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A Minimum Action Method with Optimal Linear Time Scaling

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Abstract. In this work, we develop a minimum action method (MAM) with optimal linear time scaling, called tMAM for short. The main idea is to relax the integration time as a functional of the transition path through optimal linear time scaling such that a direct optimization of the integration time is not required. The Feidlin-Wentzell action functional is discretized by finite elements, based on which h-type adaptivity is introduced to tMAM. The adaptive tMAM does not require reparametrization for the transition path. It can be applied to deal with quasi-potential: 1) When the minimal action path is subject to an infinite integration time due to critical points, tMAM with a uniform mesh converges algebraically at a lower rate than the optimal one. However, the adaptive tMAM can recover the optimal convergence rate. 2) When the minimal action path is subject to a finite integration time, tMAM with a uniform mesh converges at the optimal rate since the problem is not singular, and the optimal integration time can be obtained directly from the minimal action path. Numerical experiments have been implemented for both SODE and SPDE examples.

AMS subject classifications: 49M25, 60H30, 65K10

Key words: Large deviation principle, small random perturbations, minimum action method, rare events, uncertainty quantification.

1 Introduction

Small random perturbations of dynamical systems can introduce rare but important events. For instance, the transitions between different stable equilibrium states of a deterministic dynamical system would be impossible if noise does not exist. Such noise-induced transitions are actually observed and critical in many physical, biological and chemical systems [16]. Examples include nucleation events of phase transitions, chemical reactions, regime change in climate, conformation changes of biomolecules, hydrodynamic instability, etc.

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When the amplitude of random perturbations is small, the Freidlin-Wentzell (F-W) theory of large deviations provides a rigorous mathematical framework to understand the effects of noise on dynamics [11]. The theory shows that the occurrence of rare events actually has a rather deterministic nature in the sense that a sharply peaked probability will be observed around the pathway that is least unlikely. The central object of F-W theory of large deviations is the F-W action functional. The minimizer of the F-W action functional provides the pathway of maximum likelihood and the corresponding minimum gives an estimate of the probability and the rate of occurrence of the rare events. The most important practical issue becomes how to seek the minimum and minimizer of the F-W action functional, which has to be addressed numerically for most cases.

In gradient systems, the most probable transition path is consistent with the minimum energy path (MEP), which is always parallel to the drift of the stochastic differential equation, and passes the separatrix through some saddle points with one-dimensional unstable manifold [19], i.e., transition states. Many algorithms have been developed to search the MEPs and transition states, including the string method [4, 6], the dimer method and its variants [14, 27], the nudged elastic band method [15], eigenvector-following-type methods [1], the gentlest ascent dynamics [7], etc., where the transition mechanism of gradient systems is usually employed to improve the numerical efficiency.

Unfortunately, there does not exists a definite transition mechanism in non-gradient systems [21, 22, 24, 26], where a direct minimization of the F-W action functional has to be considered. The F-W action functional is defined on a finite time interval, which can capture rare events defined on the specified time scale. The original minimum action method (MAM) [5] was constructed to deal with this case. However, the time scale of some random events increases exponentially as the amplitude of noise decreases, such as transitions between two critical points. Then we need to consider the quasi-potential, where the integration time in the F-W action functional becomes an optimization parameter and the optimal integration time can be infinite. There are several algorithms to deal with quasi-potential. The most general algorithm is the geometric MAM (gMAM) [13], which demonstrates that under proper constraints the F-W action functional can be reformulated with respect to a scaled arc length. The integration time then disappears in the optimization problem and will be recovered by the mapping between time and arc length after the most probable path is obtained. Another minimum action method, called adaptive MAM (aMAM) [20], was constructed for the F-W action functional formulated in time. The key observation of aMAM is that if the optimal integration time is infinite, the most probable transition path can be well resolved through reparametrization or remeshing using a finite but large integration time. Since the integration time must be prescribed, aMAM is not able to deal with the quasi-potential if the optimal integration time is finite. The aMAM was reformulated in [23, 25] within the framework of finite element method to enhance the numerical efficiency and robustness.

In this work, we develop a minimum action method to deal with quasi-potential formulated with respect to time instead of arc length. We choose to work with time instead of arc length because it can be more flexible, from the algorithm point of view, to deal