Sampling rare trajectories using stochastic bridges

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The most uncommonly occurring events in stochastic systems are often the most consequential. Instances where this unlikely-yet-important combination occurs include fade-outs of epidemics, the extinction of species in ecology, the dynamics of biological switches, large fluctuations in chemical reactions and the detection or prediction of rare natural disasters such as earthquakes, storms or heavy rains. The broad range of these applications justifies the considerable recent effort expended on developing sampling algorithms for rare events in models of stochastic phenomena.

We present a new method that constructs an ensemble of stochastic trajectories that are constrained to have fixed start and end points (so-called stochastic bridges). We then show that by carefully choosing a set of such bridges and assigning an appropriate statistical weight to each bridge, one can focus more processing power on the rare events of a target stochastic process while faithfully preserving the statistics of these rare trajectories.

Given a target process defined by the transition probabilities $P(x', t+\delta t|x, t)$ and initial condition $x(t=0) = x_0$, the key components of the algorithm are: 1) build an associate process with transition probabilities

$$\tilde{P}(x', t-\delta t|x, t) = P(x, t|x', t-\delta t)\frac{P(x', t-\delta t|x_0, 0)}{P(x, t|x_0, 0)}. \quad (1)$$

Where $P(x, t|x_0, 0)$ is the probability of the target process to be in state x at time t given the initial condition $x(t=0) = x_0$. By construction, the rates in Eq. (1) will generate the stochastic bridges backwards in time. 2) Once the ensemble of bridges is generated with Eq. (1), we recover the statistics of the target process thanks to the relation

$$\mathcal{P}(\mathcal{T}) = \tilde{\mathcal{P}}(\mathcal{T})P\left(x_{\tau}, T|\, x_0, 0\right). \quad (2)$$

With $\mathcal{P}(\mathcal{T})$ and $\tilde{\mathcal{P}}(\mathcal{T})$ the probabilities of sampling a particular path $\mathcal{T}$ with the target and associated process respectively. We can apply the same ideas to any Markov process irrespectively to the continuous or discrete nature of the time and the states. See details of the method in [1].

Our approach does not require the noise in the model to be weak, and it generates uncorrelated and unbiased transition paths. Having access to the ensemble of stochastic paths unveils the whole statistical description of the transition between meta-stable states, making it possible to obtain entire distributions of first-passage times or other characteristics in simulations. For example, in Fig. 1, we show the use the stochastic bridges to sample extinction paths and their statistics in the Susceptible-Infected-Susceptible (SIS) model.

We envisage that the method that we have developed will have applications in myriad systems where sampling rare events is important. We imagine that it can also be used as a numerical aid to intuit when the WKB method will be accurate and useful. The approach presented here can also be extended to sample stochastic trajectories constrained to pass through more than two desired points.

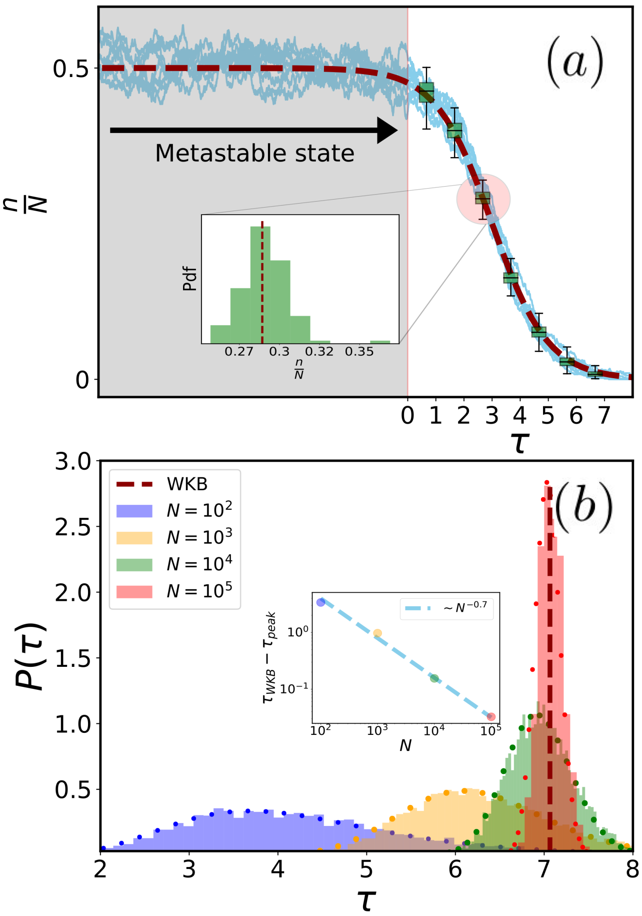

Fig. 1. Extinction paths for the SIS model ($\beta = 2, \gamma = 1$). (a) Paths leading to extinction from a common starting point $\frac{n}{N} = 1 - \frac{\gamma}{\beta} = 0.5$ to $n = 0$ for $N = 10^3$. The WKB instanton is shown as a dashed line. The time $\tau = 0$ corresponds to the point where the WKB instanton crosses $n/N = 0.48$. Boxes indicate the median and first quartiles, and error bars the observed range of the ensemble of stochastic paths. The inset shows the distribution of n/N at time $\tau = 2.8$. (b) Distribution of transition times for extinction trajectories from the quasi-stationary state towards the absorbing state. Dots show fits to log-normal distributions. The inset shows that the modes τ_{peak} of these fits approach the value predicted from the WKB instanton, with $|\tau_{\text{WKB}} - \tau_{\text{peak}}| \sim N^{-0.7}$.

[1] Aguilar, J., Baron, J. W., Galla, T., and Toral, R., *Sampling rare trajectories using stochastic bridges*,rXiv preprint arXiv:2112.08252 (2021).