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An adaptive high-order minimum action method

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ABSTRACT

In this work, we present an adaptive high-order minimum action method for dynamical systems perturbed by small noise. We use the *hp* finite element method to approximate the minimal action path and nonlinear conjugate gradient method to solve the optimization problem given by the Freidlin–Wentzell least action principle. The gradient of the discrete action functional is obtained through the functional derivative and the moving mesh technique is employed to enhance the approximation accuracy. Numerical examples are given to demonstrate the efficiency and accuracy of the proposed numerical method.

1. Introduction

Dynamical systems are often subject to random perturbations since noise is ubiquitous in nature. Even when these random perturbations have a small amplitude, they can produce a profound effect on the long time dynamics by inducing rare but important events. A large number of interesting phenomena in physics, chemistry and biology such as phase transitions, biological switches and chemical reactions, etc., are examples of such noise-induced rare events [13].

When the random perturbations are small, the Freidlin–Wentzell theory of large deviations provides a rigorous mathematical framework for us to understand how the transitions occur and how frequent they are. The transition pathways between metastable sets in a dynamical system often have a rather deterministic nature. As the noise amplitude decreases to zero, the events for successful transitions between metastable sets have a sharply peaked probability around a certain deterministic path that is least unlikely. Special features of such a path tell us crucial information about the mechanism of the transition. One class of examples that have been well studied for a long time are the gradient systems, for which the vector field is the gradient of a potential function. In gradient systems, the most probable transition path is the minimum energy path (MEP), which passes through the basin boundary between the stable states at some saddle points with one dimensional unstable manifold [16,20]. For non-gradient systems we need to consider the action functional instead of the energy, which is the central object to the Freidlin–Wentzell theory. The minimizer of the action functional provides the most probable transition path; the minimum of the action functional provides an estimate of the probability and the rate of occurrence of the transition. Thus an important practical task is to compute the minimum and minimizer of the action functional.

A large number of numerical algorithms have been designed for gradient systems. Some popular algorithms include the string method [2,4], nudged elastic band method [12], eigenvector-following-type method (e.g. [1]) as well as the dimer method [9], which usually take advantage of the fact that in gradient systems the transition paths are always parallel to the drift term of the stochastic differential equation. For general (non-gradient) systems, we need to minimize directly

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the Freidlin–Wentzell action functional and available algorithms include the minimum action method [3], the adaptive minimum action method [18] and the geometric minimum action method [8]. Compared to gradient systems, the transition mechanism in non-gradient systems is usually much more subtle, since the phase space may display a very complicated structure, where invariant sets can be fixed points, as well as limit cycles, tori or even chaotic strange attractors. We refer to [19,21] for the study of the Lorenz system and the Kuramoto–Sivashinsky equation, where it is demonstrated that the minimum action method can be a valuable tool to explore the phase space and study the transition mechanism in non-gradient systems.

In this work, we develop an adaptive high-order minimum action method by coupling the *hp* finite element approximation and a preconditioned nonlinear conjugate gradient optimization solver. In the finite element framework, the gradient of the action functional is formulated straightforwardly with respect to the functional derivative. To enhance the accuracy, we employ the moving meshing technique to adjust the temporal discretization adaptively. The methodology is general and can be easily applied to both gradient and non-gradient dynamical systems.

This paper is organized as follows. In Section 2 we briefly describe the problem and the theoretical background. We present the developed numerical method in Section 3. In Section 4, we examine the accuracy and efficiency of the method using dynamical systems given by an ordinary differential equation and a partial differential equation, respectively. Some discussions are given in Section 5.

2. Problem description and theoretical background

We consider random perturbations of dynamical systems. Let the random process $X_t = X(t) : \mathbb{R}_+ \to \mathbb{R}^n$ defined by the following stochastic ordinary differential equation (SODE):

$$dX_t = b(X_t)dt + \sqrt{\varepsilon}\,dW_t, \tag{1}$$

where W_t is a standard Wiener process in $\mathbb{R}^n$ and ε is a small positive parameter. Let $\phi(t) \in \mathbb{R}^n$ be an absolutely continuous function defined for $t \in [0,T]$. The Wentzell–Freidlin theory tells us that the probability of $X(t)$ passing through the δ-tube about ϕ on $[0,T]$ is

$$\Pr(\rho(X,\phi) < \delta) \approx \exp\left(-\frac{1}{\varepsilon}S_T(\phi)\right) \tag{2}$$

with $\rho(\phi,\varphi) = \sup_{t\in[0,T]}|\phi(t) - \varphi(t)|$, $|\cdot|$ indicates the ℓ_2 norm in $\mathbb{R}^n$, and $S_T(\phi)$ is the action functional of ϕ on $[0,T]$, defined as

$$S_T(\phi) = \frac{1}{2}\int_0^T L(\dot{\phi},\phi)\,dt, \tag{3}$$

where $L\left(\dot{\phi},\phi\right) = \left|\dot{\phi} - b(\phi)\right|^2$. In general, we have the following large deviation principle

$$\lim_{\varepsilon\to 0}\varepsilon\log\Pr(X\in A) = -\min_{\phi\in A}S_T(\phi), \tag{4}$$

where A is a particular set of random events. Thus, in analogy with the Laplace's method, the basic contribution to $\Pr(X \in A)$ is given by the neighborhood of the minimum of $S_T(\phi)$ when ε is small enough. The minimizer ϕ^*, which satisfies $S_T(\phi^*) = \min_{\phi\in A}S_T(\phi)$ is also called the "minimal action path" (MAP).

Different definitions of the set A in Eq. (4) correspond to many important phenomena that occur in dynamical systems. For example,

- If we are interested in the probability of $X(t)$ connecting one point a_1 and the other point a_2 in the phase space due to the random perturbations, A can be defined as

$$A = \{X(0) = a_1, X(T) = a_2\}.$$

The MAP will be the most probable path for the transition from a_1 to a_2 in the sense that the probability of the system taking all the other paths decays exponentially with respect to the noise amplitude ε according to the large deviation principle. Note that when a_1 and a_2 are attractors, it is more appropriate to define the set A as

$$A = \{X(-\infty) = a_1, X(\infty) = a_2\}.$$

We keep a finite time interval here mainly due to the numerical approximation discussed later.

- If a_1 and a_2 are two adjacent stable states in gradient systems, the MAP will be consistent with the minimum energy path (MEP), which passes through the basin boundary between a_1 and a_2 at a certain saddle point with one-dimensional unstable manifold.
- If there exists dynamics between a_1 and a_2, the MAP will be the path given by the dynamics corresponding to a zero action functional, which implies that the MAP is also helpful for us to study the structure of the phase space. For instance, if a_1 and a_2 are two unstable fixed points and the MAP has a zero action functional, we can conclude that there exists a heteroclinic orbit between a_1 and a_2, which is given exactly by the MAP.