Sampling of Stochastic Differential Equations using the Karhunen–Loève Expansion and Matrix Functions

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Abstract

We consider linearizations of stochastic differential equations with additive noise using the Karhunen–Loève expansion. We obtain our linearizations by truncating the expansion and writing the solution as a series of matrix-vector products using the theory of matrix functions. Moreover, we restate the solution as the solution of a system of linear differential equations. We obtain strong and weak error bounds for the truncation procedure and show that, under suitable conditions, the mean square error has order of convergence $O\left(\frac{1}{m}\right)$ and the second moment has a weak order of convergence $O\left(\frac{1}{m}\right)$, where $m$ denotes the size of the expansion. We also discuss efficient numerical linear algebraic techniques to approximate the series of matrix functions and the linearized system of differential equations. These theoretical results are supported by experiments showing the effectiveness of our algorithms when compared to standard methods such as the Euler–Maruyama scheme.

1 Introduction

Many applications of machine learning are in domains that can be modelled using a stochastic differential equation (SDE) with additive noise. The diverse array of examples across many domains includes epidemiology \cite{4}, weather forecasting \cite{6}, finance \cite{7}, and gene expression \cite{17}. In the past decade, advances in computing power have led to renewed interest in this topic from the machine learning and uncertainty quantification communities \cite{16}.

There are two common tasks when using such models. First, the forwards propagation of uncertainty from the parameters of the SDE into the output allows one to calculate the expected solution of a system, its variance, confidence intervals around the solution, or indeed its entire probability distribution \cite{12}. Second, estimating the most likely parameters of a hypothesized SDE from observations using Bayesian inference is becoming increasingly common \cite{3}. Both tasks rely heavily upon the ability to efficiently sample different realizations from these SDEs and typically use Monte Carlo approaches (e.g. \cite{8}, \cite{9}, \cite{14}).
The SDEs underlying many of these applications is a multidimensional Ornstein-Uhlenbeck process. For example a particle of dust floating in gas exhibits Brownian motion, but if there is an additional convective force generated by airflow then this Ornstein-Uhlenbeck process can be described by the linear SDE

\[ \dot{u}(t) = Lu(t) + BdW_t, \]  

(1.1)

where \( u(t) \) is the position of the particle, \( L \) describes the convection, and \( BdW_t \) describes the stochasticity. Multidimensional Ornstein–Uhlenbeck processes of the form (1.1) that arise from parabolic partial differential equations have also been considered [11].

The primary goal of this research is to increase the speed with which samples can be generated from multidimensional Ornstein-Uhlenbeck processes by exploiting a connection with matrix functions. Although we focus on the Ornstein-Uhlenbeck process, our approach can be extended to other stochastic processes.

A matrix function is an operator \( f : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n} \) which generalizes useful properties of its scalar equivalent. For example, the matrix exponential is

\[ \exp(A) = \sum_{k=0}^{\infty} \frac{A^k}{k!}. \]

This generalizes many of the useful properties of the scalar exponential, for example \( \exp(2A) = \exp(A)^2 \). This property forms the basis of the popular scaling and squaring method used to compute the exponential in practice [1].

The remainder of this work is organized as follows. In section 2, we introduce our approach on a deterministic semilinear ODE and derive results that are used throughout the rest of the analysis. Next, in section 3, we apply our approach to a SDE with additive noise. We define our numerical method in section 4 and derive error bounds on the expected truncation error introduced. In section 5, we reformulate our numerical method as a single matrix–vector product involving the matrix exponential and implementation strategies. Numerical experiments are given in section 6 with concluding remarks in section 7.

## 2 Deterministic differential equations

We begin by deriving our approach for a deterministic semilinear differential equation before introducing the additional complexity of the stochastic terms. In brief, we want to relate the solution of the semilinear differential equation

\[ \dot{u}(t) = Lu(t) + g(t), \quad u(0) = u_0 \in \mathbb{R}^n, \quad L \in \mathbb{R}^{n \times n}, \]

(2.1)

to matrix functions when the nonlinear function \( g(t) \) is approximated by a finite dimensional Fourier series. The approach is reminiscent of [11, Thm. 2.1]. To this end, we consider the Fourier series of the nonlinear function \( g : \mathbb{R} \to \mathbb{R}^n \),

\[ g(t) = \sum_{k=0}^{\infty} a_k \cos(c_k t) + b_k \sin(c_k t), \]

where \( a_k, b_k \in \mathbb{R}^n \) and \( c_k \in \mathbb{R}, \quad k \geq 1 \).
2.1 Truncated system and matrix functions

Now we can replace \( g(t) \) in the semilinear equation (2.1) by a truncated Fourier series expansion

\[
g(t) \approx g_N(t) = \sum_{k=0}^{N} a_k \cos(c_k t) + b_k \sin(c_k t) \tag{2.2}
\]

to obtain the approximative ODE

\[
\dot{u}_N(t) = Lu_N(t) + g_N(t), \quad u_N(0) = u_0 \in \mathbb{R}^n. \tag{2.3}
\]

The error introduced by this truncation will be bounded in the proceeding subsection. Using the variation-of-constants formula, the solution of (2.3) is

\[
u_N(t) = e^{tL}u_0 + \sum_{k=1}^{N} \left( \int_0^t e^{(t-s)L} \cos(c_k s) \, ds \right) a_k + \left( \int_0^t e^{(t-s)L} \sin(c_k s) \, ds \right) b_k, \tag{2.4}
\]

where \( \varphi^\cos_{k,t} \) and \( \varphi^\sin_{k,t} \) denote the functions

\[
\varphi^\cos_{k,t}(z) = \int_0^t e^{(t-s)z} \cos(c_k s) \, ds,
\]

\[
\varphi^\sin_{k,t}(z) = \int_0^t e^{(t-s)z} \sin(c_k s) \, ds.
\]

These functions are clearly analytic on the whole complex plane and for \( z \in \mathbb{C} \) satisfy

\[
\varphi^\cos_{k,t}(z) + i \varphi^\sin_{k,t}(z) = \int_0^t e^{(t-s)z} e^{i c_k s} \, ds = e^{tz} - e^{i z c_k} \frac{1}{z - i c_k}. \tag{2.5}
\]

We call \( \varphi^\cos_{k,t} \) and \( \varphi^\sin_{k,t} \) the trigonometric \( \varphi \) functions. If we consider the real and imaginary parts of (2.5) separately, we can make the following definition of the (scalar versions of the) trigonometric \( \varphi \) functions without an integral.

**Definition 1.** Let \( (\lambda_k)_{k=1}^\infty \) be a sequence of real numbers. Then the trigonometric \( \varphi \) functions corresponding to the sequence \( (\lambda_k)_{k=1}^\infty \) are defined for \( z \in \mathbb{C} \) and \( t \in \mathbb{R} \) by

\[
\varphi^\cos_{k,t}(z) = \frac{ze^{zt} - z \cos(\lambda_k t) + \lambda_k \sin(\lambda_k t)}{z^2 + \lambda_k^2}, \tag{2.6}
\]

and

\[
\varphi^\sin_{k,t}(z) = \frac{\lambda_k e^{zt} - \lambda_k \sin(\lambda_k t) - z \cos(\lambda_k t)}{z^2 + \lambda_k^2}. \tag{2.7}
\]
2.2 Bound for the truncation error

At this point we have shown how one can form an approximation to our original differential equation by truncating a Fourier series expansion of the nonlinear term (2.3) and using matrix functions (2.4). In this section we analyze the convergence of the approximate solution \( u_N(t) \) as \( N \) grows.

Our analysis requires the use of the numerical range \( \mathcal{F}(A) \) of a matrix \( A \in \mathbb{C}^{n \times n} \), which is defined as
\[
\mathcal{F}(A) = \{ x^*Ax : x \in \mathbb{C}^n, \|x\|_2 = 1 \}.
\]
We also require the related notion of the logarithmic norm of a matrix \( A \), defined as
\[
\mu(A) = \max \{ \Re z : z \in \mathcal{F}(A) \}.
\]
Using these, we state the following bound for the norm of the matrix functions \( \varphi_{k,t}^{\cos}(A) \) and \( \varphi_{k,t}^{\sin}(A) \).

**Lemma 2.** Let \( A \in \mathbb{R}^{n \times n} \), \( (\lambda_k)_{k=1}^\infty \subset \mathbb{R} \) and let the corresponding \( \varphi_{k,t}^{\cos}(z) \) and \( \varphi_{k,t}^{\sin}(z) \) be defined as in (2.6) and (2.7). Suppose \( d(i\lambda_k, \mathcal{F}(A)) > 0 \), where \( d(c, X) \) denotes the Euclidean distance of \( c \in \mathbb{C} \) from the set \( X \). Then,
\[
\|\varphi_{k,t}^{\cos}(A)\| \leq \frac{1 + e^{t\mu(A)}}{d(i\lambda_k, \mathcal{F}(A))},
\]
and the same bound holds for \( \|\varphi_{k,t}^{\sin}(A)\| \).

**Proof.** From the representation (2.5) we see that
\[
\varphi_{k,t}^{\cos}(A) = \Re \left( (e^{tA} - e^{i\lambda_k t}I)(A - i\lambda_k I)^{-1} \right)
\]
and similarly \( \varphi_{k,t}^{\sin}(A) \) is given by the imaginary part. To bound (2.8), we use the well known bounds \( \|e^A\|_2 \leq e^{\mu(A)} \) (see e.g. [20, Sec. 14]), and \( \|(zI - A)^{-1}\| \leq d(z, \mathcal{F}(A))^{-1} \).

To illustrate the utility of this bound, we give a short example of how one can bound \( \|\varphi_{k,t}^{\cos}(A)\| \) and a second example which applies this lemma to bound the truncation error \( \|u(t) - u_N(t)\| \).

**Example.** Let \( A \in \mathbb{R}^{n \times n} \) be a negative semi-definite matrix (i.e. \( \mathcal{F}(A) \subset \mathbb{R}_{\leq 0}, \mu(A) \leq 0 \)) and let \( (\lambda_k)_{k=1}^\infty \subset \mathbb{R} \setminus \{0\} \). Then using the lemma above, we have
\[
\|\varphi_{k,t}^{\cos}(A)\| \leq \frac{1}{|\lambda_k|}.
\]

**Example 2.** Let \( A \in \mathbb{R}^{n \times n} \) be a negative semi-definite matrix and let \( g(t) = f(t)p, \) \( p \in \mathbb{R}^n \), where \( f(t) \) is a \( 2\ell \)-periodic "sawtooth wave", i.e.,
\[
f(t) = \frac{t}{2\ell}, \quad 0 \leq t \leq 2\ell.
\]
In this case \( f(t) \) has the Fourier series defined by \( b_k = -\frac{1}{k\pi} \), \( c_k = \frac{k\pi}{\ell} \). Furthermore, let \( u(t) \) denote the solution of (2.1) and \( u_N(t) \) that of (2.3). Then using the lemma above we have

\[
\|u(t) - u_N(t)\|^2 \leq \sum_{k=N}^{\infty} \frac{1}{k^2} \|\varphi_k^\sin(A)\| \|p\| \leq \frac{\|p\|\ell}{\pi^2(N-1)}.
\]

3 Approximation of the Itô integral using the Karhunen–Loéve expansion

In the previous section we were focused on deterministic differential equations in order to explain our approach. We are now ready to consider a linear differential equation with an additive stochastic term by applying the same methodology.

Let us consider the stochastic differential equation

\[
dX_t = LX_t + BdW_t,
\]

where \( X_t \in \mathbb{R}^n \), \( L \in \mathbb{R}^{n \times n} \) and \( W_t \) is the standard Wiener process. The exact solution is given by (see [10, Sec. 4.8])

\[
X_t = e^{tL}X_0 + \int_0^t e^{(t-s)L}BdW_s,
\]

where the stochastic integral is defined here as the Itô integral. That is,

\[
\int_0^t f(s) dW_s = \lim_{n \to \infty} \sum_{[t_{i-1}, t_i] \in \pi_\ell} f(t_{i-1})(W_{t_i} - W_{t_{i-1}}),
\]

where \( \pi_\ell \) is a sequence of partitions of \([0, t]\) with mesh size going to zero as \( \ell \to \infty \), i.e.

\[
\pi_\ell = \{[t_0, t_1], \ldots, [t_{\ell-1}, t_\ell] \}
\]

such that \( 0 = t_0 < t_1 < \ldots < t_\ell = t \). We note that for equation (3.1) the Itô and the Stratonovich definitions are actually equivalent.

To relate the stochastic process to the nonlinear function \( g(t) \) used in the previous section, we proceed by replacing \( W_t \) with its Karhunen–Loéve expansion

\[
W_t = \sqrt{2} \sum_{k=1}^{\infty} Z_k \frac{\sin(\lambda_k t)}{\lambda_k},
\]

where \( \lambda_k = (k - 1/2)\pi \) and \( Z_k \) are independent normally distributed vector valued random variables with zero mean and unit variance. This also means that each component \((Z_k)_i\), \( 1 \leq i \leq n \), of the vectors \( Z_k \) are independent \( N(0, 1) \) distributed random variables.
To obtain a practical method we approximate the Brownian motion $W_t$ by the truncated Karhunen–Loéve expansion

$$W_t \approx W^m_t := \sqrt{2} \sum_{k=1}^{m} Z_k \frac{\sin(\lambda_k t)}{\lambda_k}.$$  

(3.3)

The truncated expansion $W^m_t$ is always differentiable with respect to $t$ and therefore

$$\int_0^t e^{(t-s)L} B dW^m_s = \sqrt{2} \sum_{k=1}^{m} \int_0^t \left( e^{(t-s)L} \left( \frac{d}{ds} \frac{\sin(\lambda_k s)}{\lambda_k} \right) ds \right) B Z_k$$

(3.4)

where the functions $\varphi_{k,t}^\cos(z)$ correspond to the sequence $(\lambda_k)_{k=1}^\infty \subset \mathbb{R}$ taken from the Karhunen–Loéve expansion. As $m$ goes to infinity the integral converges in the $L^2$ sense, the proof of which follows from the Wong–Zakai theorem [18], [22], [23]. For the convergence properties of general bases we refer to the appendix of [13].

We are now ready to present the solution to our stochastic differential equation in terms of matrix functions. For the proof of the following theorem we refer to [21, Sec. 2].

**Theorem 3.** The solution of (3.1) has the representation

$$X_t = e^{tL} X_0 + \sqrt{2} \sum_{k=1}^{\infty} \varphi_{k,t}^\cos(L) B Z_k,$$

(3.5)

where $Z_k$ are independent $\mathcal{N}(0, 1)$ distributed vector valued random variables, the functions $\varphi_{k,t}^\cos$ are defined by the coefficients $\lambda_k$ of the Karhunen–Loéve expansion of $W_t$ and equation (2.6), and where the convergence is in $L^2$ and uniform in $t$.

From the representation (3.5) we may deduce the following properties. The proof is left to the appendix.

**Theorem 4.** We have

1. $\mathbb{E}(X_t) = e^{tL} X_0$.

2. $\mathbb{E}(\|X_t\|^2) = \|e^{tL} X_0\|^2 + 2 \sum_{k=1}^{\infty} \|\varphi_{k,t}^\cos(L) B\|^2_F$, where $\| \cdot \|_F$ is the Frobenius norm.

For the special case when $L$ is a normal operator we have the following.

**Corollary 5.** Suppose $B = c I$ for some $c \in \mathbb{R}$ and that $L \in \mathbb{R}^{n \times n}$ is normal, i.e. unitarily diagonalizable. Then,

$$\mathbb{E}(\|X_t\|^2) = \|e^{tL} X_0\|^2 + 2c^2 \sum_{k=1}^{\infty} \sum_{\lambda \in \Lambda(L)} \left| \varphi_{k,t}^\cos(\lambda) \right|^2,$$

where $\Lambda(L)$ denotes the spectrum of $L$.

**Proof.** The claim follows from Theorem 4, the fact that for all $A \in \mathbb{R}^{n \times n}$, $\|A\|_F^2 = \sum_i \sigma_i^2$, where $\sigma_i$’s are the singular values of $A$, and from the fact that for normal matrices the singular values equal the absolute values of the eigenvalues. \qed
4 Numerical method and its analysis

In Theorem 3 we expressed the solution to our stochastic differential equation as an infinite sum of matrix functions. To evaluate this numerically we will approximate this by a finite sum of matrix functions

\[ X^m_t = e^{tL}X_0 + \sqrt{2} \sum_{k=1}^{m} \varphi_{k,t}^{\cos}(L)BZ_k. \] (4.1)

To simplify the discussion, let us assume that \( L \) is negative semidefinite for the moment. In this case, the strong mean squared error has the following bound.

**Theorem 6.** Let the linear operator \( L \in \mathbb{R}^{n \times n} \) in (3.1) be negative semidefinite. The error introduced by the approximation (4.1) with \( m \) terms satisfies the following theorem, of which proof is in the appendix.

\[
E(\|X_t - X^m_t\|^2) = 2 \sum_{k=m+1}^{\infty} \|\varphi_{k,t}^{\cos}(L)B\|^2_F \leq \frac{2\|B\|^2_F}{\pi^2} \frac{n}{m-1}. 
\]

For the second moment of the norm of \( X^m_t \), analogously to Theorem 4, we have the following result.

**Lemma 7.** \( X^m_t \) satisfies the following

\[
E(\|X^m_t\|^2) = \|e^{tL}X_0\|^2 + 2 \sum_{k=1}^{m} \|\varphi_{k,t}^{\cos}(L)B\|^2_F. 
\]

It is easy to see that the weak error \( ||E(X_t - X^m_t)|| \) is always zero. For the weak error of the second moment of the solution we get the following bound, which is a direct consequence of Theorem 4 and Lemma 7.

**Theorem 8.** The following weak error bound holds:

\[
E(||X_t||^2) - E(||X^m_t||^2) = 2 \sum_{k=m+1}^{\infty} \|\varphi_{k,t}^{\cos}(L)B\|^2_F \leq \frac{2\|B\|^2_F}{\pi^2} \frac{n}{m-1}. 
\]

Theorem 6 shows that the method has the same strong order of convergence \( \frac{1}{2} \) as the Euler–Maruyama method in the sense that it converges pathwise as \( O(1/\sqrt{m}) \) with respect to the number of time steps \( m \). Similarly, Theorem 8 indicates that the second moment of the norm of the numerical solution has a weak order of convergence \( 1 \) (see [10] for the definitions).

4.1 Sectorial matrices

The above bounds can be easily generalized to coefficient matrices \( L \) which are sectorial. This means that the numerical range of \( L \) lies within a cone of a given angle opening to the
left. These matrices often occur following spatial discretizations of parabolic PDEs that lead to nonsymmetric or nonnormal coefficient matrices $L$, e.g. in advection diffusion equations.

Let $\alpha \in [0, \frac{\pi}{2})$ and define

$$S_\alpha := \{0\} \cup \{ z \in \mathbb{C} : |\text{Arg}(-z)| \leq \alpha\},$$

i.e., $S_\alpha$ is a cone of angle $2\alpha$ with its vertex in origin. Using this notation we give the following definition.

**Definition 9.** Let $\alpha \in [0, \frac{\pi}{2})$ and $\gamma \in \mathbb{R}$. The matrix $L$ is called sectorial with half-angle $\alpha$ and vertex $\gamma$ if the numerical range $\mathcal{F}(L - \gamma I)$ is contained in $S_\alpha$.

If $L$ is sectorial with vertex $\gamma$ and half-angle $\alpha$, and if $\lambda \in \mathbb{R}$ such that $i\lambda \not\in S_\alpha$, then by simple geometry it can be shown that

$$\frac{1}{d(i \lambda, \mathcal{F}(L))} \leq \frac{1}{|\lambda| \cos \alpha - \gamma \sin \alpha}.$$

### 4.2 The Brownian bridge and other stochastic processes

Another example of where our theory can be applied is the Brownian bridge $B_t = W_t - tW_1$, which can be represented as the series

$$B_t = \sqrt{2} \sum_{k=1}^{\infty} Z_k \frac{\sin(\lambda_k t)}{\lambda_k},$$

where the $Z_k$ are vectors with elements drawn from a normal $\mathcal{N}(0,1)$ distribution and $\lambda_k = \pi k$. Note that this is identical to the Karhunen–Loève expansion for standard Brownian motion \[3.2\], except that in the previous case $\lambda_k = (k - 1/2)\pi$. One can trivially adapt the results from the previous sections to this, and similar, stochastic processes in order to work with a range of different models.

### 4.3 Gaussian Processes

We remark that the solution of the linear SDE is a Gaussian process so that it is uniquely determined by its mean and covariance which satisfy a vector valued linear differential equation and a matrix valued Lyapunov differential equation, respectively [16, Sec. 6]. Thus, our proposed sampling method can be seen as a way to avoid the expensive solving of the matrix valued differential equations. Moreover, changing the initial value of the system affects only the first term $e^{tL}X_0$ which allows efficient sampling also in the case the initial value $X_0$ is a random variable.

### 5 Evaluation using matrix functions

We next describe different approaches for evaluating the approximation $X^n_t$ given in (4.1) using matrix functions.
5.1 Diagonalization of $L$

We first investigate the case where $L$ is diagonalizable, i.e., $L = VDV^{-1}$ where $D \in \mathbb{C}^{n \times n}$ is diagonal. Then we can rewrite the numerical approximation (2.4) as

$$u_N(t) = e^{tL}u_0 + \sqrt{2}V \sum_{k=1}^{m} \varphi_{k,t}^{\text{cont}}(tD)V^{-1}Z_k.$$  \hspace{1cm} (5.1)

The drawback of this approach is that not all matrices $L$ are diagonalizable and, even if such a decomposition exists, it will destroy any structure such as sparsity in $L$ and requires large amounts of memory for larger matrices. The computation is also rather expensive (around $25n^3$ flops). However, if $L$ is sufficiently small and diagonalizable it may be worth doing the initial diagonalization to speed up the subsequent sampling.

An important special case is normal $L$. This means that $L$ is unitarily diagonalizable, i.e., there exists a unitary $V \in \mathbb{C}^{n \times n}$ such that $L = VDV^*$ for some diagonal $D$. If the elements of $Z_k \in \mathbb{R}^n$ are i.i.d. normally distributed with variance 1, then so are the elements of the vector $V^*Z_k$ \[13\] Thm. 2.1.2.]. This implies that instead of (5.1) we may use the simplified sampling formula

$$u_N(t) = e^{tL}u_0 + \sqrt{2}V \left( \sum_{k=1}^{m} \varphi_{k,t}^{\text{cont}}(tD)\tilde{Z}_k \right),$$ \hspace{1cm} (5.2)

where the elements of the vectors $\tilde{Z}_k$ are i.i.d. normally distributed with variance 1.

5.2 Linearization of the truncated SDE

We next consider methods for a general $L$. These methods can also exploit the possible sparsity of $L$. We start by considering the truncated series (2.2) and denote the vector of the first $N$ basis functions by $y_N(t)$,

$$y_N(t) = \begin{bmatrix} \cos(c_1t) \\ \vdots \\ \cos(c_Nt) \\ \sin(c_1t) \\ \vdots \\ \sin(c_Nt) \end{bmatrix}. \hspace{1cm} (5.3)$$

Using this notation it is clear that $y_N(t)$ satisfies the system of differential equations

$$\dot{y}_N(t) = \begin{bmatrix} 0 & C_N \\ -C_N & 0 \end{bmatrix} y_N(t), \hspace{0.5cm} y_N(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

where $C_N = \text{diag}(c_1, \ldots, c_N)$ and $1 = [1 \ldots 1]^T$. This allows us to rewrite $y_N(t)$ as

$$y_N(t) = \exp \left( t \begin{bmatrix} 0 & C_N \\ -C_N & 0 \end{bmatrix} \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \hspace{1cm} (5.4)$$

Each realization of the SDE \[8_{31}\] is simply a special case of the deterministic equation analyzed in section \[2\]. Indeed, we see that the solution presented in Theorem \[3\] is a special
case of (2.4). In order to compute our approximation to the solution efficiently we must be able to evaluate matrix–vector products of the form \( \varphi_{k,t}(A) v \) and \( \psi_{k,t}(A) v \). We reformulate this solution in terms of the matrix exponential.

To begin our reformulation, let us define \( A_N, B_N \in \mathbb{R}^{n \times N} \) by
\[
A_N = \begin{bmatrix} a_1 & \cdots & a_N \end{bmatrix} \quad \text{and} \quad B_N = \begin{bmatrix} b_1 & \cdots & b_N \end{bmatrix}.
\]
When \( y_N(t) \) is defined as in (5.3), we see that
\[
g_N(t) = [A_N \quad B_N] y_N(t) = [A_N \quad B_N] \exp \left( t \begin{bmatrix} 0 & -C_N \\ C_N & 0 \end{bmatrix} \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix}
\]
Using this, we obtain the following result with proof left to the appendix (see also Thm. 2.1 in [1]).

**Theorem 10.** Let \( L \in \mathbb{R}^{n \times n} \), \( g_N(t) \) be the partial Fourier series defined by the coefficients \( a_k, b_k, c_k \), and let \( u_N(t) \) be the solution of (2.3). Then,
\[
u_N(t) = \begin{bmatrix} I_n & 0 \end{bmatrix} \exp \left( t \begin{bmatrix} L & A_N \\ 0 & 0 \end{bmatrix} B_N \begin{bmatrix} 0 & -C_N \\ C_N & 0 \end{bmatrix} \right) \begin{bmatrix} u_0 \\ 1 \end{bmatrix}
\]
where \( 1 = [1 \ \ldots \ 1]^T \).

For a more specific example, let us consider the stochastic differential equation
\[
\dot{u}_N(t) = Lu_N(t) + dW_t^N,
\]
where \( dW_t^N \) denotes the truncated Karhunen–Loève expansion of the Weiner process [8,9]. This is a special case of Theorem 8 where \( B = I_n \). For this particular problem, if \( Z_N \in \mathbb{R}^{n \times N} \) is a matrix with independent elements drawn from a normal \( \mathcal{N}(0,1) \) distribution, we would have \( A_N = [0, \ldots, 0] \), \( B_N = \sqrt{2} Z_N \), and \( C_N = \text{diag} \left( \frac{1}{\pi}, \ldots, (N - \frac{1}{2}) \pi \right) \).

Since we have now simplified the computation of the solution into the product of the matrix exponential multiplied by a vector one can take advantage of many efficient methods for its computation. As an example we mention the scaling and squaring method [1] and the Krylov subspace methods [15]. The best method for computing \( u_N(t) \) for any particular problem will depend largely upon the matrix \( L \) (i.e. whether \( L \) is small and dense or large and sparse) and the accuracy required in the final solution.

We next consider a specific approach which exploits the fact that only the matrix \( B_N \) changes when using the expression (5.5) to evaluate samples of \( X_t^m \).

### 5.2.1 Sylvester equation approach

Since only the matrix \( B_N \) changes for each realization of \( X_t^m \), it is only the \((1,2)\)-block of size \( n \times 2N \) in the exponential (5.5) that changes for each \( X_t^m \). We have the following result which can be used to efficiently compute the \((1,2)\)-block. The proof is given in the appendix.

\[
\dot{u}_N(t) = Lu_N(t) + dW_t^N,
\]
Lemma 11. Let $L \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$ and $C \in \mathbb{R}^{m \times m}$. Then,

$$\exp \left( t \begin{bmatrix} L & B \\ 0 & C \end{bmatrix} \right) = \begin{bmatrix} e^{tL} & X(t) \\ 0 & e^{tC} \end{bmatrix},$$

where $X(t)$ satisfies the Sylvester equation

$$LX(t) - X(t)C = e^{tL}B - Be^{tC}. \quad (5.6)$$

When sampling, we set $C = \begin{bmatrix} 0 & -C_N \\ C_N & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 0 & B_N \end{bmatrix}$. Notice that $C$ has purely imaginary eigenvalues, so that if $A$ has its spectrum on the left half-plane, for example, the spectra of $A$ and $C$ are well separated and the Sylvester equation (5.6) always has a solution. This strategy has also been mentioned in [5, p.248].

6 Numerical experiments

We are now ready to test our novel methods against the Euler–Maruyama and backward Euler–Maruyama scheme. We use two illustrative stochastic differential equations to compare the methods. The first one is a small dimensional equation so that the diagonalization approach described in Sec. 5.1 can be used. Moreover, the equation is non-stiff so we compare it to the explicit Euler–Maruyama scheme. The second SDE is a large-dimensional stiff equation, and we compare the Sylvester equation based approach of Sec. 5.2.1 to the backward Euler–Maruyama scheme. As a metric for comparison we use the weak convergence of the second order moment $\mathbb{E} \|X_t\|^2$.

All experiments in this section were performed on a laptop machine with an Intel Core i5 (3.1 GHz) with 16GB of RAM. Computations were performed with MATLAB 2016b.

The sampling errors of the computed quantities decay like $1/\sqrt{N}$, where $N$ is the size of the sample. For details, see [10, Sec. 1.9]. Thus, when comparing the convergences of different methods, attention has to be paid to the selection of large enough $N$.

The MATLAB code for the experiments is provided in the supplementary material.

6.1 Turbulent diffusion

For our first example we consider the following small example of turbulent diffusion taken from Kloeden and Platen [10, Sec. 7]. For variables $V_t^{(1)}, V_t^{(1)} \in \mathbb{R}^3$, the equations describing the system are given by

$$dV_t^{(1)} = \left( -\frac{1}{T_1} V_t^{(1)} - \beta (V_t^{(1)} - V_t^{(2)}) \right) dt + \sigma_1 dW_t^{(1)}$$

$$dV_t^{(2)} = \left( -\frac{1}{T_2} V_t^{(2)} + \beta (V_t^{(1)} - V_t^{(2)}) \right) dt + \sigma_2 dW_t^{(2)},$$

where $\sigma_1, \sigma_2, T_1, T_2$ are constants that determine the behaviour of the system. This 6 dimensional system can be reformulated into a single equation: if we denote $V = [V^{(1)}, V^{(2)}]^T$ then

$$dV_t = \begin{bmatrix} -\frac{1}{T_1} + \frac{\beta}{T_1} & \beta T_2 \\ \beta T_1 & -\frac{1}{T_2} + \frac{\beta}{T_2} \end{bmatrix} V_t + \begin{bmatrix} \sigma_1 T & 0 \\ 0 & \sigma_2 T \end{bmatrix} dW_t. \quad (6.1)$$
Figure 1: First two components of a single trajectory $V^m_t$ with $m = 1000$ time discretization points. The black dots depict the initial and end points, starting at $[1 \ 1]^T$.

We observe that the system is of the form (3.1) with a symmetric coefficient matrix $L$. This allows us to apply the efficient sampling formula (5.2) based on the diagonalization of normal matrices (see section 5.1).

Our aim is to compare this diagonalization procedure based upon the Karhunen–Loève expansion to the Euler–Maruyama time-stepping scheme

$$V_{i+1} = V_i + \Delta t LV_i + B\Delta W_i,$$

where $\Delta W_i$’s are independent normally distributed random variables with covariance $\Delta t I_n$. The coefficient matrices $L$ and $B$ are given in (6.1).

For this experiment we set the parameters $T_1 = T_2 = 0.5$, $\sigma_1 = \sigma_2 = 1$, and $\beta = 2$. The initial value is set to $V_0 = [1 \ 1 \ldots \ 1]^T$. To give some insight into the typical behaviour a fluid particle might have under these conditions, we have plotted a single particle trajectory (projected onto a 2D plane) in Figure 1. This trajectory was computed using the Euler–Maruyama scheme with $m = 1000$ time discretization points.

We denote by $m$ both the number of time discretization points in the Euler–Maruyama method and the length of the Karhunen–Loève expansion. We evaluate the KL expansion based method for values $m = 10, 20, 40, 80, 160, 320, 640, 1280, 2560$. The Euler–Maruyama method is evaluated for $m = 10, 20, 40, 80, 160, 320$. In Figure 2 we denote by $X^m_t$ the approximation of both methods.

For each estimate of $\mathbb{E}(\|X^m_t\|^2)$ we draw $10^7$ samples and the reference value $\mathbb{E}(\|X_t\|^2)$ is computed in high precision using the expression given in Corollary 5. There is little difference between the two approaches in terms of their convergence, but the Karhunen–Loève approach (using the sampling method described in section 5.1) is much more efficient: both runtimes
Figure 2: Compute times vs. the weak error $|E(\|X_t\|^2) - E(\|X^m_t\|^2)|$ for the KL-expansion based method for different lengths of the expansion and Euler–Maruyama method with different number of time steps. Each estimate of $E(\|X^m_t\|^2)$ is an average of $10^7$ samples.

scale linearly with the sample size but the Karhunen–Loève approach is around 10 times faster.

6.2 A finite difference discretization of a heat equation with additive noise

In our second experiment we consider a one dimensional stochastic partial differential equation

$$\frac{\partial}{\partial t} y(x,t) = \varepsilon \frac{\partial^2}{\partial x^2} y(x,t) + \alpha \frac{\partial}{\partial x} y(x,t) + \beta \frac{\partial^2 W}{\partial t \partial x},$$

$y(0,x) = y_0(x), \quad 0 \leq x \leq 1,$

$y(t,0) = y(t,1) = 0, \quad t \geq 0.$

Here $\frac{\partial^2 W}{\partial t \partial x}$ denotes mixed second order derivative of the so called Brownian sheet \[2\]. The initial value $y_0(x)$ is given by

$$y_0(x) = \begin{cases} 2x, & \text{if } 0 \leq x \leq \frac{1}{2} \\ 2 - 2x, & \text{if } \frac{1}{2} \leq x \leq 1. \end{cases}$$

Spatial discretization using finite differences leads to the SDE (see e.g. [2])

$$dX = LX \, dt + \frac{\beta}{\sqrt{\Delta x}} dW, \quad X(0) = X_0, \quad (6.2)$$
where \( \Delta x = L/(n+1) \), \( L = \varepsilon \Delta_n + \alpha \nabla_n \),

\[
\Delta_n = \frac{1}{(\Delta x)^2} \begin{bmatrix} -2 & 1 \\ 1 & \ddots & \ddots \\ \ddots & \ddots & 1 & -2 \\ 1 & \ddots & \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \end{bmatrix}, \quad \nabla_n = \frac{1}{2\Delta x} \begin{bmatrix} 1 \\ -1 \\ \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots \\ -1 \\ \end{bmatrix},
\]

and \( X_0 \in \mathbb{R}^n \) is the discretization of the initial value \( y_0(x) \). We set \( n = 200, \varepsilon = 0.1, \alpha = -1.0, \beta = 0.1 \), and integrate up to \( t = 0.4 \). Figure 3 depicts 4 random samples and the expectation at \( t = 0.4 \).

We evaluate each realization of the truncated KL-expansion using the augmented exponential and Sylvester equation technique described in Section 5.2. This means that at each step we solve a Sylvester equation of the form (A.1). As the coefficient matrix is sparse, the Sylvester equation is efficiently solved by vectorizing the equation and reusing the sparse LU factors throughout the sampling process.

As the SDE (6.2) is now stiff (see [10]), we compare it to the backward Euler–Maruyama method

\[
X_{i+1} = (I - \Delta tL)^{-1}X_i + B\Delta W_i, \quad (6.3)
\]

where \( \Delta W_i \)'s are independent normally distributed random vectors with covariance \( \Delta tI_n \) and \( B = \frac{\beta}{\sqrt{\Delta x}} I_n \).

In the implementation of the backward Euler–Maruyama method, we use a precomputed sparse LU-factorization for \( I - \Delta tL \) to evaluate the time steps.

We evaluate the KL expansion based method for the expansion length \( m = 1, 2, \ldots, 2^5 \). The backward Euler–Maruyama method is evaluated for number of time steps \( m = 50, 100, \ldots, 800 \). In Figure 4 we denote by \( X^m_t \) the approximation of both methods.
Figure 4: Compute times vs. the relative weak error $\frac{|E(\|X_t\|^2) - E(\|X^m_t\|^2)|}{E(\|X_t\|^2)}$ for the KL-expansion based method and backward Euler–Maruyama method with different number of time steps. Each estimate of $E(\|X^m_t\|^2)$ is an average of $10^5$ samples.

The Karhunen–Loéve approach (using the Sylvester equation approach described in Sec. 5.2.1) is again more efficient (see Figure 4). However, although both methods have the weak order of convergence $O(\frac{1}{m})$, the compute time of KL approach grows quadratically with $m$ which explains the difference in the slopes of the lines in Figure 4. Here improvements could be made, e.g., for evaluating the right hand side of the Sylvester equation (A.1).

7 Conclusions

We have proposed a novel approach for sampling linear SDEs which exploits matrix functions and efficient numerical linear algebraic subroutines. Moreover, we have provided a convergence theory for the method which shows both the strong and weak convergence speeds. In numerical examples we showed that the method is very competitive both for non-stiff and stiff systems of equations, when comparing against the Euler–Maruyama and backward Euler–Maruyama method, respectively. As future work, we are interested in optimizing the various linear algebraic subproblems using Krylov subspaces, for example. Furthermore, our approach should be generalizable to inhomogeneous linear SDEs (see e.g. [16, Sec. 6]).
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A Proofs

Theorem 4. We have

1. \( \mathbb{E}(X_t) = e^{tL}X_0 \).

2. \( \mathbb{E}(\|X_t\|^2) = \|e^{tL}X_0\|^2 + 2 \sum_{k=1}^{\infty} \|\varphi_{k,t}^{\cos}(L)B\|^2_F \), where \( \| \cdot \|_F \) is the Frobenius norm.

Proof. We see from (3.4) that for all \( m > 0 \)

\[
\mathbb{E}\left( \int_0^t e^{(t-s)L}B dW_s^m \right) = \sqrt{2} \sum_{k=1}^{m} \varphi_{k,t}^{\cos}(L)B \mathbb{E}(Z_k) = 0
\]

which implies the first claim.

Since the elements of \( Z_i \)'s are i.i.d. \( \mathcal{N}(0,1) \) - distributed, it is easily verified that for all \( A \in \mathbb{R}^{n \times n} \) we have \( \mathbb{E}(Z_i^T A Z_j) = \delta_{ij} \text{tr}(A) \), where \( \text{tr}(A) \) denotes the trace of \( A \). Thus, it follows from (3.5) that

\[
\mathbb{E}\|X_t\|^2 = \|e^{tL}X_0\|^2 + 2 \sum_{k=1}^{\infty} \mathbb{E}\left( \left( \varphi_{k,t}^{\cos}(L)BZ_k \right)^T \varphi_{k,t}^{\cos}(L)BZ_k \right)
\]

\[
= \|e^{tL}X_0\|^2 + 2 \sum_{k=1}^{\infty} \text{tr}\left( \left( \varphi_{k,t}^{\cos}(L)B \right)^T \varphi_{k,t}^{\cos}(L)B \right).
\]

The second claim follows then the fact that for all \( A \in \mathbb{R}^{n \times n} \), \( \text{tr}(A^T A) = \|A\|^2_F \). \( \square \)
Theorem 6. Let the linear operator \( L \in \mathbb{R}^{n \times n} \) in (3.1) be negative semidefinite. The error introduced by the approximation (4.1) with \( m \) terms satisfies

\[
E \left( \| X_t - X^m_t \|^2 \right) = 2 \sum_{k=m+1}^{\infty} \| \varphi_{k,t}^\cos(L) B \|^2_F \leq \frac{2 \| B \|^2}{\pi^2} \frac{n}{m-1}.
\]

Proof. From the representation (3.5) and (4.1), it follows that

\[
E \left( \| X_t - X^m_t \|^2 \right) = E \left( \sqrt{2} \sum_{k=m+1}^{\infty} \varphi_{k,t}^\cos(L) B Z_k \right)^2.
\]

Following the lines of the proof of Theorem 4, we see

\[
E \left( \| X_t - X^m_t \|^2 \right) = 2 \sum_{k=m+1}^{\infty} \| \varphi_{k,t}^\cos(L) B \|^2_F.
\]

For all \( A \in \mathbb{R}^{n \times n} \) it holds that \( \| A \|_F \leq \sqrt{m} \| A \|_2 \), and therefore

\[
E \left( \| X_t - X^m_t \|^2 \right) \leq 2n \| B \|^2 \sum_{k=m+1}^{\infty} \| \varphi_{k,t}^\cos(L) \|^2.
\]

Using Lemma 2 to bound \( \| \varphi_{k,t}^\cos(L) \| \) gives

\[
\sum_{k=m+1}^{\infty} \| \varphi_{k,t}^\cos(L) \|^2 \leq \sum_{k=m+1}^{\infty} \frac{1}{((k - \frac{1}{2}) \pi)^2}
\]

\[
\leq \sum_{k=m}^{\infty} \frac{1}{(k \pi)^2}
\leq \int_{m-1}^{\infty} \frac{1}{(\pi x)^2} dx
\leq \frac{1}{\pi^2(m-1)}.
\]

Theorem 10. Let \( L \in \mathbb{R}^{n \times n} \), \( g_N(t) \) be the partial Fourier series defined by the coefficients \( a_k, b_k, c_k \), and let \( u_N(t) \) be the solution of (2.3). Then,

\[
u_N(t) = [I_n \ 0] \exp \left( t \left[ \begin{array}{cc} L & A_N & B_N \\ 0 & 0 & -C_N \\ 0 & C_N & 0 \end{array} \right] \right) \left[ \begin{array}{c} u_0 \\ 1 \\ 0 \end{array} \right]
\]

where \( 1 = [1 \ldots 1]^T \).
Proof. The claim follows from the fact that for any square matrices $X_1$ and $X_2$ \[\text{pp. 248}\]

\[
\exp \left( t \begin{bmatrix} X_1 & X_3 \\ 0 & X_2 \end{bmatrix} \right) = \begin{bmatrix} e^{tX_1} & \int_0^t e^{(t-s)X_1}X_3 e^{sX_2} \, ds \\ 0 & e^{tX_2} \end{bmatrix}.
\]

We can select $X_1 = L$, $X_2 = \begin{bmatrix} 0 & -C_N \\ C_N & 0 \end{bmatrix}$, and $X_3 = [A_N, B_N]$ before combining this result with the substitution

\[
\exp \left( t \begin{bmatrix} 0 & -C_N \\ C_N & 0 \end{bmatrix} \right) = \begin{bmatrix} \cos(t C_N) & -\sin(t C_N) \\ \sin(t C_N) & \cos(t C_N) \end{bmatrix}.
\]

\[\square\]

Lemma 11. Let $L \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$ and $C \in \mathbb{R}^{m \times m}$. Then,

\[
\exp \left( t \begin{bmatrix} L & B \\ 0 & C \end{bmatrix} \right) = \begin{bmatrix} e^{tL} & X(t) \\ 0 & e^{tC} \end{bmatrix},
\]

where $X(t)$ satisfies the Sylvester equation

\[
LX(t) - X(t)C = e^{tL}B - Be^{tC}.
\] (A.1)

Proof. Since every matrix commutes with its exponential, it holds

\[
\begin{bmatrix} L & B \\ 0 & C \end{bmatrix} \begin{bmatrix} e^{tL} & X(t) \\ 0 & e^{tC} \end{bmatrix} = \begin{bmatrix} e^{tL} & X(t) \\ 0 & e^{tC} \end{bmatrix} \begin{bmatrix} L & B \\ 0 & C \end{bmatrix}.
\]

The $(1,2)$-block of this matrix equation gives the Sylvester equation (A.1). \[\square\]