Mathematics > Probability

Multi-level Monte Carlo for continuous time Markov chains, with applications in biochemical kinetics

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We show how to extend a recently proposed multi-level Monte Carlo approach to the continuous time Markov chain setting, thereby greatly lowering the computational complexity needed to compute expected values of functions of the state of the system to a specified accuracy. The extension is non-trivial, exploiting a coupling of the requisite processes that is easy to simulate while providing a small variance for the estimator. Further, and in a stark departure from other implementations of multi-level Monte Carlo, we show how to produce an unbiased estimator that is significantly less computationally expensive than the usual unbiased estimator arising from exact algorithms in conjunction with crude Monte Carlo. We thereby dramatically improve, in a quantifiable manner, the basic computational complexity of current approaches that have many names and variants across the scientific literature, including the Bortz-Kalos-Lebowitz algorithm, discrete event simulation, dynamic Monte Carlo, kinetic Monte Carlo, the n-fold way, the next reaction method,the residence-time algorithm, the stochastic simulation algorithm, Gillespie's algorithm, and tau-leaping. The new algorithm applies generically, but we also give an example where the coupling idea alone, even without a multi-level discretization, can be used to improve efficiency by exploiting system structure. Stochastically modeled chemical reaction networks provide a very important application for this work. Hence, we use this context for our notation, terminology, natural scalings, and computational examples.

Comments:	Improved description of the constants in statement of Theorems
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