Contracting Arbitrary Tensor Networks: general approximate algorithm and applications in graphical models and quantum circuit simulations

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We present a general method for approximately contracting tensor networks with an arbitrary connectivity. This enables us to release the computational power of tensor networks to wide use in optimization, inference, and learning problems defined on general graphs. We show applications of our algorithm in graphical models, specifically on estimating free energy of spin glasses defined on various graphs, where our method largely outperforms existing algorithms including the mean-field methods and the recently proposed neural network based methods. We further apply our method to the simulation of random superconducting quantum circuits, and demonstrate that with a trade off of negligible truncation errors, our method is able to simulate large quantum circuits which are out of reach of the state-of-the-art simulation methods.

As a powerful method to alleviate the curse of dimensionality in high dimensional modeling and data analysis, the tensor networks find wide applications in many areas of science and technology. In quantum many-body physics, tensor networks on lattices including the matrix product states (MPS) [1, 2], and the projected entangled pair states (PEPS) [3] have great success in the study of strongly correlated systems; in statistical mechanics, calculation of the partition function can be naturally converted to a tensor network contraction problem [4]; in computer science, the number of solutions of constraint satisfaction problems can be computed via tensor networks [5]; in data science, tensor networks and tensor decompositions are important tools for data compression and dimensionality reduction [6]; recently, tensor network methods have been successfully extended to machine learning, in compressing a neural network [7], giving an efficient image classifier [8], and working as generative models in the unsupervised learning [9, 10].

Despite its wide use, however, the capability of the tensor networks is so far limited to either small-dimensional systems where the exact contraction is tractable, or high-dimensional systems only on regular lattices with local interactions, where there exist efficient contraction algorithms e.g. the renormalization group [4, 11–13], and the block decimation [14]. On general systems with long range interactions and irregular connectivity (such as the graphs depicted in Fig. 1), the tensor network method is rarely applied, due to the intractability of efficient contraction: to best of our knowledge, there is no general method exists for approximately contracting arbitrary tensor networks. This sets limitations on applying tensor networks to many areas such as graphical models, statistical inference, and machine learning problems.

In this work we aim to break this limitation. We propose a general method for approximately contracting tensor networks on an arbitrary graph, based on a method we term as MPS calculus: the initial tensors as well as intermediate tensors produced during the tensor contractions are represented, compressed, and operated using the matrix product states in the canonical form. This allows us to deal with large intermediate tensors which can not be stored in the memory in its original form. During the contraction process we iteratively detect low-rank structures and apply low-rank approximations to reduce the space and time complexities of the contraction, using approaches analogous to the density matrix renormalization group (DMRG) [11], until the final result, a scalar \( Z \), is obtained. We show applications of our method in graphical models, where \( Z \) represents the normalization factor of the joint distribution of a large number of random variables (i.e., the partition function in physics), and application in quantum circuits where \( Z \) represents single amplitude of a qubit string.

Contracting arbitrary tensor network.— Exactly contracting arbitrary network belongs to the class of \#P hard problems. In [15], it has been proved that the time complexity of contracting a tensor network is exponential in the tree width of the corresponding line graph. In practice the difficulties we typically encounter in the contracting process is creating large intermediate tensors that can not be stored in the memory.

Our idea is to represent every tensor in the network to a matrix product state in the canonical form, and do contractions and low-rank approximations based on the MPS representations. The matrix product state, also known as the Ten-
A tensor Train in mathematics [16], is a one dimensional tensor network composed of three-way tensors (and matrices in the boundary). The MPS has been widely applied to quantum many body problems, especially in one dimension. An obvious advantage of MPS is the parameter efficiency: a n-way tensor $\mathcal{A} \in \mathbb{C}^{\chi^n}$ can be approximated by a MPS of virtual bond dimension $\chi$ with only $(n-2)d\chi^2 + 2d\chi$ parameters, for example the sequential singular value decompositions [16], or DMRG [11]. With a large-enough $\chi$, the MPS can faithfully represent the original tensor hence give an exact result. With limited computational resources, one would restrict the bond dimensions, and introduce a certain error. The amount of error depends on how many low-rank structures there are in the underlying raw tensor $\mathcal{A}$. We refer to [17] for introductions of tensor network and the matrix product states.

The contraction in the MPS calculus is processed by eliminating edges in the tensor network one by one. By eliminating we mean merging two tensors to a single tensor by summing over the common index of them. As an example, consider merging two tensors $\mathcal{A} = [a_{ijk}]$ and $\mathcal{B} = [b_{j\mu\nu}]$ into tensor $C = [c_{j\mu\nu}]$, where tensors are all in the MPS representation formulated as

$$a_{ijk} = \sum_{\alpha} \sum_{\beta} a^{(1)}_{\alpha j} a^{(2)}_{\alpha \beta k} a^{(3)}_{\beta}, \quad b_{j\mu\nu} = \sum_{\alpha} \sum_{\beta} b^{(1)}_{\mu \alpha \beta} b^{(2)}_{\beta \nu} b^{(3)}_{\beta\nu}.$$  (1)

To ensure that summing over the index $i$ results to another MPS, we first do swap on $\mathcal{A}$ to switch the indices $i$ and $k$, which is formulated as

$$a_{ijk} = \sum_{\alpha} a^{(1)}_{\alpha j} a^{(2)}_{\alpha \beta k} = \sum_{\alpha} a^{(1)}_{\alpha j} a^{(2)}_{\alpha \beta k} a^{(3)}_{\beta}.$$  (2)

where $a^{(23)}_{\alpha \beta}$ are elements of the tensor created by contracting the index $\beta$; and the last step of the above equation requires the singular value decomposition, which could introduce truncations in the singular values. Similarly, we apply the swap operation also on tensor $\mathcal{B}$, to switch indices of $i$ and $\mu$, giving

$$b_{j\mu\nu} = \sum_{\beta} b^{(1)}_{\mu \beta} b^{(2)}_{\beta \nu} b^{(3)}_{\beta\nu}.$$  (3)

The swap operation switches the positions of two indices in the original tensor, by switching two adjacent tensors in the mps, with a similar functionality as the swap gate in the quantum information [18]. This operation increases entanglements of the MPS, and the maximum bond dimension could be increased to $d\chi$, where $\chi$ denotes the virtual bond dimension of the MPS and $d$ is the dimension of the physical indices, e.g. $i$ in the previous formulas. If $d\chi$ is greater than $\chi$, the preset limit on the virtual bond dimension, we canonicalize the MPS then truncate the bond dimension to $\chi$ during the singular value decomposition.

After performing the swap operations on both tensors, we can see that the index $i$ locates at the tail position of the MPS representation of $\mathcal{A}$ and at the head position of the MPS representation of $\mathcal{B}$. Thus summing over index $i$ results to a longer MPS $C$. Notice that after the contraction, the obtained tensor $C$ could have two indices, say $j$ (with bond dimension $d_j$) and $k$ (with bond dimension $d_k$) linked together to another tensor $D$, due to existence of a triangle with three end tensors being $\mathcal{A}, \mathcal{B},$ and $\mathcal{D}$. In this case we move indices $j$ and $k$ to adjacent positions using the swap operations and merge the two corresponding tensors to a 3-way tensor with a larger physical bond dimension $d_jd_k$. If it exceeds $\chi$, pre-set maximum physical bond dimension, we canonicalize both $C$ and $D$, then do SVD together with a truncation on singular values to reduce the bond dimension from $d_jd_k$ to $\chi$.

During the contraction process, the operations swap, contraction, and merge, are repeated until the overall tensor network is finally contracted to a scalar $Z$. A pictorial representation of the whole process is sketched in Fig. 2 and detailed in the Appendices, by taking a simple example of contracting a tensor network with $5$ four-way tensors.

An important problem of the tensor network contraction is how to choose the edge order to eliminate one by one, which we refer to as contraction order. Markov and Shi [15] showed that the optimal contraction order can be obtained using the optimal tree decomposition of the line graph corresponding to the tensor network. However finding the optimal tree decomposition for a general graph is a NP-hard problem, so usually one needs heuristic algorithms to find a good tree decomposition. Also notice that even equipped with the order given by the optimal tree decomposition, the algorithms for exact contraction in general is still an exponential algorithm with computational complexity grows exponentially with the tree width of the line graph. In this work, we consider the approximate contraction using polynomial algorithms. In contrast with the exact contraction, the dimension of the intermediate tensors in our scheme are hard to predict, because whether there are low-rank structures that we can use to reduce the dimensionalities is not known a priori. Here we adopt a greedy algorithm for sequentially selecting an edge from all remaining edges, which minimizes the dimension of the obtained tensor.

Our algorithm takes two parameters, the maximum physical bond dimension $\chi$, and the maximum virtual bond dimension $\chi$ of the MPSes. The space complexity of algorithm is bounded above by $O(\chi^2)$, and the time complexity is dominated by singular value decompositions adopted in the swap operations, which is $O(\chi^2\chi^2)$. Apparently, our algorithm is a polynomial algorithm which is able to contract arbitrary tensor networks, with a limited amount of computational resources. Moreover, our method enjoys efficient compression scheme analogous to the DMRG method, which allows dynamically adjusting dimensions of the tensors. Then a question naturally arises is whether it is possible to use our method with a reasonable bond dimension to deal with systems encoding strong entanglements which are induced by long range interactions? In the following text we will give two applications of our algorithms, the inference and learning in the graphical models, and the simulation of quantum circuits, to partially answer the question.

Applications to graphical models— Graphical models are important tools for representing joint probability distribu-
tions over a large number of random variables that interact with each other. It combines concepts and methodologies in physics, statistics, computer science, and machine learning, and finds important applications in many fields in science and engineering. Without loss of generality, in this article we use very classic example of the graphical model, the Ising model and spin glasses in the statistical physics to demonstrate the power of our method. In this problem, the joint probability of \( n \) spins \( s \in \{\pm 1\}^n \) follows the Boltzmann distribution

\[
P(s) = \frac{1}{Z} \exp(-\beta E(s)),
\]

where \( E(s) \) is the energy function of a configuration \( s \), \( \beta = 1/T \) is the inverse temperature and \( Z \) is the partition function. Given a problem instance, an essential problem is computing the free energy \( F = -\frac{1}{\beta} \ln Z \). Based on an accurate estimation of the free energy, the observables such as magnetizations and correlations, even the unbiased samples, can be obtained based on the free energy estimate. However, computing free energy belongs to the class of \#P hard problem hence there is hopeless to find polynomial algorithms for solving it exactly. In physics, many approximate algorithms have been developed. These include Markov Chain Monte Carlo (MCMC) based methods [19], mean-field methods which parametrize a variational distribution, then optimize the parameters by minimizing the variational free energy. Recently in [20], the mean-field methods are extended by employing the variational autoregressive neural networks as a variational distribution, which in principle has a strong expressive power.

Any probability distribution over discrete variables is a tensor, thus every graphical model can be converted to a tensor network by introducing copy tensors on each node of the graph, and matrices (or tensors) on each edges (or multi-body factor) of the (factor) graph. The computation of the partition function \( Z \) naturally translates to contraction of the tensor network defined exactly on the same graph. As an example, consider the celebrated pairwise Ising spin glass models with \( n \) variables, its energy function is defined as \( E(s) = -\sum_{i\neq j \in E} J_{ij} s_i s_j \), with \( E \) denoting set of edges, and \( J_{ij} \) denoting couplings between two spins \( i \) and \( j \). The partition function can be written formally as

\[
Z = \sum_s \prod_{(i,j) \in E} e^{\beta J_{ij} s_i s_j} = \operatorname{Tr}(\mathcal{A}^{(1)} \times \mathcal{A}^{(2)} \times \cdots \times \mathcal{A}^{(n)}),
\]

where the symbol \( \times \) represents contraction of tensors \( \{\mathcal{A}^{(i)}\} \), each of which is given by contracting a copy tensor with matrices defined on the edges connected to node \( i \)

\[
\mathcal{A}^{(i)} = I_{d_i \times d_i} \times B_{\partial i \times \partial i} \times B_{\bar{\partial} i \times \bar{\partial} i} \times \cdots \times B_{\bar{\partial} i \times \bar{\partial} i}.
\]

Here \( I_{d_i \times d_i} \) is a copy tensor, i.e. a diagonal tensor with order equal to the degree (number of neighbors) \( d_i \) of node \( i \), with 1 on the diagonal entries and zero on the other entries. \( \partial i \) denotes the set of neighbors of node \( i \), and the matrix \( B_{\partial i \times \partial i} \) is a \( 2 \times 2 \) matrix with \([\cosh(\beta J_{ij})/2]^{1/2} + [\sinh(\beta J_{ij})/2]^{1/2}\) on the diagonal and \([\cosh(\beta J_{ij})/2]^{1/2} - [\sinh(\beta J_{ij})/2]^{1/2}\) on the off-diagonal entries. It is also worth noting that on graphical models with variables taking \( q \) possible values, the converted tensors \( \{\mathcal{A}^{(i)}\} \) on the graph nodes are all of rank \( q \). Indeed they are of Canonic Multidic format (CP) [21] with (CP) rank \( q \), and can be exactly converted to the matrix product state with bond dimension \( q \) [16].

After converting the graphical model to a tensor network, our contraction algorithm, MPS calculus, can be directly applied to computing free energy of the problem defined on arbitrary lattices. Observe that when the graphical model is a tree, our algorithm will perform edge eliminations iteratively on leaves of the tree because this minimizes the size of the intermediate tensor. The edge eliminating on edges connecting two leaves is equivalent to variable elimination from leaves to the root of the tree, which is nothing but the belief propagation algorithm, hence is exact on a tree graphical model. On other graphs, our algorithm might generate error \( \epsilon_{\text{SVD}} \), from the truncation of singular values during the SVDs. Empirically we observe that the error \( \epsilon_{\text{SVD}} \) is several magnitude smaller than the error of the obtained free energy \( \epsilon_F \), but so far it is not clear to us how to relate the two errors analytically. We subject to numerical experiments to demonstrate the performance of our algorithm.

The experiments are carried out using the Ising models and spin glasses on various of topologies, including two dimensional lattices, random graphs, small-world graphs, and complete graphs. Our results are compared against mean-field methods including the Naïve mean-field (NMF), Thouless-Anderson-Palmer equations (TAP), Belief propagation (BP), and the neural network based variational autoregressive networks (VAN). On the 2-D lattice without the external field, the graph is planar so there are exact solutions. However on the other graphs we have to adopt exponential algorithms to compute exact free energy values for the evaluations. For the SK model with a finite size we enumerate all \( 2^n \) configurations for computing the free energy, this restricts the system
size to $n = 20$ spins in our experiments. For systems on the random graphs and small-world networks, we use an exact algorithm based on the feedback set of the underlying graph. The feedback set of the graph is a subset of the nodes such that after removing them, the remaining graph is composed of trees. So we only need to enumerate the all possible configurations of the feedback set, then compute the free energy by using the enumerated configurations weighted by contributions of remaining trees of the graph which can be calculated exactly. Details of the algorithm can be found in [23]. With this method, we can handle exact solutions of Ising spin glasses on 3-regular random graphs with 80 nodes, and on small-world graphs with 70 nodes in a reasonable amount of time.

The results are shown in Fig. 3. On the left panel, the model is the ferromagnetic Ising model on a 16 × 16 lattice with open boundary condition. It shows that the belief propagation (BP) gives relatively poor results due to presence of short loops in the lattice, and the variational autoregressive networks equipped with convolution neural networks (Cov VAN) works much better than mean-field methods, which is consistent with [20]. In the second and third panels, the model is a spin glass model defined on regular random graphs and small-world graphs respectively. We can see that in the random graphs, the belief propagation (Bethe) works well, almost as good as the VANs, because the conditional independence assumptions of the belief propagation is a good approximation in random graphs. However in the small-world network the belief propagation performs much worse than VAN due to short loops. In the last panel the model is the Sherrington-Kirkpatrick model on a complete graph, where VAN significant outperforms traditional mean-field methods, in consistent with [20]. In all of the experiments, we can see that our method outperforms all mean-field methods and the neural-network based methods, to a large margin. In regular random graphs, small-world networks, and the SK model, the accuracy is only limited by the machine precisions ($10^{-10}$). In all experiments we choose $\hat{D} = 50$, $\hat{\chi} = 500$, the computational time of our method in computing each point of the graph is of few seconds, indicating that our method is much faster than the mean-field methods which requires converging message passing equations, and the neural network based methods which require quite long time and an access to GPU. More results about the dependence of the bond dimensions, as well as the list of corresponding computational time, can be found at the appendices.

With the free energy being computed accurately, we can use it to compute macroscopic observables such as magnetizations, correlations, even the likelihood of data, by taking derivatives of the free energy, which is straightforward to compute using the back-propagation technique in the machine learning, even through SVDs [24]. This convenience immediately gives our method an ability to perform learning tasks using graphical models. In the appendix we give a simple example of using our method to learn a generative model using hand-written digits of the MNIST dataset.

**Application to quantum circuit simulations**

The problem of computing free energy of graphical models is similar to the problem of computing single amplitude estimate of a superconducting quantum circuit [25], which can be treated as a graphical model with complex couplings and temperature. Classic simulation of quantum circuits is important for verifying and evaluating the computational advances of the quantum computers. So far there are mainly two distinct styles for quantum circuit simulations. The first style is straightforward, based on storing and evolving the state vector, and can handle circuits with arbitrary depth but less than 50 qubits, due to the memory bottleneck. The second style converts the quantum circuit to a tensor network then exactly contract it
based on an heuristic contraction order e.g. given by tree decomposition of the line graph of the tensor network [15, 26–28]. This method can handle circuits with a large number of qubits, but a relatively lower depth than the first style, because the computational complexity grows exponentially in the circuit depth $d$.

Recently, equipped with advanced developments of super conducting quantum devices, Google [29] claimed that they have achieved the quantum supremacy by demonstrating that sampling from random quantum circuits requires few seconds on their quantum circuits but 10,000 years on the fastest classical super computers. However one should notice that the 10,000-year time is estimated based on exact simulation of Google’s super conducting quantum circuit, which is however noisy by itself. Thus an important open question is whether approximate simulations of quantum circuits could beat the noisy quantum device of Google? This apparently requires advanced studies of approximate algorithms for simulating quantum circuits which is lacking so far.

Our method applies to single-amplitude simulation of quantum circuits directly with any kind of connectivities such as two-dimensional lattice, and random regular graphs as considered in the QAOA [30], after converting the initial state, the measurement qubit string, as well as the gates into tensors. The key difference between our method and methods for quantum circuit simulation is that by detecting low-rank structures in the circuit, our method heavily reduces the computational complexity. Although this introduces SVD truncation errors, we will illustrate that at least in the shallow circuits the error is almost negligible. We perform experiments using standard random circuits on two dimensional lattices [26–28], which iteratively apply single-qubit gates and two-qubit Controlled-Z gates to the initial $|0, 0, ..., 0\rangle$ state, and finally measure the amplitude of a specific qubit string. The generation protocol is described in detail in the Appendices. We evaluate the performance of our method against the recently developed state-of-the-art exact tensor contraction methods [28] which has a precisely predictable space and time complexity. So in comparisons we do not have to run their algorithm which may require a supercomputer. We run our algorithm on a workstation with 64 Gigabytes memory. With depth $d = 8$, our algorithm can handle circuits with at most $40 \times 40 = 1600$ qubits with SVD accumulated truncation error $\epsilon_{\text{SVD}} \leq 10^{-12}$ within an hour, with a much smaller computational complexity that than that of [28] as compared in Fig. 4. The right panel of the Fig. 4 indicates that the method of [28] already costs at least 64 GB memory for storing the largest intermediate tensor with $L = 31$, and even requires 32 TB memory for handling $L = 40$. We note that so far our algorithm can not handle the circuit with a large depth such as Google’s circuit [29] with a small SVD error, because the current implementation of our algorithm only works on a single workstation, this prevents us from using a large bond dimension.

**FIG. 4.** Computational time (left) and memory usage (right) of our algorithm in contracting random quantum circuits with depth $d = 8$, and compared with time and space complexity of an exact tensor network method for quantum circuit simulation proposed in [28] (Guo et. al.). We ran our algorithm on a workstation with 64 GB memory (as indicated by the red dashed line). The blue lines in the figure are estimated using the precise time and space complexity of the exact algorithm [28] which are also indicated by the formulas in the figure. The memory usage is calculated based on double precision complex number. Each red point in the left panel is averaged over 10 random circuits, the error bars are much smaller than the symbol size.

In this work we adopted the greedy contraction order which minimizes the size of the intermediate tensor after current truncation. The contraction order can be improved, we put this into future work. The MPS representation of tensors in our method naturally supports distributed storage, it is interesting to see how large a quantum circuit we can simulate, if a super computer is accessible to our algorithm. Another interesting development is deeply exploring the learning capability of our scheme (via back propagation) in the learning of quantum circuits. We hope more advanced arbitrary tensor network contraction methods inspired by our approach could fully release the numerical computational power of tensor networks to wider applications in science and engineering.

A python implementation of our method and algorithm, together with the datasets used in our experiments, are available at [31].

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Detailed description of the contraction process

The pseudo code of the algorithm is listed in the Algorithm 1. In the Algorithm list, the connectivity of the tensor network is denoted by a graph $\mathcal{G}$, its vertex set is denoted by $\mathcal{V}$, and its edge set is denoted by $\mathcal{E}$; the notation $D_{ij}$ represents the dimension of the bond $(i,j)$. We also give a simple example by contracting a tensor network composed of 5 nodes, each of which is a four-way tensor connecting to each other, with the step-by-step contraction process illustrated in Fig. 5.

Algorithm 1 MPS calculus

| Input: Tensor networks with tensors $\mathcal{A}^{(1)}...\mathcal{A}^{(n)}$, and the connectivity graph $\mathcal{G}(<\mathcal{V},\mathcal{E})$; the maximum physical bond dimension $\tilde{D}$, the maximum virtual bond dimension $\chi$. |
| Output: Contraction result $Z$. |

Convert every tensor to the MPS representation.

while $|\mathcal{V}| > 1$ do

$$(i,j) \leftarrow \arg \min_{(i,j) \in \mathcal{E}} \left[ \sum_{b,c,y} \log(D_{by}) + \sum_{b,d,v} \log(D_{bv}) - 2 \log(D_{vi}) \right]$$

Move the local tensor corresponding to the edge $(i,j)$ in the $\mathcal{A}^{(0)}$ to the tail position of the MPS representation.

Move the local tensor corresponding to the edge $(i,j)$ in the $\mathcal{A}^{(0)}$ to the head position of the MPS representation.

Merge two MPSes $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(0)}$ by contracting the edge $(i,j)$ that connects them.

$E \leftarrow E \setminus (i,j)$

for $k \in \partial i$ do

$E \leftarrow E \setminus ((j,k))$

if $k \in \partial i$ then

Do swap operations to move the duplicated $(i,k)$ edges to the adjacent positions in the MPS $\mathcal{A}^{(0)}$.

merge the adjacent local tensors, so that the two edges are combined, with a larger bond dimension $D_{hi}$.

if $D_{hi} > \tilde{D}$ then

Canonicalize $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(0)}$.

Contract two tensors connected by the edge $(i,k)$.

Do SVD on the unfolded matrix of the obtained tensor, and perform truncation on singular values to reduce $D_{hi}$ to $\tilde{D}$.

end if

else

$E \leftarrow E \cup \{(i,k)\}$

end if

end for

$\mathcal{V} \leftarrow \mathcal{V} \setminus \{j\}$.

end while

Return $Z = \mathcal{A}^{(0)}$

Canonical form of the MPS

During the contraction process, each original tensor is converted to a MPS in the canonical form. The canonical form eliminates the redundant gauge degrees of freedom of the MPS representation. Considering a three-way tensor $\mathcal{R}$ in right canonical form, it follows $\sum_{\mu,\nu} \mathcal{R}_{\mu \rho \nu}(\mathcal{R})_{\rho \beta \nu} = \delta_{\nu}^{\alpha}$ as described in graphic language in Fig. 6. In a canonical form, all tensors except a certain one are isometry, this gives several conveniences including computing the norm of the MPS, and computing simple-point and two-point measurements, etc. To our algorithm, the most important advantage is that once we need to do approximation between two connected MPSes by truncating the corresponding bond dimension, the canonical form transfers the local SVD truncations to a more global truncations involving the two MPSes, rather than involving only the two local tensors.

Dependences of the bond dimension $\tilde{D}$ in the graphical model experiments

In our experiments on graphical models, $\tilde{D}$ affects not only the running time but also the overall performance of the algorithm. In Fig. 7 we show how the results are influenced by changing the maximum physical bond dimension $\tilde{D}$. The experimental settings are identical to the main text. First, as expected, it is clearly shown that the relative error becomes smaller as $\tilde{D}$ increasing for most situations. The only exception is with $\tilde{D} = 50$ on the 20-spin SK model, where the results have no difference compared to $\tilde{D} = 20$. This means $\tilde{D} = 20$ is large enough to deal with the 20-spin SK model at the $\beta$ range considered here. In Fig. 8, time usage of our algorithm with different $\tilde{D}$ are shown. Since a bigger $\tilde{D}$ results to larger tensors, the time usage
FIG. 5. Detailed process of contracting a tensor network with 5 nodes, each of which is a four-way tensor, as sketched in Fig. 2. The scissor symbols in the figures indicate applying SVDs on the matrices unfolded from the tensors. The tensors in the step (1) are the original four-way tensors connected to each other, forming a fully connected pentagon. The step (2) shows the MPS representation transformed from (1); the arrow indicates contracting two MPSes, that is, annihilating one color. As an example, the green MPS and the purple MPS is contracted to a longer purple MPS in (3). The steps (3) – (5) show the swap operation between two tensors in the purple MPS. To accomplish swapping, we contract two purple tensors first, then apply the SVD on the contracted tensor as shown in (3) and (4). Note that in (5), we keep the canonical form of the MPS. In steps (6) – (8), the swap operation is repeated until two tensors connecting the same pair of colors are switched to adjacent positions. In steps (9) and (10), we finish the first merge step by contracting two tensors indicated by the arrow, producing a thick bond between red and purple MPSes. The steps (10) – (14) represent the merge between the purple-and-brown MPS pair and the purple-and-blue MPS pair. The steps (14) – (22) depict the procedure mentioned above repeatedly until a scalar left in the end of the whole contraction process.

FIG. 6. Illustration of the canonical form.

naturally increases. But for some cases, a bigger $\bar{D}$ occasionally changes the contraction order and avoid some approximation operations, leading to a lower running time than a smaller $\bar{D}$.

FIG. 7. Relative error of free energy on different models with varies $\bar{D}$ values, the experiment setting are identical to Fig. 3
Learning of graphical model using tensor networks

Generative learning in the unsupervised learning models the joint distribution of random variables in the given data and generates new samples from the learnt distribution. It is an important task in modern machine learning [33] and find wide applications in many areas of artificial intelligence. Fashion generative models include variational autoencoders (VAE) [34], normalizing flows [35–37], autoregressive models [38, 39] and generative adversarial networks (GANs) [40]. Here, we focus on a classical generative model known as the Boltzmann machine [41] with no hidden variables, which is also known as the inverse Ising model which is the maximum entropy model given the pairwise measurement of data. Using this example we demonstrate that our method for contracting the Ising model can be directly used for learning tasks. The objective function of the learning using an Ising model is the the negative log-likelihood $L$, which we aim to minimize:

$$L = - \frac{\log P(\mathbf{X})}{N} = - \frac{\log \prod_i P(x_i)}{N}$$

$$= - \frac{\beta}{N} \sum_{(mn) \in E} J_{mn} x_m x_n - \frac{\beta}{N} \sum_m h_m x_m + \log Z$$

(6)

In the last equation, $\mathbf{X}$ is the dataset, $x_i$ is the $i$-th data, $N$ is the size of dataset and $E$ represents edges of graphical model we employ. In classical machine learning method, the partition function $\log Z$ appearing in the log-likelihood is difficult to compute, and people usually use approximated method such as the contrastive divergence. Fortunately our method provides a relatively fast and accurate way to calculate $\log Z$. Essentially, by setting the derivative of $L$ with parameters $J_{mn}$ (couplings) and $h_m$ (external fields) to be zero, we can get

$$\beta C_{data} = \frac{\beta}{N} \sum_i x_i x_i = \beta C_{model} = \frac{\partial \log Z}{\partial J_{mn}}$$

$$\beta M_{data} = \frac{\beta}{N} \sum_i x_i = \beta M_{model} = \frac{\partial \log Z}{\partial h_m}.$$  

(7)

The model parameters \{\textit{J}_{mn}\} and \{\textit{h}_m\} can be learnt by matching the moments of the model with the moments of data. We emphasize that, here we do not even need to calculate the correlations and magnetizations, because the gradient on $J_{mn}$ and $h_m$ can be estimated directly by taking derivative of the loss function by using the back-propagation algorithm. Then the learning can be carried out by utilizing a modern deep learning optimizer such as the stochastic gradient descent (SGD) [42] and the ADAM [43] to update the parameters.

As a demonstration, we perform experiments on the handwritten digits of the MNIST dataset [44] to show how to learn an Ising model from data using our TN method combined with the back-propagation algorithm. For preparation, we reshape $28 \times 28$ binarized images to $14 \times 14$ for faster contractions. Our graphical model is based on 2D square lattice with additional diagonal connections and second nearest neighbors connections. As an demonstration, we use only first five images of MNIST as training set for learning the model.

After training through stochastic gradient descent, the Ising model displays the similar distribution as the empirical distribution of the training data, and we can generate images by sampling from the distribution that our model has learned. Here we adopt traditional Markov Chain Monte Carlo (MCMC) to sample from the model, the samples are shown in Fig. 9. We can see that the images are well presented and similar to the training images. The negative loglikelihood obtained is 2.41 which is very close to the lower bound ln 5 = 1.61.

FIG. 8. Time consumptions of the tensor network contraction algorithm in Fig. 3.
FIG. 9. MCMC samples of Ising model learnt from 5 handwritten images of the MNIST dataset.

Protocol for generating random quantum circuits

The random quantum circuits with depth $d$ used in our experiments are generated as follows:

1. Apply a Hadamard gate to each qubit.
2. Apply controlled-Z gates organized in one of the eight layouts as shown in Fig. 10 once a time alternatively, then apply a randomly chosen gate from $\{T, X^{1/2}, Y^{1/2}\}$ to each qubit which is not acted by the CZ gates.
3. Repeat steps 2 for $d - 1$ times.
4. Apply a Hadamard gate to each qubit.

FIG. 10. Choices of the two-qubit-gate layers in generating random quantum circuits.