Hyperbolic periodic orbits in nongradient systems and small-noise-induced metastable transitions

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Summary. We study how small-noise-induced metastable transitions in nongradient systems may differ from those in gradient systems. These transitions utilize structures in certain deterministic systems, which are not necessarily the original one with noise removed. Such structures include hyperbolic periodic orbits (which are generally absent in gradient systems) and the associated heteroclinic orbits. Numerical methods for identifying these structures are also provided.

Freidlin-Wentzell action minimization

Rare dynamical events induced by small noise can be important. Freidlin-Wentzell large deviation theory provides an assessment of likelihoods of such events: consider

$$dX = f(X)dt + \sqrt{\epsilon}dW,$$

where $X \in \mathbb{R}^d$, $\epsilon \ll 1$, and W is a d-dimensional Wiener process. The theory states, as $\epsilon \to 0$ and given boundary condition $X(0) = x_a$ and $X(T) = x_b$, the probability density of a solution $X(\cdot)$ is formally asymptotically equivalent to $\exp(-S_T[X]/\epsilon)$, where the action functional is given by

$$S_T[X] := \frac{1}{2}\int_0^T \|\dot{X}(s) - f(X(s))\|^2 ds, \text{ if } X \in H^1; \infty \text{ otherwise.}$$

Since $\epsilon \ll 1$, the transition probability is characterized by the minimizer of the action. In addition, in many situations T is not known, and it is thus natural to also minimize over all $T > 0$. If one does so, the minimum is generally achieved when $T \to \infty$ [2]. Therefore, we seek minimizers of $S_\infty[\cdot]$ with boundary conditions. Such minimizers will be called maximum likelihood paths (MLPs). Also, we will be working with metastable transitions, i.e., x_a and x_b are two stable fixed points in the noise-less system $\dot{X} = f(X)$.

If the system is gradient, i.e., $f = -\nabla V$, it is known that a MLP between two local minima of V coincides with a Minimum Energy Path (MEP), which is everywhere parallel to ∇V and computable by numerical methods such as String method [3]. In addition, it is known that an MEP has to cross the separatrix at a saddle point.

Metastable transitions in nongradient systems

Unfortunately, a theory is incomplete for nongradient systems, which are nevertheless important because they model many practical problems such as Langevin models of mechanical systems in constant temperature environment, stochastic fluid models, and various coarse-grained systems. In fact, irreversible diffusion processes cannot be generated by gradient systems.

To better understand nongradient systems, we make a small step by showing the followings: unlike in gradient systems, MLP does not have to cross a saddle point, and in fact there may be no saddle point at all. The second simplest limit set, namely periodic orbit, may be present on the separatrix and utilized by the metastable transition. More specifically, for a class of nongradient systems dubbed ‘orthogonal-type’, the transition rate is characterized by a barrier height like in the gradient case, and given a saddle point or a hyperbolic periodic orbit that locally attracts on the separatrix, there is a unique associated local minimum action and an explicitly defined path that achieves this action. Interestingly, periodic-orbit-crossing MLPs differ significantly from a saddle-crossing MLP, as their arc-lengths are infinite and there are infinitely many of them, even if there is only one periodic orbit. On the other hand, for a non-orthogonal-type nongradient system, numerically obtained local MLPs also cross saddles or periodic orbits, but multiple local MLPs with different actions may correspond to the same separatrix crossing location.

Orthogonal-type nongradient systems and a finite-dimensional example

A nongradient system in $\mathbb{R}^d$ is called an orthogonal-type, if $f = -\nabla V + b$ for some V and b satisfying $\nabla V(x) \cdot b(x) = 0$ for all $x \in \mathbb{R}^d$. Suppose the noise-free system (i.e. $\epsilon = 0$) contains two stable fixed points x_a and x_b and the closures of their basins of attractions cover the entire space. Assume there is at least one saddle point x_s or hyperbolic periodic orbit $x_{PO}(t)$ that is attracting on the separatrix, and there is a heteroclinic orbit from x_a to x_s or a point on $x_{PO}(t)$ in an auxiliary dynamical system $\dot{X} = \nabla V(X) + b(X)$. Then a local minimizer of the Freidlin-Wentzell action corresponds to the concatenation of two heteroclinic orbits, which can be formally represented by the solution X^* to

$$\dot{X} = \begin{cases} +\nabla V(X) + b(X) & (t \leq 0) \\ -\nabla V(X) + b(X) & (t \geq 0) \end{cases},$$
$$X(-\infty) = x_a, \quad X(\infty) = x_b, \quad X(0) \in \{x_{PO}(t) \big| t \in \mathbb{R}\},$$

and the action local minimum is $2(V(X^*(0)) - V(x_a))$.

As an example, consider the transition from $(0,0,-1)$ to $(0,0,1)$ in

$$\begin{cases} dx = \left((1-z^2)\frac{x}{\sqrt{x^2+y^2}} - x - y \right) dt + \sqrt{\epsilon} dW_1 \\ dy = \left((1-z^2)\frac{y}{\sqrt{x^2+y^2}} - y + x \right) dt + \sqrt{\epsilon} dW_2 \\ dz = \left(z - z^3 \right) dt + \sqrt{\epsilon} dW_3 \end{cases},$$

where the separatrix is the $z = 0$ plane, on which the only attractor is a periodic orbit $x^2 + y^2 = 1$. Figure 1 illustrate a numerically approximated MLP; only one is shown but there are infinitely many MLPs as the system has a rotational symmetry. Also, the true MLP is infinity long because heteroclinic orbits rotate infinity near the periodic orbit. The exact minimum action can be theoretically shown to be 0.5.

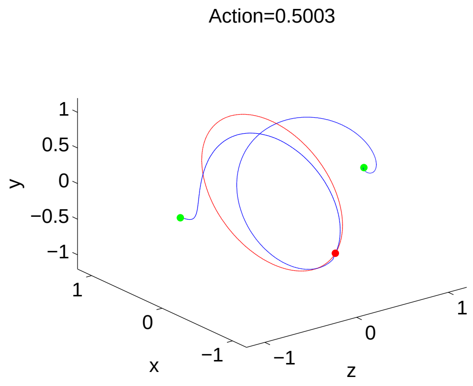

Figure 1: A finite length approximation of an MLP.

An infinite-dimensional non-orthogonal-type example

An example not of orthogonal-type is sheared Allen-Cahn SPDE on 2-torus:

$$\phi_t = \kappa \Delta \phi + \phi - \phi^3 + c \sin(2\pi y) \partial_x \phi + \sqrt{\epsilon} \eta.$$

Figure 2 and 3 illustrate a periodic orbit in this system and a numerically obtained MLP. Although unproved, this MLP was verified numerically to still go through a periodic orbit.

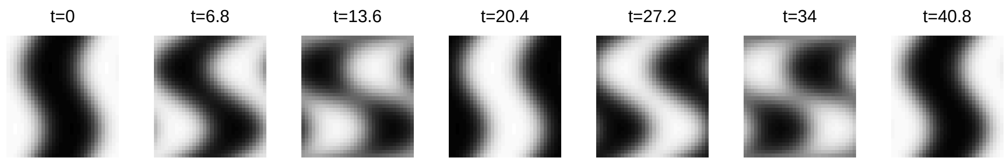

Figure 2: Snapshots of a hyperbolic periodic orbit in sheared Allen-Cahn.

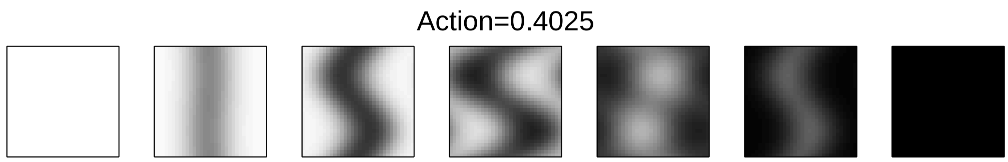

Figure 3: A local MLP in sheared Allen-Cahn that crosses separatrix at a point on a periodic orbit.

Numerical tools

Two numerical methods play critical roles in this study. One of them identifies hyperbolic periodic orbits, based on a variation of String method [ER07]. The other numerically computes MLPs by supplementing the geometric Minimum Action Method [Heymann & Vanden-Eijnden. CPAM 2008] with information about the separatrix crossing location, such as the periodic orbit computed by the first method.

Acknowledgment

This work was supported by NSF grant DMS-1521667. The problem was set up by Eric Vanden-Eijnden, with whom the author gratefully had multiple stimulating discussions.

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