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Short Communication

Locally accurate matrix product approximation to thermal states

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Classical simulation of quantum many-body systems is a fundamental problem in computational physics. One difficulty is that a generic many-body state cannot even be represented in polynomial space because the dimension of the Hilbert space grows exponentially with the system size. Fortunately, many physically interesting states are non-generic and structured. It may be possible to avoid the "curse of dimensionality" by exploiting their structure.

In one-dimensional quantum systems such as spin chains, matrix product state (MPS) methods, including the celebrated density matrix renormalization group, are popular and numerically powerful [1]. As the name suggests, an MPS is a data structure representing a many-body state by products of matrices. The dimension of the matrices is called the bond dimension, which determines the space complexity or the number of parameters in the MPS.

Consider a system in thermal equilibrium. In textbooks and courses, we learned that the system at temperature $T = 1/\beta$ is in a mixed state described by the density operator

$$\sigma_\beta := e^{-\beta H}/Z, \quad Z := \mathrm{tr} e^{-\beta H}, \tag{1}$$

where H is the Hamiltonian and Z is the partition function.

Since MPS methods are widely used, it is important to understand their empirical success in simulating the thermal properties of one-dimensional systems with short-range interactions. In a remarkable sequence of papers [2–5], σ_β is proved to be efficiently approximated by a matrix product operator (MPO) [6–8], which is a straightforward generalization of MPS to operators. Let $\tilde{O}(x) := O(x \log x)$. The best known result is

Theorem 1. [5] *Consider a chain of N spins governed by a local Hamiltonian H. There exists an MPO ϱ with bond dimension*

$$e^{\tilde{O}\left(\beta^{2/3}+\sqrt{\beta \log \frac{N}{\varepsilon}}\right)}, \tag{2}$$

such that $\|\varrho - \sigma_\beta\|_1 \leqslant \varepsilon$, where $\|X\|_1 := \mathrm{tr}\sqrt{X^\dagger X}$ is the trace norm.

Remark 1. See Refs. [2–4] for analogues of this theorem in two and higher spatial dimensions.

In practice, we may not have to increase the bond dimension with the system size N. An extreme example is the infinite imaginary time-evolving block decimation algorithm [9], which yields a translationally invariant matrix product representation of σ_β directly in the thermodynamic limit. It is empirically observed that a constant bond dimension is sufficient for computing expectation values of local observables. This observation cannot be explained by Theorem 1, where the bond dimension (2) grows with the system size N and diverges in the thermodynamic limit $N \to +\infty$.

In this paper, we prove that there exists an MPO with bond dimension

$$e^{\tilde{O}\left(\beta^{2/3}+\sqrt{\beta \log \frac{1}{\epsilon}}\right)}, \tag{3}$$

such that all local properties of σ_β are approximated to accuracy ϵ. For the constant β, the bond dimension (3)

- is independent of N. This justifies the common practice of using a constant bond dimension in the numerical simulation of thermal properties.
- grows slower than any power law in $1/\epsilon$, e.g., $\ll 1/\epsilon^{0.001}$, as $\epsilon \to 0^+$. This explains the empirical observation that high precision can be achieved with a small or moderate bond dimension.

As a side remark, Refs. [10–14] constructed locally accurate matrix product approximations to pure states with low entanglement.

We now state our results formally. Consider a chain of N spins with local dimension d.

Definition 1. (Matrix product operator) Let $\{\hat{O}_j\}_{j=0}^{d^2-1}$ be a basis of the space of linear operators on the Hilbert space of a spin. Let

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$\{D_i\}_{i=0}^N$ with $D_0 = D_N = 1$ be a sequence of positive integers. An MPO has the form

$$\rho = \sum_{j_1 j_2 \cdots j_N = 0}^{d^2-1} \left(A_{j_1}^{(1)} A_{j_2}^{(2)} \cdots A_{j_N}^{(N)}\right) \hat{O}_{j_1} \otimes \hat{O}_{j_2} \otimes \cdots \otimes \hat{O}_{j_N}, \tag{4}$$

where $A_{j_i}^{(i)}$ is a matrix of size $D_{i-1} \times D_i$. Define $\max_{0 \leqslant i \leqslant N} D_i$ as the bond dimension of the MPO ρ.

Consider a local Hamiltonian

$$H = \sum_{i=1}^{N-1} H_i, \quad \|H_i\| \leq 1, \tag{5}$$

where H_i represents the nearest-neighbor interaction between spins at positions i, $i+1$, and $\|\cdot\|$ is the operator norm. The thermal state σ_β at inverse temperature β is given by Eq. (1).

Theorem 2. *There exists an MPO ρ with bond dimension (3) such that*

$$|\mathrm{tr}(\rho \hat{O}) - \mathrm{tr}(\sigma_\beta \hat{O})| \leqslant \epsilon \tag{6}$$

for any local observable $\hat{O}$ with $\|\hat{O}\| \leq 1$.

Proof. See the Supplementary materials.

In conclusion, we have proved that in one-dimensional quantum systems with short-range interactions, a thermal state at inverse temperature β has an MPO representation with bond dimension (3) such that all local properties are approximated to accuracy ϵ. This justifies the common practice of using a constant bond dimension in the numerical simulation of thermal properties.

Notes Very recently, I became aware of a related work by Alhambra and Cirac [15], which constructed locally accurate tensor network approximations to thermal states and time evolution in any spatial dimension. Specializing to thermal states in one dimension, my method and results are different from theirs. Their proof consists of two steps:

1. Construct "local approximations" assuming exponential decay of correlations.
2. Merge local approximations using the "averaging trick" of Refs. [11–13].

The proof of Theorem 2 uses neither of these ingredients. Different from Eq. (5) in Result 1 of Ref. [15], the bond dimension (3) does not depend on the correlation length and grows slower than any power law in $1/\epsilon$ as $\epsilon \to 0^+$ for constant β. This solves an open problem in the conclusion section of Ref. [15].

Conflict of interest

The author declares that he has no conflict of interest.

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Appendix A. Supplementary materials

Supplementary materials to this article can be found online at https://doi.org/10.1016/j.scib.2021.08.011.

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