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Improved simulation techniques for first exit time of neural diffusion models

Hasan Alzubaidi[*]   Tony Shardlow[†]

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Abstract

We consider the fixed and exponential time-stepping Euler algorithms, with boundary tests, to calculate the mean first exit times (MFET) of two one-dimensional neural diffusion models, represented by the Ornstein–Uhlenbeck (OU) process and a stochastic space-clamped FitzHugh–Nagumo (FHN) system. The numerical methods are described and the convergence rates for the MFET analysed. A boundary test improves the rate of convergence from order one half to order one. We show how to apply the Multi Level Monte Carlo (MLMC) method to an Euler time stepping method with boundary test and this improves the Monte Carlo computation of the MFET.

Keywords: first exit time; fixed time-step Euler method; exponential time-stepping Euler algorithm; FitzHugh–Nagumo model; Ornstein–Uhlenbeck process.

1   Introduction

A noisy neural model is a system of stochastic differential equations (SDEs) that models the membrane potential of a single neuron. There has been significant interest in studying the so-called First Exit Time (FET) of the membrane potential through a constant firing threshold, since the time to the first spike is believed to hold significant information about the stimulus properties; see Tuckwell and Wan (2005); Tuckwell (1988); Giraudo and Sacerdote (1998). In this paper, we study the errors in the numerical computation of the mean FET (MFET) for the Ornstein–Uhlenbeck (OU) model studied by Lánský and Lánská (1994) and for the stochastic version of the space-clamped FHN system studied by Tuckwell *et al.* (2003).

[*]Department of Mathematics, University College in Qunfudah, Umm Al-Qura University, Saudi Arabia. `hmzubaidi@uqu.edu.sa`

[†]Department of Mathematical Sciences, University of Bath, Bath BA2 7AY, UK.   `t.shardlow@bath.ac.uk`.

The simplest method for approximating the MFET is to employ a time stepping method to generate an approximate path and step until the path crosses the threshold. This gives an approximate exit time and a Monte Carlo method can be used to approximate the MFET. This method suffers from two sources of error: the systematic error inherent from the time-stepping and the Monte Carlo sampling error. We choose the Euler (or Euler–Maruyama) time-stepping method with fixed and exponentially distributed time steps and discuss ways to reduce both sources of error.

We first discuss the systematic error for the Euler method with fixed time step Δt. The error in the MFET, say H_b, through a constant threshold boundary, b, produced using the Euler method has two undesirable properties. First, the error is $O(\Delta t^{1/2})$ and converges slowly compared to $O(\Delta t)$ rate for other Euler type approximations. Second, the method overestimates the MFET because there is no possibility that the threshold is reached between time steps. Mannella (1999) dealt with this situation by applying a boundary test. Later, Gobet (2000) proved that this test combined with the Euler method improves the weak order of convergence from $O(\Delta t^{1/2})$ to $O(\Delta t)$ in the evaluation of a smooth functional of $X(t)$ conditioned on $t < H_b$. Our numerical experiments for the OU and stochastic FHN models suggest also that the MFET is approximated with $O(\Delta t)$.

In addition to fixed time steps, we investigate the Euler method with i.i.d time steps taken from the exponential distribution as introduced by Jansons and Lythe (2003). This leads to a convenient method for approximating the MFET and experiments show $O(\Delta t)$ accuracy when a boundary test is incorporated.

Giles (2008a,b) introduced the Multi Level Monte Carlo (MLMC) method, using simulations on a sequence of grids and arranging the calculations so many cheap coarse grid and fewer fine grid calculations are made, to reduce computation time while keeping the same level of accuracy as a conventional Monte Carlo method. In approximation of averages of solutions to SDEs at finite times, this leads to a reduction in the work required from $O(\epsilon^{-3})$ to $O(\epsilon^{-2}|\log \epsilon|^2)$ for a given accuracy ϵ. Recently Higham *et al.* (2012) analysed the MLMC method for exit time problems and showed the method can be used with the Euler method with fixed time stepping to improve performance. We also apply MLMC to the computation of MFET and include a boundary test. We show MLMC improves performance on some examples and appears to have the same rate

of convergence as the Monte Carlo method. When MLMC is used without boundary tests as in Higham *et al.* (2012), the performance does improve (relative to a Monte Carlo simulation without boundary tests) but not to an extent that is competitive with boundary tests. Exponential time stepping is not easily adapted to MLMC.

The paper is organized as follows. In Section 2, the MFET problem is formulated and necessary notations are introduced. In Section 3, we carefully define the exponential and fixed time stepping Euler methods and the associated boundary tests. In Section 4, we include numerical experiments concerning the OU and FHN equations, in order to investigate the convergence of the methods. Section 5 covers the MLMC method and Section 6 contains our conclusions and some ideas for future work.

2 Problem formulation

Let $X(t)$, $t \geq 0$, be a stochastic process satisfying the stochastic differential equation (SDE)

$$dX(t) = \mu(X(t))dt + \sigma dW(t), \quad X(0) = x \in \mathbf{R}, \tag{1}$$

where $W(t)$ is a standard one-dimensional Wiener process on a probability space $(\Omega, \mathcal{F}, \mathbf{P})$. The constant $\sigma^2 > 0$ represents the diffusion and the function $\mu \colon \mathbf{R} \to \mathbf{R}$ represents the drift and is assumed to satisfy regularity conditions, sufficient to guarantee the existence and uniqueness of the solution to (1); e.g., (Kloeden and Platen, 1999, Theorem 4.5.3). Define now the first exit time $H_b(x)$ and mean first exit time $T(x)$ through a fixed point $b \in \mathbf{R}$ by

$$H_b(x) = \inf\{t \geq 0 : X(t) = b\}, \qquad T(x) = \mathbf{E}[H_b], \quad -\infty < x < b,$$

where $\mathbf{E}$ denotes expectation with respect to $\mathbf{P}$. It is well known that $T(x)$ obeys the boundary value problem (Karlin and Taylor (1981))

$$LT(x) = -1, \quad -\infty < x < b, \tag{2}$$

$$\lim_{a \to -\infty} T(a) = 0, \qquad T(b) = 0,$$

where the generator

$$L = \mu(x)\frac{d}{dx} + \frac{1}{2}\sigma^2\frac{d^2}{dx^2}.$$

Explicit solutions of first exit problems are limited to a few simple cases and numerical techniques are required to approximate solutions.

We use the following standard notations: $N(\mu, \sigma^2)$ for the Gaussian distribution with mean μ and variance σ^2, $U(a, b)$ for the uniform distribution on $[a, b]$, and $\text{Exp}(\lambda)$ for the exponential distribution with rate λ.

3 Simulation techniques

Consider the standard Euler method for approximating the solution $X(t_n)$ of (1) at time $t_n = n\Delta t$ by X_n defined by

$$X_{n+1} = X_n + \mu(X_n)\Delta t + \sigma\sqrt{\Delta t}\,\eta_n \tag{3}$$

and $X_0 = x$, where Δt is the fixed time step and $\eta_n \sim N(0, 1)$ i.i.d. The simplest method for approximating the MFET $T(x)$ is to calculate

$$T(x) \approx \frac{1}{M} \sum_{m=1}^{M} \min\{t_n : X_n^m \geq b \text{ or } n = N\} \tag{4}$$

where X_n^m, $m = 1, \ldots, M$, are i.i.d samples of the Euler approximation X_n and N is a maximum number time steps. We also define the Euler method with boundary test. First, let

$$P_{x,b,y} = \exp\left(\frac{-2(b-x)(b-y)}{\sigma^2 \Delta t}\right). \tag{5}$$

Then, if $x, y < b$ and Y obeys

$$dY = \mu(x)dt + \sigma dW(t), \qquad Y(0) = x$$

where we freeze the drift, $P_{x,b,y} = \mathbf{P}(Y(t) = b$, some $0 < t < \Delta t$ given $Y(\Delta t) = y)$. We expect $P_{x,b,y}$ is a good approximation to the probability of an excursion in the interval $[t_n, t_{n+1}]$ by the solution $X(t)$ of (1) given $X(t_n) = x$ and $X(t_{n+1}) = y$. This motivates the *time stepping Euler method with boundary test*, given as follows:

- The trajectories $\{X_n : n = 0, 1, 2, \cdots, N\}$ are generated according to equation (3).

- Generate $u_n \sim U(0, 1)$ i.i.d and say that an excursion during the time step $(t_n, t_{n+1}]$ is detected if $u_n < P_{x,b,y}$ for $x = X_n$ and $y = X_{n+1}$.

- We repeat the time stepping until an excursion is detected or $n = N - 1$ is reached and output t_{n+1} as the exit time.

We approximate the MFET by the average of the exit time t_{n+1} over M independent samples as in (4).

3.1 Exponential Euler method with boundary test

Under the exponential time stepping method (Jansons and Lythe (2003, 2000)), in place of a fixed time step Δt, we take time steps δt_n that are i.i.d $\text{Exp}(\lambda)$ random variables, where the rate $\lambda > 0$ plays the role of discretisation parameter. If $\tau \sim \text{Exp}(\lambda)$ and independent of $W(t)$, then $Y(\tau) = \mu\tau + \sigma W_\tau$ has density

$$p(x) = \int_0^\infty \frac{1}{\sqrt{2\pi\sigma^2 t}} e^{-(x-\mu t)/2\sigma^2 t} \lambda e^{-\lambda t} \, dt = \frac{\lambda}{\sigma^2} \frac{1}{N} \times \begin{cases} e^{-|x|(N+F)}, & x\mu < 0, \\ e^{-|x|(N-F)}, & \text{otherwise,} \end{cases}$$

for $F = \mu/\sigma^2$ and $N = \sqrt{F^2 + \nu^2}$ and $\nu^2 = 2\lambda/\sigma^2$. Note that

$$\mathbf{P}(\mu Y(\tau) > 0) = (N + F)/2N \tag{6}$$

and $Y(\tau)$ given $\pm\mu Y(\tau) > 0$ has distribution $\text{Exp}(N \mp F)$ and thus $Y(\tau)$ is easily sampled. We see then that the Euler method with exponential time steps is given by $X_{n+1} = X_n + Y(\tau)$, where $\mu = \mu(X_n)$.

To include the boundary test, let

$$\tilde{P}_{x,b,y} = e^{-2N(x)(b-\max\{x,y\})}, \qquad x, y < b. \tag{7}$$

In (Jansons and Lythe, 2003, (3.7)), it is shown that $\tilde{P}_{x,b,y} = \mathbf{P}(Y(t) > b, \text{ some } 0 \le t \le \tau)$ and this probability leads to the following *exponential time stepping Euler algorithm with boundary test* for simulating $X(t)$.

- Let u_n, p_n be pairwise independent random variables with $u_n \sim U(0, 1)$ and $p_n \sim \text{Exp}(1)$.

- Given the value of $X_n \approx X(t_n)$, we generate the value of $X_{n+1} \approx X(t_{n+1})$ for $t_{n+1} = t_n + \delta t_n$ as

$$X_{n+1} = X_n + \left(N(X_n) - s(X_n)F(X_n)\right)^{-1} s(X_n)p_n, \tag{8}$$

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where $F(X) = \sigma^{-2}\mu(X)$, $N(X) = \sqrt{F(X)^2 + \nu^2}$, $s(X) = \text{sign}(\frac{1}{2}(1 + \frac{F(X)}{N(X)}) - u_n)$. Note that $(N(X_n) - s(X_n)F(X_n))^{-1}p_n \sim \text{Exp}(N \pm F)$ and $\mathbf{P}(s(X_N)p_n > 0) = (N + F)/2N$.

- Substituting $x = X_n$, $y = X_{n+1}$ in (7), we say an excursion is detected in $(t_n, t_{n+1}]$ if $z_n < e^{-2N(X_n)(b - \max\{X_n, X_{n+1}\})}$, where $z_n \sim \mathbf{U}(0,1)$ i.i.d.

- Repeat the time stepping until an excursion is detected or the maximum number of time steps N is reached and output the number of steps taken n.

Notice that t_n or δt_n are never explicitly generated. The MFET is computed from the average number of steps n multiplied by the mean time step $\mathbf{E}\delta t_n = 1/\lambda$.

When σ is small, it is advantageous to replace the update rule (8) with

$$X_{n+1} = \begin{cases} X_n + \frac{1}{2\lambda}\mu(X_n)\delta_n + \frac{\sigma}{\sqrt{2\lambda}}\delta_n, & u_n < \frac{1}{2}\left(1 + \frac{\mu(X_n)}{\sqrt{2\lambda\sigma^2}}\right), \\ X_n + \frac{1}{2\lambda}\mu(X_n)\delta_n - \frac{\sigma}{\sqrt{2\lambda}}\delta_n, & \text{otherwise}, \end{cases} \tag{9}$$

for $\delta_n \sim \exp(1)$ i.i.d. This is quite natural as $\mathbf{E}\delta_n/2\lambda = \text{Var}(\delta_n/\sqrt{(2\lambda)})$ reflects the usual $\Delta t = \text{Var}(\sqrt{\Delta t}\eta_n)$ we have for Euler's rule with fixed time stepping. The term u_n gives a small correction, so that in the limit $\lambda \to 0$, where (9) is dominated by the $(\sigma/\sqrt{2\lambda})\delta_n$ term and $\mathbf{P}(\mu(X_n)(X_{n+1} - X_n) > 0)$ tends to $\frac{1}{2}(1 + \frac{\mu(X_n)}{\sqrt{2\lambda\sigma^2}})$, the update rule (9) agrees with (6); i.e.,

$$\frac{N + F}{2N} = \frac{1}{2} + \frac{1}{2N/F} \to \frac{1}{2}\left(1 + \frac{\mu(X_n)}{\sqrt{2\lambda\sigma^2}}\right) \quad \text{as } \lambda \to \infty.$$

It is also derived in (Jansons and Lythe, 2003, (4.16)) in a limit $\lambda/\sigma^2 \to \infty$.

4 Numerical experiments

We employ the simulation techniques described above in two neurobiological examples, the Ornstein–Uhlenbeck and FitzHugh–Nagumo models.

4.1 Ornstein–Uhlenbeck (OU) model

The simplest stochastic leaky integrate and fire (LIF) model for describing the behaviour of nerve membranes is the Ornstein–Uhlenbeck (OU) process (Lánský and Ditlevsen (2008)). It is used

to approximate the subthreshold membrane potential of a nerve cell receiving random synaptic inputs and is given by the SDE

$$dX(t) = \big(-\alpha X(t) + \eta \big) dt + \sigma dW(t), \quad X(0) = x, \tag{10}$$

where the constants η and σ reflect the input signal and its variability, resulting from the stochastic dendritic currents that are caused by the action potential of other neurons or by external stimulation in sensory neurons. The time membrane constant $\frac{1}{\alpha} = CR > 0$ governs the spontaneous decay of the membrane potential to its resting state, where R and C are the membrane resistance and its capacitance respectively. The spiking activity of the OU model is identified by the FET of the membrane potential through a constant boundary. In the OU model, the neuron emits a spike whenever the firing threshold $(b > x)$ is reached, and then the membrane potential is reset to its equilibrium potential, which is conveniently set to zero (Ditlevsen and Ditlevsen (2008)). Unlike more complex models such as the Hodgkin–Huxley model and the FHN model, the action potential is not a part of the OU model; only its time generation is considered and so we have to impose the threshold condition.

The action potential $X(t)$ given by the OU model is Gaussian with

$$\mathbf{E}[X(t)] = \frac{\eta}{\alpha} + \Big(x - \frac{\eta}{\alpha} \Big) e^{-t\alpha}, \qquad \mathrm{Var}[X(t)] = \frac{\sigma^2}{2\alpha} \Big(1 - e^{-2t\alpha} \Big).$$

For $t \to \infty$, the asymptotic mean depolarization is $\frac{\eta}{\alpha}$ and thus we have two firing regimes for the OU model. The first is called suprathreshold firing and occurs when $\frac{\eta}{\alpha} > b$ and the neuron produces spikes even in the absence of noise. The other is called subthreshold firing and is caused only by the random fluctuations of the depolarization when $\frac{\eta}{\alpha} < b$ (Lánský and Ditlevsen (2008)). The neuron, therefore, never fires when $\sigma = 0$. We are interested here in exploring the effect of noise on the spiking activity of the OU model and so we limit ourselves to the second regime, in particular when there is an absence of input $(\eta = 0)$.

The spiking activity of the OU model is measured by the first exit time of the membrane potential and it is interesting to calculate the MFET $T(x)$. From Siegert (1951), $T(x)$ is given by the integral

$$T(x) = \sqrt{\frac{\pi}{\alpha \sigma^2}} \int_x^b \Big(1 + \mathrm{erf}\Big(\frac{z\sqrt{\alpha}}{\sigma} \Big) \Big) \exp \Big(\frac{z^2 \alpha}{\sigma^2} \Big) dz, \tag{11}$$

where $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$ is the error function. In §4.3, we evaluate the integral in (11) using

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`quad` in MATLAB, to gain a reference solution to $T(x)$ and compute errors for the numerical methods in §3.

4.2 FitzHugh–Nagumo (FHN) model

Consider a space-clamped FHN system

$$
\begin{aligned}
dX &= \big(f(X(t), Y(t)) + I\big)dt + \sigma dW(t) \\
dY &= \beta\big(X(t) - \gamma Y(t)\big)dt,
\end{aligned}
\tag{12}
$$

with initial conditions $X(0) = x$ and $Y(0) = y$. $X(t)$ represents the voltage variable and $Y(t)$ the recovery variable. $W(t)$ is a standard Wiener process, σ is a noise parameter and I is a constant input current. f is the cubic function

$$
f(X, Y) = kX(X - c)(1 - X) - Y, \quad 0 < c < 1.
$$

c should be set to less than $\frac{1}{2}$ in order to obtain suitable suprathreshold responses, as in Tuckwell *et al.* (2003). γ and β are positive constants.

We are interested in finding the MFET for $X(t)$ through a constant threshold b. The recovery variable Y is practically unaffected during the elementary stages of the interspike interval, and therefore the system (12) can be reduced to a one-dimensional equation by considering $Y(t) = y$ to be a constant. The system then takes the form

$$
dX = \big(f(X(t), y) + I\big)dt + \sigma dW(t),
\tag{13}
$$

with initial condition $X(0) = x \in (-\infty, b)$. To determine a reference solution $T(x)$ for computing errors, we solve the boundary value problem (2) for $\mu(x) = f(x, y) + I$, with the boundary condition $T(a) = 0$ for $a = -100$, using the MATLAB function `bvp_4C`. This allows us to compute errors and evaluate the effectiveness of the numerical methods of §3.

4.3 Summary of simulation results

The random time step δt has expectation $\mathbf{E}[\delta t] = \frac{1}{\lambda}$ and this is used in the exponential time stepping algorithm as an equivalent to Δt in the fixed time stepping algorithm when we plot errors against a discretisation parameter. The cpu time is normalised by the number of samples.
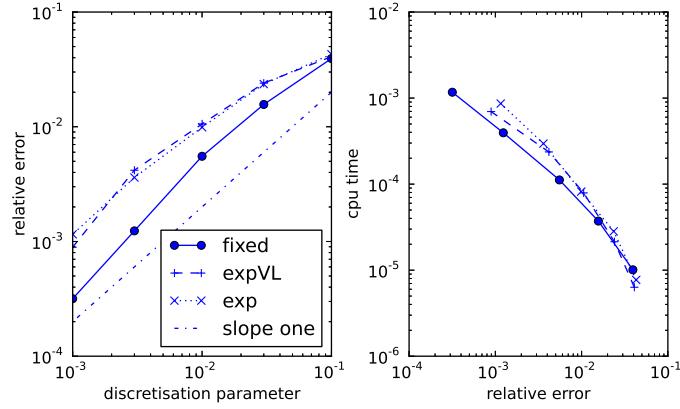
Figure 1: Plots of the relative error against discretisation parameter $\Delta t = 1/\lambda$ and cpu time against relative error for the OU model with initial data $x = 0$, dissipation $\alpha = 1$ and noise $\sigma = \sqrt{2}$. The threshold $b = 1$ and the number of samples $M = 10^6$. `fixed` is the fixed time stepping Euler method with boundary test; `exp` is the exponential time stepping Euler method with boundary test; and `expVL` is the variant of `exp` defined by (9). The reference solution $T = 2.0934$ is used for computation of the relative errors.
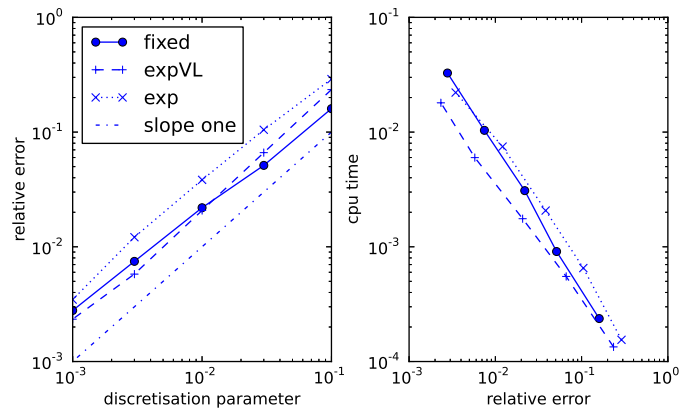

Figure 2: Similar to Figure 1, except for noise level $\sigma = 0.5$ and reference solution $T = 56.59426$.
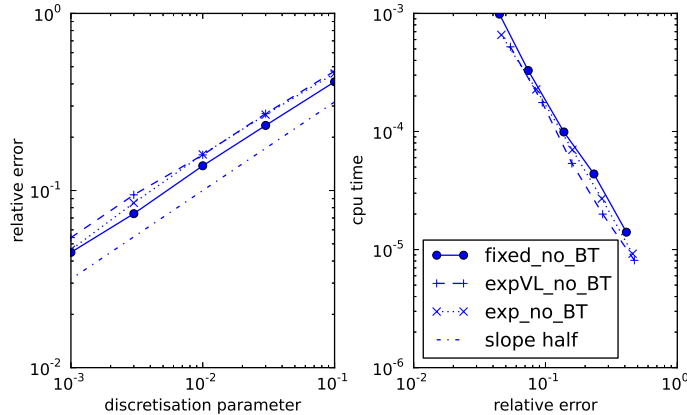
Figure 3: Similar to Figure 1, except the simulations are performed without the boundary tests. Notice that compared to Figure 1, the lines have slope half rather than slope one and the computations are much less accurate (contrast the scale on the error axis).

OU We consider two cases of the OU process with parameters $\alpha = 1, b = 1$ with the noise levels $\sigma = \sqrt{2}$ and $\sigma = 0.5$. The model becomes significantly more difficult as $\sigma \to 0$ as the noise must exit from a potential well and the exit time grows like e^{1/σ^2} and indeed we see $T(0)$ increases by a factor of 25 in reducing σ from $\sqrt{2}$ to 0.5.

We present computations of the systematic error for both the fixed and exponential time stepping Euler methods with and without boundary test in Figures 1–3 for $\sigma = \sqrt{2}$ and $\sigma = 0.5$. In order to avoid any influence from statistical errors, M is chosen as 10^6 and, in this case, the error bars which represent the statistical errors are smaller than the plotted symbols and can be neglected. Figures 1–2 show that the systematic error is proportional to $\Delta t = 1/\lambda$. In contrast, in Figure 3, we see that without the boundary test, the systematic errors are proportional to $\Delta t^{1/2} = (1/\lambda)^{1/2}$. Notably, when a smaller σ is chosen in Figure 2, the exponential time stepping method in its `expVL` variant (i.e., using (9)) is most accurate for a given amount of CPU time as this method takes advantage of the small noise.

FHN We choose the parameters $c = 0.1$, $k = 0.5$, $I = 1.5$, and $\sigma = 0.25$. The initial values are $x = 0$ and $y = 1$. To avoid any influence from the sampling errors, M is chosen as 10^6. Figure 4
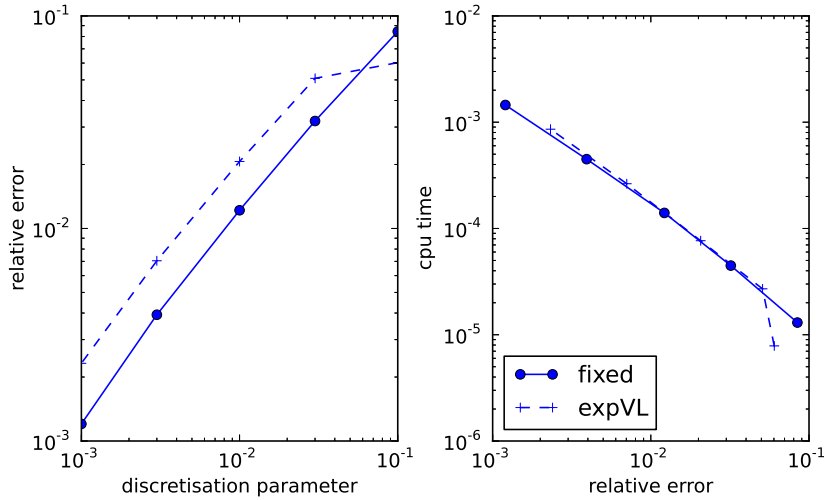
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Figure 4: Plots of the relative error against discretisation parameter $\Delta t = 1/\lambda$ and cpu time against relative error for the FHN model with initial data $x = 0$ and noise $\sigma = 0.25$. The threshold $b = 2$ and the number of samples $M = 10^6$. `fixed` is the fixed time stepping Euler method with boundary test; `expVL` is the variant of `exp` defined by (8). The reference solution $T = 2.5677$ is used for computation of the relative errors.

displays the error in the computed MFET of the FHN model as a function of $\Delta t = \frac{1}{\lambda}$ and again we see the error scales linearly with the discretisation parameter. For a given amount of cpu time, both the exponential and fixed time stepping methods achieve similar levels of accuracy.

5 Multi Level Monte Carlo

We now discuss the Multi Level Monte Carlo (MLMC) method of Giles (2008a,b) for improving the the Monte Carlo calculation. To describe MLMC, fix $\gamma = 2$ and $\Delta t_0 > 0$ and introduce time steps $\Delta t_k = \gamma^{-k} \Delta t_0$ for $k = 1, \ldots, \ell$. Let ϕ_k be the approximation to the exit time $H_b(x)$ by the
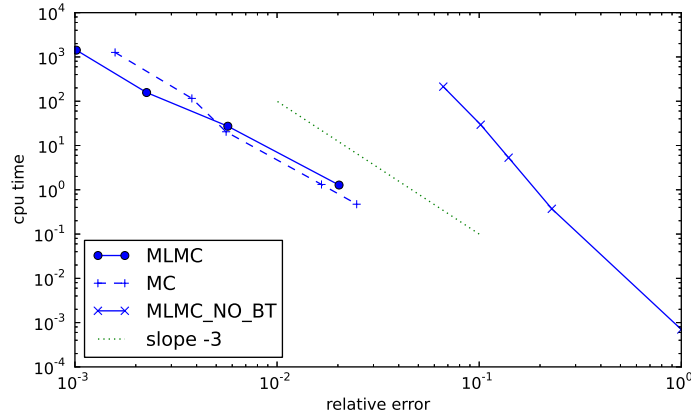
Figure 5: Plots of cpu time against relative error for the computation of the MFET of the OU process with $\alpha = 1$, $x = 0$, $b = 1$ and noise level $\sigma = \sqrt{2}$ as the smallest time step Δt_ℓ is varied. The MLMC is applied with critical time step $\Delta t_c = 0.05$ and $M_k = 50 \Delta t_\ell^{-2} \sqrt{\text{Var}(\delta_k) \Delta t_k}$. Three lines are shown: MLMC is the MLMC algorithm incorporating the boundary test (8); MLMC_NO_BT is the MLMC algorithm without the boundary test; and MC denotes the MLMC with $\ell = 0$ levels (conventional Monte Carlo). Notice that MLMC and MC are achieving the same levels of accuracy for a given CPU time and the cpu time is proportional to the error^{-3}. Without the boundary test, the algorithm is significantly less accurate.
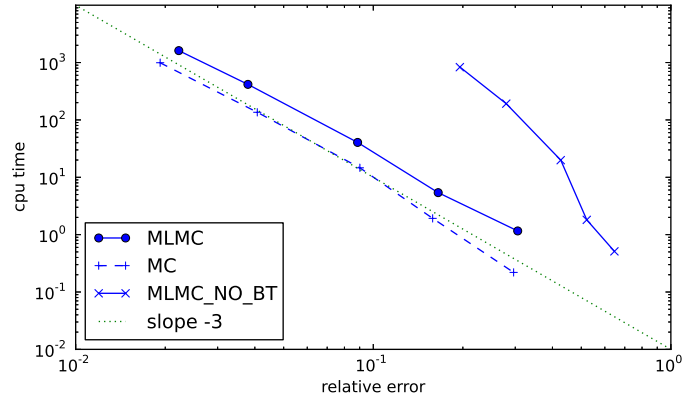
Figure 6: Plots of cpu time against relative error for the computation of the MFET of the OU process with $\sigma = 0.5$. The MLMC is applied with $\Delta t_c = 0.1$ and $M_k = \Delta t_\ell^{-2} \sqrt{\mathrm{Var}(\delta_k)\Delta t_k}$
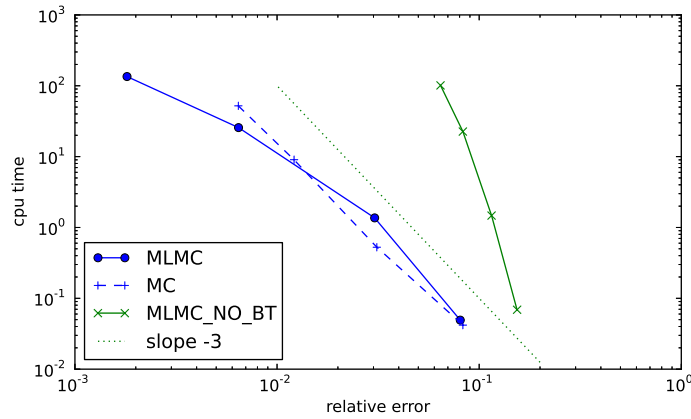

Figure 7: Plots of cpu time against relative error for the computation of the MFET of the FHN example. Three methods are tried, as in Figure 5. The MLMC is applied with $\Delta t_c = 0.1$ and $M_k = 100\Delta t_\ell^{-2} \sqrt{\mathrm{Var}(\delta_k)\Delta t_k}$.

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Euler method with time step Δt_k and consider the telescoping sum

$$\mathbf{E}[\phi_\ell] = \mathbf{E}[\phi_0] + \sum_{k=1}^{\ell} \mathbf{E}[\delta_k], \quad \delta_k = \phi_k - \phi_{k-1}.$$

In conventional Monte Carlo, we approximate $\mathbf{E}[\phi_\ell]$ by the mean of M i.i.d samples of ϕ_ℓ. The accuracy is proportional to $\sqrt{\text{Var}(\phi_\ell)/M_\ell}$ and to achieve an accuracy ϵ we require $M_\ell = O(\text{Var}(\phi_\ell)/\epsilon^2)$. In MLMC, we evaluate the expression on the right hand side, computing $\mathbf{E}[\phi_0]$ as the sample average of ϕ_0 using M_0 samples and computing $\mathbf{E}[\delta_k]$ using M_k samples. By choosing $M_k = \text{const} \times \epsilon^{-2}\sqrt{\text{Var}(\delta_k)\Delta t_k}$ for small parameter ϵ, we minimises the variance of the MLMC estimator for a given computational cost (see Giles (2008b)). When δ_k is the difference of ϕ_k, ϕ_{k-1} that are approximate exit times for the same sample path $X(t)$, we expect $\text{Var}(\delta_k)$ to be small and high accuracy can be achieved with less work by choosing $M_k \ll M_0$. Thus, we use far fewer samples of δ_k for k that require a small time step and we achieve an algorithm that requires less computational time. This scheme has been rigorously justified in the weak approximation of SDEs at finite times and accuracy ϵ can be achieved with $O(\epsilon^{-2}|\log \epsilon|^2)$ work, which compares favourably to the naive Monte Carlo that requires $O(\epsilon^{-3})$ work. Recently, Higham *et al.* (2012) analysed a MLMC method for the computation of the MFET using a fixed time step Euler method *without a boundary test* and showed the complexity is reduced from $O(\epsilon^{-4})$ to $O(\epsilon^{-3}|\log \epsilon|)$.

We introduce now a version of the MLMC method that works with the fixed time stepping Euler method with boundary test. Notice that the exponential time stepping method is not naturally set up to be used with MLMC, as the time steps Δt_k need to be replaced by exponential random variable parameters λ_k and the random variables u_n, p_n, z_n understood at the different levels. The effectiveness of MLMC depends on the size of $\text{Var}(\delta_k)$ for $\delta_k = \phi_k - \phi_{k-1}$ and this is reduced by computing ϕ_k, ϕ_{k-1} using the "same" random variables. For the Brownian increments, this is easily achieved by choosing the increments η_n, η_{n+1} on the fine level for the intervals $[t_n, t_{n+1}], [t_{n+1}, t_{n+2}]$. The corresponding increment on the coarse level over $[t_n, t_{n+2}]$ is found by adding the fine level increments and choosing $\eta_n + \eta_{n+1}$. We are simply mimicking the property that $W(t_{n+2}) - W(t_n) = (W(t_{n+2}) - W(t_{n+1})) + (W(t_{n+1}) - W(t_n))$.

We need to achieve the same effect with the boundary test and this is less straightforward. First, let X_n, X_{n+1}, X_{n+2} be the fine approximation at times t_n, t_{n+1}, t_{n+2} respectively and let Y_n, Y_{n+2} be the coarse approximation at t_n, t_{n+2}. Let $p_{f1} = P_{X_n, X_{n+1}}$, $p_{f2} = P_{X_{n+1}, X_{n+2}}$, and $p_c = P_{Y_n, Y_{n+2}}$; then the boundary tests on the first fine level and the coarse level are as follows:

Generate a random variable $u_n \sim U(0,1)$; then an excursion is detected on

$$\text{the fine level } (t_n, t_{n+1}] \text{ if } u_n < p_{f1},$$

$$\text{the coarse level } (t_n, t_{n+2}] \text{ if } u_n < p_c.$$

The choice of boundary test on the second fine level should be chosen to occur with probability p_{f2} and to use the same uniform random variable u_n. Accordingly, we say an excursion is detected on

$$\text{the fine level } (t_{n+1}, t_{n+2}] \text{ if } p_{f1} \le u_n < p_{f1} + p_{f2} - p_{f1} p_{f2},$$

which occurs with probability p_{f2} given no excursion on the first fine level ($u_n \ge p_{f1}$). This choice of boundary test preserves the distribution of ϕ_k (whether computed for δ_{k+1} or δ_k) and maximises the chance that any excursions that occur happen on both fine and coarse levels, so that the fine and coarse approximation will do the same thing most of the time and $\text{Var}(\delta_k)$ will be reduced.

We give the results of experiments with MLMC for the computation of mean first exit times for the OU and FHN models, in comparison to conventional Monte Carlo (case $\ell = 0$) and the MLMC with no boundary test (as in Higham *et al.* (2012)). In each case, we increase the accuracy by reducing the smallest time step Δt_ℓ and setting $M_k = \text{const} \times \Delta t_\ell^{-2} \sqrt{\text{Var}(\delta_k) \Delta t_k}$ (the variance of δ_k is approximated by a sample variance). The number of MLMC levels ℓ is the largest ℓ such that $\Delta t_0 \le \Delta t_c$, for some critical time step Δt_c, to ensure stability of the underlying integrator. Figures 5–6 shows numerical experiments with the OU process (10) with parameters $\sigma = \sqrt{2}$ and $\sigma = 1/2$ respectively (as before $\alpha = 1$, $b = 1$ and we compute $T(0)$). The relative error shows the root mean square average of relative errors taken from ten repetitions. Figure 7 shows numerical experiments with the FHN example and model parameters as in Figure 4.

Broadly speaking, the MLMC method shows a similar rate of convergence to the Monte Carlo method when the underlying method includes a boundary test, though in Figures 6–7 it is more efficient. The key step in improving the efficiency is to include the boundary test as this improves the cost of achieving order accuracy ϵ from $O(\epsilon^{-4})$ to $O(\epsilon^{-3})$. The experiments do not exhibit the same degree of improvement as the weak approximation at a finite time. This is because $\text{Var}(\delta_k)$ behaves experimentally as $O(\Delta t_k^{1/2})$, whilst in weak weak approximation at a finite time it behaves like $O(\Delta t_k)$. One reason for this is samples of exit times are unbounded, and samples of δ_k can be arbitrarily large. If an excursion is detected at the fine level but not at the coarse level, the coarse level may perform a large deviation and so δ_k is often large.

6 Conclusion

We used the fixed and exponential time-stepping Euler methods with boundary tests to approximate the MFET for one-dimensional diffusion neural models, represented by the OU and stochastic FHN models. We found the fixed time-stepping algorithm with Mannella's boundary test improved the order of convergence in the MFET from one half to one, which coincides with previous results, such as those in Jansons and Lythe (2003) and Buchmann (2005). There is not yet a rigorous proof of this rate of convergence, though Gobet (2000) addresses a number of related problems with due rigour. We discussed a variant of the exponential time-stepping for small noise; however, this problem remains difficult due to the exponentially large exit times.

Finally, we introduced a new MLMC method that allows the use of boundary tests in the underlying time stepping method. Recent work of Higham *et al.* (2012) uses the fixed step Euler method without a boundary test, but the complexity of the method is $O(\epsilon^{-3}|\log \epsilon|)$ and is not competitive with a Monte Carlo calculation that incorporates a boundary test with complexity $O(\epsilon^{-3})$. Though it was hoped the development of a MLMC for time stepping methods with boundary tests would give similar improvement in efficiency, we discovered the proposed MLMC method has a very similar computational cost to the standard Monte Carlo method. The limiting feature is the variation of the difference between fine and coarse levels, which is too high and severely restricts the potential gains of MLMC. This study is restricted to simulations in dimension $d = 1$, where the boundary test is simple to implement. For domains in higher dimensions, the boundary test is more difficult to formulate and its effectiveness depends on the boundary being relatively smooth (see Gobet (2000); Jansons and Lythe (2005)). In such cases, where the boundary tests are unavailable or complicated to implement, the MLMC method does give a route to improving the computation of mean exit times.

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