

Quantics-TT preconditioned and DMRG methods in high-dimensional quantum and stochastic computations

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Abstract

Modern methods of tensor-product decomposition allow an efficient data-sparse approximation of functions and operators in higher dimensions [7]. The recent quantics-TT (QTT) tensor model allows to represent the multidimensional data with log-volume complexity [3, 4, 5]. Combined with the preconditioned and DMRG-type iterative methods this approach leads to efficient solvers for multi-dimensional boundary-value, spectral and dynamical problems, which are free of the “curse of dimensionality”. We discuss the theoretical rank bounds for representation of multivariate functions and operators, including examples of potential energy surfaces (PES). The preconditioned and DMRG-type iterative methods of the log-volume complexity are discussed. Numerical results for high-dimensional spectral problems in molecular dynamics and preconditioned QTT truncated iterations in SPDEs are presented.

References

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