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Understanding tensor and tensor decompositions with application to the chemical master equation

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Tensors are multidimensional arrays that can play a key role in the representation of big data. Decompositions of higher-order tensors have applications in biochemistry, signal processing, data mining, neuroscience, and elsewhere. Building on earlier decompositions (such as canonical/parallel factor (CANDECOMP/PARAFAC), Tucker or its variants), recent research efforts have been devoted to the tensor-train (TT) or quantized tensor train (QTT) to optimize the storage in some large high-order tensors that arise naturally in different scientific fields. Computations with the decomposed tensors, however, raise the sort of challenges reminiscent of the vast complications that arose when new algorithms had to be designed to tackle large sparse matrices to emulate the tasks that were assumed for small dense matrices. But those challenges also point to the prospect of promising research to offer new insights into solving classic problems. We will consider the chemical master equation as an illustrative application that involves an extremely large matrix exponential function that would be infeasible to handle without recasting through tensor-trains decompositions.

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