Improving Heun's method for additive noise SDEs

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Introduction

We consider stochastic differential equations (SDEs) with the form:

$$dy_t = f(y_t)\,dt + \sigma\,dW_t, \tag{1}$$

where the solution $y = \{y_t\}_{t\in[0,T]}$ takes its values in $\mathbb{R}^d$, the function (also known as the "vector field") $f : \mathbb{R}^d \to \mathbb{R}^d$ is sufficiently regular (e.g. globally Lipschitz continuous and with linear growth), $\sigma \in \mathbb{R}^{d\times w}$ is a $d \times w$ matrix and W denotes a w-dimensional Brownian motion.

As one might expect, many well-known SDEs have additive noise:

- The Ornstein–Uhlenbeck process ($f(y) = a(b - y)$ with $a, b \in \mathbb{R}$)
- Overdamped Langevin dynamics ($f = -\nabla U$ where $U : \mathbb{R}^d \to \mathbb{R}$)
- Underdamped Langevin dynamics

$$dQ_t = P_t\,dt, \quad dP_t = -\nabla U\big(Q_t\big)\,dt - \nu P_t\,dt + \sqrt{\frac{2\nu}{\beta}}\,dW_t.$$

Introduction

In general, (1) cannot be solved exactly and must be approximated.

The two most popular methods for solving additive noise SDEs are:

1. The Euler-Maruyama method [1, 2, 3]. For additive noise SDEs, this method coincides with the higher order Milstein's method.

$$Y_{n+1}^{\mathsf{EM}} := Y_n^{\mathsf{EM}} + f\big(Y_n^{\mathsf{EM}}\big)(t_{n+1} - t_n) + \sigma\big(W_{t_{n+1}} - W_{t_n}\big). \tag{2}$$

2. Heun's method [2, 4, 5, 7], which involves two evaluations of f.

$$\begin{aligned}
\widetilde{Y}_{n+1}^{\mathsf{H}} &:= Y_n^{\mathsf{H}} + f\big(Y_n^{\mathsf{H}}\big)(t_{n+1} - t_n) + \sigma\big(W_{t_{n+1}} - W_{t_n}\big), \\
Y_{n+1}^{\mathsf{H}} &:= Y_n^{\mathsf{H}} + \frac{1}{2}\Big(f\big(Y_n^{\mathsf{H}}\big) + f\big(\widetilde{Y}_{n+1}^{\mathsf{H}}\big)\Big)(t_{n+1} - t_n) + \sigma\big(W_{t_{n+1}} - W_{t_n}\big).
\end{aligned} \tag{3}$$

We note that each increment of the Brownian motion over $[t_n, t_{n+1}]$ is independent and distributed as $\big(W_{t_{n+1}} - W_{t_n}\big) \sim N\big(0, (t_{n+1} - t_n) I_d\big)$.

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Definition (Strong convergence)

A numerical solution Y for (1) is said to converge in a strong sense with order α if there exists a constant $C > 0$ such that

$$\left\| Y_N - y_T \right\|_{L^2(\mathbb{P})} \leq C h^{\alpha}, \tag{4}$$

for all sufficiently small step sizes $h = \frac{T}{N}$, where we define $\| \cdot \|_{L^2(\mathbb{P})}$ as

$$\| \cdot \|_{L^2(\mathbb{P})} := \sqrt{\mathbb{E}\left[\| \cdot \|_2^2 \right]}.$$

Definition (Weak convergence)

A numerical solution Y for (1) is said to converge in a weak sense with order β if for any polynomial p there exists $C_p > 0$ such that

$$\left| \mathbb{E}\left[p\left(Y_N\right)\right] - \mathbb{E}\left[p\left(y_T\right)\right] \right| \leq C_p h^{\beta}, \tag{5}$$

for all sufficiently small step sizes $h = \frac{T}{N}$.

Introduction

Table: Convergence rates for the Euler-Maruyama and Heun methods

	Number of vector field evaluations per step	Type of convergence		
		Strong	Weak	$\sigma = 0$
Euler-Maruyama	1	$O(h)$	$O(h)$	$O(h)$
Heun	2	$O(h)$	$O(h^2)$	$O(h^2)$

We note that for Heun's method to achieve a second order rate of weak convergence, we require further smoothness assumptions on f (for example, f' and f'' to be bounded and Lipschitz continuous).

Question

Can we modify these numerical methods to improve performance?

The non-Markov Euler-Maruyama method

The following non-Markov version of the Euler-Maruyama method is considered in [6, 7] for when $f = -\nabla U$ and the SDE (1) is ergodic.

$$Y_{n+1}^{\mathsf{NEM}} := Y_n^{\mathsf{NEM}} + f\big(Y_n^{\mathsf{NEM}}\big)h + \frac{1}{\sqrt{2}}\sigma\big(\xi_n + \xi_{n+1}\big), \tag{6}$$

where $h = \frac{T}{N}$ and $\{\xi_n\}$ are iid random variables with $\xi_n \sim N\big(0, hI_d\big)$.

Whilst this method has first order weak convergence on a finite time horizon, it achieves second order convergence in the limit as $t \to \infty$.

Moreover, this non-Markovian Euler-Maruyama method has shown superior performance at targeting the SDE's stationary distribution than Heun's method.

A Heun-based stochastic Runge-Kutta method

The following stochastic Runge-Kutta (SRK) method given in [4] achieves both strong order 1.5 and weak order 2.0 convergence.

$$\begin{aligned}
\widetilde{Y}_{n+1}^{\mathsf{RK}} &:= Y_n^{\mathsf{RK}} + \frac{3+\sqrt{6}}{6}\sigma W_n + \sigma H_n, \\
\widehat{Y}_{n+1}^{\mathsf{RK}} &:= Y_n^{\mathsf{RK}} + f\big(Y_n^{\mathsf{RK}}\big)h + \frac{3-\sqrt{6}}{6}\sigma W_n + \sigma H_n, \\
Y_{n+1}^{\mathsf{RK}} &:= Y_n^{\mathsf{RK}} + \frac{1}{2}\Big(f\big(\widetilde{Y}_{n+1}^{\mathsf{RK}}\big) + f\big(\widehat{Y}_{n+1}^{\mathsf{RK}}\big)\Big)h + \sigma W_n, \qquad (7)
\end{aligned}$$

where $h = \frac{T}{N}$ and $H_n \sim N\big(0, \frac{1}{12}hI_d\big)$ is independent of $W_n \sim N\big(0, hI_d\big)$. Moreover, H_n can be defined from $\{W_t\}_{t\in[t_n,t_{n+1}]}$ (see [8] for details).

$$\begin{aligned}
W_n &:= W_{t_{n+1}} - W_{t_n}, \\
H_n &:= \frac{1}{h}\int_{t_n}^{t_{n+1}} \Big(W_t - W_{t_n} - \frac{t-t_n}{h}\big(W_{t_{n+1}} - W_{t_n}\big)\Big)\,dt.
\end{aligned}$$

AdHoc method (Additive-noise Heun with one computation)

Instead of adapting the Euler-Maruyama method to be high order, we slightly alter Heun's method by reusing vector field evaluations.

Definition (The AdHoc method)

We construct a numerical solution $Y = \{Y_n\}_{n\geq 0}$ for the SDE (1) by setting $Y_0 = \widetilde{Y}_0 = y_0$ and for $n \geq 0$ defining Y_{n+1} from $\big(Y_n, f\big(\widetilde{Y}_n\big)\big)$ as

$$\widetilde{Y}_{n+1} := Y_n + f\big(\widetilde{Y}_n\big)(t_{n+1} - t_n) + \sigma\big(W_{t_{n+1}} - W_{t_n}\big),$$

$$Y_{n+1} := Y_n + \frac{1}{2}\Big(f\big(\widetilde{Y}_n\big) + f\big(\widetilde{Y}_{n+1}\big)\Big)(t_{n+1} - t_n) + \sigma\big(W_{t_{n+1}} - W_{t_n}\big). \quad (8)$$

This numerical method was inspired by the asynchronous leapfrog ODE solver [9, 10] which uses just one evaluation of f per step.

For simplicity, we will use a fixed step size h (i.e. $t_n = hn$ for $n \geq 0$).

AdHoc method (Additive-noise Heun with one computation)

Since we store $f(\widetilde{Y}_n)$, we only have to evaluate $f(\widetilde{Y}_{n+1})$ in each step.

Therefore the AdHoc method evaluates $f(\cdot)$ once per step and thus has the same computational cost as the Euler-Maruyama method.

Of course, this comes at a price and the resulting approximation is likely to be less accurate than Heun's method (for a given step size).

Based on our intuition and some numerical evidence, we conjecture that the AdHoc method will generally outperform Euler-Maruyama.

The AdHoc method (strong convergence)

For the error analysis, it suffices to compare against Heun's method.

We assume f is twice continuously differentiable with its derivatives f' and f'' globally bounded. We shall define $M := \sup_{y\in\mathbb{R}^d} \|f'(y)\|_2 < \infty$.

Theorem (Local error estimate for AdHoc and Heun methods)

Let $h_{\max} \in (0,1)$ be fixed. Then there exists a constant C_1 such that

$$\begin{aligned}\|Y_{n+1} - Y_{n+1}^H\|_{L^2(\mathbb{P})}^2 &\leq \Big(1 + \frac{1}{2}\big(1+4M^2\big)h_n + M^2 h_n^2\Big)\|Y_n - Y_n^H\|_{L^2(\mathbb{P})}^2 \\ &\quad + \frac{1}{2}M^2\big(1+2M^2h_n^2\big)\big(2h_n + h_n^2\big)\|\widetilde{Y}_n - Y_n^H\|_{L^2(\mathbb{P})}^2,\end{aligned}$$

$$\begin{aligned}\|\widetilde{Y}_{n+1} - Y_{n+1}^H\|_{L^2(\mathbb{P})}^2 &\leq \Big(1 + \frac{1}{2}h_n\Big)\|Y_n - Y_n^H\|_{L^2(\mathbb{P})}^2 \\ &\quad + 3M^2\big(h_n + h_n^2\big)\|\widetilde{Y}_n - Y_n^H\|_{L^2(\mathbb{P})}^2 + C_1 h_n^3,\end{aligned}$$

for $h_n = t_{n+1} - t_n \leq h_{\max}$.

The AdHoc method (strong convergence)

Sketch Proof.

The result follows by a direct calculation that uses certain moment bounds for Heun's method (i.e. $\sup_{n\geq 0} \mathbb{E}\big[\|Y_n^{\mathsf{H}}\|_2^2\big] < \infty$). We start with

$$
\begin{aligned}
&\|Y_{n+1} - Y_{n+1}^{\mathsf{H}}\|_{L^2(\mathbb{P})}^2 \\
&\quad = \|Y_n - Y_n^{\mathsf{H}}\|_{L^2(\mathbb{P})}^2 + \left\|\frac{1}{2}\Big(f\big(\widetilde{Y}_n\big) - f\big(Y_n^{\mathsf{H}}\big) + f\big(\widetilde{Y}_{n+1}\big) - f\big(\widetilde{Y}_{n+1}^{\mathsf{H}}\big)\Big)h_n\right\|_{L^2(\mathbb{P})}^2 \\
&\qquad\quad + \mathbb{E}\Big[\Big\langle Y_n - Y_n^{\mathsf{H}}, \Big(f\big(\widetilde{Y}_n\big) - f\big(Y_n^{\mathsf{H}}\big) + f\big(\widetilde{Y}_{n+1}\big) - f\big(\widetilde{Y}_{n+1}^{\mathsf{H}}\big)\Big)h_n\Big\rangle\Big] \\
&\quad \leq \Big(1 + \frac{1}{2}h_n\Big)\|Y_n - Y_n^{\mathsf{H}}\|_{L^2(\mathbb{P})}^2 \\
&\qquad\quad + \frac{1}{4}\Big\|\Big(f\big(\widetilde{Y}_n\big) - f\big(Y_n^{\mathsf{H}}\big) + f\big(\widetilde{Y}_{n+1}\big) - f\big(\widetilde{Y}_{n+1}^{\mathsf{H}}\big)\Big)\Big\|_{L^2(\mathbb{P})}^2\big(2h_n + h_n^2\big),
\end{aligned}
$$

where the last line follows by Youngs's inequality. We then apply the triangle inequality before using the Lipschitz continuity of f.

The AdHoc method (strong convergence)

Sketch Proof. (continued)

The second inequality can be similarly shown, expect we now take an $\mathscr{F}_{t_n}$-conditional expectation within the inner product and apply

$$\begin{aligned} f\big(\widetilde{Y}^{\mathsf{H}}_{n+1}\big) &= f\big(Y^{\mathsf{H}}_n + f\big(Y^{\mathsf{H}}_n\big)h_n + \sigma W_n\big) \\ &= f\big(Y^{\mathsf{H}}_n\big) + f'\big(Y^{\mathsf{H}}_n\big)\big(f\big(Y^{\mathsf{H}}_n\big)h_n + \sigma W_n\big) + R^{\mathsf{H}}_n, \end{aligned}$$

where the remainder term R^{H}_n is given by

$$R^{\mathsf{H}}_n = \int_0^1 (1-r) f''\big(Y^{\mathsf{H}}_n + r\big(f\big(Y^{\mathsf{H}}_n\big)h_n + \sigma W_n\big)\big)\, dr\, \big(f\big(Y^{\mathsf{H}}_n\big)h_n + \sigma W_n\big)^{\otimes 2},$$

which can be estimated since f'' and the second moment of Y^{H}_n are bounded. Since we take an $\mathscr{F}_{t_n}$-conditional expectation of $f\big(\widetilde{Y}^{\mathsf{H}}_{n+1}\big)$, the W_n term will disappear and we can apply the boundedness of f'.

The AdHoc method (strong convergence)

From these estimates, it follows that there exists $C_0 > 0$ such that

$$\begin{aligned}
&\| Y_{n+1} - Y_{n+1}^{\mathsf{H}} \|_{L^2(\mathbb{P})}^2 + \| \widetilde{Y}_{n+1} - Y_{n+1}^{\mathsf{H}} \|_{L^2(\mathbb{P})}^2 \\
&\qquad \leq (1 + C_0 h_n)\Big(\| Y_n - Y_n^{\mathsf{H}} \|_{L^2(\mathbb{P})}^2 + \| \widetilde{Y}_n - Y_n^{\mathsf{H}} \|_{L^2(\mathbb{P})}^2 \Big) + C_1 h_n^3.
\end{aligned}$$

Since $Y_1 = Y_1^{\mathsf{H}}$ and $\| \widetilde{Y}_1 - Y_1^{\mathsf{H}} \|_{L^2(\mathbb{P})}^2 \sim O(h^3)$, it is now easy to show:

Theorem (Global error estimate for AdHoc and Heun methods)

Let $h_{\max} \in (0,1)$ be fixed. Then there exists a constant C such that

$$\| Y_n - Y_n^{H} \|_{L^2(\mathbb{P})}^2 + \| \widetilde{Y}_n - Y_n^{H} \|_{L^2(\mathbb{P})}^2 \leq C h^2.$$

for $0 \leq n \leq N$, where Y, Y^H are computed with a step size $h \leq h_{\max}$.

The AdHoc method (weak convergence)

So by the triangle inequality, we obtain the following error estimate

$$\| Y_n - y_{t_n} \|_{L^2(\mathbb{P})} \leq \| Y_n^{\mathsf{H}} - y_{t_n} \|_{L^2(\mathbb{P})} + O(h).$$

Since Heun's method converges strongly for (1) with first order [2], it follows that the AdHoc method also has $O(h)$ strong convergence.

However, it is ongoing research to quantify the weak convergence of the method. In our numerical experiment, we will see that the AdHoc method can demonstrate second order weak convergence!

Open question

What is the weak convergence rate of the AdHoc method?

The ASH method (Additive-noise Shifted Heun)

Definition (The ASH method)

We construct a numerical solution $Y^{\mathsf{S}} = \{Y_n^{\mathsf{S}}\}_{n\geq 0}$ for the SDE (1) by setting $Y_0^{\mathsf{S}} := y_0$ and for each $n \geq 0$ defining Y_{n+1}^{S} from Y_n^{S} as

$$\widetilde{Y}_{n+1}^{\mathsf{S}} := Y_n^{\mathsf{S}} + \frac{3-\sqrt{6}}{6}\sigma W_n + \sigma H_n,$$

$$\widehat{Y}_{n+1}^{\mathsf{S}} := \widetilde{Y}_{n+1}^{\mathsf{S}} + f\big(\widetilde{Y}_{n+1}^{\mathsf{S}}\big)h_n + \frac{\sqrt{6}}{3}\sigma W_n,$$

$$Y_{n+1}^{\mathsf{S}} := Y_n^{\mathsf{S}} + \frac{1}{2}\Big(f\big(\widetilde{Y}_{n+1}^{\mathsf{S}}\big) + f\big(\widehat{Y}_{n+1}^{\mathsf{S}}\big)\Big)h_n + \sigma W_n, \tag{9}$$

where $h_n = t_{n+1} - t_n$ and $\big(W_n, H_n\big)$ are independent random vectors:

$$W_n \sim N\big(0, h_n I_d\big),$$

$$H_n \sim N\Big(0, \frac{1}{12}h_n I_d\Big).$$

The ASH method (Additive-noise Shifted Heun)

The word "shifted" refers to us modifying Y_n^{S} before evaluating $f(\cdot)$.

Unsurprisingly, the above method has the same Taylor expansion as the SRK method (7) when we exclude the $O(h^{2.5})$ remainder terms.

$$\begin{aligned}
Y_{n+1}^{\mathsf{S}} \approx Y_n^{\mathsf{S}} + f\big(Y_n^{\mathsf{S}}\big)h_n + \sigma W_n \\
&+ \sigma f'\big(Y_n^{\mathsf{S}}\big)\bigg(\frac{1}{2}h_n W_n + h_n H_n\bigg) + \frac{1}{2}f'\big(Y_n^{\mathsf{S}}\big)f\big(Y_n^{\mathsf{S}}\big)h_n^2 \\
&+ \sigma^2 f''\big(Y_n^{\mathsf{S}}\big)\bigg(\frac{5}{24}W_n^{\otimes 2} + \frac{1}{4}W_n \otimes H_n + \frac{1}{4}H_n \otimes W_n + \frac{1}{2}H_n^{\otimes 2}\bigg)h_n.
\end{aligned}$$

Therefore it also converges with strong order 1.5 and weak order 2.0.

However the new method uses two evaluations of f instead of three!

Numerical example: Scalar anharmonic oscillator

We consider the following scalar SDE,

$$dy_t = \sin\left(y_t\right)dt + dW_t,$$

with $y_0 = 1$ and define the following error estimators:

$$S_N := \sqrt{\mathbb{E}\left[\left(Y_N - Y_T^{\text{fine}}\right)^2\right]},$$

$$E_N := \left|\mathbb{E}\left[Y_N\right] - \mathbb{E}\left[Y_T^{\text{fine}}\right]\right|,$$

$$V_N := \left|\mathbb{E}\left[Y_N^2\right] - \mathbb{E}\left[\left(Y_T^{\text{fine}}\right)^2\right]\right|,$$

where the expectations are approximated by Monte-Carlo simulation and Y_T^{fine} is the numerical solution of (1) obtained at the time $T = 1$ using Heun's method with a "fine" step size of $\frac{h}{10}$.

We will compute both Y_N and Y_T^{fine} using the same Brownian paths.

Numerical example: Scalar anharmonic oscillator

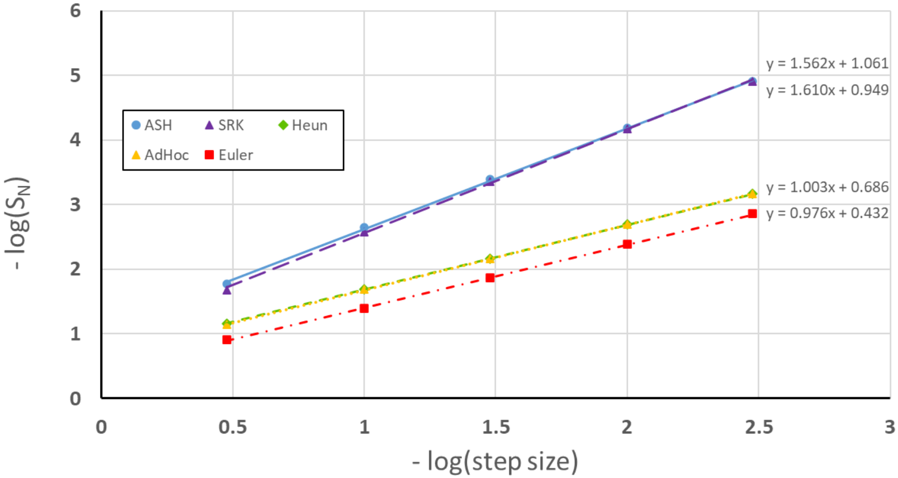

Figure: S_N computed with 1,000,000 sample paths using a fixed step size.

Numerical example: Scalar anharmonic oscillator

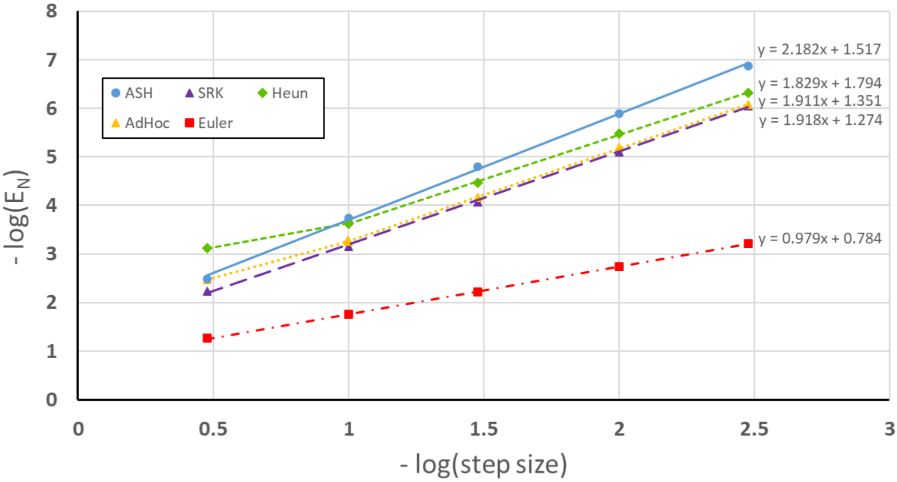

Figure: E_N computed with 1,000,000 sample paths using a fixed step size.

Numerical example: Scalar anharmonic oscillator

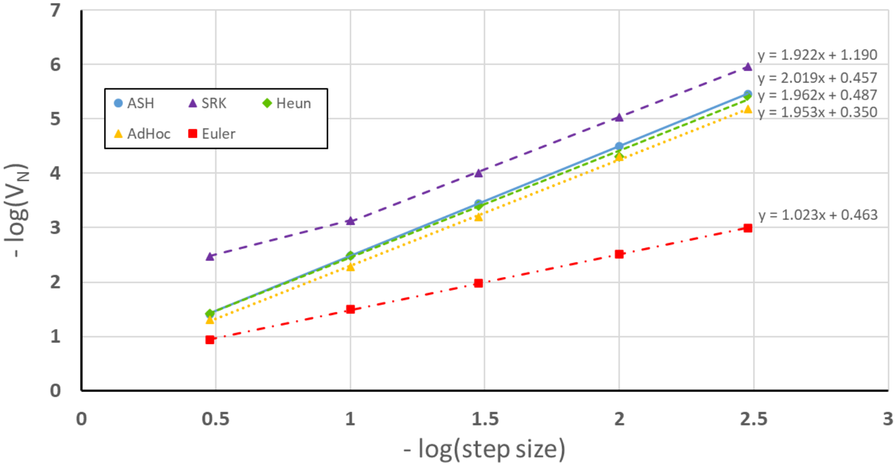

Figure: V_N computed with 1,000,000 sample paths using a fixed step size.

Future work

- Can AdHoc outperform the Euler-Maruyama method in high-dimensional settings?

  (for example, in Stochastic gradient Langevin dynamics)

- What is the order of weak convergence for approximate Heun?

- Are there extensions of AdHoc that converge for general SDEs?

- Does the AdHoc method converge if we use variable step sizes?

- Could ASH extend to SDEs with scalar or commutative noise?

Thank you
for your attention!

References I

[1] D. J. Higham, *An algorithmic introduction to numerical simulation of stochastic differential equations*, SIAM Review, vol. 43, no. 3, pp. 525–546, 2001.

[2] P. E. Kloeden and E. Platen, *Numerical Solution of Stochastic Differential Equations*, Springer, 1992.

[3] O. Butkovsky, K. Dareiotis, M. Gerencsér, *Approximation of SDEs - a stochastic sewing approach*, arxiv.org/abs/1909.07961, 2020.

[4] G. N. Milstein and M. V. Tretyakov, *Stochastic Numerics for Mathematical Physics*, Springer, 2004.

[5] K. Burrage, P. M. Burrage and T. Tian, *Numerical methods for strong solutions of stochastic differential equations: an overview*, Proceedings of the Royal Society A, vol. 460, no. 2041, 2004.

References II

[6] B. Leimkuhler and C. Matthews, *Rational construction of stochastic numerical methods for molecular sampling*, Applied Mathematics Research eXpress 2013, A, vol 1, pp. 34–56, 2013.

[7] B. Leimkuhler, C. Matthews and M. V. Tretyakov, *On the long-time integration of stochastic gradient systems*, Proceedings of the Royal Society A, vol. 470, no. 2170, 2014.

[8] J. Foster, T. Lyons and H. Oberhauser, *An optimal polynomial approximation of Brownian motion*, SIAM Journal on Numerical Analysis, vol. 58, no. 3, pp. 1393–1421, 2020.

[9] U. Mutze, *An asynchronous leapfrog method*, Mathematical Physics Preprint Archive 2008, no. 197, web.ma.utexas.edu/mp_arc/c/08/08-197.pdf, 2008.

[10] U. Mutze, *An asynchronous leapfrog method II*, arxiv.org/abs/1311.6602, 2013.