A List Based Algorithm for Large Deviation Functions

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***Short Abstract* — The method of large deviation functions has seen a growing interest in the last ten years. It provides a formalism for the treatment of dynamical phase transitions in systems far from equilibrium. While there is no universal framework for the analytical calculation of large deviation functions, the numerical treatment of such problems is far from established. Existing methods are usually either very cumbersome or computationally very expensive. Here, we offer an alternative procedure, which promises to alleviate some of these issues.**

***Keywords* — Large deviation functions, fluctuation theorems, non-equilibrium systems.**

As the analog of the free energy for dynamical trajectories, the large deviation function plays a central role in the statistical mechanics of systems far from equilibrium. We have identified numerical issues that can arise when the model of interest evolves according to a continuous-time dynamics. This analysis motivates the introduction of an algorithm in which a list of previously visited states is used to re-sample the distribution of interest. We have analyzed the convergence properties of our algorithm in detail and we have demonstrated its application to the single-site zero-range process and the many-site totally asymmetric exclusion process.

Additionally, we have expanded on the theoretical foundation of the large deviations approach. Most of the model examples in literature involve discrete state Markovian systems. We demonstrated how to generalize the notion of large deviation functions to problems driven by a Langevin dynamics. The implications of the corresponding "modified" Langevin equation were considered, together with some simple examples. Finally, the potential applications of this approach as a means of speeding up transition path sampling were considered.

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