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

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Review

This work is concerned with computational methods for continuous time Markov chains. The setting is the one pertaining to mesoscopic chemical kinetics, where the so-called "random time change" or "operational time" representation in terms of unit-rate Poisson processes is employed.

The paper proposes a multilevel Monte Carlo (MLMC) method based on the forward Euler method for continuous time Markov chains (traditionally called the "tau-leap method"). In the setting of continuous stochastic processes, MLMC is a general methodology for determining expectation values of functionals of the stochastic process, provided that time can be discretized. In essence, the idea is to use a combination of coarser time discretizations to gain in efficiency by performing more work at a coarser level where sampling is computationally fast. In the current paper an exact simulation is used at the finest level so as to avoid the discretization error. An unbiased estimate is therefore produced.

Perhaps the most important contribution lies in the two algorithms (Algorithm 2 and 3) which shows how two trajectories, differently discretized but obtained from the same Poisson process, can be simulated in a consistent fashion.

Theoretical results predicting the performance of the resulting MLMC method are also derived. The analysis is performed under the assumption of global Lipschitz constants. Computational experiments indicate that the method behaves slightly better than predicted and the authors speculate that a sharper theoretical analysis might explain why this is the case. An interesting idea which is presented in the final example of the paper is to use model reduction techniques when defining the coarser levels. The benefit is that reduced models are typically less stiff and hence less expensive to simulate.

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