Finding Most Probable Transition by Freidlin-Wentzell Theory

Molei Tao

Control and Dynamical Systems, California Institute of Technology

mtao@caltech.edu

Abstract

Freidlin-Wentzell theory tells the probability of a given trajectory in a stochastic dynamical system. The most probable transition path between arbitrary configurations is obtained by minimizing rate functional under constraints. An analytical solver, as well as a semi-analytical general solver based on a newly proposed discrete Freidlin-Wentzell theory, are presented. Langevin system in which noise is degenerate is specifically investigated.

1. Freidlin-Wentzell Theory

FREIDLIN-WENTZELL THEORY is a Large Deviation Theory on path space [1] briefly reviewed as following:
Given a stochastic dynamical system

$$d\boldsymbol{X}_\epsilon(t)=\boldsymbol{b}(\boldsymbol{X}_\epsilon)dt+\epsilon^{1/2}\boldsymbol{\sigma}(\boldsymbol{X}_\epsilon)d\boldsymbol{W}(t), \tag{1}$$

there is a rate functional over $\mathcal{C}^n[0,T]$ defined as follows:

$$I(\boldsymbol{\phi})=\int_0^T J(\boldsymbol{\phi}(t),\dot{\boldsymbol{\phi}}(t))dt, \tag{2}$$

where $\boldsymbol{\phi}(0)=\boldsymbol{x}$, and

$$J(\boldsymbol{x},\boldsymbol{y})=\frac{1}{2}(\boldsymbol{y}-\boldsymbol{b}(\boldsymbol{x}))^T\boldsymbol{A}^{-1}(\boldsymbol{x})(\boldsymbol{y}-\boldsymbol{b}(\boldsymbol{x})), \tag{3}$$

assuming diffusion matrix $\boldsymbol{A}=\boldsymbol{\sigma}\boldsymbol{\sigma}^T$ is uniformly positive definite.

The rate functional describes the asymptotic behavior of large deviation, in the sense that, given $\boldsymbol{X}_\epsilon(t)$ being the solution propagated from $\boldsymbol{X}_\epsilon(0)=\boldsymbol{x}$,

$$P(\sup_{0\le t\le T}|\boldsymbol{X}_\epsilon(t)-\boldsymbol{\phi}(t)|<\delta)\sim exp(-\epsilon^{-1}I(\boldsymbol{\phi})),\epsilon\to 0 \tag{4}$$

for any small $\delta>0$.

Therefore, one seeks for a $\boldsymbol{\phi}(t)$ in certain path space which minimizes the rate functional as the most probable path. If one is interested in transition between configurations, the path space could be $\{\phi\in\mathcal{C}[0,T]|\phi(0)=\boldsymbol{A},\phi(T)=\boldsymbol{B}\}$ or $\bigcup_{T>0}\{\phi\in\mathcal{C}[0,T]|\phi(0)=\boldsymbol{A},\phi(T)=\boldsymbol{B}\}$.

2. Langevin System

Approaches based F-W Theory such as String Method [2] solve for most probable transition path in system where the noise is non-degenerate. On the other hand, systems such as Langevin incorporate the effect of noise in such a way that noise is degenerate:

$$d\boldsymbol{q}=\boldsymbol{p}dt \tag{5}$$

$$\boldsymbol{m}d\boldsymbol{p}=-\nabla V(\boldsymbol{q})dt-c\boldsymbol{p}dt+\epsilon^{1/2}\boldsymbol{\sigma}dW \tag{6}$$

The temperature T of this system satisfies $\frac{2c}{\epsilon\sigma^2}=\frac{1}{kT}$. Therefore, F-W Theory describes only the asymptotics at $T\to 0$. However, the discrete Freidlin-Wentzell we proposed applies for any temperature.

The corresponding integrand of rate functional I could be shown by Large Deviation Theory as

$$J(\boldsymbol{q},\boldsymbol{p})=\frac{1}{2}(\boldsymbol{m}\dot{\boldsymbol{p}}+c\boldsymbol{p}+\nabla V(\boldsymbol{q}))^2, if\ \boldsymbol{p}=\dot{\boldsymbol{q}}$$
$$=\infty, otherwise \tag{7}$$

Therefore we study the following constrained variational problem for the most probable transition:

$$\begin{aligned}\delta I&=0\\ I&=\int_0^T\frac{1}{2}(\boldsymbol{m}\dot{\boldsymbol{p}}+c\boldsymbol{p}+\nabla V(\boldsymbol{q}))^2dt\\ \boldsymbol{p}&=\dot{\boldsymbol{q}}\\ \boldsymbol{q}(0)&=A,\\ \boldsymbol{q}(T)&=B\end{aligned} \tag{8}$$

In molecular dynamics, for example, one is actually more interested in an alternative version which takes the Gibbs-Boltzmann distribution of kinetic energy into account, because otherwise the solution will always be the Newtonian path whose initial velocity is big enough to overcome all energy barrier on its way, and it will render $I()$ zero. Instead of "minimizing" I, one "minimizes" $\mathcal{A}=\frac{I}{2ckT}+\frac{\boldsymbol{p}(0)^T\boldsymbol{m}\boldsymbol{p}(0)}{2kT}$ under same constraints. Notice that the probability will change as temperature changes but the optimal path won't.

3. Analytical Solver

The approach is: fix $\boldsymbol{p}(0)$, solve the variational problem without end point constraint by Hamilton-Pontryagin principle [3], optimize among solutions which satisfy end point constraint, optimize w.r.t. $\boldsymbol{p}(0)$.

Hamilton-Pontryagin introduces a Lagrange multiplier λ on the cotangent space

$$0=\delta\int_0^T\frac{1}{2}\parallel m\dot{p}+\nabla V(q)+cp\parallel_2^2+\lambda(p-\dot{q})dt \tag{9}$$

It leads to the following ODE system which describes solutions to the variational problem:

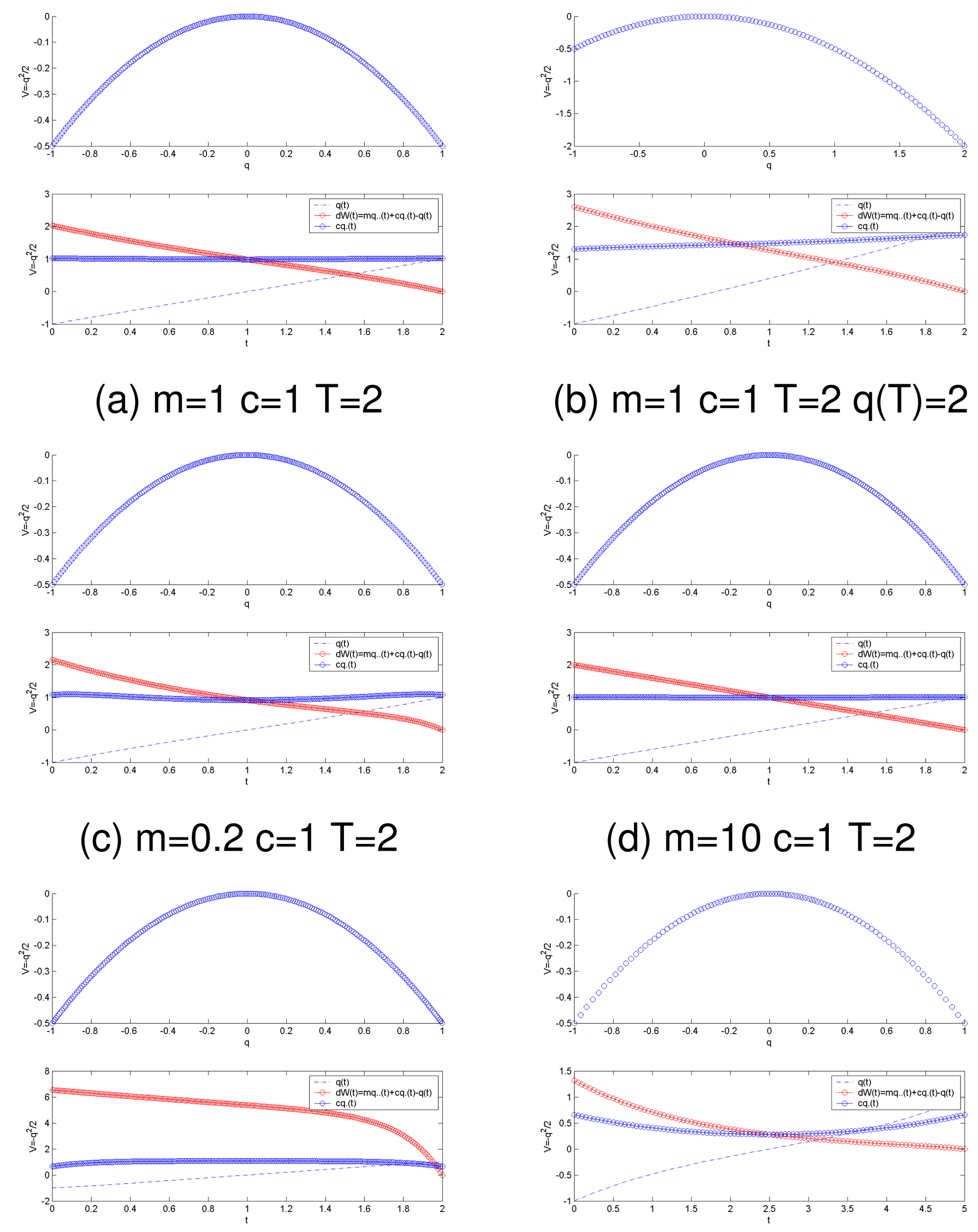
$$\begin{aligned}-(m\ddot{p}+c\dot{p}+\nabla\nabla V(q)\dot{q})m\ +(m\dot{p}+cp+\nabla V(q))c+\lambda&=0\\ (m\dot{p}+cp+\nabla V(q))\nabla\nabla V(q)+\dot{\lambda}&=0\\ p&=\dot{q}\end{aligned} \tag{10}$$

One set of sufficient initial conditions is $q(0),\dot{q}(0),\ddot{q}(0),\dddot{q}(0)$, and $q(t)$ will be a function of them. The first two are known, and the last two need to satisfy $q(T)=B$. One optimizes I under this constraint to get the most-probable path given $\dot{q}(0)$, then minimizes $\mathcal{A}$ as a function of $\dot{q}(0)$.

When the potential is quadratic, analytical solution to the ODE system exists, and the constrained "minimization" could be solved analytically.

4. Results and Discussions

It is of interest to understand how a particle under random perturbations goes over a potential barrier. The analytical solver shows the optimal way is not solely by initial momentum nor solely noise random perturbation, but instead the joint effort, which is independent on temperature, but dependent on inertia, damping coefficient and transition time.



(a) m=1 c=1 T=2 (b) m=1 c=1 T=2 q(T)=2

(c) m=0.2 c=1 T=2 (d) m=10 c=1 T=2

(e) m=1 c=5 T=2 (f) m=1 c=1 T=5

Figure 1: *Optimal transition paths through 1D quadratic potential barrier. q(0)=-1, q(T)=1 unless specified.*

Many interesting phenomena could be observed from the solutions. For example, larger c leads to more initial random kick, more global noise contribution, less initial velocity and less initial kinetic energy; larger m leads to slightly less initial random kick, slightly more global noise contribution, slightly less initial velocity and more initial kinetic energy, while smaller m makes the velocity fluctuates more; larger T leads to less initial random kick, less global noise contribution, less initial velocity and less initial kinetic energy; q(t) is symmetric if q(0) and q(T) are symmetric, and noise still pushes the particle forward after getting over the sumit; etc.

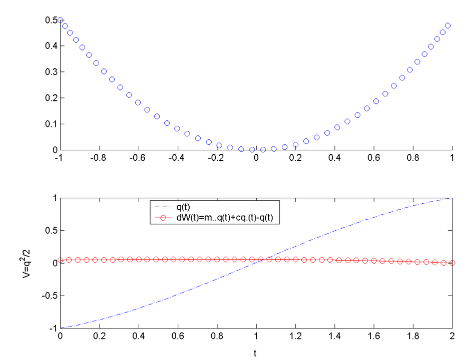


Figure 2: *Optimal transition paths through 1D quadratic potential well. q(0)=-1, q(T)=1.*

Interestingly, noise still contributes to passing potential well optimally as shown above.

5. Discrete Freidlin-Wentzell and Semi-Analytical Solver

In most situations, the ODE system couldn't be solved analytically, and nor could the constrained optimization problem. To solve it numerically one has to be careful because discretization scheme matters, and one still wants to use the "least" action principle. How to discretize the action functional or the ODE system is sophisticated.

We discretize the action intrinsically. The Langevin SDE could be discretized by Stochastic Variational Integrator [4], and the probability for any realization of the obtained Stochastic Difference Equation could hence be written as a discrete (finite dimensional) action/rate function. The problem turns into minimizing

$$\sum_{j=1}^{DOF}[(he^{\frac{ch}{m_j}}\frac{dU}{dq_j}(q_0)-(p_j)_0+e^{\frac{ch}{m_j}}\frac{m_j}{h}((q_j)_1-(q_j)_0))^2+\sum_{k=1}^{N-1}(he^{\frac{ch}{m_j}}\frac{dU}{dq_j}(q_k)-\frac{m_j}{h}((q_j)_k-(q_j)_{k-1})+e^{\frac{ch}{m_j}}\frac{m_j}{h}((q_j)_{k+1}-(q_j)_k))^2] \tag{11}$$

as a function of vector q_1, ..., q_{N-1} with p_0, q_0, q_N fixed.

One could use least action principle to turn it into a nonlinear solving problem. The problem is still hard to solve after this due to the high nonlinearity. Shooting method and other ways are under investigation to attack this problem.

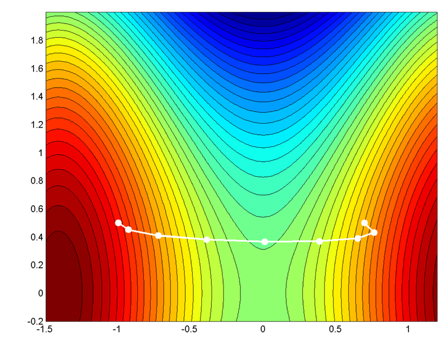


Figure 3: *Toy example: Optimal transition on 2D 4th-order potential landscape (from left to right).*

References

[1] M. I. Freidlin and A. D. Wentzell. *Random Perturbations of Dynamical Systems.* Springer-Verlag, New York, 1984.

[2] W. E, W. Ren, and E. Vanden-Eijnden. String method for the study of rare events. *Phys. Rev. B*, 66:052301, 2002.

[3] N. Bou-Rabee. *Hamilton-Pontryagin Integrators on Lie Groups.* PhD thesis, California Institute of Technology, USA, 2007.

[4] N. Bou-Rabee and H. Owhadi. Boltzmann-Gibbs Preserving Stochastic Variational Integrator. arXiv:0712.4123.

Dynarum Workshop, February 2008, California Institute of Technology. To be published.