Tensor-Based Approximation of the Stationary Solution to the Chemical Master Equation

Brandon M. Reid[1] and Roger B. Sidje[1]

***Short Abstract* — We can model the dynamics of certain cellular processes via the chemical master equation. Analyzing the system becomes especially burdensome as the number of chemical species being tracked increases. Numerous recent attempts have been made to alleviate this so-called curse of dimensionality using tensors (i.e., multidimensional arrays), because tensor-based approaches have been found to scale linearly with species count. We develop tensor-based strategies to approximate the probability distribution in the long run, after the transient behavior of the system has dissipated, with an emphasis on constructing iterative methods that scale efficiently as more chemical species are introduced to the system.**

***Keywords* — chemical master equation, stationary solution, limiting behavior, iterative methods, tensors**

I. Motivation

THE chemical master equation yields a system of linear equations that is frequently represented in matrix form:

$$A\mathbf{p} = \dot{\mathbf{p}}$$

where A is the n x n sparse transition rate matrix and $\mathbf{p}$ is an n x 1 vector enumerating the (time-dependent) probability of the n possible chemical configurations of the system. The derivative of the probability vector, $\dot{\mathbf{p}}$, will simply be the zero vector when the system is in statistical equilibrium. Solving such a system using traditional methods requires $O(n^3)$ steps [1]. Numerous approaches have been implemented to arrive at a solution more efficiently, but they tend to suffer from the curse of dimensionality to varying extents.

II. Tensor Approach

In recent years, tensors have been touted as a means of vastly reducing the computational burden involved in analyzing systems modeled by the chemical master equation. A straightforward means of converting the problem from matrix format to tensor format is to reconfigure $\mathbf{p}$ into a multidimensional array of dimension

$$n_1 \times n_2 \times \ldots \times n_d$$

where $n_j - 1$ is the maximum copy number of the j^{th} chemical species and d is the number of chemical species being tracked in the system [2-3]. The transition matrix A is likewise reformatted to tensor form and a multiplication operation relating A and $\mathbf{p}$ is defined accordingly.

Unlike the matrix formulation, tensor representation holds the advantage of preserving in its structure information concerning the underlying geometry of the system. Vast computational savings are realized when the multidimensional arrays are factored into a low-rank approximation using methods such as tensor train decomposition [4-8]. Tensor-based approaches have already been applied to the study of the chemical master equation's stationary solution [9]. Here, we present new iterative techniques to approximate the stationary solution using tensors and compare their computational efficiency to more traditional methods.

[1]The University of Alabama, Department of Mathematics, Box 870350, Tuscaloosa, AL 35487. breid@crimson.ua.edu, roger.b.sidje@ua.edu.

References

[1] Terry J. Frankcombe and Sean C. Smith. Fast, scalable master equation solution algorithms. III. direct time propagation accelerated by a diffusion approximation preconditioned iterative solver. The Journal of Chemical Physics, 119(24):12729{12740, Dec 2003.

[2] Huy D. Vo and Roger B. Sidje. An adaptive solution to the chemical master equation using tensors. The Journal of Chemical Physics, 147(4):044102, Jul 2017.

[3] Markus Hegland and Jochen Garcke. On the numerical solution of the chemical master equation with sums of rank one tensors. 52, 08 2011.

[4] Evrim Acar, Daniel M. Dunlavy, and Tamara G. Kolda. A scalable optimization approach for fitting canonical tensor decompositions. Journal of Chemometrics, 25(2):67-86, February 2011.

[5] Brett W. Bader and Tamara G. Kolda. Efficient MATLAB computations with sparse and factored tensors. SIAM Journal on Scientific Computing, 30(1):205{231, December 2007.

[6] Vladimir Kazeev, Mustafa Khammash, Michael Nip, and Christoph Schwab. Direct solution of the chemical master equation using quantized tensor trains. PLoS Computational Biology, 10(3):e1003359, Mar 2014.

[7] Tamara G. Kolda and Jimeng Sun. Scalable tensor decompositions for multi-aspect data mining. In ICDM 2008: Proceedings of the 8th IEEE International Conference on Data Mining, pages 363-372, December 2008.

[8] I. V. Oseledets. Tensor-train decomposition. SIAM Journal on Scientific Computing, 33(5):2295-2317, 2011.

[9] Vladimir Kazeev and Christoph Schwab. Tensor approximation of stationary distributions of chemical reaction networks. SIAM Journal on Matrix Analysis and Applications, 36(3):1221-1247, Jan 2015.