MULTILEVEL APPROACH TO EFFICIENT GRADIENT CALCULATION IN STOCHASTIC SYSTEMS

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ABSTRACT

Gradient estimation in Stochastic Differential Equations is a critical challenge in fields that require dynamic modeling of stochastic systems. While there have been numerous studies on pathwise gradients, the calculation of expectations over different realizations of the Brownian process in SDEs is occasionally not considered. Multilevel Monte Carlo offers a highly efficient solution to this problem, greatly reducing the computational cost in stochastic modeling and simulation compared to naive Monte Carlo. In this study, we utilized Neural Stochastic Differential Equations as our stochastic system and demonstrated that the accurate gradient could be effectively computed through the use of MLMC.

1 INTRODUCTION

Gradient estimation in the dynamic modeling of stochastic systems has always been a critical challenge in various fields. In these systems, calculating the gradient of underlying Stochastic Differential Equations (SDEs) requires consideration of different realizations of the Brownian process. Despite extensive research on pathwise gradients, the calculation of expectations over different realizations of the Brownian process in SDEs is occasionally overlooked.

This is where Multilevel Monte Carlo (MLMC) comes in as a highly effective solution to this problem. By greatly reducing the computational cost in stochastic modeling and simulation compared to naive Monte Carlo (MC), it offers a more efficient way to estimate gradients. It has been shown that to achieve an accuracy of $\epsilon$, MC simulations would require a computational cost of $O(\epsilon^{-3})$. However, with MLMC, this cost can be reduced to $O(\epsilon^{-2})$ under certain conditions [Giles 2015], making it a much more efficient solution for gradient estimation in SDEs.

In this study, we explore the use of Neural Stochastic Differential Equations (Neural SDEs) as a stochastic system and demonstrate the effectiveness of the MLMC approach in accurately computing the gradient. Also, we show that using MLMC not only reduces the computational cost compared to naive MC simulations but also helps improve training in the LatentSDE model.

2 BACKGROUND

2.1 Neural SDEs

SDEs are a generalization of ODEs, and Neural SDEs are often used to model the dynamics of stochastic systems [Liu et al. 2019]. They are defined as input-injected SDEs in either Itô or Stratonovich forms. Our consideration of systems follows the structure in Kidger et al. [2021]:

$$Z_0 = \zeta_\theta(X), \quad dZ_t = f_\theta(t, X, Z_t) \, dt + g_\theta(t, X, Z_t) \, dW_t, \quad Y_t = \ell_\theta(Z_t),$$

(1)

where $\zeta_\theta$, $f_\theta$, and $g_\theta$ are neural networks, and $\ell_\theta$ is affine.
The training process for Neural SDEs can be generalized by minimizing the expected objective, $\mathcal{L}(Y)$, over different realizations of the Brownian process $W_t$. It can be achieved by solving a nonlinear program while optimizing parameters for the system, $\theta$. We can write down the nonlinear program constrained to the Neural SDE as equation [2]

$$
\min_{\theta} \mathbb{E}_{x} \left[ \mathbb{E}_{W} \left[ \mathcal{L}(Y) \right] \right]
\text{s.t. } dZ_t = f_\theta \left( t, X, Z_t \right) \, dt + g_\theta \left( t, X, Z_t \right) \, dW_t
Z_0 = \zeta_\theta (X), \quad Y_t = \ell_\theta (Z_t)
$$

We can solve equation [2] via stochastic gradient descent, where we need to calculate $\frac{d}{d\theta} \mathbb{E}_{W} \left[ \mathcal{L}(Y) \right]$ (Bottou [2010]) and the SGD iteration has assumptions of $\mathcal{L}$ being Lipschitz such that $\mathbb{E}_{W} \left[ \frac{d}{d\theta} \mathcal{L}(Y) \right] = \frac{d}{d\theta} \mathbb{E}_{W} \left[ \mathcal{L}(Y) \right]$. Therefore the exact gradient for the Neural SDE can be estimated by calculating the expectation of pathwise gradients $\frac{d}{d\theta} \mathcal{L}(Y)$ for each of the simulated independent Brownian process.

### 2.2 Pathwise Gradients Calculation for SDEs

There is an extensive amount of work on pathwise sensitivities analysis. The forward pathwise approach is an intuitive pathwise gradient calculation method for SDEs (Gobet & Munos [2005]). However, it scales poorly in computational cost with the number of parameters or state dimensions. Giles & Glasserman (2006) proposed a discrete version of the backward adjoint sensitivity method, which calculates the same value with the forward implementation but with computational savings. The stochastic adjoint method (Li et al. [2020]) resolved the memory burden by generalizing the adjoint method to stochastic dynamics defined by SDEs to recover the value of the state $z_t$.

### 2.3 Multilevel Monte Carlo

Giles (2008) proposed MLMC that reduces the order of complexity of MC simulations. When we want to estimate $\mathbb{E}_{W} \left[ \frac{d}{d\theta} \mathcal{L}_L(Y) \right]$, there is a sequence $\frac{d}{d\theta} \mathcal{L}_0(Y), \ldots, \frac{d}{d\theta} \mathcal{L}_{L-1}(Y)$, with increasing accuracy and cost. Then, we can use equation [3] as an unbiased estimator for $\frac{d}{d\theta} \mathbb{E}_{W} \left[ \mathcal{L}_L(Y) \right]$.

$$
\mathbb{E}_{W} \left[ \frac{d}{d\theta} \mathcal{L}_L(Y) \right] = \mathbb{E}_{W} \left[ \frac{d}{d\theta} \mathcal{L}_0(Y) \right] + \sum_{\ell=1}^{L} \mathbb{E}_{W} \left[ \frac{d}{d\theta} \mathcal{L}_{\ell}(Y) - \frac{d}{d\theta} \mathcal{L}_{\ell-1}(Y) \right]
$$

**Theorem 2.1** (Complexity Theorem). For a real-valued random variable $\frac{d}{d\theta} \mathcal{L}(Y)$, we let $\frac{d}{d\theta} \mathcal{L}^\dagger(\tilde{Y})$ be the corresponding approximation using the discretization at level $l$, i.e. with $2^l$ steps of width $h_l = 2^{-l}T$.

If there exists independent estimators $\tilde{U}_l$ of computational complexity $C_l$ based on $M_l$ samples and there are positive constants $\alpha \geq \frac{1}{2} \min(1, \beta), \beta, c_1, c_2, c_3, c_4$ such that

$$
A1 : \mathbb{E} \left[ \tilde{U}_l \right] = \begin{cases} 
\mathbb{E} \left[ \frac{d}{d\theta} \mathcal{L}_0(\tilde{Y}) \right] & \text{if } l = 0 \\
\mathbb{E} \left[ \frac{d}{d\theta} \mathcal{L}_l(\tilde{Y}) - \frac{d}{d\theta} \mathcal{L}_{l-1}(\tilde{Y}) \right] & \text{if } l > 0
\end{cases}
$$

$$
A2 : \mathbb{E} \left[ \frac{d}{d\theta} \mathcal{L}(\tilde{Y}) - \frac{d}{d\theta} \mathcal{L}(Y) \right] \leq c_1 h_l^\alpha
$$

$$
A3 : \mathbb{V} \left[ \tilde{U}_l \right] \leq c_2 h_l^\beta M_l^{-1}
$$

$$
A4 : C_l \leq c_3 M_l h_l^{-1}
$$

Then there is a constant $c_4$ such that for any $\epsilon < e^{-1}$, there are values for $L$ and $(M_l)_{l=0,\ldots,L}$ resulting in a multilevel estimator $\hat{U} = \sum_{l=0}^{L} \tilde{U}_l$ with a mean-square-error $\text{MSE} = \mathbb{E} \left[ (\hat{U} - \mathbb{E} \left( \frac{d}{d\theta} \mathcal{L}(Y) \right))^2 \right] < \epsilon^2$ with a complexity $C$ bounded by
Assume we want to estimate the gradient value \( \nabla V \) and define the multilevel estimators as

\[
\tilde{V} = \frac{1}{M} \sum_{i=1}^{M} \frac{d}{d\theta} \hat{L}(\hat{Y})^{(i)}.
\]

We can write the mean square error (MSE) of the estimation as in equation 6

\[
\mathbb{E}[(\tilde{S} - V)^2] = \frac{1}{M} \mathbb{V}(\frac{d}{d\theta} \hat{L}(\hat{Y})) + (\mathbb{E}\left[\frac{d}{d\theta} \hat{L}(\hat{Y})\right] - \mathbb{E}\left[\frac{d}{d\theta} L(Y)\right])^2
\]

The first term represents the variance of the estimator due to Monte Carlo sampling and the second term represents the bias due to the discretization. With any solver with weak order of convergence of 1, such as Milstein method (Milstein, 1994), we need \( O(\epsilon^{-1}) \) time steps and \( O(\epsilon^{-2}) \) samples to achieve MSE \( O(\epsilon^2) \). Therefore, the total computational cost is \( C = O(\epsilon^{-3}) \) (Duffie & Glynn, 1995).

### Computational Complexity of Multilevel Monte Carlo

By following the basic settings of MLMC and using discretization method to approximate the gradient value, we can write the multilevel approximation of the gradient as

\[
\mathbb{E}_{W} \left[ \frac{d}{d\theta} L(Y) \right] \approx \mathbb{E}_{W} \left[ \frac{d}{d\theta} \hat{L}(\hat{Y}) \right] = \mathbb{E}_{W} \left[ \frac{d}{d\theta} \hat{L}_{0}(\hat{Y}) \right] + \sum_{i=1}^{L} \mathbb{E}_{W} \left[ \frac{d}{d\theta} \hat{L}_{l}(\hat{Y}) - \frac{d}{d\theta} \hat{L}_{l-1}(\hat{Y}) \right],
\]

Also, we can define the multilevel estimators as

\[
\tilde{L}_0 = M_0^{-1} \sum_{i=1}^{M_0} \frac{d}{d\theta} \hat{L}_0(\hat{Y})^{(i)}
\]

\[
\tilde{L}_l = M_l^{-1} \sum_{i=1}^{M_l} \left( \frac{d}{d\theta} \hat{L}_l(\hat{Y})^{(i)} - \frac{d}{d\theta} \hat{L}_{l-1}(\hat{Y})^{(i)} \right)
\]

Using the complexity theorem [2], we can get the computational complexity of MLMC by estimating the order of convergence \( \alpha \) and \( \beta \). This can be derived analytically with some assumptions as in the theorem [2]. On the other hand, we can conduct simulation experiments to estimate the \( \alpha \) and \( \beta \). In the experiments, we approximate \( \tilde{U} \) with \( \mathbb{E} \left[ \frac{d}{d\theta} \hat{L}_f - \frac{d}{d\theta} \hat{L}_c \right] \) for computational efficiency, where the fine discretizations \( \hat{L}_f \) uses \( N_f(l) = 2^l \) fine time steps and the coarse discretizations \( \hat{L}_c \) uses \( N_c(l) = 2^{l-1} \) (Burgos, 2014). Let our system be a Neural SDE as in equation 1 and \( M_l \) be the
Table 1: Estimated Complexity

<table>
<thead>
<tr>
<th>Estimator</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>Complexity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loss Value</td>
<td>$\approx 1.00$</td>
<td>$\approx 2.03$</td>
<td>$O(\epsilon^{-2})$</td>
</tr>
<tr>
<td>Gradient for $f_\theta$</td>
<td>$\approx 0.97$</td>
<td>$\approx 1.87$</td>
<td>$O(\epsilon^{-2})$</td>
</tr>
<tr>
<td>Gradient for $g_\theta$</td>
<td>$\approx 0.97$</td>
<td>$\approx 1.94$</td>
<td>$O(\epsilon^{-2})$</td>
</tr>
<tr>
<td>Gradient for $z_0$</td>
<td>$\approx 0.97$</td>
<td>$\approx 1.95$</td>
<td>$O(\epsilon^{-2})$</td>
</tr>
</tbody>
</table>

number of path simulations for each of the levels to estimate $\mathbb{E}\left[\hat{U}_l\right]$ and $V_l = M_lV\left[\hat{U}_l\right]$. Also by assuming

$$
\mathbb{E}\left(\hat{U}_l\right) = O\left(h^\alpha\right)
$$

$$
V_l = O\left(h^\beta\right),
$$

we can estimate the empirical bounds, which approximate the order of convergence, $\alpha$ and $\beta$, with

$$
\log_2 \mathbb{E}\left[\hat{U}_l\right] \sim \alpha \log_2 (h) \sim -l\alpha
$$

$$
\log_2 V_l \sim \beta \log_2 (h) \sim -l\beta.
$$

The table 1 shows the $\alpha$ and $\beta$ of our system after the experiments, and the figure B.3 shows the values of $\mathbb{E}\left[\hat{U}_l\right]$ and $V_l$ for different levels. We can compute the complexity $C$ with 5 and conclude that the total computational complexity is $O(\epsilon^{-2})$ for all gradients with respect to $f_\theta$, $g_\theta$, and $z_0$.

4 Experiment Results and Discussion

To compare the performance of various simulation methods in gradient calculation, we utilized the Latent SDE from Li et al. (2020) as our evaluation method. We trained the Latent SDE on a 3D Stochastic Lorenz Attractor process to confirm that the acquired posterior can accurately reproduce the training data and that the obtained priors are not deterministic. (See C for details)

Figure 1: Training Loss: MC Simulation Comparison

Figure 4 shows that integrating MC simulations in the Latent SDE improves performance by accurately calculating gradients. The training time per epoch is similar for both Latent SDE and MC simulation, as parallelization is used to expand samples during training, which only increases memory complexity. However, by integrating MLMC, the computational cost of MC simulation is further reduced. This means that Latent SDE in combination with MLMC achieves similar or even better performance with less computational cost.
REFERENCES


A ADDITIONAL BACKGROUND

A.1 INTERCHANGE OF DIFFERENTIATION AND EXPECTATION FOR $\mathcal{L}$

If the following equation is assumed to hold, then the pathwise derivative becomes an unbiased estimator for the true gradient value.

\[
\mathbb{E}_W \left[ \frac{d}{d\theta} \mathcal{L}(Y) \right] = \frac{d}{d\theta} \mathbb{E}_W [\mathcal{L}(Y)]
\]

(11)

The below assumptions (A1-A3) are sufficient to ensure that the equation [11] holds. Details of the proofs can be found in Glasserman (2004).

- A1: At each $\theta$, $\frac{d}{d\theta} \mathcal{L}(Y_i)$ exists with probability 1, for all $i = 1, \ldots, m$.
- A2: $\mathcal{L}(Y)$ exists with probability 1 and is given by

\[
\frac{d}{d\theta} \mathcal{L}(Y) = \sum_{i=1}^{T} \frac{\partial \mathcal{L}(Y(\theta))}{\partial Y_i} \frac{d}{d\theta} \mathcal{L}(Y_i)
\]

- A3: There exists a constant $k_f$ such that for all $x, y \in \mathbb{R}^m$

\[|\mathcal{L}(x) - \mathcal{L}(y)| \leq k_f \|x - y\|
\]

A.2 STRONG ITO-TAYLOR APPROXIMATIONS

The theorem A.1 was first introduced in Kloeden & Platen (1992) to demonstrate the convergence of strong Ito-Taylor approximations. This theorem has been modified from the version presented by Burgos (2014).

Theorem A.1. We consider the case where $Z_t \in \mathbb{R}^d$ and $W_t$ is a 1-dimensional Brownian motion. $(f_k)_{(k=1, \ldots, d)}$ and $(g_k)_{(k=1, \ldots, d)}$ are the different components of the coefficients $f$ and $g$ in the following SDE: on $[0, T]$.

\[
dZ(t) = f(Z, t)dt + g(Z, t)dW_t
\]

We let

\[
K^0 = \frac{\partial}{\partial t} + \sum_{k=1}^{d} f_k \frac{\partial}{\partial Z_k} + \frac{1}{2} \sum_{k, l=1}^{d} g_k g_l \frac{\partial^2}{\partial Z_k \partial Z_l}
\]

(12)

Assuming that

- A1: $f(Z, t)$ is $C^{(1,1)}(\mathbb{R}^d \times \mathbb{R}^+)$ and $g(Z, t)$ is $C^{(2,1)}(\mathbb{R}^d \times \mathbb{R}^+)$
- A2: (uniform Lipschitz condition): there exists a constant $C_1 > 0$ such that for all $x, y \in \mathbb{R}^d$

\[\|f(y, t) - g(x, t)\| + \|f(y, t) - g(x, t)\| + \|K^1 g(y, t) - K^1 g(x, t)\| \leq C_1 \|y - x\|
\]

- A3 (linear growth bound): There exists a constant $C_2$ such that for $x \in \mathbb{R}^d$,

\[\|f(x, t)\| + \|K_0 f(x, t)\| + \|K_1 f(x, t)\| + \|g(x, t)\| + \|K_0 g(x, t)\| + \|K_1 g(x, t)\| + \|K_0 K_1 g(x, t)\| + \|K_1 K_1 g(x, t)\| \leq C_2 (1 + |x|)
\]

- A4 (additional Lipschitz-like condition): there exists a constant $C_3$ such that for all $x \in \mathbb{R}^d$ and $s, t \in \mathbb{R}^+$, $\|g(x, t) - g(x, s)\| \leq C_3 (1 + |x|) \sqrt{|t - s|}$
Then for each \( m > 0 \),

\[
\mathbb{E} \left( \sup_{0 < t < T} \| Z_t \|^m \right) < \infty
\]

Using the Milstein discretisation \( \left( \tilde{Z}_n \right)_{n=0,...,N} \), we define the following continuous time interpolant on each time step \([t_n, t_{n+1}]\) \((n = 0, \ldots, N - 1)\) and each dimension \( k = 1, \ldots, d \) as

\[
\tilde{Z}_{P_k}(t) = \tilde{Z}_{n_k} + f_k \left( \tilde{Z}_{n_k}, t_n \right) (t - t_n) + g_k \left( \tilde{Z}_{n_k}, t_n \right) (W_t - W_n) + \frac{1}{2} \sum_{l=1}^{k} g_l \frac{\partial g_k}{\partial Z_l} \left( \tilde{Z}_{n_k}, t_n \right) \left( (W_t - W_n)^2 - (t - t_n) \right)
\]

then for each \( m > 0 \), there exists a constant \( C_m \) such that

\[
\mathbb{E} \left( \sup_{0 < t < T} \| Z_t - \tilde{Z}_P(t) \|^m \right) < C_m h^m
\]

and

\[
\mathbb{E} \left( \sup_{0 < t < T} \| \tilde{Z}_P(t) \|^m \right) < C_m
\]

**Proof.** See theorem 10.6.3 and corollary 10.6.4 in [Kloeden & Platen, 1992]. \(\blacksquare\)

## B Details of Computational Complexity for MLMC

### B.1 Complexity Theorem

The theorem 2.1 was originally presented by [Giles, 2008] and later improved upon by [Cliffe et al., 2011]. The version of the theorem that appears in this paper, which was taken from [Burgos, 2014], replaces the original payoff, \( P \), with \( \frac{d}{d \theta} \mathcal{L}(Y) \) to align with the notations used in our work.

### B.2 Details of Numerical Simulation

We constructed a minimal Neural SDE to evaluate the expected value and variance of the multilevel estimator for computational complexity in our numerical experiments. In both figures, \( B.2 \), the term \( L_f - L_c \) represents the multilevel estimator for the true loss value \( \mathcal{L} \). For the gradient estimators, each of \( dL_f/df - dL_c/df, dL_f/dq - dL_c/dq, \) and \( dL_f/dX_0 - dL_c/dX_0 \) represents the estimator for the gradient of the drift(\( f \)), the diffusion(\( g \)), and the input to the SDE, \( X_0 \), respectively.

![Figure 2: Calculating \( E(U_i) \) and \( V_i \) for Estimating Complexity](image-url)
B.3 Analytical Derivation of Computational Complexity

**Theorem B.1.** We consider an output of a stochastic system $Z_t$ on the time interval $[0, T]$ and a smooth Lipschitz loss function $L$ with a loss value of $L(Z_T)$. We assume that $Z_t$ follows an Itô process as described by equation [1] that the coefficients of the diffusion $f_0$ and $g_0$ satisfy conditions $A1$ to $A4$ of theorem [A.1] and that $g_0 > 0$. Then, the multilevel estimators of the gradients with respect to the loss $L(Z_T)$ have an accuracy $\epsilon$ at a cost $O(\epsilon^{-2})$

**Proof.** See chapter 4 in [Burgos (2014)].}

C Details on Experiments for Latent SDE

The prior and the approximated posterior are parameterized using SDEs as

$$
d\tilde{Z}_t = h(\tilde{Z}_t, t) \, dt + g(\tilde{Z}_t, t) \, dW_t,
$$
$$
dZ_t = f(Z_t, t) \, dt + g(Z_t, t) dW_t,
$$

where $h$, $f$, and $g$ are Lipschitz and both have same initial values of $z_0$.

With prior and approximate posterior defined as in Equation [13], the latent SDE can be constructed as outlined in [1]. The KL divergence between the prior and approximate posterior, which both have the same diffusion function, $g$, is finite and can be calculated by sampling paths from the approximate posterior process, as shown in [Li et al. (2020)]. The formula for the evidence lower bound (ELBO) is

$$
\log(p(x_1, x_2, \ldots, x_N|\theta)) \geq \mathbb{E}_{Z_t} \left[ \sum_{i=1}^{N} \log p(x_{t_i} | z_{t_i}) - \int_{0}^{T} \frac{1}{2} |u(z_t, t)|^2 \, dt \right],
$$

where $u : \mathbb{R}^d \times [0, T] \rightarrow \mathbb{R}^m$ satisfies

$$
\sigma(z, t)u(z, t) = h_\theta(z, t) - h_\theta(z, t),
$$

and the expectation is calculated based on the approximate posterior process that has been defined.

Other detailed explanations of the training process, such as the choice of optimizer and architecture of latent SDE, can be found in [Kidger (2022)].

**Algorithm 1 Latent SDE**

**Input:** Data $\{x_i\}_{i=1, \ldots, N}$ and times $\{t_i\}_{i=1, \ldots, N}$

$z_0 = \text{Encoder}\{x_i\}$

$\mu_{z_0}, \sigma_{z_0} = \text{Linear}(z_0)$

$z_0 \sim N(\mu_{z_0}, \sigma_{z_0})$

$\{z_i\}, D_{ki} = \text{SDESolve}(f, h, g, z_0, (t_0 \ldots t_N))$

$\tilde{x}_i = \text{Linear}(\{z_i\})$ for all $i = 1, \ldots, N$

**Return:** $\{\tilde{x}_i\}_{i=1, \ldots, N}$

We trained on the dataset sampled from stochastic Lorenz attractor SDE defined as:

$$
y \sim N(0, I_{3 \times 3})
$$
$$
dy_1(t) = a_1(y_2(t) - y_1(t)) \, dt + b_1y_1(t) \, dw(t)
$$
$$
dy_2(t) = (a_2y_1(t) - y_1(t)y_3(t)) \, dt + b_2y_2(t) \, dw(t)
$$
$$
dy_3(t) = (y_1(t)y_2(t) - a_3y_3(t)) \, dt + b_3y_3(t) \, dw(t),
$$

with $a_1 = 10, a_2 = 28, a_3 = \frac{8}{3}, b_1 = 0.1, b_2 = 0.28, b_3 = 0.3$ following the work of [Kidger (2022)].

We obtained samples at intervals of 0.05 from time 0 to 2. To conform with the preprocessing
techniques used in previous studies [Li et al., 2020], we normalized the data by computing the mean and standard deviation for each dimension. We then added Gaussian noise with a mean of zero and a standard deviation of 0.01 to corrupt the data.