Rare Event Sampling using Multicanonical Monte Carlo

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Since Metropolis *et al.* (1953), dynamic Monte Carlo methods have been used for calculation of canonical averages in statistical physics (and path integrals in field theories). However, they are universal tools for sampling from multivariate non-Gaussian/discrete distributions with unknown normalization constants, hence should be useful in problems in other fields.

We have been interested in applications of dynamic Monte Carlo methods to rare event sampling and calculation of large deviation probabilities. Examples include:

- Sampling rare events in random matrices and networks [1, 2]
- Sampling rare trajectories in chaotic dynamical systems [3, 4]
- Numerical studies on Griffiths singularity [5]

To treat these examples using dynamic Monte Carlo, the physical energy in usual simulations should be replaced by a quantity that characterizes rare events; for example, when we are interested in large deviation in the largest eigenvalue $\lambda^{\max}$ of random matrices, we use $\lambda^{\max}$ as a fictitious energy in a Monte Carlo simulation.

Slow mixing of the Markov chain caused by local optima is common in these applications. Extended ensemble methods such as replica exchange algorithm or multicanonical algorithms are useful for avoiding this difficulty. Among them, the Wang-Landau algorithm, which directly gives tails of the density of states in an efficient way, is particularly convenient for our purpose.

In this talk, we will discuss selected examples of our studies on rare event sampling using dynamic Monte Carlo, as well as earlier studies on this subject.

[1] Saito, N., Iba, Y., and Hukushima, K. (2010): Multicanonical sampling of rare events in random matrices, arXiv:1002.4499v1.

[2] Saito, N. and Iba, Y. (2010): Probability of graphs with large spectral gap by multicanonical Monte Carlo, arXiv:1003.1023.

[3] Yanagita,T, and Iba, Y. (2009): Exploration of order in chaos using the replica exchange Monte Carlo method, Journal of Statistical Mechanics, P02043.

[4] Kitajima, A. and Iba, Y. (2010): Multicanonical sampling of rare trajectories in chaotic dynamical systems, arXiv:1003.2013.

[5] Hukushima, K. and Iba, Y. (2008): A Monte Carlo algorithm for sampling rare events: Application to a search for the Griffiths singularity, Journal of Physics: Conference Series, 95, 012005.