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Probability evolution method for exit location distribution

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ABSTRACT

The exit problem in the framework of the large deviation theory has been a hot topic in the past few decades. The most probable escape path in the weak-noise limit has been clarified by the Freidlin–Wentzell action functional. However, noise in real physical systems cannot be arbitrarily small while noise with finite strength may induce nontrivial phenomena, such as noise-induced shift and noise-induced saddle-point avoidance. Traditional Monte Carlo simulation of noise-induced escape will take exponentially large time as noise approaches zero. The majority of the time is wasted on the uninteresting wandering around the attractors. In this paper, a new method is proposed to decrease the escape simulation time by an exponentially large factor by introducing a series of interfaces and by applying the reinjection on them. This method can be used to calculate the exit location distribution. It is verified by examining two classical examples and is compared with theoretical predictions. The results show that the method performs well for weak noise while may induce certain deviations for large noise. Finally, some possible ways to improve our method are discussed.

1. Introduction

Noise is usually considered to be annoying and may be ignored in most of the cases. However, during the past few decades, it has exhibited incredible roles on the phenomena of stochastic resonance (SR) [1] and coherence resonance (CR) [2], which has aroused broad interest in a variety of disciplines. SR shows that under some certain strength of noise, the amplitude of the external signal can be significantly enhanced. On the other hand, even for arbitrarily small noise, the response can be carried away from the asymptotic stable equilibrium position for sufficiently large time [3]. The latter can be of great relevance to the reliability of engineering structures on the problem of first passage failure [4]. In the framework of large deviation theory, Freidlin and Wentzell [3] applied the concept of action functional attached to each sample path to investigate the exit problem. They showed that in the weak-noise limit, the exit from a domain must take place along an extremal of the action functional with overwhelming probability. In other words, for sufficiently small noise, the escape paths rarely happen, but when they escape, the paths escape with high probability along the pathway that is least unlikely. That makes rare events predictable and noise less noisy. This elegant theory has also been verified by abundant experiments by Dykman, McClintock and their coworkers [5–7].

To accurately depict the whole exit process, the probability density function, which is the solution of the corresponding Fokker–Planck–Kolmogorov (FPK) equation, should be solved. This is not always an easy task even for low dimensional dynamical systems. Analytical results can only be obtained under some restrict circumstances, e.g. detailed balance or generalized stationary potential [8]. Thus, other approximation methods should be introduced to uncover some characteristics of a specific exit problem. These characteristics include most probable escape path (MPEP), mean first passage time (MFPT), exit location distribution (ELD), etc. Dykman et al. [5] defined the prehistory probability density to describe the distribution of paths ending at the final state from which they evolve the system backwards in time. The ridge along the top of the distribution of this quantity corresponds to the MPEP of the given system. The action plot method [9] is introduced by Beri et al. which is actually a topological method which enumerates the trajectories starting from a small neighboring area of the initial position. The trajectory with least action will be chosen as the MPEP. Other methods such as the geometric minimum action method (gMAM) [10] and the ordered upwind method (OUM) [11] are also very efficient in calculating the MPEP. These methods have been shown for accuracy and consistency in the excitable system [12]. In real physical systems, the noise strength cannot be arbitrarily small. The MPEP and ELD may be modified for finite noise inten-

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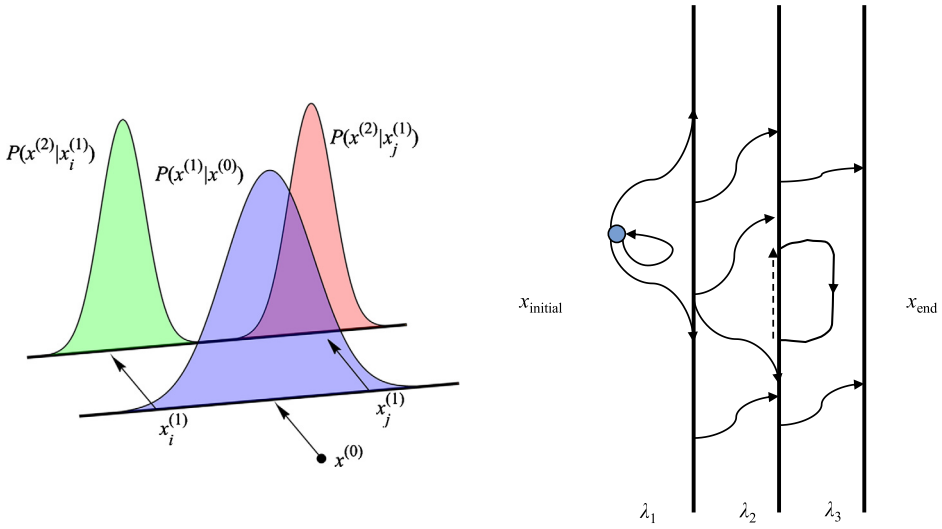

Fig. 1. Illustration of the probability evolution method. Left panel: the probability evolution example. The superscript represents the label of the interface and the subscript represents the point on the interface. The blue, green and red patches represent the transition probability distribution from the point in the previous interface to the next interface. Right panel: the sampling paths between the interfaces λ_i. The dashed arrow represents the reinjection. Details are in the text. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

sities, e.g. noise-induced shift [13,14] and saddle-point avoidance [15].

To obtain the exit location distribution for finite noise strengths, if the explicit theoretical expression cannot be calculated, direct Monte Carlo (brute force) simulation may be a good candidate which first comes to one's mind. However, when noise is small enough, the MFPT grows exponentially as noise approaches zero [16]. As a matter of fact, one is forced to waste considerable time on uninteresting dynamical behaviors until the final escape happens. Researchers have been looking for methods to accelerate the process. In order to speed up the sampling process, Allen et al. [17] presented the forward flux sampling (FFS) technique first applying in biochemical networks. This method employs several nonintersecting interfaces in phase space between the initial and final states and generates rare paths in a ratchetlike manner [18]. By using similar ideas, the barrier method [19] and milestoning [20–23] also apply interfaces to accelerate simulations. Glowacki et al. [24] introduced an even simpler method named boxed molecular dynamics which can efficiently calculate the free energy profiles. These methods are very popular in molecular dynamics (MD) simulations. Based on the knowledge of the MPEP in theory in the weak-noise limit, Beri et al. [14] used the dynamic importance sampling (DIMS) to keep the trajectory on the stable manifold of the MPEP whenever the trajectory leaves a small neighborhood of it. Crooks and Chandler [25] realized another side of the coin by directly sampling the noise process. Recently, Han et al. [26] applied the generalized cell mapping (GCM) method to the exit location distribution problem which showed quite satisfactory agreement between the theory and numerical simulation.

In this paper, we propose a method named as probability evolution method (PEM) to calculate the ELD by combining the advantages of the FFS method and the fast Monte Carlo simulations used by Bandrivskyy et al. in Ref. [27]. The structure of this paper is as follows. In Section 2, the PEM is illustrated and is compared with previous methods. It is applied to two classical examples in Section 3 and is validated by theoretical results. Finally, discussions and conclusions are given in Section 4.

2. Method

As is in the FFS method, PEM also applies several nonintersecting interfaces between the initial (equilibrium points, limit cycles, chaotic attractors, etc.) and final (saddle points, limit cycles, chaotic saddles, etc.) states. Different to the FFS method, the calculation between different interfaces is independent and the sample paths are not necessary to be reserved. The detailed process goes as follows. We take the stable equilibrium point being the initial state as an example. As is in Fig. 1, we start N_1 samples from the equilibrium and only record the final position of the path at the first interface λ_1. The transition probability distribution (TPD) can be calculated as $P\left(x^{(1)}|x^{(0)}\right)$ (the superscripts represent the label of the interfaces). By starting N_{i+1} samples at each point of the interface λ_i, say the kth point $x_k^{(i)}$, for each sample, whenever the path crosses λ_i due to relaxation, it will be reinjected back to the initial position $x_k^{(i)}$ [see the dashed arrow in Fig. 1]. As above, the final position of the path at λ_{i+1} will be recorded. The TPDs for all the points from λ_i to λ_{i+1} can be obtained as $P\left(x^{(i+1)}|x^{(i)}\right)$. Note that $P\left(x^{(i+1)}|x^{(i)}\right)$ is a matrix and each row is a TPD of a point in λ_i to the interface λ_{i+1}. By using the reinjection, the time cost for a point to reach the next interface or boundary can be reduced by an exponentially large factor as stated in Ref. [27]. It should be remarked that this manipulation will induce errors since paths may go across the interface several times before they finally reach the next one. However, for small noise intensities, the error can be reduced because paths other than the MPEP shrink as the noise intensity decreases. In other words, the dispersion of the prehistory probability density shrinks with the decreasing noise [5,28,29]. In the end, the TPD from the initial to final state is obtained as follows:

$$P\left(x^{(\text{end})}|x^{(0)}\right) = \prod_{i=0}^{n} P\left(x^{(i+1)}|x^{(i)}\right) \tag{1}$$

where n is the number of the interfaces while $i = 0$ and $i = n + 1$ represent the initial and final states, respectively.

Apart from the reduction of the time cost by an exponentially large factor, the direct advantage of this method is the independence of the calculation for the TPD between different interfaces and between different points. It's the most essential difference between FFS and PEM, whereby for the former, the sample paths are allowed to step across the previous interface without the reinjection and the sample paths are fully recorded. So for FFS, the recorded information is the whole pathway. While for PEM, the

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