High order numerical simulation of the underdamped Langevin diffusion

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Introduction

The underdamped Langevin diffusion is given by the following SDE:

$$dQ_t = P_t \, dt, \tag{1}$$

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

where $Q, P \in \mathbb{R}^d$ will represent the position and velocity of a particle moving in a potential $U : \mathbb{R}^d \to \mathbb{R}$ under the influence of a frictional force (with coefficient $\nu > 0$) along with a stochastic force given by a d-dimensional Brownian motion W (and inverse temperature β).

The underdamped Langevin equation can be viewed as an extension of Newton's second law and is a key model in statistical mechanics. ([1] is a detailed textbook that surveys these scientific applications)

Introduction

Recently this equation has been applied to computational statistics as, under mild conditions on the potential (see [2] for more details), the process admits a stationary measure with the following density:

$$\varphi(q,p) \propto \exp\left(-\beta\left(U(q) + \frac{1}{2}\|p\|^2\right)\right).$$

Hence by setting U equal to the log density of a target distribution, it is possible to generate samples by simulating a Langevin diffusion.

In practice, (1) can not be solved exactly and must be approximated.

Introduction

Our strategy for discretizing the underdamped Langevin equation is

1. Replace the Brownian motion W by a piecewise linear path $\widehat{W}$.

2. Along each piece of $\widehat{W}$ we can approximate (1) using the ODE:

$$d\widehat{Q}_t = \widehat{P}_t\,dt, \tag{3}$$

$$d\widehat{P}_t = f\big(\widehat{Q}_t\big)\,dt - \nu\widehat{P}_t\,dt + \sigma\,d\widehat{W}_t, \tag{4}$$

   where $f := -\nabla U$ and $\sigma := \sqrt{\frac{2\nu}{\beta}}$.

3. In each step, discretize (3) and (4) with a suitable ODE solver.

Piecewise linear discretization of Brownian motion

To construct the path $\widehat{W}$, we shall use the below theorem from [3].

Theorem (Brownian motion as a cubic with independent noise)

Consider a standard Brownian motion W over the unit interval $[0,1]$. Let $\widetilde{W}$ be the (unique) cubic polynomial with a root at 0 such that

$$\int_0^1 u^k \, d\widetilde{W}_u = \int_0^1 u^k \, dW_u, \quad \text{for } \; k = 0, 1, 2.$$

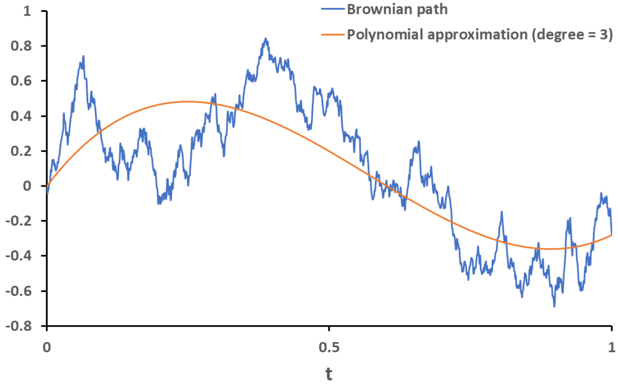
Then

$$W = \widetilde{W} + Z,$$

where Z is a centred Gaussian process independent of the cubic $\widetilde{W}$.

Piecewise linear discretization of Brownian motion

Therefore, the cubic polynomial $\widetilde{W}$ is an unbiased estimator for W.



The piecewise linear path $\widehat{W}$ will be designed to resemble this cubic.

Piecewise linear discretization of Brownian motion

Theorem (Pathwise approximation of the cubic polynomial $\widetilde{W}$)

There exists a piecewise linear path $\widehat{W}$ on $[0,1]$ and $a > 0$ such that:

1. $\widehat{W}_0 = 0$.
2. $\widehat{W}$ *has three pieces which connect at* $\frac{1}{2}\left(1 \pm a\right)$.
3. $\displaystyle\int_0^1 u^k \, d\widehat{W}_u = \int_0^1 u^k \, d\widetilde{W}_u$, *for* $k = 0, 1, 2, 3$.

Proof.

Note that for any fixed $a \in \left(0, 1\right)$, the first three integral conditions and $\widehat{W}_0$ are enough to uniquely determine the piecewise linear path.

Hence, the idea of the proof is to derive a necessary condition for a.

Piecewise linear discretization of Brownian motion

Proof. (continued)

Using the orthogonality of the Legendre polynomials, it follows that

$$\begin{aligned}\int_0^1 \left(20u^3 - 30u^2 + 12u - 1\right) d\widehat{W}_u &= \int_0^1 \left(20u^3 - 30u^2 + 12u - 1\right) d\widetilde{W}_u \\ &= \int_0^1 \left(20u^3 - 30u^2 + 12u - 1\right)\left(\widetilde{W}_u\right)' du \\ &= 0.\end{aligned}$$

On the other hand, the above integral can be explicitly computed as

$$\begin{aligned}\int_0^1 \left(20u^3 - 30u^2 + 12u - 1\right) d\widehat{W}_u \\ = \frac{1}{8}\left(5a^3 + 5a^2 - a - 1\right)\left(\widehat{W}_1 - \widehat{W}_{\frac{1}{2}(1+a)} - \widehat{W}_{\frac{1}{2}(1-a)}\right).\end{aligned}$$

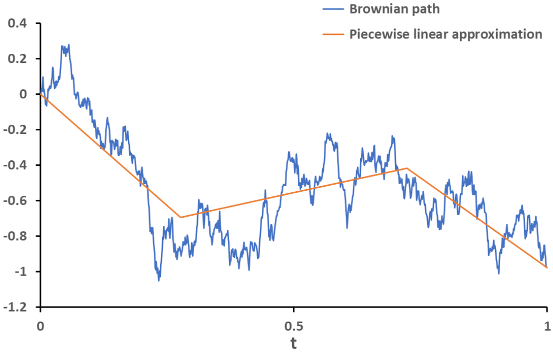
Piecewise linear discretization of Brownian motion

Proof. (continued)

So in order for $\widehat{W}$ to exist, the constant a must satisfy the equation

$$5a^3 + 5a^2 - a - 1 = 0.$$

Therefore by setting $a = \frac{\sqrt{5}}{5}$, we can construct the desired path. $\square$



Piecewise linear discretization of Brownian motion

In practice, $\widehat{W}$ can be generated on $[s,t]$ using the random variables

$$W_{s,t} := W_t - W_s,$$
$$H_{s,t} := \frac{1}{h}\int_s^t W_{s,u} - \frac{u-s}{h}W_{s,t}\,du,$$
$$K_{s,t} := \frac{1}{h^2}\int_s^t \left(W_{s,u} - \frac{u-s}{h}W_{s,t}\right)\left(\frac{1}{2}h - (u-s)\right)du,$$

where $h = t - s$.

It is straightforward to prove that $\left(W_{s,t}, H_{s,t}, K_{s,t}\right)$ are independent and uniquely determine the cubic polynomial $\widetilde{W}$ (see [3] for details).

Furthermore $W_{s,t} \sim N\big(0,h\big)$, $H_{s,t} \sim N\big(0,\frac{1}{12}h\big)$ and $K_{s,t} \sim N\big(0,\frac{1}{720}h\big)$.

Piecewise linear discretization of Brownian motion

Theorem (Pathwise approximation of the Brownian motion W)

Let $\widehat{W}$ be the piecewise linear path on $[s,t]$ with three pieces which connect the points (s, W_s), $(s + Ah, B)$, $(t - Ah, C)$, (t, W_t) given by

$$A = \frac{1}{2} - \frac{1}{2\sqrt{5}},$$

$$\frac{1}{2}\big(B + C\big) = W_s + \frac{1}{2}W_{s,t} + \frac{1}{1-A}H_{s,t},$$

$$\frac{1}{2}\big(B - C\big) = \frac{6}{1-A}K_{s,t} - \frac{1}{2}\big(1-2A\big)W_{s,t}.$$

Then $\widehat{W}$ matches the increment $W_{s,t}$, the time areas $(H_{s,t}, K_{s,t})$ and

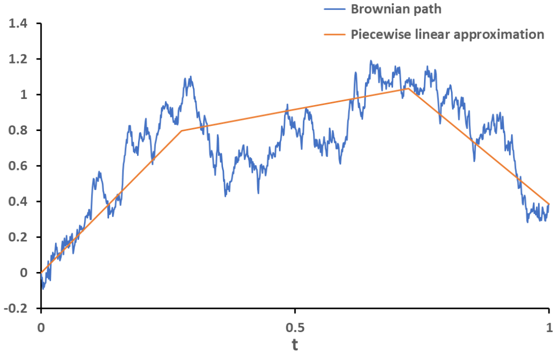
$$\int_s^t (u-s)^2\,\widehat{W}_{s,u}\,du = \mathbb{E}\left[\int_s^t (u-s)^2\,W_{s,u}\,du \,\middle|\, W_{s,t}, H_{s,t}, K_{s,t}\right].$$

Piecewise linear discretization of Brownian motion

Proof.

The result is a direct consequence of the previous two theorems. □

When approximating the underdamped Langevin diffusion on $[0, T]$, we shall generate $\widehat{W}$ on the uniform grid $\triangle_N$ with mesh size $h = \frac{T}{N}$.



Approximation of underdamped Langevin diffusion by ODEs

Recall that the underdamped Langevin equation is the SDE given by

$$dQ_t = P_t\,dt, \tag{5}$$

$$dP_t = f(Q_t)\,dt - \nu P_t\,dt + \sigma\,dW_t. \tag{6}$$

Provided that f is twice differentiable, we have the Taylor expansion

$$\begin{aligned}\begin{pmatrix} Q_t \\ P_t \end{pmatrix} = \begin{pmatrix} Q_s \\ P_s \end{pmatrix} &+ (\cdots)\,h + (\cdots)\,W_{s,t} + (\cdots)\int_s^t W_{s,u}\,du + (\cdots)\,h^2 + (\cdots)\,h^3 \\ &+ (\cdots)\int_s^t\int_s^u W_{s,v}\,dv\,du + (\cdots)\int_s^t\int_s^u\int_s^v W_{s,r}\,dr\,dv\,du \\ &+ (\cdots)\int_s^t\int_s^u\int_s^v (r-s)\,dW_r\,dv\,du + O(h^4),\end{aligned}$$

where $(\cdots)$ are terms involving the vector fields and their derivatives.

Approximation of underdamped Langevin diffusion by ODEs

Similarly, $(\widehat{Q}, \widehat{P})$ will also have this expansion but with $\widehat{W}$ integrals.

By the previous theorem, these integrals are approximated optimally using $\widehat{W}$ (in an $L^2(\mathbb{P})$ sense) and hence gives the local error estimate

Theorem

Provided the vector field f and its first two derivatives are bounded and Lipschitz continuous, there exist constants $C_1, C_2 > 0$ such that

$$\mathbb{E}\left[\left\|\begin{pmatrix} Q_t \\ P_t \end{pmatrix} - \begin{pmatrix} \widehat{Q}_t \\ \widehat{P}_t \end{pmatrix}\right\|^2\right] \leq \left(1 + C_1 h\right)\mathbb{E}\left[\left\|\begin{pmatrix} Q_s \\ P_s \end{pmatrix} - \begin{pmatrix} \widehat{Q}_s \\ \widehat{P}_s \end{pmatrix}\right\|^2\right] + C_2 h^7, \quad (7)$$

for sufficiently small h.

Approximation of underdamped Langevin diffusion by ODEs

Sketch Proof.

We derive (7) from the Taylor expansions of $\big(Q_t, P_t\big)$ and $\big(\widehat{Q}_t, \widehat{P}_t\big)$.

The first term in the estimate follows using the Lipschitz continuity.

Therefore it is helpful to consider the case when $\big(Q_s, P_s\big) = \big(\widehat{Q}_s, \widehat{P}_s\big)$. As the $O\big(h^{\frac{7}{2}}\big)$ integrals in both expansions have mean zero, we have

$$\mathbb{E}\left[\begin{pmatrix} Q_t \\ P_t \end{pmatrix} - \begin{pmatrix} \widehat{Q}_t \\ \widehat{P}_t \end{pmatrix}\right] \sim O(h^4). \tag{8}$$

It's important that the above quantity is strictly smaller than $O\big(h^{\frac{7}{2}}\big)$ so that large (but unbiased) terms disappear in the full expansion of

$$\mathbb{E}\left[\left\|\begin{pmatrix} Q_t \\ P_t \end{pmatrix} - \begin{pmatrix} \widehat{Q}_t \\ \widehat{P}_t \end{pmatrix}\right\|^2\right].$$

Sketch Proof. (continued)

The explicit calculation required to derive (7) is lengthy but follows the typical argument for $L^2(\mathbb{P})$ error estimation (see [4] for details).

The key idea is that the leading error terms are $O\big(h^{\frac{7}{2}}\big)$ but unbiased. So by squaring and taking an expectation, the terms that cannot be estimated using Lipschitz continuity will have a size of $O\big(h^7\big)$. $\square$

The above theorem then leads to the following global error estimate

Theorem (Strong convergence rate of the ODE approximation)

Suppose that $\big(\widehat{Q},\widehat{P}\big)$ *was obtained on* $[0,T]$ *using a uniform grid* $\triangle_N$ *with mesh size* $h=\frac{T}{N}$ *and an initial value* $\big(Q_0,P_0\big)=\big(\widehat{Q}_0,\widehat{P}_0\big)$*. Then*

$$\left\|\begin{pmatrix}Q_T\\ P_T\end{pmatrix}-\begin{pmatrix}\widehat{Q}_T\\ \widehat{P}_T\end{pmatrix}\right\|_{L^2(\mathbb{P})}\sim O\big(h^3\big).$$

Approximation of underdamped Langevin diffusion by ODEs

Similarly, by comparing the two Taylor expansions we can show that

Theorem (Weak convergence rate of the ODE approximation)

Suppose that $(\widehat{Q}, \widehat{P})$ *was obtained on* $[0, T]$ *using a uniform grid* $\triangle_N$ *with a mesh size of* $h = \frac{T}{N}$ *and the initial value* $(Q_0, P_0) = (\widehat{Q}_0, \widehat{P}_0)$*. Then for any polynomial* p*, there exists a constant* $C_p > 0$ *such that*

$$\left|\mathbb{E}\left[p\begin{pmatrix} Q_T \\ P_T \end{pmatrix}\right] - \mathbb{E}\left[p\begin{pmatrix} \widehat{Q}_T \\ \widehat{P}_T \end{pmatrix}\right]\right| \leq C_p h^3,$$

for all sufficiently small step sizes h*.*

Remark

The ODE driven by $\widehat{W}$ gives a third order numerical method for (1).

Discretization of the underdamped Langevin ODE

Since the ODE driven by $\widehat{W}$ is a third order approximation, it should be discretized using a numerical method that is at least third order.

Due to the structure of (3, 4), we can apply Runge-Kutta-Nyström (RKN) methods, which are explicitly designed for ODEs of the form

$$
\begin{aligned}
y'' &= F(t, y), \\
y(0) = y_0, &\quad y'(0) = y_0',
\end{aligned}
\tag{9}
$$

In addition, we wish for the RKN method to be symplectic since the underdamped Langevin equation is a stochastic Hamiltonian system.

Fortunately, the RKN method proposed by [5] has these properties.

Discretization of the underdamped Langevin ODE

To propagate the numerical solution over $[s,t]$, we use the variables

$$\begin{pmatrix} y_u \\ x_u \end{pmatrix} := \begin{pmatrix} e^{\frac{1}{2}\nu(u-s)}\widehat{Q}_u \\ e^{\nu(u-s)}\widehat{P}_u \end{pmatrix}, \qquad \forall u \in [s,t],$$

to represent the system (3, 4) using the following second order ODE

$$\frac{d^2 y}{du^2} = \frac{1}{4}\nu^2 y + e^{\frac{1}{2}\nu(u-s)}\left(f\big(e^{-\frac{1}{2}\nu(u-s)}y\big) + \sigma\,\frac{d\widehat{W}}{du}\right), \tag{10}$$

$$y_s = \widehat{Q}_s, \qquad y_s' = \widehat{P}_s + \frac{1}{2}\nu\,\widehat{Q}_s.$$

We can apply RKN methods on the intervals where $\frac{d\widehat{W}}{du}$ is constant.

Discretization of the underdamped Langevin ODE

For the numerical example, we will use the below numerical method.

Definition (A third order three-stage symplectic RKN method)

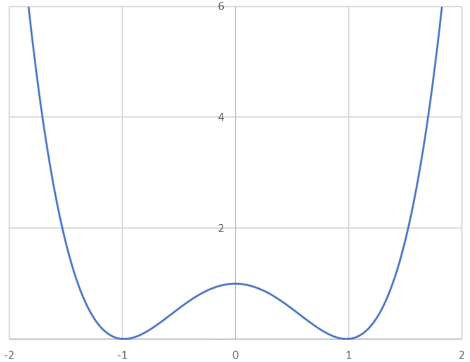
This method is presented in [5] and defined by the Butcher tableau:

$$
\begin{array}{c|ccc}
0 & & & \\
0.630847693 & 0.164217030 & & \\
0.536704894 & 0.139710559 & -0.103005664 & \\
\hline
 & 0.260311692 & 0.4039053382 & -0.164217030 \\
 & 0.260311692 & 1.094142798 & -0.354454490
\end{array}
$$

Numerical example: A particle in a double-well potential

For the numerical experiment, we shall consider a scalar double-well potential with the same parameters used in the first example of [6]:

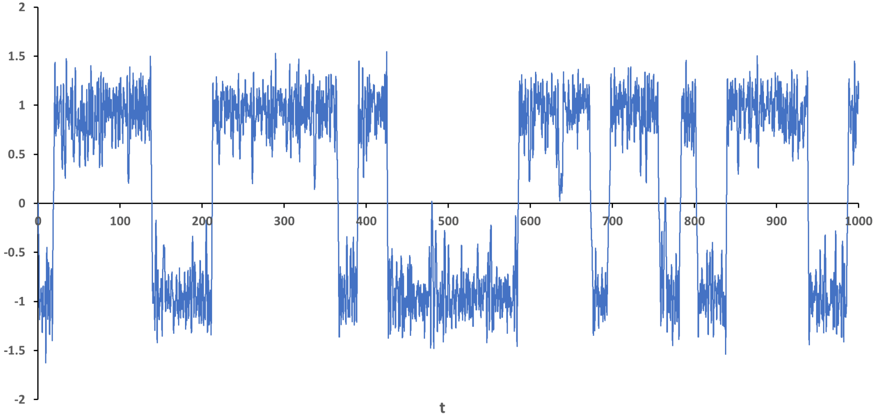
$$U(q) = \left(q^2 - 1\right)^2,$$



$$\nu = 1, \quad \beta = 3, \quad \left(Q_0, P_0\right) = 0.$$

Numerical example: A particle in a double-well potential

A sample path of the Langevin diffusion obtained by discretizing (3)



Numerical example: A particle in a double-well potential

Let $\widehat{Q}_T$ be the approximate position at time T computed with $h = \frac{T}{N}$.

We examine the strong and weak convergence using the estimators:

$$S_N := \sqrt{\mathbb{E}\Big[\big(\widehat{Q}_T - Q_T^{\text{fine}}\big)^2\Big]}, \tag{11}$$

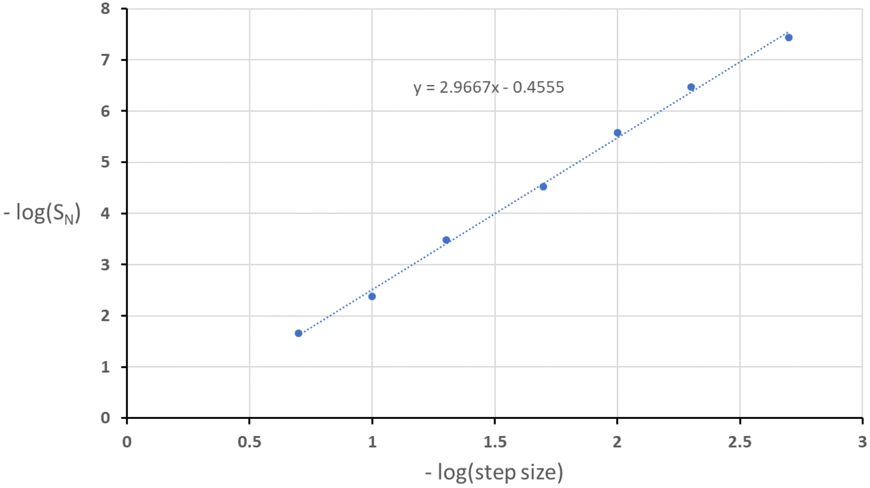
$$E_N := \Big|\mathbb{E}\big[\widehat{Q}_T^2\big] - \mathbb{E}\big[\big(Q_T^{\text{fine}}\big)^2\big]\Big|, \tag{12}$$

where the expectations are approximated by Monte-Carlo simulation and Q_T^{fine} denotes the numerical solution of (1) obtained at time T using the proposed method with a “fine” step size of $\min\left(\frac{h}{25}, \frac{T}{50000}\right)$.

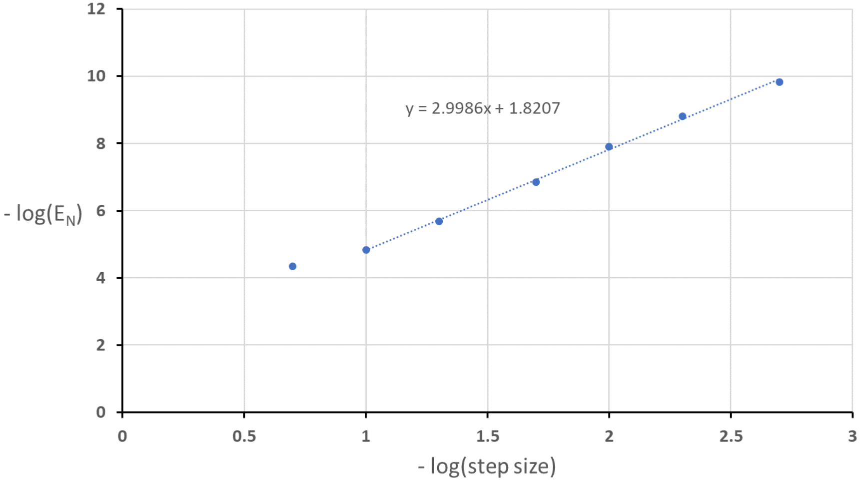
We will compute both $\widehat{Q}_T$ and Q_T^{fine} using the same Brownian paths.

For the numerical experiment, we shall use a time horizon of $T = 10$.

Numerical example: A particle in a double-well potential



Numerical example: A particle in a double-well potential



Future work

- How well does the proposed numerical method approximate the stationary distribution of the underdamped Langevin diffusion?
- Is this method practical for problems within Bayesian statistics?
- What are best ODE solvers for discretizing the system (3), (4)?
- Can this methodology be improved by using variable step sizes?

Thank you
for your attention!

References I

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