Tensor Renormalization Group with Randomized Singular Value Decomposition

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An algorithm of the tensor renormalization group is proposed based on a randomized algorithm for singular value decomposition. Our algorithm is applicable to a broad range of two-dimensional classical models. In the case of a square lattice, its computational complexity and memory usage are proportional to the fifth and the third power of the bond dimension, respectively, whereas those of the conventional implementation are of the sixth and the fourth power. The oversampling parameter larger than the bond dimension is sufficient to reproduce the same result as full singular value decomposition even at the critical point of the two-dimensional Ising model.

I. INTRODUCTION

Tensor networks are becoming powerful tools in the study of strongly correlated condensed matter physics [1 2]. A classical example is the density matrix renormalization group [3 4], which can be viewed as a variational method based on a one-dimensional tensor network, i.e., the matrix product state. Its higher-dimensional generalization, such as the projected entangled pair state (PEPS) [5] and projected entangled simplex state (PESS) [6], is quite successful. In classical systems, the partition functions can be expressed as tensor networks [8 9], so that the physical properties of the systems can be obtained by the contraction of tensor networks.

One of the main goals of developing tensor network algorithms is to find efficient and accurate methods for contracting tensor networks. Real-space renormalization by coarse-graining tensor networks, including the tensor renormalization group (TRG) [10] method and its derivatives [9 11 15], is an efficient numerical method for the contraction of tensor networks. However these methods require huge computational time and memory usage even though they are polynomially proportional to the system size. Thus complexity reduction without loss of accuracy is desired.

Decomposition and contraction are major parts of most tensor network methods. The former splits a tensor into two tensors. In general, exact decomposition requires a huge computational cost and memory because of the large bond dimension between the two tensors. To avoid this problem, an approximation based on singular value decomposition (SVD) is often used. One can keep the bond dimension finite by truncating small singular values. Therefore, what is really necessary in most cases is a partial SVD, rather than a full SVD. Actually, however, truncation after a full SVD is a frequently used procedure, despite it having a different (worse) computational complexity than the partial SVD. This is partially due to the lack of efficient and easy-to-use libraries supporting partial SVD on the latest parallel machines.

One of the partial SVD algorithms is the Arnoldi method, which is an iterative algorithm based on the Krylov subspace [16]. To create the Krylov subspace, this method iterates matrix-vector products. However, a matrix-vector product is generally less efficient than a matrix-matrix product because the memory band-width becomes narrow on the latest massively parallel machines.

Recently, a partial SVD algorithm based on the low-rank approximation using a randomized algorithm was proposed, which was called randomized singular value decomposition (RSVD) [17]. To obtain a projector to the subspace spanned by singular vectors corresponding to leading singular values, a random matrix is multiplied to a target matrix to be decomposed. The computational efficiency of matrix-matrix products is the advantage of RSVD over the Arnoldi method, although their computational costs are of the same order. In Refs. [18 19], the RSVD was applied to the time-evolving block-decimation (TEBD) [20 21] method based on a matrix product state, which is a one-dimensional tensor network, and its speed-up compared with full SVD was confirmed. However, this method does not reduce computational complexity with respect to the matrix size.

In this paper, we apply RSVD to a two-dimensional tensor network and investigate its efficiency and accuracy. Especially, we focus on the TRG method [10], one of the simplest real-space renormalization schemes, and propose a scheme of TRG using RSVD. Its computational complexity scales as \( O(\chi^5) \) with the bond dimension \( \chi \), while the original TRG method is \( O(\chi^6) \). Although using the partial SVD is vital in reducing the order of the complexity, SVD is not the only part that yields the \( \chi^6 \) dependence. Therefore, as we discuss below, we need an alternative scheme for the whole procedure of TRG to reduce the order. Its memory usage is also reduced from \( O(\chi^4) \) to \( O(\chi^3) \).

This paper is organized as follows. In the next section, we propose our scheme of TRG with RSVD. We also briefly review the original TRG method and the RSVD.
algorithm. In the third section, we report benchmark results of our method on the two-dimensional Ising model. We show the scaling of computational time and dependence of its accuracy on the oversampling parameter for RSVD. The performance of the power iteration scheme is also investigated. The last section is devoted to the summary.

II. ALGORITHMS

A. Tensor Renormalization Group

First, we review the TRG method for a translation invariant tensor network on a square lattice. Let us consider that the local tensors $T^{(0)}_i$ are located on each lattice site. A contraction of all local tensors gives the partition function as

$$Z = \text{Tr} \prod_i T^{(0)}_{x,y,z',y'}. \tag{1}$$

where $i$ runs over all lattice sites, and the operation Tr is to sum over all the tensor indices. By redefining a lattice site, adding auxiliary degrees of freedom, and/or taking a local summation, various short-range interaction models on a two-dimensional periodic lattice can be cast into a nearest-neighbor-interaction model on a square lattice, for which the tensor can be expressed, in general, as

$$T^{(0)}_{x,y,z',y'} = \sum_s W_{sx} W_{syy} W^*_{sx}, \tag{2}$$

where $W$ is the square root of the local Boltzmann factor,

$$\sum_x W_{sx} W^{*}_{s',x} = \exp (-\beta h_{s,s'}). \tag{3}$$

Here, $\beta = 1/T$ is the inverse temperature and $h_{s,s'}$ denotes the local Hamiltonian. Classical models with continuous degrees of freedom can also be represented as a finite-dimension tensor network with high accuracy [22].

The TRG method consists of two key steps, decomposition and contraction. In the first step of TRG, the local tensor is approximated by the product of two third-order tensors in two ways, as shown in Fig. 1(a),

$$T^{(n)}_{x,y,z',y'} \simeq \sum_{i=1}^{\chi} S^{[3]}_{x,y,i} S^{[1]}_{y,i}, \tag{4}$$

$$T^{(n)}_{x,y,z',y'} \simeq \sum_{i=1}^{\chi} S^{[2]}_{x,y',i} S^{[4]}_{y',i}, \tag{5}$$

where $\chi$ denotes the maximum bond dimension which determines the accuracy of the algorithm. The truncation based on the singular value decomposition, $T_{x,y,z',y'} = \sum_i s_i U_{xy,i} V^*_{x',y',i}$ provides minimum error defined by the Frobenius norm. We assume that the singular values $s_i$

satisfy $s_1 \geq s_2 \geq \cdots$. The decomposed tensors $S^{[1]}$ and $S^{[3]}$ are calculated as

$$S^{[3]}_{x,y,i} = \sum_{x=1}^{\chi} \sqrt{s_i} U_{xy,i} \tag{6}$$

$$S^{[1]}_{y,i} = \sum_{y=1}^{\chi} \sqrt{s_i} V^*_{x,y',i}. \tag{7}$$

The other tensors, $S^{[2]}$ and $S^{[4]}$, are obtained by SVD of a matrix $T_{x,y',x,y} = T_{x,y,x,y'}$. In the second step, we calculate the renormalized tensor by the contraction of four third-order tensors, as shown in Fig. 1(b),

$$T^{(n+1)}_{x,y,z',y'} \simeq \sum_{x,y,z',y'} S^{[1]}_{x,y,1} S^{[2]}_{x,y',1} S^{[3]}_{x,y,i} S^{[4]}_{y',i}. \tag{8}$$

The resulting tensor network tilts by 45 degrees and the lattice spacing increases by a factor of $\sqrt{2}$.

The computational cost to obtain all the singular values and vectors scales as $O(\chi^6)$, while the partial SVD takes $O(\chi^5)$ cost. We note that the computational cost of contraction in Eq. (8) also scales as $O(\chi^6)$. Thus, we need to reduce both the computational costs of tensor decomposition and construction. The memory usage of the original TRG algorithm scales as $O(\chi^4)$.

B. Randomized algorithm for SVD

In this subsection, we briefly review the randomized algorithm for singular value decomposition (RSVD) [17]. Let us consider an $m \times n$ matrix $A$ to be decomposed. The goal is to obtain the leading $k$ singular values and corresponding singular vectors of $A$.

The first stage of RSVD is to obtain the low-rank approximation of $A$ as

$$A \simeq QQ^\dagger A. \tag{9}$$

Here the basis matrix $Q$ is an $m \times (k + p)$ matrix whose columns are orthogonal, i.e. $Q^\dagger Q$ is the identity matrix.
We introduce the oversampling parameter $p$ which determines the accuracy of RSVD. The optimal solution of $Q$ that minimizes the Frobenius distance $\|A - QQ^\dagger A\|$ is given by the matrix whose columns are the left singular vectors corresponding to the leading $(k + p)$ singular values.

To obtain the basis matrix $Q$, we use an $n \times (k + p)$ random matrix $\Omega$. Reorthogonalization of an $m \times (k + p)$ matrix $Y \equiv AQ$ by QR decomposition ($Y = QR$) or the Schmidt orthogonalization provides the matrix $Q$. The columns of a random matrix $\Omega$ will be linearly independent with high probability. If the rank of $A$ is $(k + p)$, the columns of $Y$ will span the image of the linear transformation induced by $A$. Thus, the reorthogonalization of $Y$ produces the orthogonal basis for the image of $A$.

In this paper, we use the standard Gaussian matrix as $\Omega$, whose components are independently drawn from the normal distribution. However, a choice of the random distribution is not essential for the accuracy of RSVD. We confirmed that the uniform distribution produced almost the same results as the Gaussian distribution. Note that the elements of $\Omega$ could be complex when the elements of $\Omega$ could be complex when the columns of a random matrix $\Omega$ will be linearly independent with high probability.

In the second stage of RSVD, we form the $(k + p) \times n$ matrix $B = Q^\dagger A$ and compute the full SVD of $B$. By dropping smaller singular values, we obtain $B \simeq U\Sigma^\\dagger V^\dagger$, where $U$ and $V$ are $(k + p) \times k$ and $n \times k$ matrices with orthonormal columns, respectively. The $k \times k$ diagonal matrix $\Sigma$ holds the largest $k$ singular values of $B$. The columns of matrix $V$ approximate the right singular vectors of $A$. Finally, we form the $m \times k$ matrix $U = Q\hat{U}$ with the left singular vectors of $A$.

The upper bound of expectation error of the low-rank approximation Eq. (9) is estimated analytically as

$$\langle \|A - QQ^\dagger A\| \rangle \leq \left(1 + \frac{k}{p - 1}\right)^{1/2}\left(\sum_{j>k} s_j^2\right)^{1/2},$$

where the angle brackets stand for expectation with respect to the Gaussian test matrix $\Omega$ [12]. The optimal solution of the $k$-rank approximation obtained by SVD has the minimum Frobenius-norm error $(\sum_{j>k} s_j^2)^{1/2}$. If the singular values decay exponentially or faster as a function of the index, the randomized algorithm provides accurate decomposition with small $p$ and its error is of order $s_{k+1}$.

The power iteration scheme improves the accuracy of low-rank approximation (9), in which $Y = A\Omega$ is replaced into $Y_{2q+1} = (AA^\dagger)^q A\Omega$ or $Y_{2q} = (AA^\dagger)^q \Omega'$. Here, $\Omega'$ is an $m \times (k + p)$ random matrix. Clearly, the upper bound of expectation error for $Y$, is proportional to $(\sum_{j>k} s_j^2)^{1/2}$. Thus the power iteration reduces the approximation error exponentially with the power $r$ while the computational cost is proportional to $r$. The following algorithm, which is algebraically equivalent to the power iteration, is useful in practice to reduce the rounding error in floating-point arithmetic. First, form $Y_1 = A\Omega$ and compute its QR decomposition $Y_1 = Q_1R_1$.

Next, repeat $2q$ times the matrix-matrix products and the QR decompositions,

$Y_{2j} = A^\dagger Q_{2j-1} = Q_{2j}R_{2j}$

$Y_{2j+1} = AQ_{2j}^\dagger = Q_{2j+1}R_{2j+1}$.

The resulting basis matrix $Q_{2q+1}$ is the same as the QR decomposition of $Y_{2q+1}$. In the case of $r = 2q$, we start from the QR decomposition of $A\Omega'$.

In the case of $(k + p) < m, n$, the computational cost of RSVD is $O(mn(k + p))$ which comes from the matrix-matrix products $A\Omega$ and $Q'A$. The QR decomposition of $Y$ and the full SVD of the matrix $B$ have a smaller cost than either one of the matrix multiplications. If the oversampling parameter $p$ is less than $O(k)$, the cost of RSVD is $O(mnk)$, which is the same as that of the Arnoldi method. The advantage of RSVD over the Arnoldi method is that a matrix-matrix product is much more efficient than a matrix-vector product because the performance of a matrix-vector product is often limited by the memory bandwidth.

In the TRG algorithm on the square lattice, the local tensor $T$ is transformed into a $\chi^2 \times \chi^2$ matrix and truncated by keeping leading $\chi$ singular values, i.e., $m = n = \chi^2$ and $k = \chi$. Therefore, the computational cost of tensor decomposition with RSVD is $O(\chi^3)$ if the oversampling parameter $p$ is at most of order $\chi$. If we utilize the power iteration scheme, the order of the computational cost increases only by a factor $r$.

C. $O(\chi^3)$ algorithm of TRG

While the cost of tensor decomposition is reduced to $O(\chi^3)$ by using partial SVD, the total cost of TRG is still $O(\chi^6)$ owing to tensor contraction in Eq. (5). The present section shows that we can reduce the total cost down to $O(\chi^5)$ by working directly with the four third-order tensors $S^{[i]}$ without actually computing the fourth-order tensor $T$. In other words, the iterative SVD techniques such as RSVD make it possible to skip the intermediate step of computing $T$ in the chain of deformation as shown Fig. 2. The key observation is that in the procedure in RSVD described in the previous section, we actually do not need the matrix elements as long as we can compute the results of the matrix operation on an arbitrary vector or matrix. In the present case, we can operate the four $S$ tensors one-by-one on a given tensor to obtain the same result as operating $T$ on it. Therefore, we do not need the explicit form of the tensor $T$. Moreover, our improved algorithm reduces the memory usage from $O(\chi^4)$ to $O(\chi^3)$.

The graphic representation of the improved TRG algorithm is shown in Fig. 3. The solid bonds have dimension $\chi$, while the double lines have dimension $\chi + p$ for the oversampling of RSVD. This figure shows how to generate $S^{[1]}_{\text{new}}$ and $S^{[3]}_{\text{new}}$ from four tensors $\{S^{[i]}\}$. The other tensors $S^{[2]}_{\text{new}}$ and $S^{[4]}_{\text{new}}$ can be obtained by connecting
Then the summations over the blocks are postponed after computational cost \( \propto \chi^5 \). For example, the computational cost of contraction of five third-order tensors is of order \( \chi^6 \) as long as the oversampling parameter \( p \) is less than or scaled as \( \chi \). As we mentioned, the cost of contraction of the tensor network without \( \Omega \) and \( Q \) is \( O(\chi^6) \). The order of contractions is important to reduce the computational cost. For example, the computational cost of \( Y = S^{[1]}(S^{[2]}(S^{[3]}(S^{[4]}\Omega))) \) scales as \( O(\chi^5) \), but \( Y = ((S^{[1]}S^{[2]}S^{[3]}S^{[4]}\Omega) \) scales as \( O(\chi^6) \).

We also note that the loop blocking technique helps reduce the memory usage of contractions. Some summation loops of indices are partitioned into small blocks and then the summations over the blocks are postponed after the other contractions. In the case of Figs. 3(a) and 3(b), memory usage is reduced to \( O(\chi^3) \) by applying this technique to the index between \( S^{[1]} \) and \( S^{[4]} \) (see the details in the Appendix). We emphasize that this technique always reduces the memory usage of intermediate tensors to at most the same order of the initial and final tensor networks.

The power iteration scheme of RSVD is applicable to this algorithm within the same order of computational cost and memory usage. We can use the similar diagrams of Fig. 3. For example, the QR decomposition of \( B (= Y_2) \) instead of SVD yields the third-order tensor \( Q_2 \) and the contraction of Fig. 3(a) by replacing \( \Omega \) by \( Q_2 \) provides the third-order tensor corresponding to \( Y_3 \).

### III. Numerical Results

To investigate the effect of randomness in RSVD and performance of the improved TRG algorithm, we calculate the free energy of the Ising model on the square lattice. The initial tensor Eq. (2) for an Ising model without an external magnetic field is given with a \( 2 \times 2 \) matrix,

\[
W \equiv \left( \frac{\sqrt{\cosh \beta J}}{\sqrt{\cosh \beta J} - \sqrt{\sinh \beta J}} \right). \tag{11}
\]

The critical temperature of this model is given by \( \beta_c J = \log(\sqrt{2} + 1)/2 \).

The relative errors of the free energy from the Onsager’s solution \( f_{\text{exact}} \) at the critical temperature in the thermodynamic limit are plotted against the oversampling parameter in Fig. 4. We iterated at least 36 TRG steps where the renormalized tensor \( T^{(36)} \) contains \( 2^{36} \).
spins. This TRG step suffices for convergence of the free energy to the thermodynamic limit at the critical temperature. The error bars denote standard deviations estimated by more than 16 independent runs. The horizontal dashed lines indicate results of the original algorithm using full SVD. As expected, the improved TRG algorithm with a larger oversampling parameter \( p \) shows a smaller error and converges toward the full SVD result. Even at the critical temperature, \( p \approx \chi \) is sufficient to provide the same results as full SVD independently of \( \chi \). In the system away from the critical temperature, much smaller \( p \) is sufficient because of the rapid decay of the singular values. The standard deviation of free energy decreases with the oversampling parameter because of the law of large numbers.

The accuracy of the power iteration scheme is shown in Fig. 5. We found that the difference in the free energy from the full SVD result exponentially decreases with the oversampling parameter \( p \) and the decay constant is proportional to the number of power iterations \( r \),

\[
|f - f_{\text{full}}| \propto e^{-\kappa r p / \chi},
\]

This fact involves the upper bound of the error of the power iteration scheme as mentioned before. We estimated the coefficient \( c = 3.60 \) at the critical temperature with \( \chi = 128 \). The value of \( c \) is nearly independent of the bond dimension. Since the power iteration scheme enhances the decay of the singular values, a smaller value of the oversampling parameter is sufficient for larger \( r \).

For \( r = 2 \), \( p \approx \chi / 8 \) achieves an accuracy comparable with \( p = \chi \) without the power iteration. For \( r = 3 \), even \( p = 0 \) is sufficient. From a viewpoint of time to solution, however, the improved algorithm without the power iteration is superior to the others. For example, in the case of \( \chi = 128 \), the elapsed time per TRG step with \((r, p) = (1, 128), (2, 16), \) and \((3, 0)\) is 85.2(1), 94.3(2), and 124.9(2) s, respectively.

The elapsed time per TRG step against bond dimension \( \chi \) is plotted in Fig. 6. Here, we set the oversampling parameter of RSVR as \( p = \chi \) and do not use the power iteration scheme of RSVR \((r = 1)\). The improved algorithm clearly follows \( \chi^5 \) scaling, while the original one with full SVD scales as \( O(\chi^6) \). We achieved \( \chi = 512 \) in the improved algorithm with the aid of the loop blocking technique. Although the most time-consuming part in the original algorithm is full SVD, the contraction in Eq. (8) also scales as \( O(\chi^6) \), as shown in Fig. 6. Thus, to achieve the \( \chi^5 \) scaling, the replacement of full SVD with partial SVD is insufficient and one needs to remove explicit construction of the fourth-order tensor. To compare the RSVR approach with other partial SVD methods with \( \chi^5 \) scaling, we consider the Arnoldi method. It can solve an SVD problem without explicit matrix or tensor construction and we confirm that TRG with the Arnoldi method also shows \( \chi^5 \) scaling. However we observe that the RSVR approach is around two times faster than TRG with the Arnoldi method which takes 164.7(4) s per TRG step for \( \chi = 128 \).

We note that computational times were measured by simulations in a single core on Intel Xeon E5-2697A (2.60 GHz) with 128 GB memory. We implemented the proposed TRG algorithm and original one by using the script...
language Python. We used NumPy and SciPy \cite{24,25}, the fundamental packages for scientific computing with Python, for numerical linear algebra. These packages call LAPACK routines \cite{26} for full SVD and QR decomposition. To compare with the present method based on RSVD, we also used a partial SVD solver in the sparse linear algebra module in SciPy, which is based on the implicitly restarted Arnoldi method through ARPACK \cite{27}.

IV. CONCLUSIONS

In summary, we proposed a scheme of the TRG algorithm with $O(\chi^5)$ computational cost. By using RSVD, we can avoid creating the fourth-order tensor. Numerical results on the two-dimensional Ising model clearly show the $\chi^5$ scaling of computational time. Our method is 100 times faster than the conventional method with full SVD for $\chi = 128$. In addition, the memory usage scales as $O(\chi^3)$ by using the loop-blocking technique.

The heaviest part in the RSVD algorithm is the matrix-matrix product. The number of floating-point operations per memory access (flops per byte, F/B) in the matrix-matrix product is proportional to the linear size of the matrices. On the other hand, the one for the matrix-vector product is of order unity. Since a narrow memory bandwidth tends to be a bottleneck in current massively parallel machines, a larger F/B is preferable. Moreover, the matrix-matrix product can be accelerated by general-purpose computing on graphics processing units and well parallelized on distributed memory. Therefore, RSVD is expected to be more efficient for a large matrix than the Krylov subspace methods including the Arnoldi method.

Tensor decomposition by SVD commonly appears in other tensor network methods and a tensor version of low-rank approximation Eq. \ref{eq:low-rank} is also a general and important technique. Although we applied RSVD only to the TRG method in this paper, it is straightforward to use randomized algorithms instead of conventional ones. Thus, we believe that randomized algorithms would be useful to reduce computational time and memory usage in many SVD-based tensor network methods.

In the present paper, we have proposed improvements on the tensor network computation by transforming the standard “contraction and decomposition” procedure into multiplication among smaller tensors. Here we emphasize that the proposed method reduced the computational complexity of the whole procedure of the TRG method including not only the SVD part but also the contraction. Since these two components dominate the computational time of most tensor network schemes, the techniques presented in this paper would be useful in improving most of the tensor network calculations in an essential way.

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Appendix: Loop blocking technique

The memory usage of contracting tensor networks can be reduced down to the same order as the largest among the order of initial and final tensors by using the loop blocking technique. For example, let us consider the contraction of Fig. 3(a),

$$Y_{x'y'} = \sum_{x_1 y_1 x_2 y_2} S_{x_1 y_1 x_2 y_2}^{[1]} S_{x_2 y_2 x_3 y_3}^{[2]} S_{x_3 y_3 x_4 y_4}^{[3]} S_{x_4 y_4 x_5 y_5}^{[4]} \Omega_{x_5 y_5}. \quad (A.1)$$

As we mentioned in the main text, the order of contractions, $S^{[1]}(S^{[2]}(S^{[3]}(S^{[4]}\Omega)))$, achieves $O(\chi^3)$ computational cost. However, some intermediate tensors such as $S^{[4]}\Omega$ are fourth order. To avoid $O(\chi^4)$ memory usage, we split the summation of the index $y_1$ between $S^{[1]}$ and $S^{[4]}$ into small blocks with a block size $\chi_b$. Assuming the bond dimension $\chi$ is divisible by the block size $\chi_b$ for simplicity, the contraction with the loop blocking technique is precisely represented as

$$Y_{x'y'} = \sum_{b=1}^{\chi/\chi_b} \left[ \sum_{x_1=1}^{\chi} \sum_{x_2=1}^{\chi} \sum_{x_3=1}^{\chi} \sum_{x_4=1}^{\chi} \sum_{x_5=1}^{\chi} \times \left( \sum_{y_2=1}^{\chi} S_{x_2 y_2 x_3 y_3}^{[2]} \left( \sum_{x_1=1}^{\chi} \sum_{x_4=1}^{\chi} S_{x_4 y_4 x_5 y_5}^{[4]} \Omega_{x_5 y_5} \right) \right) \right]. \quad (A.2)$$

Clearly, the memory usage of intermediate tensors is reduced to $O(\chi_b \chi^3)$. Thus, it is $O(\chi^3)$ if the block size $\chi_b$ is of order unity. Our simulations in this paper typically used $\chi_b = 8$, which reduced the memory usage with $\chi = 512$ from 550 to 8.6 GB.

Although splitting one loop is enough in this case, one needs to block several loops in more complicated contractions. We note that the loop blocking technique does not change the computational cost.
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