Global optimization of MPS and applications to quantum-inspired numerical analysis

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The expressivity and efficiency of tensor networks (TNs) make them ideal tools to develop quantum-inspired algorithms. We revise the problem of operator diagonalization with TNs for quantum-inspired methods for numerical analysis [1,2]. We use matrix product operators (MPO) to represent partial differential equations (PDEs), while matrix product states (MPS) for their solution, based on the encoding of functions in a quantum register [3]. We focus on: (i) imaginary-time evolution, (ii) gradient-descent, (iii) linear algebra approximate diagonalization, and (iv) DMRG-like optimization. We implement methods (i)-(iii) in a framework of approximate linear algebra, concluding that time-evolution is costlier than simple gradient descent. We upgrade gradient descent to work in a Krylov basis of n_v arbitrary vectors, formulating a variant of the Arnoldi method that outperforms (i) and (ii). We benchmark it to DMRG and vector-based Arnoldi using the 2D squeezed harmonic oscillator. We find that, while DMRG performs exponentially better in single-shot experiments (Fig.1(a)), Arnoldi matches it in accuracy and execution time when using a renormalization strategy (Fig. 2) and can be generalized to MPOs of greater depth. This shows its power to address large scale optimization problems, not only in quantum-inspired numerical analysis, but also in other many-body and quantum chemistry applications. MPS-based methods present an exponential advantage in memory when compared to vectors (Fig. 1(b)), evidencing the benefits of quantum-inspired methods for large dimensional problems.

References

[1] García-Molina, P., et al., arXiv:2303.09430 (2023).
[2] García-Ripoll, J. J, Quantum, 5 (2021) 431.
[3] García-Molina, P., et al., Phys. Rev. A 105 (2022), 012433.

Figures

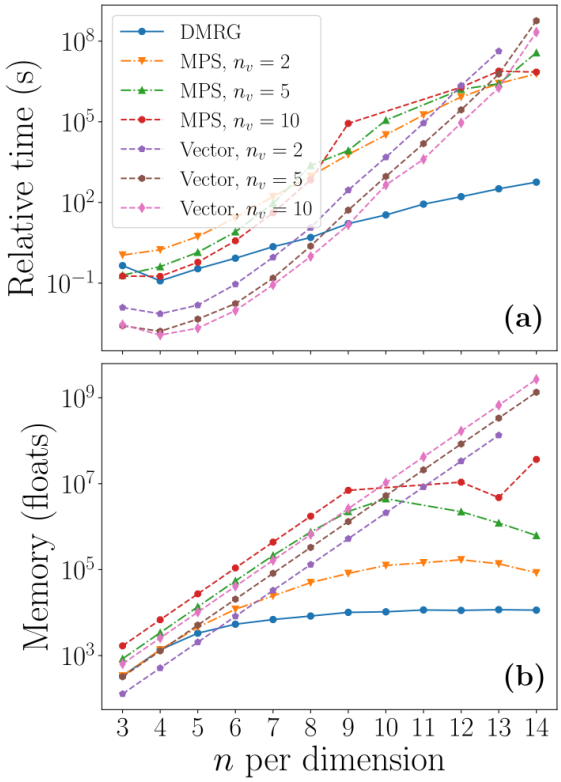

Figure 1: Single-shot results for DMRG and Arnoldi (MPS and vectors) for 2^n points per dimension. (a) Relative execution time with respect to n = 3. (b) Memory.

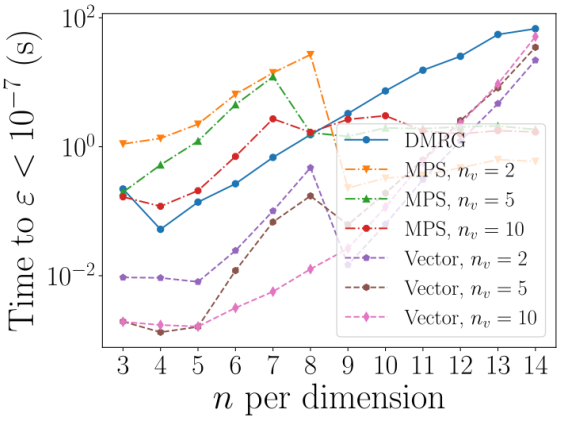

Figure 2: Time to energy error ε < 1e-7 for DMRG and Arnoldi (MPS and vectors) with renormalization for 2^n points per dimension.