Guided simulation of conditioned chemical reaction networks

Frank van der Meulen
Department of Mathematics, Vrije Universiteit Amsterdam, The Netherlands
f.h.van.der.meulen@vu.nl

Coauthor(s): Marc Corstanje

Let X be a chemical reaction process, modeled as a multi-dimensional continuous-time Markov jump process. Assume that at given times $0 < t_1 < \cdots < t_n$, linear combinations $v_i = L_i X(t_i)$, $i = 1, \ldots n$ are observed for given matrices L_i.

I will show how to sample the process conditioned on hitting the states $v_1, \ldots, v_n$ by a change of measure on the law of the unconditioned process. Sufficient conditions for this change of measure are presented. I will comment on the efficiency of the proposed approach using numerical examples.

The mathematical framework used is applicable to wider classes of stochastic processes, such as diffusion processes on Euclidean space or on a manifold. I will shortly outline the more general setting.

[1] Corstanje, Marc & Van der Meulen, Frank (2023). *Guided simulation of conditioned chemical reaction networks.* arXiv preprint arXiv:2312.04457.

[2] Corstanje, Marc; Van der Meulen, Frank; Schauer, Moritz; & Sommer, Stefan (2024). *Simulating conditioned diffusions on manifolds.* arXiv preprint arXiv:2403.05409.