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Sampling the probability of rare events

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ABSTRACT

Blue moon sampling is a widely-used technique for the sampling of rare events, e.g., the conformational transitions in biomolecules. The idea behind it is to constrain a system to those regions in state space that would be rarely visited otherwise (i.e., once in a blue moon). The probability distribution of the rare events is eventually reconstructed by an appropriate reweighting of the constrained trajectories [1]. Yet there has been (and still is) some confusion about how the weight is affected by the presence of momenta or velocities in the system. In point of fact reweighting is also an issue for first-order systems (e.g., Brownian motion) as can be explained by the often ignored difference between constrained systems and systems with infinitely stiff restraints which each give rise to completely different probability distributions.

We present a novel hybrid Monte-Carlo algorithm for sampling the Gibbs distribution of a mechanical system that is subject to configuration constraints [2]. Using the ordinary Metropolis-Hastings acceptance rule together with a standard symplectic integrator for constrained systems (e.g., SHAKE or RATTLE) we can prove that the dynamics is ergodic and samples the correct distribution without bias (i.e., for any stable stepsize in the numerical integration). As an example we consider sampling issues in the optimal prediction of the conformation dynamics of a small biomolecule. We briefly discuss extensions to Brownian motion and Langevin dynamics, and the problem of convergence indicators [3].

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