

# TENSOR TECHNIQUES FOR CMES

THE AUTHOR

The first and more basic is the finite state projection (FSP)<sup>1</sup>. When the CME describes a chemical reaction network that has a finite copy numbers (the system is closed and does not create species), the FSP method provides an exact analytical solution. When the system is allowed to have a large or even infinite variation of copy numbers, the FSP method truncates the state-space of the CME given a precision. This precision is quantified by the mass of probability that “leaves” the state-space due to jumps to out of it. The algorithm tries to expand the state-space until it reaches the precision, but at the cost of computing the whole probability at each trial. Another methods as sliding windows<sup>2</sup> that are based on the probability of jumping out of the state-space in a given interval of time. The difference is that the state-space is “slid” according to such probabilities and iteratively.

More recent advances try to address the curse of dimensionality using tensor decomposition techniques<sup>3</sup>. In special, the called “tensor-train” decomposition, found by Oseledets<sup>4</sup> (cf. a more comprehensive review<sup>5</sup>). The main idea is to decompose the tensors obtained from the CME operator and the state-space probabilities into product of lower-rank tensors, achieving a lower complexity for the evaluation of the evolution and a lower storage cost<sup>6</sup>. The technique has been used for solving the chemical master equation<sup>7</sup>

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<sup>1</sup>Munsky, B., & Khammash, M. (2006). The finite state projection algorithm for the solution of the chemical master equation. *The Journal of Chemical Physics*, 124(4), 044104. doi:10.1063/1.2145882

<sup>2</sup>Wolf, V., Goel, R., Mateescu, M., & Henzinger, T. A. (2010). Solving the chemical master equation using sliding windows. *BMC Systems Biology*, 4(1), 42. doi:10.1186/1752-0509-4-42

<sup>3</sup>Kolda, T. G., & Bader, B. W. (2009). Tensor Decompositions and Applications. *SIAM Review*, 51(3), 455–500. doi:10.1137/07070111x

<sup>4</sup>Oseledets, I. V. (2009). A new tensor decomposition. *Doklady Mathematics*, 80(1), 495–496. doi:10.1134/s1064562409040115

<sup>5</sup>Oseledets, I. V. (2011). Tensor-Train Decomposition. *SIAM Journal on Scientific Computing*, 33(5), 2295–2317. doi:10.1137/090752286

<sup>6</sup>Gelss, P. (2017). The Tensor-Train Format and Its Applications: Modeling and analysis of chemical reaction networks, catalytic processes, fluid flows, and Brownian dynamics. Dissertation, Freie Universität Berlin.

<sup>7</sup>Ion, I. G., Wildner, C., Loukrezis, D., Koeppl, H., & De Gersem, H. (2021). Tensor-train approximation of the chemical master equation and its application for parameter inference. *The Journal of Chemical Physics*, 155(3), 034102. doi:10.1063/5.0045521.

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