Second Renormalization of Tensor-Network States

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We propose a second renormalization group method to handle the tensor-network states or models. This method reduces dramatically the truncation error of the tensor renormalization group. It allows physical quantities of classical tensor-network models or tensor-network ground states of quantum systems to be accurately and efficiently determined.

One of the biggest challenges in physics is to develop accurate and efficient methods that can solve many currently intractable problems in correlated quantum or statistical systems. While the density matrix renormalization group (DMRG) has proven to be a powerful numerical tool for the study of strongly correlated systems in one dimension, applications to two or higher dimensions are hampered by accuracy. Quantum Monte Carlo simulations, on the other hand, are not limited by the dimensionality, but are hamstrung by the minus sign problem for fermionic or frustrated spin systems. To resolve these difficulties, increasing interest has recently been devoted to the study of the tensor-network states or models\textsuperscript{1, 2, 3, 4, 5}. In statistical physics, all classical lattice models with local interactions, such as the Ising model, can be written as tensor-network models. To investigate these tensor-network models, Levin and Nave proposed a tensor renormalization group (TRG) method\textsuperscript{3}. They showed that the magnetization obtained with this method for the Ising model on triangular lattice agrees accurately with the exact result.

In a quantum system, a tensor-network state\textsuperscript{1, 2} presents a higher-dimensional extension of the one-dimensional matrix-product state\textsuperscript{6} in the study of DMRG\textsuperscript{7}. It captures accurately the nature of short-range entanglement of a quantum system and is believed to be a good approximation of the ground state. In a recent work, we have developed a projection method to determine accurately and systematically the tensor-network ground state wavefunction for an interacting quantum Hamiltonian\textsuperscript{1}. In the evaluation of its expectation values, we adopted the TRG method of Levin and Nave\textsuperscript{3}. From the calculation, we found that the TRG can indeed produce qualitatively correct results. However, the truncation error in the TRG iteration grows rapidly with the bond dimension of local tensors (\(D\)). This leads to a big error in the calculation of expectation values. In particular, the ground state energy and other physical quantities oscillate strongly with increasing \(D\), indicating that the truncation error of the TRG is too big to produce a converging result in the large \(D\) limit.

In this Letter, we propose a novel renormalization group scheme to solve the above problem. In the TRG method of Levin and Nave, the singular-value spectra of an \(M\)-matrix defined by a product of two neighboring local tensors is renormalized in the truncation of basis space. This can be thought as the first renormalization to the tensor-network state. However, this renormalization does not consider the influence of other tensors (denoted as the environment hereafter) to the \(M\)-matrix. It presents a local rather than global optimization of the truncation space. The role of environment is to modify the truncation space by reweighing the singular-value spectra of \(M\). We will introduce a systematical method to study this renormalization effect of environment. This method, as will be demonstrated below, improves significantly the accuracy of results. We will call it the second renormalization group method of tensor-network states, abbreviated as SRG.

To understand how our method works, let us first consider how the tensor-network state is renormalized in the TRG\textsuperscript{3}. We start with a classical tensor-network model on honeycomb lattices whose partition function is defined by

\[
Z = \text{Tr} \prod_{i \in b, j \in w} T^a_{x_i, y_i, z_i} T^b_{x_j, y_j, z_j},
\]

where \('b/w'\) stands for the black/white sublattice shown in Fig. 1. \(T^a_{x_i, y_i, z_i}\) and \(T^b_{x_j, y_j, z_j}\) are the two tensors of rank three defined on the black and white sublattices, respec-
where $N = D^2$. The singular value decomposition is then applied to decouple this matrix into the following form

$$M_{ij,kl} = \sum_{m} T_{mj,k}^{a} T_{ml,i}^{b}, \quad \text{(2)}$$

where $U$ and $V$ are two $N \times N$ unitary matrices. $\Lambda = (\Lambda_1, \cdots, \Lambda_N)$ is a semi-positive diagonal matrix arranged in descending order, $\Lambda_1 \geq \Lambda_2 \geq \cdots \geq \Lambda_N$.

The next step is to truncate the basis space and retain $D_{\text{cut}} (\leq N)$ largest singular values and the corresponding vectors. $M$ is then replaced by an approximate expression

$$M_{ij,kl} \approx \sum_{m=1}^{D_{\text{cut}}} U_{ij,m} \Lambda_{m} V_{kl,m}, \quad \text{(3)}$$

The corresponding truncation error is defined by

$$\varepsilon(\Lambda) = \frac{\sum_{m>D_{\text{cut}}} \Lambda_{m}}{\text{Tr}\Lambda}. \quad \text{(4)}$$

Eq. (4) minimizes the truncation error of $M$. However, it does not consider the influence of the rest of lattice (i.e. environment) to $M$. In real systems, what needs to be minimized is acturally the truncation error of the partition function $Z$. This means that the truncation error is only locally minimized by the TRG. For the spin-1/2 Ising model with $D = 2$, the truncation error is generally very small except in the vicinity of the critical point. However, if the bond degrees of freedom $D$ becomes large, the truncation error increases dramatically. This may cause a big error in the final result.

**FIG. 2:** (a) To form the $M$ matrix by tracing out the common bond indices of tensors $T^{a}$ and $T^{b}$. (b) To perform the singular value decomposition defined by Eq. (3).

The TRG starts by rewiring a pair of tensors with singular value decomposition as shown in Fig. 2. To do this, let us contract a pair of neighboring tensors to form a $N \times N$ matrix $M$ defined by

$$M_{ij,kl} = \sum_{m} T_{mj,k}^{a} T_{ml,i}^{b}, \quad \text{(2)}$$

where $N = D^2$. The singular value decomposition is then applied to decouple this matrix into the following form

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The next step is to truncate the basis space and retain $D_{\text{cut}} (\leq N)$ largest singular values and the corresponding vectors. $M$ is then replaced by an approximate expression

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Eq. (4) minimizes the truncation error of $M$. However, it does not consider the influence of the rest of lattice (i.e. environment) to $M$. In real systems, what needs to be minimized is acturally the truncation error of the partition function $Z$. This means that the truncation error is only locally minimized by the TRG. For the spin-1/2 Ising model with $D = 2$, the truncation error is generally very small except in the vicinity of the critical point. However, if the bond degrees of freedom $D$ becomes large, the truncation error increases dramatically. This may cause a big error in the final result.

**FIG. 3:** Configuration of an environment lattice (a) and that after one TRG iteration (b).

To understand this more clearly, let us rewrite the partition function (1) as

$$Z = \text{Tr} M M^{e} = \sum_{ij,kl} M_{ij,kl} M_{kl,ij}^{e}, \quad \text{(6)}$$

where $M^{e}$ is the contribution from the environment lattice defined in Fig. 3. $M^{e}$ is defined by tracing out all bond indices in the environment lattice excluding those connecting with the two vertices on which $M$ is defined. This formula indicates that to reduce the error in $Z$, one needs to minimize the truncation error of $M M^{e}$, rather than that of $M$.

**FIG. 3:** Configuration of an environment lattice (a) and that after one TRG iteration (b).

In the minimization of the truncation error of $M M^{e}$, it is better to treat the row $ij$ and column $kl$ indices of $M$ as symmetrically as possible. To do this, let us first...
Again, and show that semi-positive diagonal matrix. Then we can define a new
Thus to minimize the error in $Z$ are arranged in descending order. Then we can truncate positive diagonal matrix whose diagonal matrix elements do a singular value decomposition for $M^c$

$$M^c = U_c \Lambda_c V_c^\dagger,$$

where $U_c$ and $V_c$ are two unitary matrices and $\Lambda_c$ is a semi-positive diagonal matrix. Then we can define a new matrix

$$\tilde{M} = \Lambda^{-1/2}_c V^\dagger_c M U_c \Lambda^{-1/2}_c,$$

and show that

$$Z = \text{Tr} \tilde{M}.$$

Thus to minimize the error in $Z$, one needs only to minimize the truncation error of $\tilde{M}$. 

Now let us take a singular value decomposition for $\tilde{M}$

$$\tilde{M} = \tilde{U} \tilde{\Lambda} \tilde{V}^\dagger.$$

Again, $\tilde{U}$ and $\tilde{V}$ are two unitary matrices. $\tilde{\Lambda}$ is a semi-positive diagonal matrix whose diagonal matrix elements are arranged in descending order. Then we can truncate the basis space by keeping the $D_{\text{cut}}$ largest singular values of $\tilde{\Lambda}$. By substituting the approximate $\tilde{M}$ back into Eq. (8), one can find that

$$M_{ij,kl} \approx \sum_{n=1}^{D_{\text{cut}}} S^a_{n,ij} S^b_{n,kl},$$

where

$$S^a = \tilde{\Lambda}^{1/2} \tilde{U}^\dagger \Lambda^{-1/2}_c V^\dagger_c,$$

$$S^b = \tilde{\Lambda}^{1/2} \tilde{V}^\dagger \Lambda^{-1/2}_c U^\dagger_c$$

are the two tensors defined in the rewired lattice. Finally one can follow the steps introduced in Ref. [3] to update tensors $T^a$ and $T^b$ in a squeezed lattice by taking the coarse grain decimation of $S^a$ and $S^b$. This completes a full cycle of SRG iteration. By repeating this procedure, one can finally obtain the value of partition function in the thermodynamic limit.

We have applied this SRG method to the spin-1/2 Ising model on triangular lattices, Fig. [4] compares the relative error of the free energy and the specific heat (lower panel) as functions of temperature for the Ising model on triangular lattices obtained using TRG (red) and SRG. $f_{\text{ex}}(T)$ is the exact result calculated using the formula given in Ref. [8]. The dotted line in the Inset is the specific heat (lower panel) as functions of temperature for the Ising model on triangular lattices obtained using TRG (red) and SRG. $f_{\text{ex}}(T)$ is the exact result calculated using the formula given in Ref. [8]. The dotted line in the Inset is the critical temperatures $T_c = 4/\ln 3$.
The number of lattice sites is $2 \times 3^{15}$. The truncation error in the SRG calculation is less than $\varepsilon_0 \sim 10^{-3}$ and $D_{\text{cut}} = D^2$. We have used the second order Trotter-Suzuki decomposition formula to improve the accuracy in the calculation of the ground state wavefunctions using the projection approach introduced in Ref. [4]. The staggered magnetization is evaluated directly from the wavefunction. For $D = 8$, the SRG results of the ground energy and the staggered magnetization per site are respectively -0.5445 and 0.2142, consistent with the results obtained by other methods [10, 11, 12]. The accuracy of these results are still not comparable with those obtained by the DMRG [13] and the quantum Monte Carlo method [14]. By considering the symmetry of the Hamiltonian, the tensor-network states with a bond dimension as large as $D \sim 20$ can in principle be handled. In that case, the SRG results will be further improved.

In conclusion, we have introduced a SRG method to improve significantly the accuracy in the TRG calculation. This method differs from the TRG by taking into account the renormalization effect of environment to the $M$-matrix, similar as the DMRG contrasting the conventional block renormalization group method. For the classical Ising model, the relative error of the free energy as well as other quantities is reduced by more than two to five orders of magnitude when $D_{\text{cut}} = 24$ and can be further reduced by increasing $D_{\text{cut}}$, in comparison with the TRG. The SRG, in combined with the projection method introduced in Ref. [4], provides an accurate and efficient tool for exploring tensor-network ground states of quantum lattice models. It will play a more and more important role in the study of highly correlated systems. The physical idea present in this work can be also generalized to apply to other physical problems where the system can be divided into two parts and the interplay between them is important. In particular, if one wants to generalize the projection method proposed in Ref. [4] to evaluate time-dependent or thermodynamic quantities, then the SRG correction to the wavefunction should be considered to minimize the accumulated Trotter and truncation errors in the iteration.

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