_{\Delta t}^{ll}) \approx \exp\left(\frac{A}{2}\right) \exp(B) \exp\left(\frac{A}{2}\right)
$$

gives strong order 2.

**Proof.** We use the Baker Campbell Hausdorff formula \[22\] for both splitting schemes:

$$
\exp A \exp B = \exp\{A + B + \frac{1}{2} [A, B] + \frac{1}{12} ([A, [A, B]] + [B, [B, A]] + \ldots) \}
$$

$$
\exp(A/2) \exp B \exp(A/2) = \exp\{A + B + \frac{1}{12} [B, B, A] - \frac{1}{24} [A, A, B] + \ldots \}
$$

(60)

where $[A, B] := AB - BA$ is the commmutator bracket from Lie algebras, and $[A, A, B] := [A, [A, B]]$, etc.

The symmetric splitting will give us a higher order method because the bracket $[A, B]$ does not show up.
Fortunately, we do not have to compute the difficult third order brackets in order to see this. It can be shown (see (123)) that

$$\exp A \exp B \left( \begin{array}{c} x \\ v \end{array} \right) \approx \left[ I + A + B + \frac{1}{2} [A, B] + \frac{1}{2} (A^2 + AB + BA + B^2) \right] \left( \begin{array}{c} x \\ v \end{array} \right)$$

$$= \left( \begin{array}{c} x(\Delta t) \\ v(\Delta t) \end{array} \right) + \left( \begin{array}{c} 0_{n \times 1} \\ 2D_x f(x)v - \Gamma f(x) + \Gamma^2 v \end{array} \right) \frac{\Delta t^2}{2}$$

$$+ \sum_{j=1}^{n} \left( -\sigma^j \right) \Delta U^j + \sum_{j=1}^{n} \left( 0_{n \times 1} \right) \frac{\Delta t \Delta W^j}{2} + \sum_{j=1}^{n} \left( 0_{n \times 1} \right) \frac{\Delta t \Delta U^j}{2},$$

where $\Delta t$ denotes the strong order $\gamma = 1$ Ito Taylor approximation. We see that $g_\alpha = f_\alpha$ for all $\alpha \in A_1$, but $g_\alpha \neq f_\alpha$ for $\alpha = (0, 0), (j, 0) \in A_2$. Therefore the naive splitting $\exp A \exp B$ of truncation 2 $D^2_{\Delta t} = A + B$ gives a strong order $\gamma = 1$ method but not a strong order $\gamma = 2$ method.

Turning now to the symmetric splitting, one can show (see (124)) that

$$\exp(A/2) \exp B \exp(A/2) \left( \begin{array}{c} x \\ v \end{array} \right) \approx \left( \begin{array}{c} I + A + B + \frac{1}{2} (A^2 + AB + BA + B^2) \end{array} \right) \left( \begin{array}{c} x \\ v \end{array} \right)$$

$$= \left( \begin{array}{c} x(\Delta t) \\ v(\Delta t) \end{array} \right) + \sum_{j=1}^{n} \left( \Gamma \sigma^j \right) \Delta U^j + \sum_{j=1}^{n} \left( 0_{n \times 1} \right) \frac{\Delta t \Delta W^j}{2} + \sum_{j=1}^{n} \left( 0_{n \times 1} \right) \frac{\Delta t \Delta U^j}{2},$$

where $\Delta t$ denotes the strong order $\gamma = 2$ Ito Taylor approximation. Then $g_\alpha = f_\alpha$ for all $\alpha \in A_2$, and the remainder term $\Delta t \Delta U^j / 2$ has variance $O(\Delta t^3)$. Therefore the symmetric splitting of truncation 2 has strong order 2.

The numerical tests in Figures 1 and 2 confirmed the convergence orders for truncation II with the naive and symmetric splittings methods can be found in the next section.
3.3. Third-order truncation

Finally, we turn to the next truncation, $D_{\Delta t}^{III} = \Delta t + \sum_{j=1}^{n} \Delta W_j \mathcal{X}_j + \sum_{j=1}^{n} \Delta U_j |\mathcal{X}_0, \mathcal{X}_j | + \sum_{j=1}^{n} \Delta V_j |\mathcal{X}_0, \mathcal{X}_j |, \mathcal{X}_0|

\Delta U_j = \frac{1}{2} [\Delta t, \Delta W_j] = \frac{1}{2} (I_{(0,j)} - I_{(j,0)}) = I_{(0,j)} - \Delta t \Delta W_j / 2

\Delta U = (\Delta U^1, \ldots, \Delta U^n)

\Delta V_j = [\Delta t, \Delta W_j, \Delta t] = \frac{1}{18} \left( 2 I_{(0,j,0)} - 2 I_{(j,0,0)} + \Delta t I_{(j,0)} - \Delta t I_{(0,j)} \right)

\Delta V = (\Delta V^1, \ldots, \Delta V^n).

This comes from [21, eq. 2.15], using the fact that $[|\mathcal{X}_0, \mathcal{X}_j |, \mathcal{X}_j |] = 0$ when $i, j \neq 0$ for additive noise. Since

\begin{align*}
\mathcal{X}_0 &= v \cdot \nabla x + (f(x) - \Gamma v) \cdot \nabla v \\
\mathcal{X}_j &= \sigma^j \cdot \nabla v \\
[\mathcal{X}_0, \mathcal{X}_j |] &= -\sigma^j \cdot \nabla x + \Gamma \sigma^j \cdot \nabla v \\
[|\mathcal{X}_0, \mathcal{X}_j |, \mathcal{X}_0 |] &= \Gamma \sigma^j \cdot \nabla x - (Df(x)\sigma^j + \Gamma^2 \sigma^j) \cdot \nabla v,
\end{align*}

we can rewrite $D_{\Delta t}^{III}$ as

\begin{equation}
D_{\Delta t}^{III} = (v \Delta t - \sigma \Delta U + \Gamma \sigma \Delta V) \cdot \nabla x + \left( (f(x) - \Gamma v) \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U - (Df(x)\sigma + \Gamma^2 \sigma) \Delta V \right) \cdot \nabla v,
\end{equation}

which gives us the ODEs

\begin{equation}
\begin{cases}
x' &= v \Delta t - \sigma \Delta U + \Gamma \sigma \Delta V \\
v' &= (f(x) - \Gamma v) \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U - (Df(x)\sigma + \Gamma^2 \sigma) \Delta V.
\end{cases}
\end{equation}

We choose not to pursue a proof of the strong convergence order of the method $X_{\Delta t} = \exp(D_{\Delta t}^{III})X_0$ due to the lengthy calculations, but rather rely on the numerical results.

For the numerical implementation, we use the splitting $D_{\Delta t}^{III} = A + B$ where,

\begin{equation}
\begin{aligned}
A &= v \Delta t - \sigma \Delta U + \Gamma \sigma \Delta V \\
B &= (f(x) - \Gamma v) \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U - (Df(x)\sigma + \Gamma^2 \sigma) \Delta V,
\end{aligned}
\end{equation}

\textbf{eq: III}

\textbf{eq: AB-III}
and the two corresponding ODEs are given by

\[ x' = v \Delta t - \sigma \Delta U + \Gamma \sigma \Delta V \]

\[ v' = 0 \]  

(68)

and

\[ x' = 0 \]

\[ v' = (f(x) - \Gamma v) \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U - (D f(x) \sigma + \Gamma^2 \sigma) \Delta V. \]

They have explicit solutions

\[ x(t) = x + t \left( v - \frac{\sigma \Delta U}{\Delta t} + \frac{\Gamma \sigma \Delta V}{\Delta t} \right) \]  

(70)

and

\[ v(t) = c_0 v + \frac{c_1}{\Delta t} \left( f(x) \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U - (D f(x) \sigma + \Gamma^2 \sigma) \Delta V \right) \]  

(71)

where \( c_0 = \exp(-\Gamma t) \) and \( c_1 = \Gamma^{-1}(I - c_0) \).

In principle, the symmetric splitting methods applied to ODEs have order 2. In order to achieve higher order of accuracy, we solve the ODEs (66) using the Neri’s splitting method [22], which consists of alternating the operators in (67) three times:

\[ \exp(D_{III}) \approx \exp(c_1 A) \exp(d_1 B) \exp(c_2 A) \exp(d_2 B) \exp(c_3 A) \exp(d_3 B) \exp(c_4 A), \]

where \( c_1 = \frac{1}{2(2 - \sqrt{2})} \), \( c_2 = \frac{1}{2} - c_1 \), \( c_3 = c_2 \), \( c_4 = c_1 \), \( d_1 = \frac{1}{2 - \sqrt{2}} \), \( d_2 = 1 - 2d_1 \), \( d_3 = d_1 \). \n
(72)

In the implementation, the term \( D f(x) \sigma \) will be approximated by a finite-difference formula,

\[ D f(x) \sigma \Delta V \approx \frac{f(x + \epsilon \sigma \Delta V) - f(x)}{\epsilon}. \]  

(73)

For practical implementations, the joint covariances of \( \Delta W, \Delta U, \) and \( \Delta V \) are needed in order to sample these mean-zero Gaussian random variables. Note that \( E(\Delta W^i \Delta W^j) = \Delta t \delta_{ij} \) for \( i, j = 1, 2, \ldots, n \), since the components of the Brownian motion are independent with mean 0 and variance \( \Delta t \). Therefore the matrix \( [E(\Delta W^2)]_{ij} := E(\Delta W^i \Delta W^j) \) satisfies \( E(\Delta W^2) = \Delta t I_{n \times n} \). Using [2] p. 223] and a considerable
amount of effort, one can calculate (see appendix)

\[
E(\Delta W^i \Delta U^j) = 0, \\
E(\Delta W^i \Delta V^j) = 0, \\
E(\Delta U^i \Delta U^j) = \frac{\Delta t^3}{12} \delta_{ij}, \\
E(\Delta U^i \Delta V^j) = -\frac{\Delta t^4}{216} \delta_{ij}, \\
E(\Delta V^i \Delta V^j) = \frac{\Delta t^5}{2430} \delta_{ij}
\]

so that

\[
\begin{pmatrix}
E(\Delta W^2) & E(\Delta W^i \Delta U^j) & E(\Delta W^i \Delta V^j) \\
E(\Delta U^i \Delta W^j) & E(\Delta U^2) & E(\Delta U^i \Delta V^j) \\
E(\Delta V^i \Delta W^j) & E(\Delta V^i \Delta U^j) & E(\Delta V^2)
\end{pmatrix} =
\begin{pmatrix}
\Delta t I_{n \times n} & 0_{n \times n} & 0_{n \times n} \\
0_{n \times n} & \frac{\Delta t^3}{12} I_{n \times n} & -\frac{\Delta t^4}{216} I_{n \times n} \\
0_{n \times n} & -\frac{\Delta t^4}{216} I_{n \times n} & \frac{\Delta t^5}{2430} I_{n \times n}
\end{pmatrix}.
\]  

(75) \text{ eq: cov}

4. Numerical tests

4.1. A one-dimensional pendulum model

In the first sets of experiments, we consider the one-dimensional pendulum model:

\[
f(x) = -\sin(x)
\]

(76)

when \(x \in \mathbb{R}\). To examine the strong order, we generate the ‘exact’ solution using the Euler-Maruyama method with very small step size \(\delta t = 2^{-18}\). In order to verify strong convergence, we used 100 realizations. Furthermore, in order to follow the same realization in the implementation of each algorithms, we first generate the Brownian motions with small step size, and then the multiple stochastic integrals are evaluated using a numerical quadrature (Simpson's rule). Notice that this is only for the purpose of examining the strong order of accuracy. In practice, one can sample the integrals using the covariance matrix (75). As can be seen from Figure[1] the order of accuracy is as expected.

4.2. Lennard-Jones cluster

The Lennard Jones model is given by

\[
f_i(x) = \sum_{j \neq i, j=1}^{n} \left(12 \left(\frac{1}{r_{ij}}\right)^{13} - 6 \left(\frac{1}{r_{ij}}\right)^7 \right) \frac{\bar{r}_{ij}}{r_{ij}}, \quad \text{where } \bar{r}_{ij} = \bar{x}_i - \bar{x}_j \in \mathbb{R}^3 \text{ and } r_{ij} = \|\bar{r}_{ij}\|_2,
\]

(77)
Figure 1: The error plot versus the time step for the pendulum model on the log-log scale. From top to bottom: Truncations I, II and III.
and \( f(x) = -\nabla E(x) \) where \( E \) is the Lennard Jones potential. For our simulations, we used 7 particles in \( \mathbb{R}^3 \).

The matrix \( \Gamma = 10I_{21 \times 21} \), and \( \sigma = \sqrt{2k_B T} \), where \( k_B T = 0.3 \), and \( T \) is the temperature, not to be confused with the final time \( T \). Initially, the atoms are arranged at the vertices of a hexagon and its center. The side length corresponds to the minimum of the Lennard-Jones potential, \( 2^{1/6} \). Notice that for this model, the function \( f(x) \) does not have bounded derivatives unless a cut-off is introduced. Nevertheless, as shown in Figure 2, the strong order of accuracy is still consistent with the results of the analysis.

![Graphs showing error plots for different truncations of the Lennard-Jones potential](image)

Figure 2: The error plot for the LJ-7 cluster on a log-log scale. From top to bottom: Truncations I, II and III.
5. Summary and discussion

In this paper, we presented the analysis of strong convergence of some numerical schemes for the Langevin equation with additive noise. This type of convergence is important for predicting the transient stage of the stochastic processes. In addition, we presented several new operator-splitting schemes based on Kunitas solution representation. In particular, we obtained algorithms with strong order up to order 3.

There are several remaining challenges in simulating algorithms for Langevin-type of equations. First, there might be multiple scales involved in the force term \( f(x) \) \[23\]. In this case, a more appropriate splitting is between the fast and slow forces, e.g., \[24\]. Secondly, the damping and diffusion coefficients can be position-dependent. Such models arise, for instance, in the dissipative-particle dynamics (DPD) \[25, 26\]. Finally, there are Langevin equations with strong stiffness, e.g., large damping coefficients. In this case, implicit algorithm are needed. These issues will be addressed in separate works.

6. Appendix

Due to the lengthy calculations in the analysis, we have included some parts of the proofs in the appendix. These details are provided here also for the interested readers who intend to implement the new algorithms.

6.1. Coefficient function computations

The coefficient function \( f_\alpha \) for a multi-index \( \alpha = (j_1, j_2, \ldots, j_l) \) is given by

\[
f_\alpha(x) = L^{j_1} L^{j_2} \cdots L^{j_l} x,
\]

\[
L^0 := \sum_{k=1}^{d} a_k \frac{\partial}{\partial x_k} + \frac{1}{2} \sum_{k,l=1}^{d} \sum_{j=1}^{m} b^{kj} b^{lj} \frac{\partial^2}{\partial x_k \partial x_l},
\]

\[
L^j := \sum_{k=1}^{d} b^{kj} \frac{\partial}{\partial x_k}, \quad j = 1, 2, \ldots, m,
\]

(78)
Observe that for the Langevin equation with additive noise,

\[
L^0 = v \cdot \nabla_x + (f(x) - \Gamma v) \cdot \nabla_v \\
L^j = \sigma^j \cdot \nabla_v
\]

\[
f_{(0)}(x, v) = L^0(x, v) = \left(L^0_x, L^0_v\right) = \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix},
\]

\[
f_{(j)}(x, v) = L^j(x, v) = (L^j_x, L^j_v) = \begin{pmatrix} 0 \\ \sigma^j \end{pmatrix}, \quad j = 1, 2, \ldots, n,
\]

\[
f_{(0, 0)}(x, v) = \left(L^0_v, L^0(f(x) - \Gamma v)\right) = \begin{pmatrix} f(x) - \Gamma v \\ Df(x)v - \Gamma(f(x) - \Gamma v) \end{pmatrix}, \quad \text{where } Df(x) \text{ is the Jacobian matrix}
\]

\[
f_{(j_1, j_2)}(x, v) = L^{j_1}(0, \sigma^{j_2}) = (0, L^{j_1} \sigma^{j_2}) = \hat{0} \quad \text{for additive noise}
\]

\[
f_{(0, j)}(x, v) = L^0(0, \sigma^j) = \hat{0}
\]

\[
f_{(j_1, j_0)}(x, v) = L^j(v, f(x) - \Gamma v) = \begin{pmatrix} \sigma^j \\ -\Gamma \sigma^j \end{pmatrix}
\]

\[
f_{(j_1, j_2, j_3)} = \hat{0} \text{ if } j_1, j_2 \neq 0 \text{ and } j_3 \in \{0, 1, \ldots, n\}
\]

\[
f_{(j_1, j_2, j_3, j_4)} = \hat{0} \text{ if } j_1, j_2, j_3, j_4 \neq 0
\]

\[
f_{(j_1, 0, 0)} = \begin{pmatrix} -\Gamma \sigma^j \\ Df(x)\sigma^j + \Gamma^2 \sigma^j \end{pmatrix} \quad \text{for all } j = 1, 2, \ldots, n \text{ where } \Gamma^2 \text{ means } \Gamma \text{ squared}
\]

\[
f_{(0, 0, 0)} = \begin{pmatrix} Df(x)v - \Gamma f(x) + \Gamma^2 v \\ D(Df(x)v)v - D[\Gamma f(x)]v + Df(x)(f(x) - \Gamma v) + \Gamma^2(f(x) - \Gamma v) \end{pmatrix}
\]

\[
f_{(j_1, j_2, 0, 0)} = \hat{0} \text{ for all } j_1, j_2 = 1, 2, \ldots, n.
\]

These are all the coefficient functions we’ll need for methods of strong order \( \leq 3 \).

6.2. Hierarchical set computations

Throughout this paper, \( \alpha \) will denote a multi-index \( \alpha = (j_1, j_2, \ldots, j_l) \) with entries \( j_k \in \{0, 1, 2, \ldots, n\} \), length \( l(\alpha) := l \), and \( n(\alpha) \) will denote the number of zero entries in \( \alpha \). In this section we focus on hierarchical sets [24 eq. 10.6.2]

\[
\mathcal{A}_\gamma := \{\alpha : l(\alpha) + n(\alpha) \leq 2\gamma \text{ or } l(\alpha) = n(\alpha) = \gamma + 0.5\}
\]
where \( \gamma \in \{0.5, 1.0, 1.5, 2.0, 2.5, 3\} \), and \( f_a \) refers to the coefficient functions for the Itô Taylor truncation corresponding to the Langevin equation with additive noise. To find \( \mathcal{A}_\gamma - \{ \alpha : f_a = 0 \} \) we will use the coefficient function calculations from the previous section. All of the following calculations were done by hand, are easily verified in the case \( n = 1 \), and generalize immediately to the case \( n \geq 1 \):

\[
A_{0.5} = \{ \alpha : l(\alpha) + n(\alpha) \leq 1 \text{ or } l(\alpha) = n(\alpha) = 1 \}
\]

\[
= \{ (j_1), (0) : j_1 = 1, 2, \cdots, n \}
\]

\[
A_{0.5} - \{ \alpha : f_a = 0 \} = A_{0.5}
\]

\[
A_1 = \{ \alpha : l(\alpha) + n(\alpha) \leq 2 \}
\]

\[
= \{ (j_1), (0), (j_1, j_2) : j_1, j_2 = 1, 2, \cdots, n \}
\]

\[
A_1 - \{ \alpha : f_a = 0 \} = \{ (j_1), (0) : j_1 = 1, 2, \cdots, n \}
\]

\[
A_{1.5} = \{ \alpha : l(\alpha) + n(\alpha) \leq 3 \text{ or } l(\alpha) = n(\alpha) = 2 \}
\]

\[
= \{ (j_1), (0), (j_1, j_2), (0, j_1), (j_1, 0, j_2), (j_1, j_2, 0), (j_1, j_2, j_3), (0, 0) : j_k = 1, 2, \cdots, n \}
\]

\[
A_{1.5} - \{ \alpha : f_a = 0 \} = \{ (j_1), (0), (j_1, 0), (0, 0) : j_1 = 1, 2, \cdots, n \}
\]

\[
A_2 = \{ \alpha : l(\alpha) + n(\alpha) \leq 4 \}
\]

\[
= \{ (j_1), (0), (j_1, j_2), (0, j_1), (j_1, 0) \}
\]

\[
\cup \{ (j_1, j_2, j_3), (0, 0), (j_1, j_2), (j_1, 0, j_2), (j_1, j_2, 0), (j_1, j_2, j_3), (0, 0) : j_k = 1, 2, \cdots, n \}
\]

\[
A_2 - \{ \alpha : f_a = 0 \} = \{ (j_1), (0), (j_1, 0), (0, 0) : j_1 = 1, 2, \cdots, n \}
\]

\[
A_{2.5} = A_2 \cup \{ l(\alpha) + n(\alpha) = 5 \text{ or } l(\alpha) = n(\alpha) = 3 \}
\]

\[
= A_2 \cup \{ (0, 0, 0), (0, 0, j_1), (0, j_1, 0) \}
\]

\[
\cup \{ (j_1, j_2, j_3), (j_1, 0, j_2), (j_1, j_2, j_3), (0, 0, j_1), (j_1, j_2, j_3), (0, 0) : j_k = 1, 2, \cdots, n \}
\]

\[
A_{2.5} - \{ \alpha : f_a = 0 \} = \{ (j_1), (0), (j_1, 0), (0, 0, 0), (j_1, 0, 0) : j_1 = 1, 2, \cdots, n \}
\]

\[
A_3 = A_{2.5} \cup \{ \alpha : l(\alpha) + n(\alpha) = 6 \}
\]

\[
= A_{2.5} \cup \{ (j_1, j_2, 0, 0), (j_1, 0, j_2, 0), (j_1, 0, 0, j_2) \}
\]

\[
\cup \{ (0, j_1, j_2, 0), (0, j_1, 0, j_2), (0, 0, j_1, j_2) \}
\]

\[
\cup \{ (0, j_1, j_2, j_3, j_4), (j_1, 0, j_2, j_3, j_4), (j_1, j_2, 0, j_3, j_4), (j_1, j_2, j_3, 0, j_4) \}
\]

\[
\cup \{ (j_1, j_2, j_3, j_4, 0), (j_1, \ldots, j_6) : j_k = 1, 2, \cdots, n \}
\]

\[
A_3 - \{ \alpha : f_a = 0 \} = A_{2.5} - \{ \alpha : f_a = 0 \} = \{ (j_1), (0), (j_1, 0), (0, 0, 0), (j_1, 0, 0) : j_1 = 1, 2, \cdots, n \}.
\]
The large index sets \( \mathcal{A}_r \) are possibly necessary for multiplicative noise, but for additive noise what we really need are the smaller index sets \( \mathcal{A}_r - \{ \alpha : f_\alpha = 0 \} \):

\begin{align*}
A_1 - \{ \alpha : f_\alpha = 0 \} &= A_{0.5} - \{ \alpha : f_\alpha = 0 \} = \{(j_1), (0) : j_1 = 1, 2, \cdots, n\} \\
A_2 - \{ \alpha : f_\alpha = 0 \} &= A_{1.5} - \{ \alpha : f_\alpha = 0 \} = \{(j_1), (0), (j_1, 0), (0, 0) : j_1 = 1, 2, \cdots, n\} \\
A_3 - \{ \alpha : f_\alpha = 0 \} &= A_{2.5} - \{ \alpha : f_\alpha = 0 \} = \{(j_1), (0), (j_1, 0), (0, 0), (j_1, 0, 0), (0, 0, 0) : j_1 = 1, 2, \cdots, n\}.
\end{align*}

6.3. Derivation of the strong order 1 Taylor approximation for the Langevin equation with additive noise

The strong order 1 (and 0.5) Itô Taylor truncation is

\[ X_{n+1} = X_n + \sum_{\alpha \in A: f_\alpha \neq 0} f_\alpha(X_n) I_\alpha, \tag{83} \]

which gives us

\[
\begin{pmatrix}
  x(\Delta t) \\
  v(\Delta t)
\end{pmatrix} = \begin{pmatrix} x & v \\ \gamma x & 0 \end{pmatrix} \Delta t + \sum_{j=1}^n \begin{pmatrix} 0 \\ \sigma \end{pmatrix} \Delta W^j. \tag{84} \]

6.4. Strong order 2 Itô Taylor approximation for the Langevin equation with additive noise

The strong order 2 (and 1.5) Itô Taylor (discrete time) approximation for

\[ dX_t = a(X_t) dt + \sum_{j=1}^n b^j dW^j \]

is then

\[ X_{n+1} = X_n + \sum_{\alpha \in A_2 - \{ \alpha : f_\alpha = 0 \}} f_\alpha(X_n) I_\alpha. \]

where the coefficient functions are given in (79) and the multiple Itô integrals \( I_\alpha \) are given by

\[ I_\alpha = \int_0^{\Delta t_1} \int_0^{\Delta t_2} \cdots \int_0^{\Delta t_l} dW_{l_1}^j dW_{l_2}^j \cdots dW_{l_l}^j. \tag{85} \]

Recall from (81) that

\[ A_2 - \{ \alpha : f_\alpha = 0 \} = \{(j_1), (0), (j_1, 0), (0, 0) : j_1 = 1, 2, \cdots, n\}. \tag{86} \]
and the relevant coefficient functions are (79)

\[ f_{(0)} = a = \begin{pmatrix} \nu \\ f(x) - \Gamma v \end{pmatrix}, \]

\[ f_{(j)} = b^j = \begin{pmatrix} 0 \\ \sigma^j \end{pmatrix}, \quad j = 1, \ldots, n, \]

\[ f_{(0,0)} = \begin{pmatrix} f(x) - \Gamma v \\ Df(x) \nu - \Gamma(f(x) - \Gamma v) \end{pmatrix}, \]

\[ f_{(j,0)} = \begin{pmatrix} \sigma^j \\ -\Gamma \sigma^j \end{pmatrix}. \] 

Then the strong order 2 Itô Taylor approximation is

\[
\begin{pmatrix} x(\Delta t) \\ v(\Delta t) \end{pmatrix} = \begin{pmatrix} x \\ v \end{pmatrix} + \begin{pmatrix} \nu \\ f(x) - \Gamma v \end{pmatrix} \Delta t + \begin{pmatrix} f(x) - \Gamma v \\ Df(x) \nu - \Gamma(f(x) - \Gamma v) \end{pmatrix} \frac{\Delta t^2}{2} + \sum_{j=1}^n \begin{pmatrix} 0 \\ \sigma^j \end{pmatrix} \Delta W^j + \sum_{j=1}^n \begin{pmatrix} \sigma^j \\ -\Gamma \sigma^j \end{pmatrix} I_{(j,0)}.
\]

6.5. Strong order 3 Itô Taylor approximation for the Langevin equation with additive noise

Building off of the previous section, the strong order 3 (and 2.5) Itô Taylor truncation (not given in [2]) requires computing coefficient functions and multiple Itô integrals for multi-indices in the hierarchical set (see (81))

\[ A^3_\alpha = \{ \alpha : f_\alpha = 0 \} = \{(j), (0), (j,0), (0,0), (j,0,0), (0,0,0) : j = 1, 2, \ldots, n \}. \] 

For this method, we just have to compute the additional coefficient functions \( f_{(0,0,0)} \) and \( f_{(j,0,0)} \), and multiple Itô integrals \( I_{(0,0,0)} \) and \( I_{(1,0,0)} \). The easiest of these four things to compute is the Riemann integral

\[ I_{(0,0,0)} = \int_0^{\Delta t} \int_0^t \int_0^s dv ds dt = \frac{\Delta t^3}{3!}. \]

For the coefficient functions, recall from (79) that

\[ f_{(j,0,0)}(x,v) = \begin{pmatrix} -\Gamma \sigma^j \\ Df(x) \sigma^j + \Gamma^2 \sigma^j \end{pmatrix} \quad \text{for all } j = 1,2,\ldots,n \]

\[ f_{(0,0,0)}(x,v) = \begin{pmatrix} \nu Df(x) - \Gamma(f(x) - \Gamma v) \\ D(Df(x) \nu - \Gamma f(x))v + Df(x)(f(x) - \Gamma v) + \Gamma^2(f(x) - \Gamma v) \end{pmatrix}. \]
Then, with $\Delta V^j := I_{(j,0,0)}$, the strong order 3 Itô Taylor approximation is

$$
\begin{align}
(\Delta t) \left( \begin{array}{c} x(t) \\ v(t) \end{array} \right) &= \left( \begin{array}{c} \frac{x(x) - \Gamma v}{Df(x)v - \Gamma f(x) - \Gamma v} \\ f(x) - \Gamma v \end{array} \right) \Delta t + \sum_{j=1}^n \frac{\sigma^j I_{(j,0)}(\Delta t)}{\Delta t^2} + \frac{\Delta t^2}{2} + \sum_{j=1}^n \sigma^j \Delta Z^j
\end{align}
$$

$$
= \sum_{j=1}^n \left( \begin{array}{c} vDf(x) - \Gamma f(x) - \Gamma v \\ Df(x)v - D(\Gamma f(x)v) + \Gamma f(x) - \Gamma v \end{array} \right) \frac{\Delta t^3}{3!} + \sum_{j=1}^n \left( \begin{array}{c} -\Gamma v \\ Df(x)\sigma^j + \Gamma^2 \sigma^j \end{array} \right) \Delta V^j.
$$

(92)

6.6. The analysis of the stochastic velocity Verlet method

Here we give a detailed proof of the following:

**Theorem 10.** The SVV algorithm has strong order 2.

**Proof.** We start with the displacement component. We compare

$$
(\Delta t) x(t) = x + v\Delta t + \frac{f(x) - \Gamma v}{2} + \sum_{j=1}^n \sigma^j I_{(j,0)}(\Delta t)
$$

i.e., the Taylor approximation with strong order 2, with the SVV method,

$$
(\Delta t) x(t) = x + v\Delta t + \frac{f(x) - \Gamma v}{2} + O(\Delta t^3) + \sum_{j=1}^n \sigma^j I_{(j,0)}(\Delta t) + \sum_{j=1}^n \int_0^{\Delta t} \int_0^t (e^{-\Gamma(t-s)} - I) \sigma^j dW^j_s dt.
$$

(93)

Setting $f_0 = g_0 = v, f_j = g_j = 0, f_{00} = g_{00} = f(x) - \Gamma v, f_{j0} = g_{j0} = \sigma^j, f_{0j} = g_{0j} = 0, f_{j1,j2} = 0$, and $g_{j1,j2} = O(\Delta t^3)$ for all $j_1, j_2 = 1,2,\ldots,n$, we see that convergence condition (14) is clearly satisfied for $\gamma = 2$ and all $\alpha \in A_2 = [(0),(j),(0,0),(0),\ldots]$. (For $\alpha = (j_1,j_2)$, the left hand side of (14) is $O(\Delta t^6)$ and the right hand side is $O(\Delta t^3)$). The remainder term $R_k, k = 0,\ldots,n_T - 1$ after the $k$th step is a discrete martingale (2) pg. 195

$$
R_k = \sum_{j=1}^n \int_{k\Delta t}^{(k+1)\Delta t} \int_{k\Delta t}^t (e^{-\Gamma(t-s)} - I) \sigma^j dW^j_s dt,
$$

(94)

and it remains to show that $R_k$ satisfies convergence condition (15) with $\gamma = 2$. To that end, first notice that $\mathbb{E}(R_k R_l) = \delta_{kl}\mathbb{E}(R_k^2)$ (where $\delta_{kl} = 1$ if $k = l$ and 0 otherwise), since the increments of the Wiener process are independent. Next, since $R_k$ is a martingale, we may apply the discrete version of Doob's lemma with $p = 2$ (2) eq. 2.3.7] to obtain an estimate for (15):

$$
\mathbb{E} \left( \max_{1 \leq m \leq n_T} \sum_{k=0}^{n-1} R_k \right)^2 \leq 4 \mathbb{E} \left( \sum_{k=0}^{n-1} R_k \right)^2
$$

by Doob's lemma

$$
\leq 4 \sum_{k=0}^{n_T} \mathbb{E}(R_k^2)
$$

since $\mathbb{E}(R_k R_l) = \delta_{kl}\mathbb{E}(R_k^2)$

$$
= 4n_T \mathbb{E}(R_k^2).
$$

(95)
Notice $e^{-\Gamma(t-s)} - I_n = O(\Delta t)\text{ones}_{n \times n}$ for $k\Delta t \leq s \leq (k+1)\Delta t$, and recall that $\mathbb{E}(I^2_{j0}) = O(\Delta t^3)$ for all $j = 1, 2, \cdots, n$ [2 pg. 172, exercise 5.2.7]. As $\mathbb{E}(I_{(j1,0)}I_{(j2,0)}) = 0$ for distinct $j_1, j_2 = 1, 2, \cdots, n$ ($W^{j1}, W^{j2}$ are independent, see [2] p. 223, eq. 5.12.7) for more details), we have

\[
\mathbb{E}(R^2_j) = \mathbb{E}\left( O(\Delta t^2) \left( \sum_{j=1}^n \sigma^j I_{(j,0)} \right)^2 \right) = O(\Delta t^2)\mathbb{E}\left( \sum_{j=1}^n \sigma^2_j I_{(j,0)}^2 \right)
\]
\[
= O(\Delta t^2) \sum_{j=1}^n \sigma^2_j \mathbb{E}(I_{(j,0)}^2) = O(\Delta t^2)O(\Delta t^3) \quad \text{since } n << n_T = O(\Delta t^2)
\]

Therefore, $\mathbb{E}\left( \max_{1 \leq m \leq n_T} \left| \sum_{k=0}^{n-1} R_k \right|^2 \right) \leq 4n_T O(\Delta t^3) = O(\Delta t^4)$, so convergence criterion [15] is satisfied for $\gamma = 2$.

For the velocity components, with $c_0 = e^{-\Gamma t}$, $c_1 = (\Gamma \Delta t)^{-1}((I - c_0)$, and $c_2 = \frac{1}{\Delta t} \int_0^{\Delta t} \Gamma^{-1}(I - e^{-\Gamma t}) \, dt$, where $I$ is the $n \times n$ identity matrix, we compare the Itô Taylor approximation with strong order 2 and the SVV algorithm,

\[
v(\Delta t) = v + (f(x(t)) - \Gamma v) \Delta t + (Df(x(t))v - \Gamma(f(x(t)) - \Gamma v)) \frac{\Delta t^2}{2} + \sum_{j=1}^n \sigma^j \Delta W^j - \sum_{j=1}^n \Gamma \sigma^j I_{(j,0)}(\Delta t)
\]
\[
v(\Delta t) = c_0 v + c_1 f(x(t)) \Delta t + c_2 (f(x(t)) - f(x)) \Delta t + \sum_{j=1}^n \int_0^{\Delta t} e^{-\Gamma(\Delta t - s)} \sigma^j \, dW^j_s
\]
\[
\quad = v + (f(x(t)) - \Gamma v) \Delta t + [Df(x(t))v - \Gamma(f(x(t)) - \Gamma v)] \frac{\Delta t^2}{2} + \sum_{j=1}^n \sigma^j \Delta W^j - \Gamma \sigma^j I_{(j,0)} + \sum_{j=1}^n \int_0^{\Delta t} (e^{-\Gamma(\Delta t - s)} - 1 + \Gamma(\Delta t - s)) \sigma^j \, dW^j_s,
\]

where the last equality is non-trivial and holds from Taylor expanding the $c$'s and $f(x(\Delta t)) = f(x)$. Setting $f_\alpha = g_\alpha$ for all $\alpha \in A_2$, we see from the calculation above that convergence criterion [14] is trivially satisfied. Next, set

\[
R_k = \sum_{j=1}^n \int_{k\Delta t}^{(k+1)\Delta t} (e^{-\Gamma(\Delta t - s)} - 1 + \Gamma(\Delta t - s)) \sigma^j \, dW^j_s, \quad k = 0, \cdots, n_T - 1,
\]

and notice that $R_k$ is a discrete martingale. Once again, $\mathbb{E}(R_k R_l) = \delta_{kl} \mathbb{E}(R^2_k)$ since Brownian increments
are independent and the Itô integrals are taken over disjoint intervals. Then we see that

\[ E(R_k^2) = \int_0^{\Delta t} (e^{-\Gamma(\Delta t - s)} - I + \Gamma(\Delta t - s))^2 ds \]  

by the Itô isometry \cite[Cor. 3.7]{27}

\[ = K \int_0^{\Delta t} s^4 ds \]  

by Taylor series approximation

\[ = \frac{K}{5} \Delta t^5 \]

\[ \Rightarrow E \left( \max_{1 \leq m \leq n_T} \left| \sum_{k=0}^{m-1} R_k \right|^2 \right) \leq 4E \left( \sum_{k=0}^{n_T-1} R_k^2 \right) \]  

by discrete Doob's lemma

\[ \leq 4E \left( \sum_{k=0}^{n_T-1} |R_k|^2 \right) \]  

since \( E(R_k, R_l) = \delta_{kl} E(R_k^2) \)

\[ = \frac{4K}{5} \sum_{k=0}^{n_T-1} E(R_k^2) \]

\[ = \frac{4K}{5} n_T \cdot O(\Delta t^5) \]

\[ = O(\Delta t^4) \]  

since \( n_T \Delta t = T \).

Therefore convergence criterion \cite{15} is satisfied with \( \gamma = 2 \).

\[ \square \]

6.7. Expansion of \( \exp \left( D_{\Delta t}^1(x, v) \right) \)

Here we derive the following formula to show the strong order convergence of the first order truncation:

\[
\exp(D_{\Delta t}^1) \left( \begin{array}{c}
  x \\
  v 
\end{array} \right) = \left( \begin{array}{c}
  x \\
  v 
\end{array} \right) + \left( \begin{array}{c}
  v \\
  f(x) - \Gamma v 
\end{array} \right) \Delta t + \left( \begin{array}{c}
  f(x) - \Gamma v \\
  Df(x)v - \Gamma(f(x) - \Gamma v) 
\end{array} \right) \frac{\Delta t^2}{2} + \sum_{j=1}^{n} \left( \begin{array}{c}
  0 \\
  \sigma_j 
\end{array} \right)^j \frac{\Delta t \Delta W^j}{2} + \text{higher order terms} \tag{100}
\]

\( \text{eq: trunc1} \)

where the higher order terms do not involve \( I_{(j,0)} \).

\[ \text{Proof.} \] Recall that \( D_{\Delta t}^1 \) is given by

\[
D_{\Delta t}^1 = \Delta t \mathcal{X}_0 + \sum_{j=1}^{n} \Delta W^j \mathcal{X}_j \tag{101}
\]
where $\mathcal{X}_0(\cdot) = D_x(\cdot)v + D_v(\cdot)(f(x) - \Gamma v)$ and $\mathcal{X}_j(\cdot) = D_v(\cdot)\sigma^j$. Observe that

\[
\mathcal{X}_0(x) = D_x(x)v + D_v(x)(f(x) - \Gamma v) = I_n v = v
\]

\[
\mathcal{X}_j(x) = D_v(x)\sigma^j = 0_{n \times n}\sigma^j = 0_{n \times 1}
\]

\[
\Rightarrow D^1_{\Delta t}(x) = \Delta t v
\]

\[
\mathcal{X}_0(v) = D_x(v)v + D_v(v)(f(x) - \Gamma v) = f(x) - \Gamma v
\]

\[
\mathcal{X}_j(v) = D_v(v)\sigma^j = \sigma^j
\]

\[
\Rightarrow D^1_{\Delta t}(v) = \Delta t \mathcal{X}_0(v) + \sum_{j=1}^{n} \Delta W^j \mathcal{X}_j(v)
\]

\[
= \Delta t(f(x) - \Gamma v) + \sum_{j=1}^{n} \sigma^j \Delta W^j
\]

\[
\Rightarrow D^1_{\Delta t}\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} D^1_{\Delta t}(x) \\ D^1_{\Delta t}(v) \end{pmatrix} = \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \Delta t + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ \sigma^j \end{pmatrix} \Delta W^j
\]
\[
\mathcal{X}_0(D^1_{\Delta t}, x) = \mathcal{X}_0(v \Delta t) = \Delta t \mathcal{X}_0(v) = \Delta t (f(x) - \Gamma v)
\]
\[
\mathcal{X}_j(D^1_{\Delta t}, x) = \Delta t \mathcal{X}_j(v) = \sigma^j \Delta t
\]
\[
\Rightarrow (D^1_{\Delta t})^2 x = \Delta t \mathcal{X}_0(D^1_{\Delta t}(x)) + \sum_{j=1}^n \Delta W^j \mathcal{X}_j(D^1_{\Delta t}(x))
\]
\[
= (f(x) - \Gamma v) \Delta t^2 + \sum_{j=1}^n \sigma^j \Delta t \Delta W^j
\]
\[
\mathcal{X}_0(D^1_{\Delta t}, v) = \mathcal{X}_0 \left( \Delta t (f(x) - \Gamma v) + \sum_{j=1}^n \sigma^j \Delta W^j \right)
\]
\[
= \Delta t \mathcal{X}_0(f(x) - \Gamma v) + \sum_{j=1}^n \Delta W^j \mathcal{X}_0(\sigma^j)
\]
\[
= \Delta t (D_x f(x) - \Gamma v) v + D_v (f(x) - \Gamma v) (f(x) - \Gamma v) + 0_{n \times 1}
\]
\[
= \Delta t D_x f(x) v - \Delta t \Gamma f(x) \Delta t^2 v
\]
\[
\mathcal{X}_j(D^1_{\Delta t}, v) = \Delta t \mathcal{X}_j(f(x) - \Gamma v) + \sum_{k=1}^n \Delta W^k \mathcal{X}_j(\sigma^k)
\]
\[
= \Delta t D_v (f(x) - \Gamma v) \sigma^j
\]
\[
= -\Delta t \Gamma \sigma^j
\]
\[
\Rightarrow (D^1_{\Delta t})^2 v = \Delta t \mathcal{X}_0(D^1_{\Delta t}, v) + \sum_{j=1}^n \Delta W^j \mathcal{X}_j(D^1_{\Delta t}, v)
\]
\[
= \Delta t \left( \Delta t D_x f(x) v - \Delta t \Gamma f(x) + \Delta t^2 v \right) + \sum_{j=1}^n \Delta W^j (-\Delta t \Gamma \sigma^j)
\]
\[
= \Delta t^2 (D_x f(x) v - \Gamma f(x) + \Gamma^2 v) + \sum_{j=1}^n (-\Gamma \sigma^j) \Delta t \Delta W^j
\]
\[
\Rightarrow (D^1_{\Delta t})^2 \left( \frac{x}{v} \right) = \left( \frac{(D^1_{\Delta t})^2 x}{(D^1_{\Delta t})^2 v} \right)
\]
\[
= \left[ \begin{array}{c}
\frac{f(x) - \Gamma v}{D_x f(x) v - \Gamma f(x) + \Gamma^2 v}
\end{array} \right] \Delta t^2 + \sum_{j=1}^n \left[ \begin{array}{c}
\sigma^j
\end{array} \right] \Delta t \Delta W^j
\]
\[
\Rightarrow \exp(D^1_{\Delta t}) \left( \frac{x}{v} \right) = \left( I + D^1_{\Delta t} + \frac{1}{2} (D^1_{\Delta t})^2 + \ldots \right) \left( \frac{x}{v} \right)
\]
\[
= \left[ \begin{array}{c}
x
\end{array} \right] + \left[ \begin{array}{c}
v
\end{array} \right] \Delta t + \sum_{j=1}^n \left[ \begin{array}{c}
0
\end{array} \right] \Delta W^j
\]
\[
+ \left[ \begin{array}{c}
f(x) - \Gamma v
\end{array} \right] \frac{\Delta t^2}{2} + \sum_{j=1}^n \left[ \begin{array}{c}
\sigma^j
\end{array} \right] \frac{\Delta t \Delta W^j}{2} + \text{higher order terms.}
\]

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6.8. Derivation of $\exp D_{\Delta t}^{\text{II}}(x,v)$

We define truncation 2 by the truncation of the Kunita solution operator $D_{\Delta t}$ after the second order brackets $[\mathcal{X}_i, \mathcal{X}_j]$:

$$D_{\Delta t}^{\text{II}} := \Delta t \mathcal{X}_0 + \sum_{j=1}^{n} \Delta W^j \mathcal{X}_j + \frac{1}{2} \sum_{i<j} [\Delta W^i, \Delta W^j] [\mathcal{X}_i, \mathcal{X}_j]$$

(104)

where $\Delta W^0 := \Delta t$,

$$[\Delta W^i, \Delta W^j] = \int_{0}^{\Delta t} W^i_t dW^j_t - \int_{0}^{\Delta t} W^j_t dW^i_t,$$

(105)

the vector fields $\mathcal{X}_i, i = 0 : n$ are defined as in the previous section, and $[A, B] = AB - BA$ is the commutator bracket from Lie algebras. For additive noise, that is, constant $\sigma$, most of the commutators $[\mathcal{X}_i, \mathcal{X}_j]$ are identically zero: indeed for $i, j = 1, 2, \cdots, n$,

$$\mathcal{X}_i \mathcal{X}_j x = \mathcal{X}_i (0_{n+1}) = 0_{n+1},$$

$$\mathcal{X}_i \mathcal{X}_j v = \mathcal{X}_i \sigma^j = 0_{n+1},$$

$$[\mathcal{X}_0, \mathcal{X}_j] x = \mathcal{X}_0 0_{n+1} - \mathcal{X}_j v$$

$$= 0_{n+1} - \sigma^j = -\sigma^j,$$

$$[\mathcal{X}_0, \mathcal{X}_j] v = \mathcal{X}_0 \sigma^j - \mathcal{X}_j (f(x) - \Gamma v) = -D_v(f(x) - \Gamma v) \sigma^j$$

$$= \Gamma \sigma^j.$$

(106)

Therefore, for additive noise, with $\Delta U^j := \frac{1}{2} [\Delta t, \Delta W^j]$, we have

$$D_{\Delta t}^{\text{II}} x = v \Delta t - \sum_{j=1}^{n} \sigma^j \Delta U^j,$$

$$D_{\Delta t}^{\text{II}} v = (f(x) - \Gamma v) \Delta t + \sum_{j=1}^{n} \sigma^j \Delta W^j + \sum_{j=1}^{n} \Gamma \sigma^j \Delta U^j,$$

$$\Rightarrow D_{\Delta t}^{\text{II}} \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} D_{\Delta t}^{\text{II}} x \\ D_{\Delta t}^{\text{II}} v \end{pmatrix}$$

$$= \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \Delta t + \sum_{j=1}^{n} \begin{pmatrix} 0_{n+1} \\ \sigma^j \end{pmatrix} \Delta W^j + \sum_{j=1}^{n} \begin{pmatrix} 0_{n+1} \\ -\sigma^j \end{pmatrix} \Delta U^j$$

(107)
\[ \mathcal{X}_0(D^{\|} x) = \mathcal{X}_0 \left( v \Delta t - \sum_{j=1}^{n} \sigma^j \Delta U^j \right) \]

\[ = \Delta t \mathcal{X}_0(v) = (f(x) - \Gamma v) \Delta t \]

\[ \mathcal{X}_j(D^{\|} x) = \Delta t \mathcal{X}_j(v) = \sigma^j \Delta t \]

\[ [\mathcal{X}_0, \mathcal{X}_j](D^{\|} x) = \Delta t[\mathcal{X}_0, \mathcal{X}_j](v) = \Delta t \Gamma \sigma^j \]

\[ \Rightarrow (D^{\|})^2 x = \Delta t \mathcal{X}_0(D^{\|} x) + \sum_{j=1}^{n} \Delta W^j \mathcal{X}_j(D^{\|} x) + \sum_{j=1}^{n} \Delta U^j [\mathcal{X}_0, \mathcal{X}_j](D^{\|} x) \]

\[ = (f(x) - \Gamma v) \Delta t^2 + \sum_{j=1}^{n} \sigma^j \Delta t \Delta W^j + \sum_{j=1}^{n} \Gamma \sigma^j \Delta t \Delta U^j \]

\[ \mathcal{X}_0(D^{\|} v) = \Delta t \mathcal{X}_0(f(x) - \Gamma v) \]

\[ = \Delta t \left[ D_x(f(x) - \Gamma v) v + D_v(f(x) - \Gamma v)(f(x) - \Gamma v) \right] \]

\[ = \Delta t \left[ D_x f(x) v - \Gamma f(x) + \Gamma^2 v \right] \]

\[ \mathcal{X}_j(D^{\|} v) = \Delta t \mathcal{X}_j(f(x) - \Gamma v) \]

\[ = \Delta t D_v(f(x) - \Gamma v) \sigma^j = -\Delta t \Gamma \sigma^j \]

\[ [\mathcal{X}_0, \mathcal{X}_j](D^{\|} v) = \Delta t[\mathcal{X}_0, \mathcal{X}_j](f(x) - \Gamma v) \]

\[ = \Delta t[\mathcal{X}_0 \mathcal{X}_j(f(x) - \Gamma v) - \mathcal{X}_j \mathcal{X}_0(f(x) - \Gamma v)] \]

\[ = \Delta t[\mathcal{X}_0(-\Gamma \sigma^j) - \mathcal{X}_j(D_x f(x) v - \Gamma f(x) + \Gamma^2 v)] \]

\[ = \Delta t[0_{n \times 1} - D_v(D_x f(x) v) \sigma^j + 0_{n \times 1} - D_v(\Gamma^2 v) \sigma^j] \]

\[ = \Delta t[-D_x f(x) \sigma^j + \Gamma^2 \sigma^j] \]

\[ \Rightarrow (D^{\|})^2 v = \Delta t \mathcal{X}_0(D^{\|} v) + \sum_{j=1}^{n} \Delta W^j \mathcal{X}_j(D^{\|} v) + \sum_{j=1}^{n} \Delta U^j [\mathcal{X}_0, \mathcal{X}_j](D^{\|} v) \]

\[ = \Delta t^2 [D_x f(x) v - \Gamma f(x) + \Gamma^2 v] - \sum_{j=1}^{n} \Gamma \sigma^j \Delta t \Delta W^j - \sum_{j=1}^{n} (D_x f(x) \sigma^j + \Gamma^2 \sigma^j) \Delta t \Delta U^j \]

\[ \Rightarrow (D^{\|})^2 \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} (D^{\|})^2 x \\ (D^{\|})^2 v \end{pmatrix} \]

\[ = \begin{pmatrix} f(x) - \Gamma v \\ D_x f(x) v - \Gamma f(x) + \Gamma^2 v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \left( \sigma^j \Delta t \Delta W^j + \sum_{j=1}^{n} \left( \Gamma \sigma^j \Delta t \Delta U^j \right) \right) \]

\[ (109) \]
\[
\exp D^{\|} \left( \frac{x}{v} \right) = \left( I + D^{\|} + \frac{1}{2} (D^{\|})^2 + \ldots \right) \left( \frac{x}{v} \right)
\]
\[
= \left( \frac{x}{v} \right) + \left( \frac{v}{f(x) - \Gamma v} \right) \Delta t + \left( \frac{f(x) - \Gamma v}{D_x f(x) - \Gamma f(x) + \Gamma^2 v} \right) \frac{\Delta t^2}{2}
\]
\[
+ \sum_{j=1}^{n} \left( \frac{0_{n \times 1}}{\sigma^j} \right) \Delta W^j + \sum_{j=1}^{n} \left( \frac{-\sigma^j}{\Gamma \sigma^j} \right) \Delta U^j + \sum_{j=1}^{n} \left( \frac{\sigma^j}{-\Gamma \sigma^j} \right) \frac{\Delta t \Delta W^j}{2}
\]
\[
+ \sum_{j=1}^{n} \left( \frac{\Gamma \sigma^j}{-D_x f(x) \sigma^j - \Gamma^2 \sigma^j} \right) \frac{\Delta t \Delta U^j}{2} + \text{higher order terms.}
\]

6.9. Baker Campbell Hausdorff Formula

The operator splitting methods are based off of the Baker Campbell Hausdorff (henceforth BCH) formulas [22, eq. 3.1]

\[
\exp A \exp B = \exp\{ A + B + \frac{1}{2} \left[ A, B \right] + \frac{1}{12} \left( \left[ A, A \right] + \left[ B, B \right], + \left[ A, B, A \right] \right) + \text{higher order brackets} \},
\]

and a second application of this formula yields the following useful formula [22, eq. (3.2)]:

\[
\exp(A/2) \exp(B \exp(A/2)) = \exp\{ A + B + \frac{1}{12} \left[ B, B \right], + \frac{1}{24} \left[ A, A, B \right] + \ldots \}.
\]

This symmetric product causes the bracket \([A, B]\) to vanish, and in terms of numerics this observation will give us a higher order method.

6.10. Convergence of naive and symmetric splittings for truncation 1

Consider the first order truncation \(D^1\) split into \(D^1 = A + B\) with

\[
A = v \Delta t \mathcal{V}_x \quad \text{and} \quad B = \left( f(x) - \Gamma v \right) \Delta t + \sigma \Delta W \mathcal{V}_x.
\]

We compute the following:

\[
Ax = D_x (v \Delta t) = I(v \Delta t) = v \Delta t
\]
\[
Av = D_x (v \Delta t) = 0_{n \times n}(v \Delta t) = 0_{n \times 1}
\]
\[
Bv = (f(x) - \Gamma v) \Delta t + \sigma \Delta W
\]
\[
Bx = D_v (x) B v = 0_{n \times n} B v = 0_{n \times 1}
\]

In general: \(A(\cdot) = D_x(\cdot) A x\) and \(B(\cdot) = D_v(\cdot) B v\)
\[(A + B)\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \Delta t + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ \sigma^j \end{pmatrix} \Delta W^j \]  
(115)

\[A^2 x = A(Ax) = D_x(Ax)Ax = D_x(v \Delta t)Ax = 0_{n \times n}Ax = 0_{n \times 1} \]

\[A^2 v = A(Av) = A0_{n \times 1} = 0_{n \times 1} \]

\[ABx = A0_{n \times 1} = 0_{n \times 1} \]

\[ABv = D_x(Bv)Ax = D_x(f(x)\Delta t)Ax = \Delta t^2 D_x f(x) v \]  
(116)

\[B^2 x = B(Bx) = B0_{n \times 1} = 0_{n \times 1} \]

\[B^2 v = B(Bv) = D_v(Bv)Bv = D_v(-\Gamma v \Delta t)Bv = -\Delta t \Gamma Bv \]

\[= (-\Gamma f(x) + \Gamma^2 v)\Delta t^2 - \Gamma \sigma \Delta t \Delta W \]

\[
\frac{1}{2} \left( [A, B] + A^2 + AB + BA + B^2 \right) \begin{pmatrix} x \\ v \end{pmatrix} = \frac{1}{2} \left( 2AB + B^2 \right) \begin{pmatrix} x \\ v \end{pmatrix} \text{ since } A^2(x, v) = 0 \\
= \begin{pmatrix} AB + \frac{1}{2} B^2 \end{pmatrix} \begin{pmatrix} x \\ v \end{pmatrix} \\
= \begin{pmatrix} 0_{n \times 1} \\ D_x f(x) v - (1/2) \Gamma f(x) + (1/2) \Gamma^2 v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ -\Gamma \sigma^j \end{pmatrix} \frac{\Delta t \Delta W}{2} \]
(117)

By the BCH formula,

\[\exp(A) \exp(B) \begin{pmatrix} x \\ v \end{pmatrix} = \left( I + A + B + \frac{1}{2} [A, B] + \frac{1}{2} (A^2 + AB + BA + B^2) \right) \begin{pmatrix} x \\ v \end{pmatrix} \\
= \begin{pmatrix} x \\ v \end{pmatrix} + \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \Delta t + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ \sigma^j \end{pmatrix} \Delta W^j \]  
(118)

\[+ \begin{pmatrix} 0_{n \times 1} \\ D_x f(x) v - (1/2) \Gamma f(x) + (1/2) \Gamma^2 v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ -\Gamma \sigma^j \end{pmatrix} \frac{\Delta t \Delta W}{2} \]

We see by comparison with the Ito Taylor approximations that the non-symmetric method above has strong order \( \gamma = 1 \) by matching terms and noticing that the multiple stochastic integral \( I_{(j,0)} \) does not show up.
As for the symmetric splitting, we first compute

\[ B Ax = D_v(Ax)Bv = D_v(v\Delta t)Bv = \Delta tBv \]
\[ = (f(x) - \Gamma v)\Delta t^2 + \sigma \Delta t \Delta W \]

\[ BA v = B0_{n \times 1} = 0_{n \times 1} \]

\[ \Rightarrow B A \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} f(x) - \Gamma v \\ 0_{n \times 1} \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} \sigma^j \\ 0_{n \times 1} \end{pmatrix} \Delta t \Delta W^j \]

and use the computations for \( A^2, AB, B^2 \) given above to obtain

\[ (A^2 + AB + BA + B^2) \begin{pmatrix} x \\ v \end{pmatrix} = 0_{2n \times 1} + \begin{pmatrix} 0_{n \times 1} \\ D_x f(x)v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} \sigma^j \\ 0_{n \times 1} \end{pmatrix} \Delta t \Delta W^j \]

\[ + \begin{pmatrix} 0_{n \times 1} \\ -\Gamma f(x) + \Gamma^2 v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ -\Gamma \sigma^j \end{pmatrix} \Delta t \Delta W^j \]

\[ = \begin{pmatrix} f(x) - \Gamma v \\ D_x f(x)v - \Gamma f(x) + \Gamma^2 v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} \sigma^j \\ -\Gamma \sigma^j \end{pmatrix} \Delta t \Delta W^j. \]

Then using the BCH formula, we get the approximation

\[ \exp(A/2) \exp(B) \exp(A/2) \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} x \\ v \end{pmatrix} + \begin{pmatrix} v \\ f(x) - \Gamma v \end{pmatrix} \Delta t + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ \sigma^j \end{pmatrix} \Delta W^j \]

\[ + \begin{pmatrix} f(x) - \Gamma v \\ D_x f(x)v - \Gamma f(x) + \Gamma^2 v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} \sigma^j \\ -\Gamma \sigma^j \end{pmatrix} \Delta t \Delta W^j. \]

By comparing again to the Ito Taylor approximations, we see that this approximation is much closer to attaining strong order \( \gamma = 2 \) than the non-symmetric splitting, but still falls short of strong order \( \gamma = 2 \), only because the multiple Ito integral \( I_{(j,0)} \) is not present.

6.11. Convergence of naive and symmetric splittings for truncation 2

Here we consider the second order truncation \( D^\Pi_{\Delta t} \) split into \( D^\Pi_{\Delta t} = A + B \). By the BCH formula in the previous section, it seems necessary to compute the brackets \( [A,B], [A,[A,B]] \) and \( [B,[B,A]] \) in order to find the strong convergence order for the naive splitting and the symmetric splitting below.
Observe that with \( A = (\nu \Delta t - \sigma \Delta U) \cdot \nabla x \) and \( B = ((f(x) - \Gamma \nu) \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U) \cdot \nabla v \), we have

\[ Ax = \nu \Delta t - \sigma \Delta U, \quad Av = 0 \]

\[ Bv = (f(x) - \Gamma \nu) \Delta t + \sigma \Delta W + \Gamma \sigma \Delta U \]

\[ A(\cdot) = D_x A \]

\[ B(\cdot) = D_v B \]

where \( D_x(\cdot) = \frac{\partial(\cdot)}{\partial x} \) and \( D_v(\cdot) = \frac{\partial(\cdot)}{\partial v} \) \((i, j = 1, 2, \ldots, n)\)

\[ Av = D_x(v) Ax = 0_{n \times n} Ax = 0_{n \times 1} \]

\[ Bx = D_v(x) Bv = 0_{n \times n} Bv = 0_{n \times 1} \]

\[ ABx = BAv = 0_{n \times 1} \]

\[ BAv = AB(x) = D_v(Ax) Bv = \Delta t I_{n \times n} Bv = \Delta t Bv \]

\[ ABv = A(Bv) = D_x(Bv) Ax = \Delta t D_x f(x) Ax \]

\[ \Rightarrow AB \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0_{n \times 1} \\ D_x f(x) v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} 0_{n \times 1} \\ -D_x f(x) \sigma_j \end{pmatrix} \Delta t \Delta U^j \]

\[ BA \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} f(x) - \Gamma v \\ 0_{n \times 1} \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} \sigma_j \\ 0_{n \times 1} \end{pmatrix} \Delta t \Delta W^j + \sum_{j=1}^{n} \begin{pmatrix} \Gamma \sigma_j \end{pmatrix} \Delta t U^j \]

\[ A^2 \begin{pmatrix} x \\ v \end{pmatrix} = 0_{2n \times 1} \]

\[ B^2 \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0_{n \times 1} \\ -\Delta t \Gamma Bv \end{pmatrix} \]

\[ (A^2 + AB + BA + B^2) \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} f(x) - \Gamma v \\ D_x f(x) v - \Gamma f(x) + \Gamma^2 v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} \sigma_j \\ -\Gamma \sigma_j \end{pmatrix} \Delta t \Delta W^j + \sum_{j=1}^{n} \begin{pmatrix} \Gamma \sigma_j \\ -D_x f(x) \sigma_j - \Gamma^2 \sigma_j \end{pmatrix} \Delta t U^j \]

\[ [A, B] \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} |A, B| x \\ |A, B| v \end{pmatrix} = \begin{pmatrix} ABx - BAx \\ ABr - BAv \end{pmatrix} = \begin{pmatrix} -B Ax \\ -\Delta t Bv \end{pmatrix} = \begin{pmatrix} -\Delta t D_x f(x) Ax \end{pmatrix} \]

\[ = \begin{pmatrix} -f(x) + \Gamma v \\ D_x f(x) v \end{pmatrix} \Delta t^2 + \sum_{j=1}^{n} \begin{pmatrix} -\sigma_j \\ 0_{n \times 1} \end{pmatrix} \Delta t \Delta W^j + \sum_{j=1}^{n} \begin{pmatrix} -\Gamma \sigma_j \\ -D_x f(x) \sigma_j \end{pmatrix} \Delta t U^j \]

\[(122)\]
Observe that the naive splitting gives

\[
\exp A \exp B \left( \frac{x}{v} \right) \approx \left[ I + A + B + \frac{1}{2} ([A,B] + A^2 + AB + BA + B^2) \right] \left( \frac{x}{v} \right)
\]

\[
= \left( \frac{x}{v} \right) + \left( \frac{v}{f(x) - \Gamma v} \right) \Delta t + \sum_{j=1}^{n} \left( \frac{0_{n \times 1}}{\sigma^j} \right) \Delta W^j + \left( \frac{0_{n \times 1}}{2D_x f(x) v - \Gamma f(x) + \Gamma^2 v} \right) \frac{\Delta t^2}{2}
\]

\[
+ \sum_{j=1}^{n} \left( \frac{-\sigma^j}{\Gamma \sigma^j} \right) \Delta U^j + \sum_{j=1}^{n} \left( \frac{0_{n \times 1}}{-\Gamma \sigma^j} \right) \frac{\Delta t \Delta W^j}{2} + \sum_{j=1}^{n} \left( \frac{0_{n \times 1}}{-2D_x f(x) \sigma^j - \Gamma^2 \sigma^j} \right) \frac{\Delta t \Delta U^j}{2}
\]

\[
\Rightarrow \exp A \exp B \left( \frac{x}{v} \right) - \left( \frac{x(\Delta t)}{v(\Delta t)} \right) = \left( \frac{0_{n \times 1}}{2D_x f(x) v - \Gamma f(x) + \Gamma^2 v} \right) \frac{\Delta t^2}{2}
\]

\[
+ \sum_{j=1}^{n} \left( \frac{-\sigma^j}{\Gamma \sigma^j} \right) \Delta U^j + \sum_{j=1}^{n} \left( \frac{0_{n \times 1}}{-\Gamma \sigma^j} \right) \frac{\Delta t \Delta W^j}{2} + \sum_{j=1}^{n} \left( \frac{0_{n \times 1}}{-2D_x f(x) \sigma^j - \Gamma^2 \sigma^j} \right) \frac{\Delta t \Delta U^j}{2}
\]

where we let \((x(\Delta t), v(\Delta t))\) denote the strong order \(\gamma = 1\) Ito Taylor approximation. We see that \(g_a = f_a\) for all \(a \in A_1\), but \(g_a \neq f_a\) for \(a = (0,0), (j,0) \in A_2\). Therefore the naive splitting \(\exp A \exp B\) of truncation \(2 D_{\Delta t}^{1} = A + B\) gives a strong order \(\gamma = 1\) method but not a strong order \(\gamma = 2\) method.

As for the symmetric splitting, observe that

\[
\exp(A/2) \exp(A/2) \left( \frac{x}{v} \right) \approx \left[ I + A + B + \frac{1}{2} (A^2 + AB + BA + B^2) \right] \left( \frac{x}{v} \right)
\]

\[
= \left( \frac{x}{v} \right) + \left( \frac{v}{f(x) - \Gamma v} \right) \Delta t + \sum_{j=1}^{n} \left( \frac{0_{n \times 1}}{\sigma^j} \right) \Delta W^j
\]

\[
+ \sum_{j=1}^{n} \left( \frac{-\sigma^j}{\Gamma \sigma^j} \right) \Delta U^j + \sum_{j=1}^{n} \left( \frac{\sigma^j}{\Gamma \sigma^j} \right) \frac{\Delta t \Delta W^j}{2} + \sum_{j=1}^{n} \left( \frac{-\Gamma \sigma^j}{-2D_x f(x) \sigma^j - \Gamma^2 \sigma^j} \right) \frac{\Delta t \Delta U^j}{2}
\]

\[
\text{and } \frac{\Delta t \Delta W^j}{2} - \Delta U^j = I_{(j,0)}(\Delta t). \text{ Therefore,}
\]

\[
\exp(A/2) \exp(A/2) \left( \frac{x}{v} \right) - \left( \frac{x(\Delta t)}{v(\Delta t)} \right) = \sum_{j=1}^{n} \left( \frac{\Gamma \sigma^j}{-2D_x f(x) \sigma^j - \Gamma^2 \sigma^j} \right) \frac{\Delta t \Delta U^j}{2},
\]

\[(125)\]

where \((x(\Delta t), v(\Delta t))\) denotes the strong order \(\gamma = 2\) Ito Taylor approximation. That is, the strong order \(\gamma = 2\) Ito Taylor approximation agrees with this method up to the terms \(\Delta t \Delta U^j\).
6.12. Covariances

Here we derive the covariances of $\Delta W, \Delta U, \Delta V$ in the multi-dimensional case, where

$$
\Delta U^i = I_{(0, i)} - \frac{\Delta t \Delta W^i}{2},
$$

$$
\Delta V^i = \frac{1}{9} \left( I_{(0, i, 0)} - I_{(i, 0, 0)} - \Delta t \Delta U^i \right).
$$

(126)

Notice $\mathbb{E}(\Delta W^i \Delta W^j) = \mathbb{E}(W^i_{\Delta t} W^j_{\Delta t}) = \Delta t \delta_{ij}$, so that $\mathbb{E}(\Delta W^2) = \Delta t I_{n \times n}$.

To find $\mathbb{E}(\Delta W \Delta U)$, we need to know $\mathbb{E}(\Delta W^i I_{(0,j)})$, since

$$
\mathbb{E}(\Delta W^i \Delta U^j) = \mathbb{E}(\Delta W^i I_{(0,j)}) - \frac{\Delta t}{2} \mathbb{E}(\Delta W^i) \Delta W^j = \mathbb{E}(\Delta W^i I_{(0,j)}) - \frac{\Delta t^2}{2} \delta_{ij}.
$$

(127)

So, we look on [2] p. 223 and find that $\mathbb{E}(\Delta W^i I_{(0,j)}) = \frac{\Delta t^2}{2} \delta_{ij}$, or verify this fact:

$$
\mathbb{E}(\Delta W^i I_{(0,j)}) = \mathbb{E} \left( W^i_{\Delta t} \int_0^{\Delta t} t dW^j_t \right) \text{ by definition}
$$

$$
= \mathbb{E} \left( W^i_{\Delta t} \left( \Delta t W^j_{\Delta t} - \int_0^{\Delta t} W^j_t dt \right) \right) \text{ integration by parts}
$$

$$
= \Delta t \mathbb{E} \left( W^i_{\Delta t} W^j_{\Delta t} \right) - \int_0^{\Delta t} \mathbb{E} (W^i_{\Delta t} W^j_t) dt
$$

$$
= \Delta t^2 \delta_{ij} - \int_0^{\Delta t} \mathbb{E} \left( \left( W^i_{\Delta t} - W^j_t \right) W^j_t \right) + \mathbb{E} \left( W^i_{\Delta t} W^j_t \right) dt
$$

$$
= \Delta t^2 \delta_{ij} - \int_0^{\Delta t} t \delta_{ij} dt \text{ since increments are independent, mean 0}
$$

$$
= \frac{\Delta t^2}{2} \delta_{ij}.
$$

(128)

Therefore,

$$
\mathbb{E}(\Delta W^i \Delta U^j) = \mathbb{E}(\Delta W^i I_{(0,j)}) - \frac{\Delta t}{2} \mathbb{E}(\Delta W^i) \Delta W^j = \frac{\Delta t^2}{2} \delta_{ij} - \frac{\Delta t^2}{2} \delta_{ij} = 0 \text{ for all } i, j = 1, 2, \ldots, n.
$$

(129)

Then also $\mathbb{E}(\Delta U^i \Delta W^j) = 0$, so that $\mathbb{E}(\Delta U \Delta W) = \mathbb{E}(\Delta U \Delta W) = 0_{n \times n}$. Next, to find $\mathbb{E}(\Delta W \Delta V)$, we first need to know $\mathbb{E}(\Delta W^i I_{(0,0)})$ and $\mathbb{E}(\Delta W^i I_{(j,0,0)})$, because

$$
\mathbb{E}(\Delta W^i \Delta V^j) = \frac{1}{9} \left( \mathbb{E}(\Delta W^i I_{(0,j,0)}) - \mathbb{E}(\Delta W^i I_{(j,0,0)}) - \Delta t \mathbb{E}(\Delta W^i \Delta U^j) \right)
$$

(130)

and we already know that $\mathbb{E}(\Delta W^i \Delta U^j) = 0$. To that end, we go to [2] p. 223 again and find $\mathbb{E}(\Delta W^i I_{(0,0)}) =$
\[ \mathbb{E}(\Delta W^i I_{(i,0,0)}) = \frac{\Delta^2}{3!} \delta_{ij}, \] or verify ourselves:

\[ \mathbb{E}(\Delta W^i I_{(i,0,0)}) = \mathbb{E}\left(W^i_\Delta \int_0^{\Delta t} \int_0^t dW^j_u ds dt \right) \quad \text{by definition} \]
\[ = \mathbb{E}\left( \int_0^{\Delta t} \int_0^t W^i_\Delta W^j_s ds dt \right) \]
\[ = \int_0^{\Delta t} \int_0^t E(W^i_\Delta W^j_s) ds dt \]
\[ = \int_0^{\Delta t} \int_0^t s \delta_{ij} ds dt \]
\[ = \int_0^{\Delta t} \frac{t^2}{2} \delta_{ij} dt \]
\[ = \frac{\Delta^3}{3!} \delta_{ij}, \quad (131) \]

\[ \mathbb{E}(\Delta W^i I_{(0,j,0)}) = \mathbb{E}\left(W^i_\Delta \int_0^{\Delta t} I_{(0,j)(t)} dt \right) \]
\[ = \int_0^{\Delta t} E\left( W^i_\Delta - W^i_t \right) I_{(0,j)(t)} + E\left( W^i_t I_{(0,j)(t)} \right) dt \]
\[ = \int_0^{\Delta t} \frac{t^2}{2} \delta_{ij} dt \]
\[ = \frac{\Delta^3}{3!} \delta_{ij}. \]

Therefore,
\[ \mathbb{E}(\Delta W^i \Delta V^j) = \mathbb{E}(\Delta V^i \Delta W^j) = 0, \quad \text{i.e.} \quad \mathbb{E}(\Delta W \Delta V) = \mathbb{E}(\Delta V \Delta W) = 0_{n \times n}. \quad (132) \]

We now seek \( \mathbb{E}(\Delta U^2) \), which will require the covariances \( \mathbb{E}(I_{(0,i)} I_{(0,j)}) \), yet to be determined, because we can write

\[ \mathbb{E}(\Delta U^i \Delta U^j) = \mathbb{E}(I_{(0,i)} I_{(0,j)}) - \Delta t \mathbb{E}(\Delta W^i I_{(0,j)}) + \frac{\Delta t^2}{4} \mathbb{E}(\Delta W^i \Delta W^j) \]
\[ = \mathbb{E}(I_{(0,i)} I_{(0,j)}) - \frac{\Delta t^3}{2} \delta_{ij} + \frac{\Delta t^3}{4} \delta_{ij} \]
\[ = \mathbb{E}(I_{(0,i)} I_{(0,j)}) - \frac{\Delta t^3}{4} \delta_{ij}. \quad (133) \]

To find \( \mathbb{E}(I_{(0,i)} I_{(0,j)}) \), use the Itô isometry:

\[ \mathbb{E}(I_{(0,i)} I_{(0,j)}) = \mathbb{E}\left( \int_0^{\Delta t} t dW^i_t \int_0^{\Delta t} t dW^j_t \right) = \int_0^{\Delta t} t^2 d t \delta_{ij} = \frac{\Delta^3}{3} \delta_{ij}. \quad (134) \]

Then
\[ \mathbb{E}(\Delta U^i \Delta U^j) = \frac{\Delta t^3}{12} \delta_{ij}, \quad \text{i.e.} \quad \mathbb{E}(\Delta U^2) = \frac{\Delta t^3}{12} I_{n \times n}. \quad (135) \]

Moving on to \( \mathbb{E}(\Delta U \Delta V) \), it is straightforward, using our previous analyses, to show

\[ 9 \mathbb{E}(\Delta U^i \Delta V^j) = \mathbb{E}(I_{(0,i)} I_{(0,j,0)}) - \mathbb{E}(I_{(0,i)} I_{(j,0,0)}) - \frac{\Delta t^4}{12} \delta_{ij}. \quad (136) \]
So, we need to find \( E(I_{(0,i)} I_{(0,j,0)}) \) and \( E(I_{(0,i)} I_{(j,0,0)}) \). Notice
\[
E(I_{(0,i)} I_{(0,j,0)}) = \mathbb{E}\left( \int_0^{\Delta t} (I_{(0,i)}(\Delta t) - I_{(0,i)}(t)) I_{(0,j,0)}(t) dt \right) + \mathbb{E}\left( \int_0^{\Delta t} I_{(0,i)}(t) I_{(0,j,0)}(t) dt \right)
\]
\[= 0 + \int_0^{\Delta t} \frac{t^3}{3} \delta_{ij} dt \]
\[= \frac{\Delta t^4}{12} \delta_{ij}, \quad (137)\]
and
\[
E(I_{(0,i)} I_{(j,0,0)}) = \mathbb{E}\left( \int_0^{\Delta t} (I_{(0,i)}(\Delta t) - I_{(0,i)}(t)) I_{(j,0,0)}(t) dt \right) + \mathbb{E}\left( \int_0^{\Delta t} I_{(0,i)}(t) I_{(j,0,0)}(t) dt \right)
\]
\[= 0 + \int_0^{\Delta t} \frac{t^3}{3!} \delta_{ij} dt \]
\[= \frac{\Delta t^4}{4!} \delta_{ij}. \quad (138)\]

Therefore \( 9E(\Delta U \Delta V) = \frac{-\Delta t^4}{4!} \delta_{ij} \), that is,
\[
E(\Delta U \Delta V) = E(\Delta V \Delta U) = \frac{-\Delta t^4}{216} \delta_{ij}. \quad (139)\]

For \( E(\Delta V^2) \), we need \( E(I_{(0,i,0)} I_{(j,0,0)}) \), \( E(I_{(0,i,0)} I_{(0,j,0)}) \), and \( E(I_{(i,0,0)} I_{(j,0,0)}) \). These higher order calculations cannot be found in [2], but we can use [2 Cor. 5.12.3] to find them:
\[
E(I_{(0,i,0)} I_{(0,j,0)}) = 2E\int_0^{\Delta t} I_{(0,i)} I_{(0,j,0)} dt \quad \text{by Cor. 5.12.3}
\]
\[= 2 \int_0^{\Delta t} \frac{t^4}{12} dt \delta_{ij} \]
\[= \frac{\Delta t^5}{30} \delta_{ij}, \quad (140)\]
and
\[
E(I_{(0,i,0)} I_{(j,0,0)}) = E\int_0^{\Delta t} I_{(0,i)} I_{(j,0,0)} dt + E\int_0^{\Delta t} I_{(0,i,0)} I_{(j,0)} dt
\]
\[= \int_0^{\Delta t} \frac{t^4}{4!} + \frac{t^4}{12} dt \delta_{ij} \]
\[= \frac{\Delta t^5}{40} \delta_{ij}, \quad (141)\]
and
\[
E(I_{(i,0,0)} I_{(j,0,0)}) = 2E\int_0^{\Delta t} I_{(i,0)} I_{(j,0,0)} dt \quad \text{by [2 Cor. 5.12.3]}
\]
\[= 2 \int_0^{\Delta t} t^4 \delta_{ij} dt \]
\[= \frac{\Delta t^5}{20} \delta_{ij}. \quad (142)\]
We have

\[
81 \Delta V^i \Delta V^j = I_{(0,i,0)} I_{(0,j,0)} - I_{(0,i,0)} I_{(0,j,0)} - \Delta t \Delta U^i I_{(0,i,0)}
- I_{(i,0,0)} I_{(0,j,0)} + I_{(i,0,0)} I_{(0,j,0)} + \Delta t \Delta U^j I_{(i,0,0)}
- \Delta t \Delta U^i I_{(0,j,0)} + \Delta t \Delta U^j I_{(i,0,0)} + \Delta t^2 \Delta U^i \Delta U^j
\]

\[
81 \mathbb{E}(\Delta V^i \Delta V^j) = \frac{\Delta t^5}{30} - \frac{\Delta t^5}{40} - 2 \Delta t \mathbb{E}(\Delta U^i I_{(0,j,0)}) + 2 \Delta t \mathbb{E}(\Delta U^j I_{(i,0,0)}) - \frac{\Delta t^5}{40} + \frac{\Delta t^5}{20} + \frac{\Delta t^5}{12}
\]

\[
= \frac{\Delta t^5}{30} - 2 \Delta t \mathbb{E}(\Delta U^i I_{(0,j,0)}) + 2 \Delta t \mathbb{E}(\Delta U^j I_{(i,0,0)}) + \frac{\Delta t^5}{12}
\]

all times \( \delta_{ij} \)

\[
\mathbb{E}(\Delta U^i I_{(0,j,0)}) = \mathbb{E}(I_{(0,i)} I_{(0,j,0)}) - \frac{\Delta t}{2} \mathbb{E}(\Delta W^i I_{(0,j,0)})
\]

\[
= \frac{\Delta t^4}{12} - \frac{\Delta t}{2} \frac{\Delta t^3}{3!}
\]

\[
= 0
\]

\[
\mathbb{E}(\Delta U^i I_{(j,0,0)}) = \mathbb{E}(I_{(0,i)} I_{(j,0,0)}) - \frac{\Delta t}{2} \mathbb{E}(\Delta W^i I_{(j,0,0)})
\]

\[
= \frac{\Delta t^4}{4!} - \frac{\Delta t}{2} \frac{\Delta t^3}{3!}
\]

\[
= -\frac{\Delta t^4}{24} \delta_{ij}
\]

\[
81 \mathbb{E}(\Delta V^i \Delta V^j) = \frac{\Delta t^5}{30} - 2 \Delta t \frac{\Delta t^4}{24} + \frac{\Delta t^5}{12}
\]

\[
= \frac{\Delta t^5}{2430} \delta_{ij}.
\]

Therefore,

\[
\mathbb{E}(\Delta V^2) = \frac{\Delta t^5}{2430} I_{n \times n}.
\]

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