Tropical Tensor Network for Ground States of Spin Glasses

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We present a unified exact tensor network approach to compute the ground state energy, identify the optimal configuration, and count the number of solutions for spin glasses. The method is based on tensor networks with the Tropical Algebra defined on the semiring of \((\mathbb{R} \cup \{-\infty\}, \oplus, \odot)\). Contracting the tropical tensor network gives the ground state energy; differentiating through the tensor network contraction gives the ground state configuration; mixing the tropical algebra and the usual algebra counts the ground state degeneracy. The approach brings together the concepts from graphical models, tensor networks, differentiable programming, and quantum circuit simulation, and easily utilizes computational power of graphical processing units (GPU). For applications, we compute the exact ground state energy of Ising spin glasses with random Gaussian couplings and fields on square lattice up to 1024 spins on a single GPU. Furthermore, we obtain exact ground state energy of ±J Ising spin glass on the chimera graph of D-Wave quantum annealer of 512 qubits in less than 100 seconds. Lastly, we investigate the exact value of the residual entropy of ±J spin glasses on the chimera graph which has not been reported before.

Introduction—Combinatorial optimization problems have fundamental theoretical interests in statistical physics and computer science. Efficient solutions to combinatorial optimization problems are also relevant to many practical applications such as operations research and artificial intelligence. A prototypical combinatorial optimization problem is finding the ground state of the Ising spin glass with the energy function

\[
E(\sigma) = -\sum_{i<j} J_{ij} \sigma_i \sigma_j - \sum_i h_i \sigma_i,
\]

where \(\{\sigma\} \in \{\pm1\}^N\) denotes a configuration of \(N\) Ising spins. Such problem arises in a broad contexts ranging from magnetic properties of dilute alloys \[1\] to probabilistic inference in graphical models \[2\]. Finding the ground state of the spin-glass is NP-hard except on some special graphs \[3\]. This implies that an efficient solution to the problem is unlikely unless \(P = NP\). Many NP problems have convenient Ising spin glass formulation \[4\]. In past decades, various approaches have been applied to such a problem, including the simulated annealing on classical computer \[5\] and quantum annealing on manufactured quantum devices \[6\].

Besides the ground state energy and configurations, counting the number of ground-state configuration is also of interest from physics and optimization perspective. The number of degeneracy characterizes the level of frustration and gives rise to residual entropy of the system at zero temperature \[7\]. For example, there can be an exponentially large number of degenerated ground states of the spin-glass such that the system exhibits finite entropy density in the thermodynamic limit. Unfortunately, counting the number of the degenerated ground state of spin glasses is \#P-complete \[8\] which can be even harder than finding the ground state.

In this paper, we present a unified approach to compute ground state energy, find out the ground state configuration, and count the ground state degeneracy of spin glasses exactly. The approach is based on the exact contraction of the tensor networks with tropical numbers which compute the spin-glass partition function directly in the zero-temperature limit. In principle, the approach is not conceptually new since there can be equivalent dynamic programming or message passing formulations. It is rather a synthesis of techniques in combinatorial optimization, graphical model, and machine learning into a unified framework in the language of tensor networks, which provides valuable insights for efficient and generic implementations. In particular, the tropical tensor network offers a general computational framework so that one can easily exploit software and hardware advances in quantum circuit simulation, automatic differentiation, and hardware accelerations. In this regard, the approach adds another example along the fruitful line of researches bridging the graphical models, tensor networks, and quantum circuits \[9–17\].

There were previous efforts of investigating low-temperature properties of spin-glasses using approximated tensor contraction methods \[17–19\]. Among other things, these approaches and related transfer matrix approach \[20,21\] face numerical issues at low temperatures due to the cancellation of tensor elements with exponential scales \[22\]. References \[23,24\] investigated residual entropy of infinite translational invariant frustrated classical spin systems by constructing tensor networks according to local rules of the ground state manifold. More closely related to the present paper, one can employ exact tensor network contraction to count the number of solutions in the constraint satisfaction problems \[25–28\]. However, the ground state energy of satisfaction problems is known to be zero in contrast to the optimization problems considered here, where minimal energy is difficult to determine.
**Tropical Tensor Network**— The tropical algebra is defined by replacing the usual sum and product operators for ordinary real numbers with the max and sum operations respectively \[ x \oplus y = \max(x, y), \quad x \odot y = x + y. \] (2)

One sees that \(-\infty\) acts as zero element for the tropical number since \(-\infty \oplus x = x \) and \(-\infty \odot x = -\infty\). On the other hand, \(0\) acts as the multiplicative identity since \(0 \odot x = x\). The \(\oplus\) and \(\odot\) operators still have the commutative, associative, and distributive properties. However, since there is no additive inverse, the \(\oplus\) and \(\odot\) operations define a semiring over \(\mathbb{R} \cup \{-\infty\}\). The semiring formulation unifies a large number of inference algorithms in the graphical models based on dynamic programming \([30,31]\). Recently, there have been efforts in combing the semiring algebra with modern deep learning frameworks with optimized tensor operations and automatic differentiation \([32,33]\).

One can consider tensor networks whose elements are tropical numbers with the algebra Eq. (2). Since the elementary operations involved in contracting tensor networks are just sum and product, contraction of tropical tensor networks is well defined. One can use such contraction to solve the ground state of the Ising spin glass. For example, consider the Ising spin glasses Eq. (1) defined on a two-dimensional square lattice, the tropical tensor network is shown in Fig. 1(a). The tensor network representation corresponds to the factor graph of the spin-glass graphical model \([30]\). There are \(2 \times 2\) tropical tensors \( [J_{ij} \text{ } -J_{ij}] \) reside on the bond connecting vertices \(i\) and \(j\), with the tensor elements being the negative coupling energies. The dots are diagonal tensors with \( \begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix} = h_i, \begin{bmatrix} 2 & 2 \\ -1 & -1 \end{bmatrix} = -h_i, \) and \(-\infty\) for all other tensor elements. In cases where the local field vanishes, these dots reduce to the copy tensor in terms of the tropical algebra which demands that all the legs have the same indices. Contraction of the tensor network under the tropical algebra gives the ground state energy of the Ising spin glass. In the contraction, the \(\oplus\) operation selects the optimal spin configuration, and the \(\odot\) operation sums the energy contribution from subregions of the graph. The intermediate tensors record the minimal energy given the external tensor indices, so they correspond to max-marginals in the graphical model \([34]\).

From the physics perspective, the tropical tensor network naturally arises from computing the zero temperature limit of the partition function \(Z = \sum_{\sigma} e^{-\beta E}\). The ground state energy, \(E^* = -\lim_{\beta \to \infty} \frac{1}{\beta} \ln Z = -\lim_{\beta \to \infty} \frac{1}{\beta} \ln \sum_{\sigma} \prod_{i \in J} e^{b_i \sigma_i \sigma_j}, \prod_{J} e^{b_J \sigma_i}, \) involves ordinary sum and product operations for the Boltzmann weights. When taking the zero temperature limit, it is more convenient to deal with the the exponents directly

\[
\lim_{\beta \to \infty} \frac{1}{\beta} \ln(e^{a_x} + e^{a_y}) = x \oplus y,
\quad \frac{1}{\beta} \ln(e^{a_x} \cdot e^{a_y}) = x \odot y,
\]

which leads to the tropical algebra Eq. (2). The tropical representation also corresponds to the logarithmic number system \([35]\) which avoids the numerical issue in dealing with exponentially large numbers on computers with finite precision numerics \([22]\).

Moreover, one can also employ the present approach to count the number of ground states at the same computational complexity of computing the ground state energy. To implement this, we further generalize the tensor element to be a tuple \((x, n)\) composed by a tropical number \(x\) and an ordinary number \(n\). The tropical number records the negative energy, while the ordinary number counts the number of minimal energy configurations. For tensor network contraction, we need the multiplication and addition of the tuple:

\[
(x_1, n_1) \odot (x_2, n_2) = (x_1 + x_2, n_1 \cdot n_2) \text{ and }
(x_1, n_1) \oplus (x_2, n_2) = \begin{cases} (x_1 \oplus x_2, n_1 + n_2) & \text{if } x_1 = x_2 \\ (x_1 \odot x_2, n_1) & \text{if } x_1 > x_2 \\ (x_1 \odot x_2, n_2) & \text{if } x_1 < x_2 \end{cases}
\]

Essentially, these two numbers in the tuple correspond to leading order and the \(O(1/\beta)\) contributions (energy and entropy) in the low-temperature expansion of the log-partition function. After contracting the tensor network, one reads out the ground state energy and degeneracy from the two elements of the tuple. In this way, one can count the number of optimal solutions exactly without explicitly enumerating the solutions \([36,37]\).

**Contract Tropical Tensor Networks**— We have formulated the computation of the ground state energy and the ground state degeneracy of the Ising spin glass Eq. (1) as a contraction of the tropical tensor network. On a tree graph, contraction of the tropical tensor network is equivalent to the max-sum algorithm \([2]\), i.e. the maximum of a posterior version of the sum-product (belief propagation) algorithm on graphical models. On a general graph, when the junction tree algorithm \([38]\) applies it can be treated as a special case of the tropical tensor network contraction algorithm using a specific contraction order utilizing a tree decomposition of the graph.

The contraction of a general tensor network belongs to the class of \(\#P\) hard problems \([39]\), so it is unlikely to find polynomial algorithms for exact contractions. Algorithmically, the
computational complexity of tensor network contraction is exponential to the tree-width of the network [9]. On a regular graph (e.g. 2–D lattice), one can easily find a good contraction order that has an optimal computational complexity. However on a general graph, a good contraction order is usually difficult to find, thus one usually relies on heuristic algorithms to identify a contraction order with low computational complexity. Ref. [9] proposed to use tree decomposition of the line graph of the tensor network, found by a branch and bound algorithm. This has been widely adopted in subsequent works on classical simulation of quantum circuits with tensor networks [14]–[16]. Recently, more advanced heuristic algorithms have been developed by combining graph partition algorithms and greedy algorithms [47]–[48].

In addition to a good contraction order, efficient linear algebra libraries are also important for the performance of the contractions. For ordinary contractions, the basic linear algebra subprograms (BLAS) library is a standard tool for performing efficient product and plus operations, and can fully release the computational power of specialized hardware such as graphical processing units (GPU) and tensor processing units. In the cases where the space complexity of the contraction is larger than the memory, the recently developed slicing technique [47]–[49] splits the whole task to many small sub-tasks which can be feed into GPU memory sequentially. For the tropical algebra, fortunately, basic operations can be inherited from standard linear algebra libraries as long as they are programmed in a generic manner to support ⊕ and ⊙ operators. When performing contractions on GPU, another important factor is memory efficiency, that is, all operations should be performed in-place without allocating extra memory. This actually shares the same demand as the simulation of quantum circuits. To this end, one can actually contract tropical tensor networks by repurposing software that is originally developed for quantum circuit simulations.

To sum up, the tropical tensor network formulation opens a way to leverage recent algorithmic and software advances in tensor network contraction for combinatorial optimization problems. Moreover, the tensor contraction formation fits nicely to the specialized hardware such as GPUs, where, as we reported below, one can actually employ low precision floating numbers (or even integer type for integral couplings) for better numerical performance and reduced memory usage.

**Obtaining the Ground States with Automatic Differentiation**

For many practical applications, it is important to obtain ground state configuration in addition to the optimal energy value of optimization problems. Given the way to compute the ground state energy of the spin glass, there are several ways to obtain the ground state configurations. The most straightforward way would be running the same energy minimization program repeatedly with perturbed fields. Since the ground state energy is a piecewise linear function of the fields, the numerical finite-difference of the energy with respect to fields suffices to determine the ground state configurations [52]. Alternatively, one can impose an arbitrary order of the spin variables and compute the conditional probability of a variable being in the ground state given the previous ones, then sample the ground state configurations according to the conditional probability [54]. Both methods need to re-run the contraction algorithm $O(N)$ times with the same memory cost as finding the ground state energy. One can nevertheless trade memory for computation time by caching intermediate contraction results and backtracking the computation for minimal energy configuration.

We employ the differentiable programming technique to differentiate through the tropical tensor network contraction [53]. To this end, we program the whole tensor network contraction in a differentiable way and compute the gradient of the contraction outcome with respect to the tensor elements using automatic differentiation (AD). We note that the general idea of differentiating through combinatorial optimization solver applies to cases beyond tropical tensor network contraction [54]. It is well known to the machine learning community that there is the time-memory tradeoff in different ways of performing the automatic differentiation to a computer program [55]. The forward mode automatic differentiation has the same time and memory cost as the finite difference approach. While in the other extreme limit, the reverse mode automatic differentiation displays the $O(1)$ computation overhead compared to the forward tensor contraction, and $O(N)$ memory overhead. The time versus memory tradeoff can be further controlled flexibly by using the checkpoint technique [55].

**Applications**

We first apply the tropical tensor network approach to the Ising spin glasses on $L \times L$ square lattices. For this tensor network with a regular structure in 2-D lattice structure shown in Fig. 1(a), the contraction order with an optimal computational complexity is to contract the network column by column from left to right. Interestingly, the computation is similar to evolving a quantum state under the action of local quantum gates, with the crucial difference that we are now dealing with nonunitary gates with the tropical algebra. Exploiting this intimate connection between tensor network contraction and quantum circuit simulation, we employ the quantum programming software Yao.jl [56] to contract this tropical tensor networks [57]. Notably, Yao.jl’s

![FIG. 2. Wall clock time for computing the ground state energy of the (a) Ising spin glass on an open square lattice with $L^2$ spins. (b) Wall clock time for computing the ground state configurations using forward (ForwardDiff.jl) on GPU and reverse mode (NiLang.jl) automatic differentiation on CPU respectively.](image-url)
generic programming implementation easily enables this unorthodox application without any modification or sacrificing performance.

As shown in Fig. 1(b), the tensor network is cast into the expectation of a tropical circuit on the state vector of $2^L$ dimension. We denote $\langle \psi_\text{init} | \psi_\text{f} \rangle = \langle 0 | 0 \rangle$ so that the initial and final states are both product states $\langle 0 | 0 \rangle^{\otimes L}$. The square symbols represent tropical gates, in which $\begin{pmatrix} J_{ij} \quad -J_{ij} \\ -J_{ij} \quad J_{ij} \end{pmatrix}$ and $\begin{pmatrix} h_i \quad -\infty \\ -\infty \quad -h_i \end{pmatrix}$ are single-site gates. The symbol $\begin{array}{cccc} a & b & c & d \end{array}$ denotes two site gate acting on neighboring sites. In fact, it is a diagonal tropical matrix $\text{diag}(J_{ij}, -J_{ij}, -J_{ij}, J_{ij})_{abcd}$, with the off-diagonal elements set to $-\infty$. The order of operation of these diagonal gates to the state vector can be arbitrary.

Figure 2(a) shows the wall clock time for computing the ground state energy of Ising spin glass on the chimera graph with $L \times L$ unit cells. Each spin-glass solver was carried out as evolution of a state with dimension $16^L \times 16$ tropical matrices which contain the couplings between the original Ising spins. Such a tensor network formulation makes better use of the bipartite structure of the chimera graph than simply grouping the 8 spins within the unit cell together [19]. After turning these tensors into local tropical gates, contraction of the tensor network can be carried out as evolution of a state with dimension $16^L$. As shown in Fig. 3(c) one can obtain the ground state energy of $8L^2 = 512$ Ising spin in 84 seconds on the Nvidia V100 GPU. This is much faster than the brute force enumeration using GPUs [62]. It is also slightly faster than the belief propagation exact solver running on 16 CPU cores used in Ref. [63].

![Fig. 3](image-url) A chimera lattice with $4 \times 4$ unit cells. Dots represent Ising spins and lines indicate couplings.

![Fig. 4](image-url) (a) A histogram of the ground state degeneracy of $\pm J$ spin glasses on the chimera graph with $L \times L$ unit cells. (b) The residual entropy density versus system size.

Next, we consider spin glass instances with $\pm J$ coupling and no external field on the chimera graph of the actual D-Wave device [6] shown in Fig. 5(a). The chimera graph consists of unit cells arranged in a square grid of the size of $L \times L$. Each unit cell contains 8 spins forming a complete bipartite graph. Each group of four spins within the unit cell connects horizontally or vertically to the spins in the neighboring unit cells.

We transform the chimera graph into a tensor network shown in Fig. 5(b) by exploiting its specific structure [61]. The red and blue circles are tropical copy tensors that represent a group of four Ising spins within each unit cell. The black tensor describes the intra-unit-cell couplings. While the red and blue squares denote the inter-cell interaction in the vertical and horizontal direction respectively. The reverse mode automatic differentiation is more efficient in this application than the forward model AD which has computational complexity proportional to the number of parameter $L^2$. However, the reverse mode AD requires caching intermediate states for backpropagation, which causes memory overheads. NiLang.jl provides machine instruction level automatic differentiation. One does not need to derive the forward rules manually, instead, he can just rewrite the original program in a reversible programming [69] style and the automatic differentiation just works. Reversible programming also provides a flexible tradeoff between space and time, so that we can differentiate a spin-glass solver up to $L = 28$ with an $O(L)$ space overhead (in the supplementary material). In Fig. 2(b), we show the timings up to $L = 24$.

For each system size, we solve 10000 random instances. (b) The residual entropy density versus system size.
use Int16 datatype for computational and memory efficiency, which is sufficient for such calculation since the energy has bounded integral values.

Finally, Figure 4(a) shows the histogram of the ground state degeneracy of the chimera spin glass instances. One observes that the distributions are unimodal and broaden as the system size enlarges. Figure 4(b) shows the residual entropy density $s = \mathbb{E}[\ln g]/(8L^2)$ where $g$ is the degeneracy and the expectation is over the 10000 random instances. The value of the residual entropy approaches to $s = 0.03$ for increasingly larger system sizes. As a comparison, this value of the entropy density is smaller than the one of the $\pm J$ square lattice Ising spin glass $s \approx 0.07$ [21, 64, 66], indicate a smaller number of degenerated ground state on the chimera graph compared to the $\pm J$ square lattice Ising spin glasses.

**Discussions**– An immediate implication of the present paper is that quantum circuit simulators can be repurposed to solve combinatorial optimization problems. This connection adds a profitable motivation for crafting efficient and generic quantum circuit simulators besides validating quantum devices. The tropical tensor network framework is general so it applies to other combinatorial optimization problems beyond Ising spin glasses considered here. One can either embed general combinatorial optimization problems to the Ising energy function or generalize the tropical tensors to have larger bond dimensions. Moreover, for specific problems one could apply specific bounds on the ground-state energy to enforce sparsity of the tropical tensors, this would link the tropical tensor network framework with the branch and bound methods. Moving forward, approximated contractions schemes for the tropical tensor networks may provide practical algorithms for optimization and counting of large instances.

A JULIA implementation of the tropical tensor network used in this paper is available at [67]. Thanks to generic programing, a minimalist working example contains only ~ 60 lines of code.

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Mapping a tensor network to a quantum circuit

We first introduce notations that used in representing a tropical circuit.

1. Starting/termination symbol

   \[ \langle - \rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \]  \hspace{1cm} (5)

2. Horizontal coupling gate

   \[ -[T] = \begin{pmatrix} J_{ij} & -J_{ij} \\ -J_{ij} & J_{ij} \end{pmatrix} \]  \hspace{1cm} (6)

3. Magnetic field gate

   \[ -[h] = \begin{pmatrix} h_i & -\infty \\ -\infty & -h_i \end{pmatrix} \]  \hspace{1cm} (7)

4. Vertical coupling gate

   \[ \begin{pmatrix} J_{ij} & -\infty & -\infty & -\infty \\ -\infty & J_{ij} & -\infty & -\infty \\ -\infty & -\infty & -\infty & -\infty \\ -\infty & -\infty & -\infty & J_{ij} \end{pmatrix} \]  \hspace{1cm} (8)

5. Copy gate

   \[ \begin{pmatrix} 0 & -\infty & -\infty & -\infty \\ -\infty & 0 & -\infty & -\infty \\ -\infty & -\infty & 0 & -\infty \\ -\infty & -\infty & -\infty & 0 \end{pmatrix} \]  \hspace{1cm} (9)

6. Cut gate

   \[ \langle \rangle = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \]  \hspace{1cm} (10)

The copy gate and cut gate are useful in mapping a general tropical tensor network to the circuit model. As an example, in Fig. 5(a), in order to arrange gates in a specific time order, we introduce an extra ancilla qubit \( 2' \) as show in (b). One can use the copy gate to store the information in qubit \( 2 \) into the ancilla qubits \( 2' \). At the end of an operation, we use the cut gate to restore the state of the ancilla qubit.

Reversible programming approach to compute gradients

It is a challenge to differentiate a generic quantum simulator with tropical numbers inside. We need to derive the backward rules for tropical quantum circuits simulation. Unlike a traditional quantum simulation program, one cannot trace back the intermediate states by applying the adjoint of gates to save memory [56].

Instead of deriving the backward rule manually, we differentiate the source codes by writing it in a reversible programming manner [51]. Due to the overhead of reversible programming, the memory usage of our reversible implementation is \( 2L \) times the original program, while the computational time is also several times slower. This overhead is acceptable in differential programming since it is comparable to the theoretical optimal of the checkpointing scheme in traditional machine learning. In Fig. 6 we illustrate the compute-copy-uncompute scheme in reversible programming. Figure 6(a) is the naive approach that caches all intermediate states in a global stack with a negligible computational time overhead. It uses approximately \( L^2 \) times more memory than the original program. Since the spin-glass solver is memory critical, a better approach is to uncompute some of the intermediate results as shown in Fig. 6(b). In Fig. 6(b), we use two stacks. A stack is a dynamic one that uncomputed in each sweep of a column. B stack is a global one, that only uncomputed when running the program backward. Both A and B are \( L \) times the size of a state vector, hence the memory overhead is \( 2L \) and the computational time overhead is \( \sim 2 \).

Although with non-negligible overhead, the reversible programming approach is still much more efficient than the for-
ward mode AD since the computational overhead of forward-mode AD is proportional to the number of parameters $L^2$. In the benchmark shown in the main text, even single thread reversible programming AD is faster than forward-mode AD on GPU by a factor of $\sim 6$. In Fig. 7, we show the optimal configuration of Ising spin-glass models on a $28 \times 28$ square lattice and a $7 \times 7$ chimera lattice.