Tensor Numerical Methods for High-Dimensional PDEs: Prospects and Limitations

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Abstract

Modern methods of rank-structured tensor decomposition allow an efficient separable approximation of multivariate functions and operators, providing linear complexity scaling in the dimension [6, 7]. The recent quantized tensor train (QTT) matrix product states technique is proved to provide the super-compressed representation of high-dimensional data with log-volume complexity [1]. The approach opens the way to efficient numerical solution of high-dimensional PDEs with linear scaling in the dimension and logarithmic scaling in the grid size [2, 3, 4, 5, 8, 9]. We discuss the asymptotically optimal low QTT-rank representations for a class of multivariate functions and operators, substantiating the computational efficiency of the QTT transform to higher dimensions. In particular, the QTT expansions for a family of discrete multidimensional Hamiltonian operators will be addressed. Numerical illustrations in electronic structure calculations, quantum molecular dynamics and stochastic PDEs are presented. We conclude with discussion on future prospects and limitations of tensor numerical methods in scientific computing.

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