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A predictor-corrector method in quantized tensor train format for the equilibrium of the chemical master equation

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It is well known that networks with complex interacting components arise in a variety of disciplines [4], and that a master equation can help describe the joint probability function of the components over time. This work focuses on the chemical master equation (CME) that results from modeling the system using a continuous-time Markov chain. It is of our interest to study the system's long-term behavior, which can be explored by computing the stationary solution to the CME. However, the number of states involved grows exponentially with the number of chemical species tracked. To cope with an extremely large or even infinite state space when solving the CME in biological problems, a potent strategy is to restrict to a finite state projection (FSP) [10] and represent the transition matrix and probability vector in quantized tensor train (QTT) [11] format, leading to savings in storage while retaining accuracy. In summary, we propose a method that further advances the efficiency of using tensor-based approaches to estimate the probability mass function when the system is in statistical equilibrium. We do so by providing a computationally inexpensive initial approximation from which to efficiently obtain a more robust estimation of the stationary solution. Our methodology is to use the reaction rate equations of the system to roughly estimate the probability function of each chemical species. This cheap estimate is then fed to a predictor-corrector pair of solvers aimed at quickly reaching equilibrium by alternating between a linear system solver (predictor) and a transient solver (corrector). Numerous techniques have been developed that leverage tensors in recent years [11, 6, 8, 7, 2, 5, 9, 12] but here we use the AMEn solver the alternating minimal energy (AMEn) algorithm [3] for the predictor part and our adaptive FSP tensor-based solver with sliding windows [1] for the corrector part.

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