Classical simulation of quantum many-body systems with a tree tensor network

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(Dated: April 1, 2022)

We show how to efficiently simulate a quantum many-body system with tree structure when its entanglement is bounded for any bipartite split along an edge of the tree. This is achieved by extending the time-evolving block decimation simulation algorithm for time evolution from a one-dimensional lattice to a tree graph, while replacing a matrix product state with a tree tensor network. As an application, we show that any one-way quantum computation on a tree graph can be efficiently simulated with a classical computer.

PACS numbers:

Introduction.— The underlying physical laws describing classical and quantum systems are quite different, which makes it generally hard to efficiently simulate a quantum many-body evolution with a classical computer. However, if the quantum evolution has certain restrictions, an efficient classical simulation may be possible. Indeed, efficient simulation algorithms are known for several restricted quantum circuit models, while a general connection between entanglement and the classical simulatability of quantum lattice models has been unveiled. In one spatial dimension (1D), for instance, the state of a quantum chain with a limited amount of entanglement between any bipartition along the chain can be efficiently described using a matrix product state (MPS). This is exploited by the density matrix renormalization group (DMRG) algorithm to find the ground state of the chain and by the time-evolving block decimation (TEBD) method to simulate an evolution in time. Furthermore, projected entangled-pair states (PEPS) have been introduced as an extension of MPS to simulate 2D systems.

In this work we consider the simulation of a quantum many-body system with a restricted amount of entanglement according to a tree structure. As in the 1D and 2D approaches mentioned above, we express the \(d^n\) complex amplitudes \(c_{i_1 \cdots i_n}\) of the state \(|\Psi\rangle\) of \(n\) qudits (or \(d\)-level quantum systems),

\[
|\Psi\rangle = \sum_{i_1=1}^{d} \cdots \sum_{i_n=1}^{d} c_{i_1 \cdots i_n} |i_1\rangle \otimes \cdots \otimes |i_n\rangle,
\]

in terms of a network of tensors, but specialize to the case where this tensor network (TN) has tree structure. Given a tree TN, we explain (i) how to simulate the response of the system to local operations and classical communication (LOCC), that is to generic manipulation of individual qudits, including adaptive unitary transformations and measurements and (ii) how to simulate time evolution. The latter is achieved by extending the TEBD algorithm, originally proposed to simulate 1D quantum lattices, so that it applies to a much broader class of states and physical situations. As in the 1D case, the key to an efficient simulation is that the amount of entanglement in the system remains sufficiently bounded during the time evolution.

From the perspective of theoretical computer science, our results imply that one-way quantum computation with a tree-graph cluster state can be efficiently simulated with a classical computer. One-way quantum computation with cluster states, an interesting alternative to the quantum circuit model, had previously been shown to be universal for quantum computation in a 2D lattice but classically simulatable in a 1D lattice. By extending the classical simulatability result to tree cluster states, we further sharpen the boundary between the complexities for classical and quantum computation.

From the perspective of computational physics, our results provide an algorithm both to find the ground state and to simulate time evolution in complex quantum systems with tree structure (see also), such as dendrimers—a class of highly branched polymers. This algorithm, based solely on tensor multiplications and singular value decompositions, also offers new ways to simulate 1D systems with long-range interactions.

Canonical form of a tree TN.— We use a TN with \(n\) open indices and tree structure, see Fig. 1, to express the \(d^n\) complex coefficients of the \(n\)-qudit state \(|\Psi\rangle\). More specifically, we consider a tree network made of tensors with only 3 indices each, the network therefore containing \(n-2\) tensors. An index connecting two tensors divides the network into two sub-trees, \(A\) and \(B\) and the \(n\) qudits into two disjoint sets. We use the term bipartition to refer only to such divisions. The rank of an index is the number of values it takes. In what follows, \(\chi\) denotes the largest rank among all indices in the network. Notice that the tree TN depends on \(O(n\chi^3)\) complex coefficients.

The Schmidt decomposition of \(|\Psi\rangle\) according to bipart-
introduce the parameter $\chi$ and where the Schmidt rank satisfies $\chi \leq \chi$. Each vertex has three edges and corresponds to a tensor with three indices. Pairs of tensors are connected in the network through a shared index, over which there is an implicit summation. (ii) Canonical form of the previous tree TN. For each bipartition, sub-trees $A$ and $B$ describe Schmidt bases, see Eq. (2). An empty circle on top of an edge represents a set of Schmidt coefficients weighting the corresponding index.

Definition. A tree TN is in the canonical form for bipartition $A : B$ if (i) the weights on the connecting index $\alpha$ correspond to the Schmidt coefficients $\{\lambda_\alpha\}$ and (ii) the sub-trees $A$ and $B$ describe a set of Schmidt bases $\{\Phi_\alpha^{[4]}\}$ and $\{\Phi_\alpha^{[6]}\}$. A tree TN is in the canonical form if it is so for all bipartitions.

**Theorem 1.** The canonical form of an n-qudit tree TN $n$ can be obtained with $O(n\chi^2)$ basic operations.

**Proof:** Given a bipartition $A : B$, $|\Psi\rangle$ can be written as

$$|\Psi\rangle = \sum_{\alpha} \lambda_\alpha |\alpha\rangle^{[4]} \otimes |\alpha\rangle^{[6]},$$

where $\langle \alpha^{|4}| \alpha^{[6]} \rangle = \delta_{\alpha\alpha'} \sum_\alpha (\lambda_\alpha)^2 = 1$ and where the Schmidt rank satisfies $\chi(4,8) \leq \chi$. We next introduce the canonical form of a tree TN, which also consists of tensors with three indices but where each index $\alpha$ shared by two tensors carries weights, see Fig. 1.

**Theorem 2.** A two-qudit reduced density matrix can be computed with $O(m^2\chi^4)$ basic operations, where $m$ is the number of tensors in the path that connects the two qudits in the tree TN. [see Fig. 2]

Second, we can arbitrarily relocate a qudit within the tree TN. This is achieved by swapping the index corresponding to this qudit with other indices in the tree.

**Theorem 3.** Swapping a qudit index of a tensor with an index of a neighboring tensor can be achieved with $O(d^2\chi^4)$ basic operations. [See Fig. 3]

Third, we can update the tree TN after a unitary gate $U$ has acted either on one qudit or on two neighboring qudits. Unitarity preserves the orthogonality of the Schmidt bases for most bipartitions, and as a result the
update process involves changing only one or two tensors. When \( U \) acts on one qudit or on two qudits that are connected to the same three-legged tensor, that tensor simply absorbs the gate through index contraction.

**Theorem 4.** Consider a two-qudit gate \( U \) acting on a pair of open indices of two tensors that are nearest neighbors in the network. The tree TN can be updated by replacing these two tensors, at a cost of \( O(d^3 \chi^3) \) basic operations. [See Fig. 4.]

**Efficient simulation with a tree TN.**— All the above manipulations require computational time (and space as well) that scales at most linearly in the number of qudits \( n \) and as a small power of the maximal Schmidt rank \( \chi \). Therefore, in those systems where the amount of entanglement across all relevant bipartitions, as characterized by \( \chi \), scales at most polynomially in \( n \), such manipulations can be implemented efficiently. This opens up a number of simulation possibilities.

For instance, we can simulate the response of the system to arbitrary local manipulation. Recall that LOCC manipulation can be decomposed as an adaptive sequence of generalized local measurements mapping pure states into pure states. Let \( \mathcal{E} \) denote one such measurement on a qudit, as characterized by a set of operators \( \{E_r\} \), where \( r \) labels the measurement outcome. Outcome \( r \) occurs with probability \( p_r = \langle \Psi \rvert E_r^\dagger E_r \rvert \Psi \rangle \), in which case the state of the system becomes \( \rvert \Psi_r \rangle = E_r \rvert \Psi \rangle / \sqrt{p_r} \). To simulate \( \mathcal{E} \), first we randomly draw an outcome \( r \) according to the probability \( p_r = \text{tr}[E_r \rho^{(1)}] \), computed from the reduced density matrix \( \rho^{(1)} \) of the qudit to be measured. Then a tree TN for \( \rvert \Psi_r \rangle \) is obtained from that of \( \rvert \Psi \rangle \) by simply absorbing operator \( E_r \) into it. The new maximal Schmidt rank \( \chi_r \) satisfies \( \chi_r \leq \chi \).

An implication of the above result is that one-way quantum computation on a tree can be efficiently simulated. This follows from the fact that a tree-graph cluster state has a very simple tree TN representation, with \( \chi = 2 \), while the manipulations involved in a one-way computation consists of LOCC.

The simulation of a time evolution according to a two-body Hamiltonian \( H = \sum_{i,j} h_{ij} \) is also possible. As in the case of a 1D system \(^4\), we expand the evolution operator \( V = \exp(-iHt) \) into a series of two-qudit unitary gates \( U \) using a Suzuki-Trotter expansion. But now, for each of these gates, we first bring the indices of the two qudits together using Theorem 3, then absorb \( U \) into the tree TN using Theorem 4, and finally bring the qudit indices back into their initial position. This generalizes the TEBD algorithm \(^4\) from 1D systems to a generic tree TN. With minimal modifications to deal with non-unitary gates, The TEBD algorithm can also be used to simulate an evolution in imaginary time according to \( V' = \exp(-iHt) \). In this way we can compute the ground state of \( H \), provided \( H \) has a finite gap \( \Delta > 0 \) in its spectrum. Recall that the expectation value of local observables, such as the energy \( E = \langle \Psi \rvert H \rvert \Psi \rangle \) or two-point correlators, can be computed from two-qudit reduced density matrices, which we can obtain using Theorem 2.

As discussed in \(^4\) for 1D systems, the use of a canon-
The tensor subnetwork in (i) is contracted into the four-legged tensor in (ii), which is then decomposed into (iii) by using a SVD (of a $d \times d$ matrix) that takes $O(d^3)$ basic operations. Notice that, as in Fig. 3, special attention is paid to first absorbing and then detaching the weights of the lateral indices. This guarantees that the resulting tree TN is in its canonical form.

A tree TN may be used to simulate a many-body system with a genuine tree structure (determined e.g. by the interaction pattern) as it is the case of dendrimers. But it can also be used to simulate a 1D system with long-range interactions, including periodic boundary conditions. Notice that when using a MPS (that is, a linear TN) to represent a 1D system, the number of tensors in the path connecting two random qudits scales as $O(n)$ and, consequently, so does the computational time to simulate a gate acting on those qudits. Instead, in a binary tree TN, see Fig. 7, the path connecting any two qudits contains at most $O(\log n)$ tensors. This shortens the time required to simulate that gate by a significant factor $\log(n)/n$.

We conclude by noticing that in this paper we have explored the most general extension of the TEBD algorithm. Indeed, it appears that a tree TN — not having closed loops — is the most general TN to which we can associate a Schmidt decomposition to each of its indices, a fundamental ingredient of the simulation algorithm.

Y.-Y. thanks A. Kitaev for introducing to him the general concept of tensor networks. L.-M. thanks S. Barrett, P. Kok, and F. Verstraete for helpful discussions. This work was supported by NSF under Awards 0323555, 0347078, and 0431476, the ARDA under ARO contracts, and the A. P. Sloan Fellowship.

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A tensor with more than three indices can be decomposed into a tree $T_N$ made of tensors with three indices each (for instance, through a sequence of SVDs).