Very Large-Scale Singular Value Decomposition Using Tensor Train Networks

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Abstract

We propose new algorithms for singular value decomposition (SVD) of very large-scale matrices based on a low-rank tensor approximation technique called the tensor train (TT) format. The proposed algorithms can compute several dominant singular values and corresponding singular vectors for large-scale structured matrices given in a TT format. The computational complexity of the proposed methods scales logarithmically with the matrix size under the assumption that both the matrix and the singular vectors admit low-rank TT decompositions. The proposed methods, which are called the alternating least squares for SVD (ALS-SVD) and modified alternating least squares for SVD (MALS-SVD), compute the left and right singular vectors approximately through block TT decompositions. The very large-scale optimization problem is reduced to sequential small-scale optimization problems, and each core tensor of the block TT decompositions can be updated by applying any standard optimization methods. The optimal ranks of the block TT decompositions are determined adaptively during iteration process, so that we can achieve high approximation accuracy. Extensive numerical simulations are conducted for several types of TT-structured matrices such as Hilbert matrix, Toeplitz matrix, random matrix with prescribed singular values, and tridiagonal matrix. The simulation results demonstrate the effectiveness of the proposed methods compared with standard SVD algorithms and TT-based algorithms developed for symmetric eigenvalue decomposition.

KEY WORDS: curse-of-dimensionality, low-rank tensor approximation, matrix factorization, symmetric eigenvalue decomposition, singular value decomposition, tensor decomposition, tensor network, matrix product operator, Laplace operator, Hankel matrix, Toeplitz matrix, tridiagonal matrix

1 Introduction

The singular value decomposition (SVD) is one of the most important matrix factorization techniques in numerical analysis. The SVD can be used for the best low-rank approximation for matrices, computation of pseudo-inverses of matrices, solution of unconstrained linear least squares problems, principal component analysis, canonical correlation analysis, and estimation of ranks
and condition numbers of matrices, just to name a few. It has a wide range of applications in image processing, signal processing, immunology, molecular biology, information retrieval, systems biology, computational finance, and so on [42].

In this paper, we propose an algorithm for computing $K$ dominant singular values and corresponding singular vectors of structured very large-scale matrices. The $K$ dominant singular vectors can be computed by solving the following trace maximization problem: given $A \in \mathbb{R}^{P \times Q}$,

$$\begin{align*}
\text{maximize}_{U,V} & \quad \text{trace}(U^TAV) \\
\text{subject to} & \quad U^TU = V^TV = I_K.
\end{align*}$$

(1)

Standard algorithms for computing the SVD of a $P \times Q$ matrix with $P \geq Q$ cost $O(PQ^2)$ for computing full SVD and $O(PK^2)$ for computing $K$ dominant singular values [4]. However, in case that $P$ and $Q$ are exponentially growing, e.g., $P = Q = I^N$ for some fixed $I$, the computational and storage complexities also grow exponentially with $N$. In order to avoid the “curse-of-dimensionality”, the Monte-Carlo algorithm [11] was suggested but its accuracy is not high enough.

The basic idea behind the proposed algorithm is to reshape (or tensorize) matrices and vectors into high-order tensors and compress them by applying a low-rank tensor approximation technique [13]. Once the matrices and vectors are represented in low-rank tensor formats such as the tensor train (TT) [33, 35] or hierarchical Tucker (HT) [12, 15] decompositions, all the basic numerical operations such as the matrix-by-vector multiplication are performed based on the low-rank tensor formats with feasible computational complexities growing only linearly in $N$ [12, 33].

On the other hand, traditional low-rank tensor approximation techniques such as the CANDECOMP/PARAFAC (CP) and Tucker decompositions also compress high-order tensors into low-parametric tensor formats [23]. Although the CP and Tucker decompositions have a wide range of applications in chemometrics, signal processing, neuroscience, data mining, image processing, and numerical analysis [23], they have their own limitations. The Tucker decomposition cannot avoid the curse-of-dimensionality, which prohibits its application to the tensorized large-scale data matrices [13]. The CP decomposition does not suffer from the curse-of-dimensionality, but there does not exist a reliable and stable algorithm for best low-rank approximation due to the lack of closedness of the set of tensors of bounded tensor ranks [6].

In this paper, we focus on the TT decomposition, which is one of the most simplest tensor network formats [10]. The TT and HT decompositions can avoid the curse-of-dimensionality by low-rank approximation, and possess the closedness property [10, 13]. For numerical analysis, basic numerical operations such as addition and matrix-by-vector multiplication based on low-rank tensor networks usually cause rank growth, so efficient rank-truncation should be followed. Efficient rank-truncation algorithms for the TT and HT decompositions were developed in [12, 33].

In order to solve large-scale optimization problems based on the TT decomposition, several different types of optimization algorithms have been suggested in the literature.

First, existing iterative methods can be combined with truncation of the TT format [27, 32, 18]. For example, for computing several extremal eigenvalues of symmetric matrices, conjugate-gradient type iterative algorithms are combined with truncation for minimizing the (block) Rayleigh quotient in [27, 32]. In the case that a few eigenvectors should be computed simultaneously, the block of orthonormal vectors can be efficiently represented in block TT format [27]. However, the whole matrix-by-vector multiplication causes all the TT-ranks to grow at the same time, which leads to a very high computational cost in the subsequent truncation step.

Second, alternating least squares (ALS) type algorithms reduce the given large optimization problem into sequential relatively small optimization problems, for which any standard optimization
algorithm can be applied. The ALS algorithm developed in [17] is easy to implement and each iteration is relatively fast. But the TT-ranks should be predefined in advance and cannot be changed during iteration. The modified alternating least squares (MALS) algorithm, or equivalently density matrix renormalization group (DMRG) method [17, 21, 35] can adaptively determine the TT-ranks by merging two core tensors into one bigger core tensor and separating it by using the truncated SVD. The MALS shows a fast convergence in many numerical simulations. However, the reduced small optimization problem is solved over the merged bigger core tensor, which increases the computational and storage costs considerably in some cases. Dolgov et al. [8] developed an alternative ALS type method based on block TT format, where the mode corresponding to the number $K$ of orthonormal vectors is allowed to move to the next core tensor via the truncated SVD. This procedure can determine the TT-ranks adaptively if $K > 1$ for the block TT format. Kressner et al. [24] further developed an ALS type method which adds rank-adaptivity to the block TT-based ALS method of Dolgov et al. [8] even if $K = 1$.

In this paper, we propose the ALS and MALS type algorithms for computing the $K$ dominant singular values of matrices which are not necessarily symmetric. The ALS algorithm based on block TT format was originally developed for block Rayleigh quotient minimization for symmetric matrices [8]. The MALS algorithm was also developed for Rayleigh quotient minimization for symmetric matrices [17, 21, 35]. We show that the $K$ dominant singular values can be efficiently computed by solving the maximization problem (1). We compare the proposed algorithms with other block TT-based algorithms which were originally developed for computing eigenvalues of symmetric matrices, by simulated experiments and a theoretical analysis of computational complexities. Moreover, we present extensive simulated experiments for various types of structured matrices such as Hilbert matrix, Toeplitz matrix, random matrix with prescribed singular values, and tridiagonal matrix. We compare the performances of several different SVD algorithms, and present the relationship between TT-ranks and approximation accuracy based on the experimental results. We show that the proposed block TT-based algorithms can achieve very high accuracy by adaptively determining the TT-ranks. It is shown that the proposed algorithms can solve very large-scale optimization problems for matrices of as large sizes as $2^{25} \times 2^{25}$ and even $2^{50} \times 2^{50}$ on desktop computers.

The paper is organized as follows. In Section 2, notations for tensor operations and TT formats are described. In Section 3, the proposed SVD algorithms based on block TT format is presented. Their computational complexities are analyzed and computational considerations are discussed. In Section 4, extensive experimental results are presented for analysis and comparison of performances of SVD algorithms for several types of structured matrices. Conclusion and discussions are given in Section 5.

## 2 Tensor Train Formats

### 2.1 Notations

We refer to [3, 23, 32] for notations for tensors and multilinear operations. Scalars, vectors, and matrices are denoted by lowercase, lowercase bold, and uppercase bold letters as $x$, $\mathbf{x}$, and $\mathbf{X}$, respectively. An $N$th order tensor $\mathbf{X}$ is a multi-way array of size $I_1 \times I_2 \times \cdots \times I_N$, where $I_n$ is the size of the $n$th dimension or mode. A vector is the 1st order tensor and a matrix is the 2nd order tensor. Tensorization refers to the process of reshaping large-scale vectors and matrices into higher-order tensors by folding each of the modes. For instance, a vector of length $P = I_1 I_2 \cdots I_N$
Figure 1: Tensor network diagrams for (a) a vector, a matrix, a 3rd order tensor, (b) the contracted product of two 3rd order tensors, (c) the tensorization of a vector, and (d) singular value decomposition of a $I \times J$ matrix.

can be reshaped into a tensor of size $I_1 \times I_2 \times \cdots \times I_N$, and a matrix of size $I_1 I_2 \cdots I_N \times J_1 J_2 \cdots J_N$ can be reshaped into a tensor of size $I_1 \times J_1 \times I_2 \times J_2 \times \cdots \times I_N \times J_N$.

The $(i_1, i_2, \ldots, i_N)$th entry of $X \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is denoted by either $x_{i_1, i_2, \ldots, i_N}$ or $X(i_1, i_2, \ldots, i_N)$.

The mode-$(M, 1)$ contracted product of tensors $A \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_M}$ and $B \in \mathbb{R}^{I_M \times J_2 \times J_3 \times \cdots \times J_N}$ is defined by

$$c_{i_1, i_2, \ldots, i_M-1, j_2, j_3, \ldots, j_N} = \sum_{i_M=1}^{I_M} a_{i_1, i_2, \ldots, i_M} b_{i_M, j_2, j_3, \ldots, j_N}. \tag{2}$$

The mode-$(M, 1)$ contracted product is a natural generalization of the matrix-by-matrix multiplication.

Tensors and tensor operations are often represented as tensor network diagrams for illustrating the underlying principles of algorithms and tensor operations [17]. Figure 1 shows examples of the tensor network diagrams for tensors and tensor operations. In Figure 1(a), a tensor is represented by a node with as many edges as its order. In Figure 1(b), the mode-(3, 1) contracted product is represented as the link between two nodes. Figure 1(c) represents the tensorization process of a vector into a 3rd order tensor. Figure 1(d) represents a singular value decomposition of an $I \times J$ matrix into the product $U \Sigma V^T$. The matrices $U$ and $V$ of orthonormal column vectors are represented by half-filled circles, and the diagonal matrix $\Sigma$ is represented by a circle with slash.

### 2.2 Tensor Train Format

A tensor $X \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is in TT format if it is represented by

$$X = X^{(1)} \odot X^{(2)} \odot \cdots \odot X^{(N-1)} \odot X^{(N)}, \tag{3}$$

where $X^{(n)} \in \mathbb{R}^{R_{n-1} \times I_n \times R_n}, n = 1, 2, \ldots, N$, are 3rd order core tensors called TT-cores, and $R_1, R_2, \ldots, R_{N-1}$ are called TT-ranks. It is assumed that $R_0 = R_N = 1$. 


Figure 2 shows the tensor network diagram for an $N$th order tensor in TT format. Each of the core tensors is represented as a third order tensor except the first and the last core tensor.

The TT format is often called the matrix product states (MPS) with open boundary conditions in quantum physics community because each entry of $X$ in (3) can be written by the products of matrices as

$$x_{i_1,i_2,...,i_N} = X^{(1)}_{i_1} X^{(2)}_{i_2} \cdots X^{(N)}_{i_N},$$

where $X^{(n)}_{i_n} = X^{(n)}(i_n : , i_{n-1} : , \ldots , i_1 : , i_{n+1}, \ldots , i_N : ) \in \mathbb{R}$ is the entry of the $n$th core tensor $X^{(n)}$. The tensor $X$ in TT format can also be written by the outer products of the fibers (or column vectors) as

$$X = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} x^{(1)}_{r_1,i_1,r_2,i_2} \circ x^{(2)}_{r_2,i_2,r_3,i_3} \circ \cdots \circ x^{(N)}_{r_{N-1},i_{N-1},1} \circ x^{(N)}_{i_N,1,1},$$

where $x^{(n)}_{r_{n-1},i_{n},r_{n}} = X^{(n)}(r_{n-1},i_{n},r_{n}) \in \mathbb{R}$ is the entry of the $n$th core tensor $X^{(n)}$. The tensor $X$ in TT format can also be written by the outer products of the fibers (or column vectors) as

$$X^{(n)} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} x^{(1)}_{r_1,i_1,r_2,i_2} \circ x^{(2)}_{r_2,i_2,r_3,i_3} \circ \cdots \circ x^{(N)}_{r_{N-1},i_{N-1},1} \circ x^{(N)}_{i_N,1,1},$$

where $\circ$ is the outer product and $x^{(n)}_{r_{n-1},i_{n},r_{n}} = X^{(n)}(r_{n-1},i_{n},r_{n}) \in \mathbb{R}$ is the mode-2 fiber of the $n$th TT-core $X^{(n)}$.

The storage cost for a TT format is $O(NIR^2)$, where $I = \max(I_n)$ and $R = \max(R_n)$, that is linear with the order $N$. Any tensor can be represented exactly or approximately in TT format by using the TT-SVD algorithm in [33]. Moreover, basic numerical operations such as the matrix-by-vector multiplication can be performed in time linear with $N$ under the assumption that the TT-ranks are bounded [33].

### 2.3 Tensor Train Formats for Vectors and Matrices

Any large-scale vectors and matrices can also be represented in TT format. We suppose that a vector $x \in \mathbb{R}^{I_1 I_2 \cdots I_N}$ is tensorized into a tensor $X \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ and consider the TT format (3) as the TT representation of $x$. That is,

$$x = \text{vec}(X)$$

where $\text{vec}(X)$ is the vectorization of $X$.
in the sense that the vectorization is the reverse process of the tensorization. We define that each entry of $\mathbf{x}$ is associated with each entry of $\mathbf{X}$ by

$$x(i_1i_2\ldots i_N) = X(i_1, i_2, \ldots, i_N),$$

where $i_1i_2\ldots i_N = i_N + (i_{N-1} - 1)J_N + \cdots + (i_1 - 1)J_2\cdots J_N$ denotes the multi-index. The vector $\mathbf{X}$ in TT format can be expressed via the Kronecker products of fibers of core tensors

$$\mathbf{x} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} x^{(1)}_{r_1, r_2} \otimes x^{(2)}_{r_2, r_3} \otimes \cdots \otimes x^{(N)}_{r_{N-1}, 1} \in \mathbb{R}^{I_1J_2\cdots I_N}, \quad (7)$$

where $x^{(n)}_{r_n-1, r_n} = \mathbf{X}^{(n)}(r_n-1, \ldots, r_n) \in \mathbb{R}^{I_n}$ is the mode-2 fiber of the $n$th TT-core $\mathbf{X}^{(n)}$.

A matrix $\mathbf{A} \in \mathbb{R}^{I_1I_2\cdots I_N \times J_1J_2\cdots J_N}$ is considered to be tensorized into a tensor $\mathbf{A} \in \mathbb{R}^{I_1 \times J_1 \times J_2 \times \cdots \times I_N \times J_N}$. As in $\textbf{(6)}$, the tensor $\mathbf{A}$ can be represented in TT format as contracted products

$$\mathbf{A} = \mathbf{A}^{(1)} \otimes \mathbf{A}^{(2)} \otimes \cdots \otimes \mathbf{A}^{(N)},$$

where $\mathbf{A}^{(n)} \in \mathbb{R}^{R_{n-1}^A \times I_n \times J_n \times R_n^A}$, $n = 1, 2, \ldots, N$, are 4th order TT-cores with TT-ranks $R_1^A, R_2^A, \ldots, R_{N-1}^A$. We suppose that $R_0^A = R_N^A = 1$. The entries of $\mathbf{A}$ can also be represented in TT format by the products of slice matrices

$$a_{i_1, j_1, i_2, j_2, \cdots, i_N, j_N} = A^{(1)}_{i_1, j_1} A^{(2)}_{i_2, j_2} \cdots A^{(N)}_{i_N, j_N}, \quad (8)$$

where $A^{(n)}_{i_n, j_n} = A^{(n)}(i_n, j_n) \in \mathbb{R}^{R_{n-1}^A \times R_n^A}$ is the slice of the $n$th TT-core $A^{(n)}$. The matrix $\mathbf{A}$ in TT format can be represented as Kronecker products of slice matrices

$$\mathbf{A} = \sum_{r_1^A=1}^{R_1^A} \sum_{r_2^A=1}^{R_2^A} \cdots \sum_{r_{N-1}^A=1}^{R_{N-1}^A} A^{(1)}_{r_1^A, r_2^A} \otimes A^{(2)}_{r_2^A, r_3^A} \otimes \cdots \otimes A^{(N)}_{r_{N-1}^A, 1} \in \mathbb{R}^{I_1J_2\cdots I_N \times J_1J_2\cdots J_N}, \quad \text{(9)}$$

where $A^{(n)}_{r_{n-1}^A, r_n^A} = A^{(n)}(r_{n-1}^A, \ldots, r_n^A) \in \mathbb{R}^{I_n \times J_n}$ is the slice of the $n$th TT-core $A^{(n)}$.

In this paper, we call the TT formats $\textbf{(7)}$ and $\textbf{(9)}$ as the vector TT and matrix TT formats, respectively. Figure 3 shows a tensor network representing a matrix of size $I_1I_2\cdots I_N \times J_1J_2\cdots J_N$ in matrix TT format. Each of the core tensors is represented as a 4th order tensor except the first and the last core tensor.
2.4 Block TT Format

A group of several vectors can be represented in block TT format as follows. Let \( \mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_K] \in \mathbb{R}^{I_1I_2\cdots I_N \times K} \) denote a matrix with \( K \) column vectors. Suppose that the matrix \( \mathbf{U} \) is tensorized into a tensor \( \mathbf{U} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_{n-1} \times K \times I_n \times \cdots \times I_N} \), where the mode of the size \( K \) is located between the modes of sizes \( I_{n-1} \) and \( I_n \) for a fixed \( n \). In block TT format, the tensor \( \mathbf{U} \) is represented as contracted products

\[
\mathbf{U} = \mathbf{U}^{(1)} \bullet \mathbf{U}^{(2)} \bullet \cdots \bullet \mathbf{U}^{(N)},
\]

where the \( n \)th TT-core \( \mathbf{U}^{(n)} \in \mathbb{R}^{R_{n-1}^U \times K \times I_n \times R_n^U} \) is a 4th order tensor and the other TT-cores \( \mathbf{U}^{(m)} \in \mathbb{R}^{R_{m-1}^U \times I_m \times R_m^U}, m \neq n \), are 3rd order tensors. We suppose that \( R_0 = R_N^U = 1 \). Each entry of \( \mathbf{U} \) can be expressed by the products of slice matrices

\[
\mathbf{u}_{i_1,i_2,\ldots,i_{n-1},k,i_{n},\ldots,i_N} = \mathbf{U}^{(1)}_{i_1} \mathbf{U}^{(2)}_{i_2} \cdots \mathbf{U}^{(n-1)}_{i_{n-1},k,i_{n}} \mathbf{U}^{(n+1)}_{i_{n+1}} \cdots \mathbf{U}^{(N)}_{i_N},
\]

where \( \mathbf{U}^{(m)}_{i_m} \in \mathbb{R}^{R_{m-1}^U \times R_m^U}, m \neq n \), and \( \mathbf{U}^{(n)}_{k,i_n} \in \mathbb{R}^{R_{n-1}^U \times R_n^U} \) are the slice matrices of the \( m \)th and \( n \)th core tensors. We note that for a fixed \( k \in \{1, 2, \ldots, K\} \), the subtensor \( \mathbf{U}^{(n)}(:,k,:) \in \mathbb{R}^{R_{n-1}^U \times I_n \times R_n} \) is of order 3, so the block TT format is reduced to the vector TT format. Thus, each column vector of \( \mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_K] \) can be written as the Kronecker products of fibers of core tensors

\[
\mathbf{u}_k = \sum_{r_1=1}^{R_{1}^U} \sum_{r_2=1}^{R_{2}^U} \cdots \sum_{r_{N-1}=1}^{R_{N-1}^U} \mathbf{u}^{(1)}_{r_1,1} \otimes \mathbf{u}^{(2)}_{r_2,1} \otimes \cdots \otimes \mathbf{u}^{(n)}_{r_{n-1},k,r_{n}} \otimes \cdots \otimes \mathbf{u}^{(N)}_{r_{N-1},1},
\]

where \( \mathbf{u}^{(m)}_{r_m-1,r_m} = \mathbf{U}^{(m)}(:,r_m) \in \mathbb{R}^{I_m}, m \neq n \), and \( \mathbf{u}^{(n)}_{r_{n-1},k,r_{n}} = \mathbf{U}^{(n)}(:,r_{n-1},k,:) \in \mathbb{R}^{I_n} \).

In this paper, we call the block TT format \([10]\) as the block-\( n \) TT format, termed by \([24]\), in order to distinguish between different permutations of modes.

Figure 4 shows a tensor network representing a matrix \( \mathbf{U} \in \mathbb{R}^{I_1I_2\cdots I_N \times K} \) in block-\( n \) TT format. We can see that the mode of size \( K \) is located at the \( n \)th TT-core. We remark that the position of the mode of size \( K \) is not fixed.

2.5 Matricization of Block TT Format

Given the block-\( n \) TT format \([10]\) of \( \mathbf{U} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times K \times I_n \times \cdots \times I_N} \), we define the contracted products of the left TT-cores by

\[
\mathbf{U} < n = \mathbf{U}^{(1)} \bullet \cdots \bullet \mathbf{U}^{(n-1)} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times R_{n-1}}
\]
and the right TT-cores by

\[ U^{>n} = U^{(n+1)} \cdots U^{(N)} \in \mathbb{R}^{R_n \times I_{n+1} \times \cdots \times I_N} \]

for \( n = 1, 2, \ldots, N \). We suppose that \( U^{<1} = U^{>N} = 1 \). The mode-\( n \) matricization of \( U^{<n} \) and the mode-1 matricization of \( U^{>n} \) are written by

\[
U^{(n)}(n) \in \mathbb{R}^{R_{n-1} \times I_1 I_2 \cdots I_{n-1}}, \\
U^{>n}(1) \in \mathbb{R}^{R_n \times I_{n+1} I_{n+2} \cdots I_N}.
\]

Note that the block-\( n \) TT tensor \( U \) is written by \( U = U^{<n} \cdot U^{(n)} \cdot U^{>n} \), where \( U^{(n)} \in \mathbb{R}^{R_{n-1} \times K \times I_n \times R_n} \). The mode-\( n \) matricization \( U_{(n)} \in \mathbb{R}^{K \times I_1 I_2 \cdots I_N} \) of \( U \) can be expressed by

\[
U_{(n)} = \left( U^{<n} \cdot U^{(n)} \cdot U^{>n} \right)_{(n)} \\
\quad = \left( U^{(n)} \times_1 (U^{<n})^T \times_4 (U^{>n})^T \right)_{(2)} \tag{13}
\]

In the same way, we consider the contraction of the two neighboring core tensors

\[
U^{(n-1,n)} = U^{(n-1)} \cdot U^{(n)} \in \mathbb{R}^{R_{n-2} \times I_{n-1} \times K \times I_n \times R_n} \tag{14}
\]

Then the block-\( n \) TT tensor \( U \) is written by \( U = U^{<n-1} \cdot U^{(n-1,n)} \cdot U^{>n} \), and we can get an another expression for the mode-\( n \) matricization as

\[
U_{(n)} = U^{(n-1,1)}_{(3)} \left( U^{<n-1} \otimes I_{I_{n-1}} \otimes I_n \otimes U^{>n}(1) \right) \in \mathbb{R}^{K \times I_1 I_2 \cdots I_N}. \tag{15}
\]

**Definition 2.1** (Frame matrix, [8, 24]). The frame matrices \( U^{\neq n} \in \mathbb{R}^{I_1 I_2 \cdots I_N \times R_n} \) and \( U^{\neq n-1,n} \in \mathbb{R}^{I_1 I_2 \cdots I_N \times R_{n-1} I_n R_n} \) are defined by

\[
U^{\neq n} = (U^{<n})^T \otimes I_n \otimes (U^{>n})^T \tag{16}
\]

and

\[
U^{\neq n-1,n} = (U^{<n-1})^T \otimes I_{I_{n-1}} \otimes I_n \otimes (U^{>n})^T. \tag{17}
\]

Hence, from (13) and (15), the matrix \( U = [u_1, u_2, \ldots, u_K] \in \mathbb{R}^{I_1 I_2 \cdots I_N \times K} \) in block-\( n \) TT format can be written by

\[
U = U^{\neq n} U^{(n)}, \quad n = 1, 2, \ldots, N, \tag{18}
\]

where \( U^{(n)} = (U^{(n)}_{(2)})^T \in \mathbb{R}^{R_{n-1} I_n R_n \times K} \), and by

\[
U = U^{\neq n-1,n} U^{(n-1,n)}, \quad n = 2, 3, \ldots, N, \tag{19}
\]

where \( U^{(n-1,n)} = (U^{(n-1,n)}_{(3)})^T \in \mathbb{R}^{R_{n-2} I_n R_n \times K} \).
2.6 Orthogonalization of Core Tensors

Definition 2.2 (Left- and right-orthogonality, [16]). A 3rd order core tensor $U^{(m)} \in \mathbb{R}^{R_m-1 \times I_m \times R_m}$ is called left-orthogonal if

$$U^{(m)}_{(3)} \left(U^{(m)}_{(3)}\right)^T = I_{R_m},$$

(20)

and right-orthogonal if

$$U^{(m)}_{(1)} \left(U^{(m)}_{(1)}\right)^T = I_{R_m-1}.$$  

(21)

We can show that the matricizations $U_{\leq n}^{(1)}$ and $U_{\geq n}^{(1)}$ have orthonormal rows if the left core tensors $U^{(1)}, \ldots, U^{(n-1)}$ are left-orthogonalized and the right core tensors $U^{(n+1)}, \ldots, U^{(N)}$ are right-orthogonalized [28]. Consequently, the frame matrices $U_{\neq n}$ and $U_{\neq n-1,n}$ have orthonormal columns if each of the left and right core tensors is properly orthogonalized. From the expressions $U = U_{\neq n} U^{(n)}$ and $U = U_{\neq n-1,n} U^{(n-1,n)}$ in (18) and (19), we can guarantee orthonormality of the columns of $U$ by orthogonalizing the TT-cores. Figure 5 shows a tensor network diagram for the matrix $U$ in block-$n$ TT format where all the core tensors are either left or right orthogonalized except the $n$th core tensor. In this case we can guarantee that the frame matrices $U_{\neq n}$ and $U_{\neq n-1,n}$ have orthonormal columns.

3 SVD Algorithms Based on Block TT Format

In this section, we describe the new SVD algorithms, which we call the ALS for SVD (ALS-SVD) and MALS for SVD (MALS-SVD).

In the ALS-SVD and MALS-SVD, the left and right singular vectors $U = [u_1, \ldots, u_N] \in \mathbb{R}^{I_1 I_2 \cdots I_N \times K}$ and $V = [v_1, \ldots, v_N] \in \mathbb{R}^{J_1 J_2 \cdots J_N \times K}$ are initialized with block-$N$ TT formats. At the $n$th iteration, we suppose that $U$ and $V$ are represented by block-$n$ TT formats

$$U = U^{(1)} \cdot U^{(2)} \cdots \cdot U^{(N)}, \quad V = V^{(1)} \cdot V^{(2)} \cdots \cdot V^{(N)},$$

where the $n$th core tensors $U^{(n)} \in \mathbb{R}^{R_{n-1}^U \times K \times I_n \times R_n^U}$ and $V^{(n)} \in \mathbb{R}^{R_{n-1}^V \times K \times J_n \times R_n^V}$ are 4th order tensors and the other core tensors are 3rd order tensors. We suppose that all the 1, 2, ..., $(n-1)$th core tensors are left-orthogonalized and all the $n+1, n+2, \ldots, N$th core tensors are right-orthogonalized.

Figure 6 illustrates the tensor network diagram representing the trace $(U^T A V)$ in the maximization problem (1). Note that the matrix $A \in \mathbb{R}^{I_1 I_2 \cdots I_N \times J_1 J_2 \cdots J_N}$ is in matrix TT format. In the
Figure 6: Tensor network diagram for the trace \((U^TAV)\) in the maximization problem (1), where 
\(U \in \mathbb{R}^{I_1 I_2 \cdots I_N \times K}\) and \(V \in \mathbb{R}^{J_1 J_2 \cdots J_N \times K}\) are matrices of orthonormal column vectors in block-n TT format and \(A \in \mathbb{R}^{I_1 I_2 \cdots I_N \times J_1 J_2 \cdots J_N}\) is a matrix in matrix TT format.

Algorithms we don’t need to compute the large-scale matrix-by-vector products \(AV\) or \(A^TU\). All the necessary basic computations are performed based on efficient contractions of core tensors.

3.1 ALS for SVD Based on Block TT Format

The ALS algorithm for SVD based on block TT format is described in Algorithm 1. From (18), the matrices \(U\) and \(V\) of singular vectors are written by

\[
U^{(n)} = U^{\neq n} U^{(n)}, \quad V^{(n)} = V^{\neq n} V^{(n)},
\]

where \(U^{(n)} = (U^{(n)})^T \in \mathbb{R}^{R_{n-1} I_n R_n^U \times K}\) and \(V^{(n)} = (V^{(n)})^T \in \mathbb{R}^{R_n^V J_n R_n^V \times K}\). Note that \((U^{\neq n})^T U^{\neq n} = I_{R_{n-1} I_n R_n^U}\) and \((V^{\neq n})^T V^{\neq n} = I_{R_n^V J_n R_n^V}\). Given that all the core tensors are fixed except the \(n\)-th core tensors, the maximization problem (1) is reduced to the smaller optimization problem

\[
\text{maximize } U^{(n)}, V^{(n)} \quad \text{subject to } (U^{(n)})^T U^{(n)} = (V^{(n)})^T V^{(n)} = I_K
\]

for \(n = 1, 2, \ldots, N\), where

\[
\Xi_n = (U^{\neq n})^T A V^{\neq n} \in \mathbb{R}^{R_{n-1} I_n R_n^U \times R_n^V J_n R_n^V}
\]

is the projected matrix. In the case that the TT-ranks \(\{R_n^U\}\) and \(\{R_n^V\}\) are small enough, the projected matrix \(\Xi_n\) has much smaller sizes than \(A \in \mathbb{R}^{I_1 I_2 \cdots I_N \times J_1 J_2 \cdots J_N}\), so that any standard and efficient SVD algorithms can be applied. In the next subsection we will describe how the reduced local optimization problem (23) can be efficiently solved. In practice, the matrix \(\Xi_n\) don’t need to
be computed explicitly. Instead, the local matrix-by-vector multiplications $\mathbf{A}_n^T \mathbf{u}$ and $\mathbf{A}_n \mathbf{v}$ for any vectors $\mathbf{u} \in \mathbb{R}^{R_n - 1 \times R_n}$ and $\mathbf{v} \in \mathbb{R}^{R_n \times 1}$ are computed more efficiently based on the contractions of core tensors of $\mathbf{U}$, $\mathbf{A}$, and $\mathbf{V}$.

Algorithm 1: ALS for SVD based on block TT format

Data: $\mathbf{A} \in \mathbb{R}^{J_1 J_2 \cdots J_N \times I_1 I_2 \cdots I_N}$ in matrix TT format, $K \geq 2$, $\delta \geq 0$

Result: Dominant singular values $\mathbf{\Sigma} = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_K)$ and corresponding singular vectors $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_K] \in \mathbb{R}^{J_1 J_2 \cdots J_N \times K}$ and $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_K] \in \mathbb{R}^{J_1 J_2 \cdots J_N \times K}$ in block-$N$ TT format. The TT-ranks are denoted by $R_1^U, R_2^U, \ldots, R_{N-1}^U$ for $\mathbf{U}$ and $R_1^V, R_2^V, \ldots, R_{N-1}^V$ for $\mathbf{V}$.

1 Initialization: $\mathbf{U}$ and $\mathbf{V}$ in block-$N$ TT format with left-orthogonalized TT-cores $\mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(N-1)}, \mathbf{V}^{(1)}, \ldots, \mathbf{V}^{(N-1)}$ and small TT-ranks $R_1^U, \ldots, R_{N-1}^U, R_1^V, \ldots, R_{N-1}^V$.

2 repeat

   for $n = N, N-1, \ldots, 2$ do right-to-left half sweep

   // Optimization

   4 Fix all the TT-cores except $\mathbf{U}^{(n)}$ and $\mathbf{V}^{(n)}$, compute $\mathbf{U}^{(n)}$ and $\mathbf{V}^{(n)}$ by solving (23).

   // Matrix Factorization and Adaptive Rank Estimation

   6 Compute $\mathbf{U}^{(n)} = \text{reshape}(\mathbf{U}^{(n)}, [R_{n-1}^U, I_n, R_n^U], K)$,
     $\mathbf{V}^{(n)} = \text{reshape}(\mathbf{V}^{(n)}, [R_n^V, J_n, R_{n-1}^V], K)$

   7 Compute $\delta$-truncated SVD: $[\mathbf{U}_1, \mathbf{S}_1, \mathbf{V}_1] = \text{SVD}_\delta \left( \mathbf{U}^{(n)}_{(1,4) \times (2,3)} \right)$,
     $[\mathbf{U}_2, \mathbf{S}_2, \mathbf{V}_2] = \text{SVD}_\delta \left( \mathbf{V}^{(n)}_{(1,4) \times (2,3)} \right)$.

   8 Update $R_{n-1}^U = \text{rank}(\mathbf{V}_1)$, $R_n^U = \text{rank}(\mathbf{V}_2)$.

   9 Update $\mathbf{U}^{(n)} = \text{reshape}(\mathbf{V}_1^T, [R_{n-1}^U, I_n, R_n^U])$, $\mathbf{V}^{(n)} = \text{reshape}(\mathbf{V}_2^T, [R_n^V, J_n, R_{n-1}^V])$.

   10 Update $\mathbf{U}^{(n-1)} = \mathbf{U}^{(n-1)} \odot \text{reshape}(\mathbf{U}_1 \mathbf{S}_1, [R_{n-1}^U, K, R_n^U])$,
     $\mathbf{V}^{(n-1)} = \mathbf{V}^{(n-1)} \odot \text{reshape}(\mathbf{V}_1 \mathbf{S}_1, [R_{n-1}^V, K, R_n^V])$.

   end

   for $n = 1, 2, \ldots, N-1$ do

     Carry out left-to-right half sweep similarly

   end

until a stopping criterion is met;

We note that the $K$ dominant singular values $\mathbf{\Sigma} = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_K)$ are equivalent to the $K$ dominant singular values of the projected matrix $\mathbf{A}_n$ in the sense that $\mathbf{\Sigma} = \mathbf{U}^T \mathbf{A} \mathbf{V} = (\mathbf{U}^{(n)})^T \mathbf{A}_n \mathbf{V}^{(n)}$. Hence, the singular values are updated at each iteration by the singular values estimated by the standard SVD algorithms for the reduced optimization problem (23).

The TT-ranks of the block TT formats are adaptively determined by separating the mode corresponding to $K$ from the $n$th core tensors by using the $\delta$-truncated SVD. For example, during the right-to-left half sweep, the $\delta$-truncated SVD decomposes unfolded $n$th core tensors as

$$
\mathbf{U}^{(n)}_{(1,4) \times (2,3)} = \mathbf{U}_1 \mathbf{S}_1 \mathbf{V}_1^T + \mathbf{E}_1 \in \mathbb{R}^{R_{n-1}^U \times K \times I_n \times R_n^U},
$$

$$
\mathbf{V}^{(n)}_{(1,4) \times (2,3)} = \mathbf{U}_2 \mathbf{S}_2 \mathbf{V}_2^T + \mathbf{E}_2 \in \mathbb{R}^{R_n^V \times K \times J_n \times R_{n-1}^V},
$$

(25)
where \( \| E_1 \|_F \leq \delta \| U^{(n)} \|_F \) and \( \| E_2 \|_F \leq \delta \| V^{(n)} \|_F \). Then, the TT-ranks are updated by \( R_U^{n-1} = \text{rank}(V_1) \) and \( R_V^{n-1} = \text{rank}(V_2) \), which are simply the numbers of columns of \( V_1 \) and \( V_2 \). The \( n \)th TT-cores are updated by reshaping \( V_1^{(n-1)} \) and \( V_2^{(n-1)} \) into tensors of proper sizes. Note that in the case that \( K = 1 \), the TT-ranks \( R_U^{n-1} \) and \( R_V^{n-1} \) cannot be increased because, for example, \( \text{rank}(V_1) = \text{rank}(U_1 S_1) \leq R_U^{n-1} \).

Figure 7 illustrates the ALS scheme based on block TT format for the first two iterations during the right-to-left half sweep. In the figure, the \( n \)th TT-core is computed by a local optimization algorithm for the maximization problem (23), and then the block-\( n \) TT format is converted to the block-(\( n-1 \)) TT format via the \( \delta \)-truncated SVD.

### 3.2 MALS for SVD Based on Block TT Format

The MALS algorithm for SVD based on block TT format is described in Algorithm 2. At the \( n \)th iteration during right-to-left half sweep, the left and right singular vectors \( U \) and \( V \) are represented in block-\( n \) TT format. From (19), the matrices \( U \) and \( V \) are written by

\[
U = U \neq n-1, n U^{(n-1,n)}, \quad V = V \neq n-1, n V^{(n-1,n)}
\]

for \( n = 2, 3, \ldots, N \), where \( U^{(n-1,n)} \in \mathbb{R}^{R_{n-2} J_{n-1} J_n R_U^{n-1} \times K} \) and \( V^{(n-1,n)} \in \mathbb{R}^{R_{n-2} J_{n-1} J_n R_V^{n-1} \times K} \) are matricizations of the merged TT-cores \( U^{(n-1)} \bullet U^{(n)} \) and \( V^{(n-1)} \bullet V^{(n)} \). Given that all the TT-cores are fixed except the \((n-1)\)th and \( n \)th TT-cores, the large-scale optimization problem (1) is reduced to

\[
\begin{align*}
\text{maximize} & \quad \text{trace} \left( U^T A V \right) = \text{trace} \left( (U^{(n-1,n)})^T \tilde{A}_{n-1,n} V^{(n-1,n)} \right) \\
\text{subject to} & \quad (U^{(n-1,n)})^T U^{(n-1,n)} = (V^{(n-1,n)})^T V^{(n-1,n)} = I_K
\end{align*}
\]
Figure 8: Illustration of the MALS scheme based on block TT format for the first two iterations during right-to-left half sweep

where

$$\tilde{A}_{n-1,n} = (U^{\neq n-1,n})^T AV^{\neq n-1,n} \in \mathbb{R}^{R_{n-2}^{U} I_{n-1} R_{n}^{U} \times R_{n-2}^{U} J_{n-1} J_{n} V_{n}}$$

is the projected matrix.

Figure 8 illustrates the MALS scheme. In the MALS, two neighboring core tensors are first merged and updated by solving the optimization problem (27). Then, the $\delta$-truncated SVD factorizes it back into two core tensors. Note that the block-$n$ TT format is transformed into the block-$(n-1)$ TT format.

3.3 Efficient Computation of Projected Matrix-by-Vector Product

In order to solve the reduced optimization problems [23] and [27], we consider the eigenvalue decomposition of the block matrices

$$\bar{B}_n = \begin{bmatrix} 0 & A_n \\ A_n^T & 0 \end{bmatrix}, \quad \bar{B}_{n-1,n} = \begin{bmatrix} 0 & \tilde{A}_{n-1,n} \\ \tilde{A}_{n-1,n}^T & 0 \end{bmatrix}.$$  

It can be shown that the $K$ largest eigenvalues of $\bar{B}_n$ correspond to the $K$ dominant singular values of the projected matrix $\bar{A}_n$, and the eigenvectors of $\bar{B}_n$ correspond to a concatenation of the left and right singular vectors of $\bar{A}_n$. See Appendix A for more detail. The same holds for $\bar{B}_{n-1,n}$ and $\tilde{A}_{n-1,n}$.

For computing the eigenvalue decomposition of the above matrices, we don’t need to compute the matrices explicitly, but we only need to compute matrix-by-vector products. Let

$$\mathbf{x} \in \mathbb{R}^{R_{n-1}^{U} I_{n} R_{n}^{U}}, \quad \mathbf{y} \in \mathbb{R}^{R_{n-1}^{V} J_{n} R_{n}^{V}}, \quad \tilde{\mathbf{x}} \in \mathbb{R}^{R_{n-2}^{U} I_{n-1} I_{n} R_{n}^{U}}, \quad \tilde{\mathbf{y}} \in \mathbb{R}^{R_{n-2}^{V} J_{n-1} J_{n} V}$$

be the given vectors. Then, the matrix-by-vector products are expressed by

$$\bar{B}_n \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} A_n \mathbf{y} \\ A_n^T \tilde{\mathbf{x}} \end{bmatrix}, \quad \bar{B}_{n-1,n} \begin{bmatrix} \tilde{\mathbf{x}} \\ \tilde{\mathbf{y}} \end{bmatrix} = \begin{bmatrix} \tilde{A}_{n-1,n} \tilde{\mathbf{y}} \\ \tilde{A}_{n-1,n}^T \tilde{\mathbf{x}} \end{bmatrix},$$  

(29)
Algorithm 2: MALS for SVD based on block TT format

Data: $\mathbf{A} \in \mathbb{R}^{I_1J_1 \cdots I_NJ_N}$ in matrix TT format, $K \geq 1$, $\delta \geq 0$

Result: Dominant singular values $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_K)$ and corresponding singular vectors $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_K] \in \mathbb{R}^{I_1J_1 \cdots I_NK}$ and $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_K] \in \mathbb{R}^{J_1J_2 \cdots J_NK}$ in block-$N$ TT format. The TT-ranks are denoted by $R_{1U}, R_{2U}, \ldots, R_{N-1U}$ for $\mathbf{U}$ and $R_{1V}, R_{2V}, \ldots, R_{N-1V}$ for $\mathbf{V}$.

Initialization: $\mathbf{U}$ and $\mathbf{V}$ in block-$N$ TT format with left-orthogonalized TT-cores $\mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(N-2)}, \mathbf{V}^{(1)}, \ldots, \mathbf{V}^{(N-2)}$ and small TT-ranks $R_{1U}, R_{2U}, \ldots, R_{N-1U}, R_{1V}, \ldots, R_{N-1V}$.

repeat
  
  for $n = N, N-1, \ldots, 2$ do right-to-left half sweep
    
    // Optimization
    Fix all the TT-cores except the $n$th and $(n-1)$th TT-cores, compute $\mathbf{U}^{(n-1,n)}$ and $\mathbf{V}^{(n-1,n)}$ by solving (27).

    Update the singular values $\Sigma = (\mathbf{U}^{(n-1,n)})^T \tilde{\mathbf{A}}_{n-1,n} \mathbf{V}^{(n-1,n)}$.

    // Matrix Factorization and Adaptive Rank Estimation
    Compute $\mathbf{U}^{(n-1,n)} = \text{reshape}(\mathbf{U}^{(n-1,n)}, [R_{n-2U}, I_{n-1}, I_n, R_{nU}, K])$, $\mathbf{V}^{(n-1,n)} = \text{reshape}(\mathbf{V}^{(n-1,n)}, [R_{n-2V}, J_{n-1}, J_n, R_{nV}, K])$.

    Compute $\delta$-truncated SVD: $[\mathbf{U}_1, \mathbf{S}_1, \mathbf{V}_1] = \text{SVD}_\delta(\mathbf{U}^{(n-1,n)}(\{1,2,5\} \times \{3,4\}))$, $[\mathbf{U}_2, \mathbf{S}_2, \mathbf{V}_2] = \text{SVD}_\delta(\mathbf{V}^{(n-1,n)}(\{1,2,5\} \times \{3,4\}))$.

    Update $R_{n-1U} = \text{rank}(\mathbf{V}_1)$, $R_{n-1V} = \text{rank}(\mathbf{V}_2)$.

    Update $\mathbf{U}^{(n)} = \text{reshape}(\mathbf{V}_1^T, [R_{n-1U}, I_n, R_{nU}])$, $\mathbf{V}^{(n)} = \text{reshape}(\mathbf{V}_2^T, [R_{n-1V}, J_n, R_{nV}])$.

    Update $\mathbf{U}^{(n-1)} = \text{reshape}(\mathbf{U}_1 \mathbf{S}_1, [R_{n-2U}, I_{n-1}, K, R_{nU}])$, $\mathbf{V}^{(n-1)} = \text{reshape}(\mathbf{U}_2 \mathbf{S}_2, [R_{n-2V}, J_{n-1}, K, R_{nV}])$.

  end

for $n = 1, 2, \ldots, N-1$ do
  
  Carry out left-to-right half sweep similarly

end

until a stopping criterion is met;
which consist of the projected matrix-by-vector products, $\vec{A}_n y, \vec{A}_n^T x, \vec{A}_{n-1} y, \vec{A}_{n-1}^T x$, and $\vec{A}_{n-1,n}^T x$.

The computation of the projected matrix-by-vector products is performed in an iterative way as follows. Let $U_{i,m}^{(m)} = U^{(m)}(:,i,m,:)$, $A_{i,m}^{(m)} = A^{(m)}(:,i,m,:)$, and $V_{j,m}^{(m)} = V^{(m)}(:,j,m,:)$ be the slice matrices of the three $m$th core tensors for $m \neq n$. Let

$$Z^{(m)} = \sum_{i,m=1}^{I_m} \sum_{j,m=1}^{J_m} U_{i,m}^{(m)} \otimes A_{i,m,J_m}^{(m)} \otimes V_{j,m}^{(m)} \in \mathbb{R}^{R_{m-1}^U R_{m-1}^A R_{m-1}^V \times R_{m-1}^A R_{m}^V R_{m}^V},$$

(30)

We define 3rd order tensors $L^{<m} \in \mathbb{R}^{R_{m-1}^U \times R_{m-1}^A \times R_{m-1}^V}$, $m = 1,2,\ldots,n$, and $R^{>m} \in \mathbb{R}^{R_{m}^U \times R_{m}^A \times R_{m}^V}$, $m = n,n+1,\ldots,N$, recursively by

$$\text{vec} (L^{<m})^T = \text{vec} (L^{<m-1})^T Z^{(m-1)} \in \mathbb{R}^{1 \times R_{m-1}^U R_{m-1}^A R_{m-1}^V}, \quad m = 2,3,\ldots,n,$$

(31)

and

$$\text{vec} (R^{>n}) = 1,$$

(32)

Recall that $(U^{(n)})^T \vec{A}_n v^{(n)} = U^T A V$, and Figure 6 illustrates the tensor network diagram for the trace of $U^T AV$. Let $U^{(n)} = [u_1^{(n)},\ldots,u_K^{(n)}]$ and $V^{(n)} = [v_1^{(n)},\ldots,v_K^{(n)}]$. From the matrix product representations of the TT block and block TT formats $[\square]$ and $[\square\square]$, we can show that the $(k_1,k_2)$th entry of $(U^{(n)})^T \vec{A}_n v^{(n)}$ is expressed by

$$(u_{k_1}^{(n)})^T \vec{A}_n v_{k_2}^{(n)} = u_{k_1}^T A v_{k_2}$$

$$= Z^{(1)} \cdots Z^{(n-1)} \sum_{i,m=1}^{I_m} \sum_{j,n=1}^{J_n} U_{k_1,i,n}^{(n)} \otimes A_{i,n,J_n}^{(n)} \otimes V_{k_2,J_n}^{(n)} \in \mathbb{R}^{R_{n+1}^U R_{n+1}^A R_{n+1}^V}$$

(33)

which is the contraction of the tensors $L^{<n}, U^{(n)}, A^{(n)}, V^{(n)}$, and $R^{>n}$. Thus, the computation of $\vec{A}_n y$ is performed by the contraction of the tensors $L^{<n}, Y, A^{(n)}$, and $R^{>n}$, where $Y \in \mathbb{R}^{R_{n-1}^U \times J_n \times R_{n}^V}$ is the tensorization of the vector $y$. In the same way, the computation of $\vec{A}_n^T x$ is performed by the contraction of the tensors $L^{<n}, X, A^{(n)}$, and $R^{>n}$, where $X \in \mathbb{R}^{R_{n-1}^U \times I_n \times R_{n}^U}$ is the tensorization of the vector $x$.

Similarly, we can derive an expression for the projected matrix $\vec{A}_{n-1}$ as

$$\begin{align*}
(u_{k_1}^{(n-1,n)})^T \vec{A}_{n-1,n} v_{k_2}^{(n-1,n)} &= \text{vec} (L^{<n-1})^T \left( \sum_{i,n=1}^{I_n} \sum_{j,n=1}^{J_n} \sum_{m=1}^{I_m} \sum_{j,m=1}^{J_m} U_{i,n,k_1,i,n}^{(n-1,n)} \otimes A_{i,n,J_n}^{(n-1)} \otimes A_{i,n,J_n}^{(n)} \otimes V_{j,n,k_2,j_n}^{(n-1,n)} \otimes V_{j,n,k_2,j_n}^{(n)} \right) \text{vec} (R^{>n})^T,
\end{align*}$$

(34)

$$\text{vec} (L^{<n-1})^T \left( \sum_{i,n=1}^{I_n} \sum_{j,n=1}^{J_n} \sum_{m=1}^{I_m} \sum_{j,m=1}^{J_m} U_{i,n,k_1,i,n}^{(n-1,n)} \otimes A_{i,n,J_n}^{(n-1)} \otimes A_{i,n,J_n}^{(n)} \otimes V_{j,n,k_2,j_n}^{(n-1,n)} \otimes V_{j,n,k_2,j_n}^{(n)} \right) \text{vec} (R^{>n})^T,$$
| Optimization | line 4: $O(K^2IR^2)$ | line 4: $O(K^2IR^2)$ |
|-------------|---------------------|---------------------|
| Factorization | line 7: $O(KI^2R^2)$ | line 7: $O(KI^2R^3)$ |
| Projected Matrix-by-Vector Products, Updating Tensor | line 4: $O(IR_AR^3) + O(I^2RA^2R^2)$ | line 4: $O(I^2R_AR^3) + O(I^3RA^2R^2)$ |
| $L^{<n}$ or $R^{>n}$ | line 9: $O(IR_AR^3) + O(I^2RA^2R^2)$ | line 9: $O(IR_AR^3) + O(I^2RA^2R^2)$ |

which is the contraction of the tensors $L^{<n-1}$, $U^{(n-1,n)}$, $A^{(n-1)}$, $A^{(n)}$, $Y^{(n-1,n)}$, and $R^{>n}$. Thus, the computation of $\tilde{A}_{n-1,n}Y$ is performed by the contraction of the tensors $L^{<n-1}$, $Y$, $A^{(n-1)}$, $A^{(n)}$, and $R^{>n}$, where $Y \in R_{R_{-2}}^{R_{-2}} \times \times \times R_{-2}^{R_{-2}}$ is the tensorization of the vector $\hat{y}$. In the same way, the computation of $\tilde{A}_{n}^{T}X$ is performed by the contraction of the tensors $L^{<n-1}$, $X$, $A^{(n-1)}$, $A^{(n)}$, and $R^{>n}$, where $X \in R_{R_{-2}}^{R_{-2}} \times \times \times R_{-2}^{R_{-2}}$ is the tensorization of the vector $\hat{x}$.

Figure 9 illustrates the tensor network diagrams for the computation of the projected matrix-by-vector products $\tilde{A}_{n}Y$ and $\tilde{A}_{n-1,n}Y$ for the vectors $y \in R_{R_{-2}}^{R_{-2}}$, and $\hat{y} \in R_{R_{-2}}^{R_{-2}}$. Based on the tensor network diagrams, we can easily specify the sizes of the tensors and how the tensors are contracted with each other.

### 3.4 Computational Complexity

Let $R = \max\{\{R_{u}\}, \{R_{v}\}\}$, $R_A = \max\{\{R_{A}\}\}$, and $I = \max\{\{I_{u}\}, \{J_{u}\}\}$. The computational complexities for the ALS-SVD and MALS-SVD algorithms are summarized in Table 1. We may assume that $K \geq I$ because we usually choose very small values for $I_{u}$ and $J_{u}$, e.g., $I = I_{u} = J_{u} = 2$. The computational complexities in Table 1 correspond to each iteration, so the total computational costs for one full sweep (right-to-left and left-to-right half sweeps) grow linearly with the order $N$ given that $R$, $R_A$, $I$, and $K$ are bounded.

Computational complexities for the projected matrix-by-vector products can be conveniently analyzed by using the tensor network diagrams in Figure 9. In Figure 9(a), the optimal order of contraction for computing $\tilde{A}_{n}Y$ is $(L^{<n}, Y, A^{(n)}, R^{>n})$, and its computational complexity is $O(IR_AR^3) + O(I^2RA^2R^2)$. If we compute the contractions in the order of $(L^{<n}, \tilde{A}^{(n)}, Y, R^{>n})$, however, the computational complexity increases to $O(I^2R_AR^3) + O(I^2RA^2R^2)$. On the other hand, an explicit computation of the matrix $\tilde{A}_{n}$ can be performed by the contraction of $(L^{<n}, \tilde{A}^{(n)}, R^{>n})$, which costs $O(I^4R_AR^3) + O(I^4RA^2R^2)$. Thus, it is recommended to avoid computing the projected matrices explicitly.

In Figure 9(b), the most efficient order of contraction for computing $\tilde{A}_{n-1,n}Y$ is $(L^{<n-1}, \tilde{Y}, A^{(n-1)}, A^{(n)}, R^{>n})$, and the computational complexity amounts to $O(I^2R_AR^3) + O(I^3RA^2R^2)$. However, if we follow the order of $(L^{<n-1}, \tilde{A}^{(n-1)}, A^{(n)}, \tilde{Y}, R^{>n})$ for contraction, it costs $O(I^4R_AR^3) + O(I^4RA^2R^2)$. Moreover, if we have to compute the projected matrix $\tilde{A}_{n-1,n}$ explicitly, its computational cost increases to $O(I^4R_AR^4) + O(I^4R_AR^4)$.

Both the ALS-SVD and MALS-SVD maintain the recursively defined left and right tensors $L^{<m}$, $m = 1, 2, \ldots, n$, and $R^{>m}$, $m = n, n+1, \ldots, N$, during iteration. At each iteration, the algorithms update the left or right tensor after the factorization step by the definitions (31) or (32). For example, during the right-to-left half sweep, the right tensor $R^{>n-1}$ is computed by the
Figure 9: Computation of the projected matrix-by-vector products (a) $\bar{A}_n y$ for ALS-SVD and (b) $\bar{A}_{n-1,n} \bar{y}$ for MALS-SVD for solving the reduced optimization problems in the ALS-SVD and MALS-SVD algorithms. (a) The computation of $\bar{A}_n y$ is carried out by the contraction of $L^{<n}$, $Y$, $A^{(n)}$, and $R^{>n}$. (b) The computation of $\bar{A}_{n-1,n} \bar{y}$ is carried out by the contraction of $L^{<n-1}$, $Y$, $A^{(n-1)}$, $A^{(n)}$, and $R^{>n}$. The efficient order of contraction is expressed by the numbers on each tensor.
Figure 10: Iterative computation of the right tensor $R^{\geq n-1}$ by the contraction of the tensors $R^{\geq n}$, $V^{(n)}$, $A^{(n)}$, and $U^{(n)}$ during the right-to-left half sweep. The optimal order of contraction is expressed by the numbers on each tensor.

The computational costs of the ALS-SVD and MALS-SVD are significantly affected by the TT-ranks of the left and right singular vectors. Even if we have good initial guesses for the left and right singular vectors $U$ and $V$, it may take much computational time until convergence if their TT-ranks are large. Therefore, it is advisable to initialize $U$ and $V$ in block TT format with relatively small TT-ranks, e.g., $R_n^U = [K/(I_{n+1} \cdots I_N)]$, $n = 1, \ldots, N$. Since both the ALS-SVD and MALS-SVD can adaptively determine TT-ranks during iteration process, they update the singular vectors very fast for the first a few sweeps and usually make good initial updates for themselves.
3.5.2 Stopping Criterion

The ALS-SVD and MALS-SVD algorithms can terminate if the relative residual decreases below a prescribed tolerance parameter $\epsilon$:

$$r = \frac{\|A^T U - V\Sigma\|_F}{\|V\Sigma\|_F} < \epsilon.$$  \(\text{(35)}\)

However, the matrix-by-vector multiplication, $A^T U$, increases the TT-ranks to the products $\{R^A_n R^U_n\}$. Then, the computational cost for the truncation of $A^T U$ is $O(NI(R^A R^U)^3)$ \([33]\). In order to reduce the computational cost, we may select a few rows, $J \subset \{1, 2, \ldots, Q\}$, of $A^T U \in \mathbb{R}^{Q \times K}$ and $V \in \mathbb{R}^{Q \times K}$, and compute an approximate relative residual by

$$r \approx \hat{r} = \frac{\|A^T(J,:)U - V(J,:)\Sigma\|_F}{\|V(J,:)\Sigma\|_F}.$$  \(\text{(36)}\)

The approximate relative residual is efficiently computed by randomly selecting several modes $N \subset \{1, 2, \ldots, N\}$ from TT tensors and determining $J$ by $J = \{j_1 j_2 \cdots j_N : j_n \not\in N, j_n \in \{1, 2, \ldots, J_n\} \text{ if } n \in N\}$.

3.5.3 Truncation Parameter

At each iteration, the $\delta$-truncated SVD is used to determine close to optimal TT-ranks and simultaneously to orthogonalize TT-cores. The $\delta$ value significantly affects the convergence rate of the ALS-SVD and MALS-SVD algorithms. If $\delta$ is small, then the algorithms usually converge fast within one or two full sweeps, but the TT-ranks may also grow largely, which causes high computational costs. In \([16]\), it was reported that a MALS-based algorithm often resulted in a rapidly increasing TT-ranks during iteration process. On the other hand, if $\delta$ is large, TT-ranks grow slowly, but the algorithms may not converge to the desired accuracy but converge to a local minimum.

We use several strategies for determining the $\delta$ value in the simulation. First, in order to make the algorithms converge, the $\delta$ value is set to be proportional to the tolerance $\epsilon$. Note that in the truncation algorithm in \([33]\) the $\delta$ value is set by $\epsilon/\sqrt{N-1} \propto \epsilon$. Second, in the case that the algorithm could not converge to the desired tolerance $\epsilon$ after the $N_{\text{sweep}}$ number of maximum sweeps, we restart the algorithm with different random initializations. In this case, the $\delta$ value may not be changed or can be decreased to, e.g., $0.25\delta$. If $K$ is not small, the algorithms usually converge in one or two full sweeps, so a small $N_{\text{sweep}}$ value is often sufficient. But if $K$ is small, e.g., $K = 2$, then the rank growth in each sweep is relatively slow and a more number of sweeps may be necessary. Third, in order to reduce the computational complexity, we use a rather large $\delta$ value at the first half sweep, for instance, $100\delta$. In this way, we can speed up the computation while not harming the convergence.

4 Numerical simulations

In numerical simulations, we computed the $K$ dominant singular values and corresponding singular vectors of several different types of very large-scale matrices. We compared the following SVD methods including two standard methods, LOBPCG and SVDS.
1. LOBPCG: The LOBPCG method can compute the $K$ largest or smallest eigenvalues of a Hermitian matrix. We applied a MATLAB version of LOBPCG to the matrix $A^T A \in \mathbb{R}^{Q \times Q}$ to compute the $K$ largest eigenvalues $\Lambda = \Sigma^2 = \text{diag}(\sigma_1^2, \ldots, \sigma_K^2)$ and corresponding eigenvectors $V \in \mathbb{R}^{Q \times K}$. Then we computed the left singular vectors by $U = AV \Sigma^{-1}$.

2. SVDS: The MATLAB function SVDS uses the Fortran package ARPACK to compute the $K$ largest eigenvalues of $B = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}$ and corresponding eigenvectors.

3. ALS-SVD, MALS-SVD: The ALS-SVD and MALS-SVD algorithms are described in Algorithms 1 and 2. For the local optimization at each iteration, we applied the MATLAB function EIGS in the way described in Section 3.3.

4. ALS-EIG, MALS-EIG: The ALS and MALS schemes are implemented for computing the $K$ largest eigenvalues of the Hermitian matrix $A^T A$ by maximizing the block Rayleigh quotient. We applied the MATLAB function EIGS for optimization at each iteration. After computing the $K$ largest eigenvalues $\Lambda = \Sigma^2$ and eigenvectors $V$, the left singular vectors are computed by $U = AV \Sigma^{-1}$.

For LOBPCG, ALS-EIG, and MALS-EIG, if $\Sigma$ is not invertible, then eigenvalue decomposition of $AA^T$ is computed to obtain the left singular vectors $U$. The ALS-EIG and MALS-EIG methods stop the iteration when

$$\|A^T AV \Sigma^1 - V \Sigma\|^2 < \epsilon^2 \|\Sigma\|^2,$$

where $\Sigma^\dagger$ is the pseudo-inverse. Then the relative residual can be controlled below $\epsilon$ as

$$\|A^T U - V \Sigma\|^2 = \|A^T AV \Sigma^{-1} - V \Sigma\|^2 < \epsilon^2 \|\Sigma\|^2.$$

We note that the computation of $A^T A$ and $U = AV \Sigma^{-1}$ is followed by the truncation algorithm to reduce the TT-ranks. If the truncation parameter value is too small, then a large TT-rank is obtained. In the simulation, we set the truncation parameter to $0.1\epsilon$ for the given tolerance parameter $\epsilon$.

We note that for the two standard methods, LOBPCG and SVDS, the matrix $A$ is in full matrix format, whereas for the block TT-based SVD methods, the matrix $A$ is in matrix TT format. In the simulations, we stopped running the two standard methods when the size of the matrix grows larger than $2^{13} \times 2^{13}$, because not only the computational time is high, but also the storage cost exceed the desktop memory capacity.

We implemented our code in MATLAB. The simulations were performed on a desktop computer with Intel Xeon CPU at 3.47GHz ($\times 2$) and 96GB of memory running Windows 7 professional and MATLAB 2014a. In the simulations, we performed 30 repeated experiments independently and averaged the results.

4.1 Random Matrix with Prescribed Singular Values

In order to measure the accuracy of computed singular values, we built matrices of rank 25 in matrix TT format by

$$A = U_0 \Sigma_0 V_0^T \in \mathbb{R}^{2^N \times 2^N},$$

...
where \( U_0 \in \mathbb{R}^{2N \times 25} \) and \( V_0 \in \mathbb{R}^{2N \times 25} \) are randomly generated left and right singular vectors in block-\( N \) TT format, and \( \Sigma_0 = \text{diag}(\sigma_{01}, \sigma_{02}, \ldots, \sigma_{0,25}) \) are singular values given by \( \sigma_{0k} = \beta^k, \ k = 0, 1, \ldots, 24 \). \( \beta \) takes values from \( \{0.2, 0.3, 0.4, 0.5, 0.6\} \). Figure 11 illustrates the 25 singular values for each \( \beta \) value. The block TT-ranks of \( U_0 \) and \( V_0 \) are set at the fixed value 5. The TT-cores of \( A \) in (38) were calculated based on the TT-cores of \( U_0 \) and \( V_0 \) as

\[
A^{(n)}_{i_n,j_n,:) = U^{(n)}_{i_n,:) \otimes V^{(n)}_{j_n,:}, \quad n = 1, 2, \ldots, N - 1,
\]

\[
A^{(N)}_{i_N,j_N,:) = \sum_{k=1}^{25} U^{(N)}_{i_k,i_N,:} \otimes V^{(N)}_{j_k,j_N,:), \quad i_n = 1, \ldots, I_n, j_n = 1, \ldots, J_n.
\]

for \( i_n = 1, \ldots, I_n, j_n = 1, \ldots, J_n \). We set \( \epsilon = \delta = 10^{-8} \) and \( K = 10 \). The relative error for the estimated singular values \( \Sigma \) is calculated by

\[
\frac{\| \Sigma - \Sigma_0 \|_F}{\| \Sigma_0 \|_F}.
\]

In Figure 12, we can see that the computational costs of the TT-based algorithms grow only logarithmically with the matrix size, whereas the times for the standard SVD algorithms grow exponentially with \( N \). Among the TT-based algorithms, the ALS-SVD and MALS-SVD show the smallest computational costs. The ALS-EIG and MALS-EIG have higher computational costs because the product \( A^T A \) increases its matrix TT-ranks and the subsequent truncation step results in high computational costs. The LOBPCG and SVDS show a fast rate of increase in the computational cost. The LOBPCG and SVDS were stopped running for larger matrix sizes than \( 2^{13} \times 2^{13} \) because of the computational cost and desktop computer memory capacity. The black dotted line shows a predicted computational time for the LOBPCG.

Figure 13 shows the performances of the four TT-based algorithms for various different \( \beta \) values for the random matrices \( A \in \mathbb{R}^{2N \times 2N} \) with \( N = 50 \). In Figure 13(a), the ALS-SVD and MALS-SVD
Figure 12: Performances for $2^N \times 2^N$ random matrices with $1 \leq N \leq 50$ and fixed $\beta = 0.5$ show the smallest computational times over all the $\beta$ values. In Figures 13(b) and (c), we can see that the ALS-SVD and MALS-SVD accurately estimate the block TT-ranks and the $K = 10$ dominant singular values. On the other hand, the ALS-EIG and MALS-EIG estimate the block TT-ranks and the singular values slightly less accurately, especially for small $\beta$ values. We note that the ALS-EIG and MALS-EIG take square roots on the obtained eigenvalues to compute the singular values.

### 4.2 A Submatrix of Hilbert Matrix

The Hilbert matrix $H \in \mathbb{R}^{P \times P}$ is a symmetric matrix with entries $h_{i,j} = (i + j - 1)^{-1}, i,j = 1,2,\ldots,P$. It is known that the eigenvalues of the Hilbert matrix decay to zero very fast. Let $H \in \mathbb{R}^{2^N \times 2^N}$. In this simulation, we consider a rectangular submatrix $A \in \mathbb{R}^{2^N \times 2^N-1}$ of the Hilbert matrix defined by

$$A = H(:, 1 : 2^{N-1}) \in \mathbb{R}^{2^N \times 2^{N-1}},$$

in MATLAB notation, in order to apply the SVD algorithms to the non-symmetric matrix $A$. In order to build the matrix TT representation of $A$, we modified and applied the explicit TT representation of the Toeplitz matrix developed in [20]. See Appendix B for details. First, we applied a DMRG-type algorithm in [17] to convert the $2^{N+1}$-vector $[1, 1, 2^{-1}, 3^{-1}, \ldots, (2^{N+1} - 1)^{-1}]^T$ to a vector TT decomposition with a relative approximation error of either $10^{-6}$ or $10^{-8}$. Figure 14 shows that a smaller approximation error results in larger matrix TT-ranks, and the matrix TT-ranks are bounded over $6 \leq N \leq 25$. However, the computational cost for the DMRG approximation algorithm grows exponentially with $N$ because the algorithm has to read the entries of the $2^{N+1}$-vector at least once.

For comparison of performances of the SVD algorithms, we set $\epsilon = 10^{-8}, \delta = 2^{\min(0, -(N-17))}\epsilon$, and $K = 10$. In Figure 15(a) the computational costs of the TT-based algorithms grow logarithmically with the matrix size. The ALS-EIG and ALS-SVD have the least computational costs because the matrix TT-ranks are relatively quite small in this simulation. We can see that the computational costs of the ALS-EIG and MALS-EIG grow slightly faster than the ALS-SVD and MALS-SVD. In Figure 15(b) we can see that the maximum block TT-ranks are decreasing in $10 \leq N \leq 17$, and they slowly increase in $17 \leq N \leq 25$. 
Figure 13: Performances for $2^N \times 2^N$ random matrices with prescribed singular values for $N = 50$ and various $\beta$ values. (a) The computational time, (b) maximum block TT-rank of right singular vectors, and (c) relative error for singular values.
Figure 14: Maximum matrix TT-rank of a submatrix $A$ of Hilbert matrix

Figure 15: Performances for the $2^N \times 2^N - 1$ submatrices of Hilbert matrices with $10 \leq N \leq 25$. (a) Computational cost, and (b) maximum block TT-rank of the right singular vectors for $K = 10$ and $10 \leq N \leq 25$. 
Figure 16: Performances for the $2^N \times 2^N$ random tridiagonal matrices for $K = 10$ and $10 \leq N \leq 50$. (a) Computational cost and (b) maximum block TT-rank of the right singular vectors.

### 4.3 Random Tridiagonal Matrix

A tridiagonal matrix is a banded matrix whose nonzero entries are only on the main diagonal, the first diagonal above the main diagonal, and the first diagonal below the main diagonal. The matrix TT representation of a tridiagonal matrix is described in Appendix [C]. We randomly generated three vectors $a, b, c$ in vector TT format with TT-ranks $R_a = R$. Then we took absolute values of the TT-cores of $a$ so that entries of $a$ had nonnegative values. Finally, we normalized the three vectors as

$$\|a\| = 2N, \|b\| = \|c\| = N,$$

and we built the $2^N \times 2^N$ tridiagonal matrix $A$ whose main diagonal is $a$, super- and sub-diagonals are $b$ and $c$. The matrix TT-ranks of $A$ are bounded by $5R$, which are largely reduced after truncation.

For performance evaluation, we set $R = 8$, $\epsilon = 10^{-8}$, $\delta = \max(10^{-11}, 2^{-\min(0, -(N-17))})$, and $K = 10$. We computed the exact relative residual (35) at each sweep for stopping criterion. In this simulation, the TT-based SVD algorithms converged within $N_{\text{sweep}} = 3$ full sweeps.

Figure [16(a)] shows that the computational costs for the TT-based SVD algorithms are growing logarithmically with the matrix size over $10 \leq N \leq 50$. The ALS-SVD and MAL-SVD have the smallest computational costs. The ALS-EIG and MAL-EIG have relatively high computational costs because the matrix TT-ranks are relatively large in this case so the truncation of $A^T A$ was computationally costly. Figure [16(b)] shows that the maximum block TT-ranks are bounded by 20 and slowly decreasing as $N$ increases. We note that in this simulation the diagonal entries of the matrices were randomly generated and the 10 dominant singular values were close to each other, similarly as the identity matrix. We conclude that the TT-based SVD algorithms can accurately compute several dominant singular values and singular vectors even in the case that the singular values are almost identical.
4.4 Random Toeplitz Matrix

Toeplitz matrix is a square matrix that has constant diagonals. A Toeplitz matrix \( A \) of size \( 2^N \times 2^N \) is generated by the entries of its first row and first column. An explicit matrix TT representation of a Toeplitz matrix is described in [20]. See Appendix B for more details. We randomly generated a vector \( \mathbf{x} = [x_1, \ldots, x_{2N+1}]^T \) in TT format with fixed TT-ranks \( R_m = R \). Then, we converted \( \mathbf{x} \) into a Toeplitz matrix \( A \in \mathbb{R}^{2^N \times 2^N} \) in matrix TT format with entries

\[
a_{i,j} = x_{2^N+i-j}, \quad i, j = 1, 2, \ldots, 2^N.
\]

(44)

The matrix TT-ranks of \( A \) are bounded by twice the TT-ranks of \( x \), i.e., \( 2R \) [20].

Since the matrix \( A \) is generated randomly, we cannot expect that the block TT-ranks of the singular vectors are bounded over \( N \). Instead, we fix the maximum of the block TT-ranks, \( R_{\text{max}} \), and compare the computational times and relative residuals of the algorithms. We set \( R = 8, \delta = 10^{-8\min(0, -(N-17))}, K = 10, \) and \( N_{\text{sweep}} = 3 \).

Figures 17(a) and (b) show the performances for \( R_{\text{max}} = 20 \) and \( 10 \leq N \leq 25 \). In Figure 17(a) we can see that the computational costs of the TT-based algorithms grow logarithmically with the matrix size because the matrix TT-ranks and the block TT-ranks are bounded. In Figure 17(b), the relative residual values remain almost constantly below 0.1. Figures 17(c) and (d) show the computational costs and relative residuals for \( 10 \leq R_{\text{max}} \leq 40 \) and \( N = 50 \). We can see that the computational cost for the ALS-SVD is the smallest and is growing the most slowly as \( R_{\text{max}} \) increases.

5 Conclusion and Discussions

In this paper, we proposed new SVD algorithms for very large-scale structured matrices based on TT decompositions. Unlike previous researches focusing only on eigenvalue decomposition (EVD) of symmetric positive semidefinite matrices [8, 17, 21, 24, 27, 32, 38], the proposed algorithms do not assume symmetricity of the data matrix \( A \). We investigated the computational complexity of the proposed algorithms rigorously, and provided optimized ways of tensor contractions for the fast computation of the singular values. We conducted extensive simulations to demonstrate the effectiveness of the proposed SVD algorithms compared with the other TT-based algorithms which are based on the EVD of symmetric positive semidefinite matrices.

Once a very large-scale matrix is represented in matrix TT format, the proposed ALS-SVD and MALS-SVD algorithms can compute the SVD in logarithmic time complexity with respect to the matrix size under the assumption that the TT-ranks are bounded. Unlike the EVD-based methods, the proposed algorithms avoid truncation of the matrix TT-ranks of the product \( A^T A \) but directly optimize the maximization problem (1). In the simulated experiments, we demonstrated that the computational costs of the EVD-based algorithms are highly affected by the matrix TT-ranks, and the proposed methods are highly competitive compared with the EVD-based algorithms. Moreover, we showed that the proposed methods can compute the SVD of \( 2^{50} \times 2^{50} \) matrices accurately even in a few seconds on desktop computers.

The proposed SVD methods can compute a few dominant singular values and corresponding singular vectors of TT-structured matrices. The structured matrices used in the simulations are random matrices with prescribed singular values, Hilbert matrix, random tridiagonal matrix, and random Toeplitz matrix. The singular vectors are represented as block TT formats, and the TT-ranks are adaptively determined during iteration process. Moreover, we also presented the case of
Figure 17: Performances for \(2^N \times 2^N\) random Toeplitz matrices. The block TT-ranks of the left and right singular vectors are constrained to be bounded by \(R_{\text{max}}\). (a) Computational cost and (b) relative residual for \(R_{\text{max}} = 20\) and \(10 \leq N \leq 25\). (c) Computational cost and (b) relative residual for \(10 \leq R_{\text{max}} \leq 40\) and \(N = 25\).
random Toeplitz matrices, where the block TT-ranks of the singular vectors are not bounded as the matrix size increases. In this case, the proposed methods computed approximate solutions based on fixed TT-ranks with reasonable approximation errors. The computational cost will be much reduced if the $\delta$-truncated SVD step is replaced with the QR decomposition.

In the simulated experiments, in the case that the TT-based ALS and MALS algorithms fall into local minimum, we restarted the algorithm with new initial block TT tensors. Moreover, we observed that not only the initializations but also the truncation parameter $\delta$ for the $\delta$-truncated SVD highly affects the convergence. If $\delta$ value is too large, then the algorithm falls into local minimum and its accuracy does not improve any more. If $\delta$ value is too small, then the TT-ranks grow fastly and the computational cost increases. If a proper $\delta$ value is selected, then the algorithms converge usually in at most 3 full sweeps. Moreover, the MALS algorithm shows faster convergence than the ALS algorithm because the TT-ranks can be increased more fastly at each iteration.

The performance of the TT-based algorithms are highly dependent on the choice of the optimization algorithms for solving the reduced local problems. In the simulations we used the MATLAB function EIGS in order to obtain accurate singular values. Moreover, for the Hilbert matrices, we had to convert a vector into a vector TT decomposition via the DMRG method, which takes an additional computational cost. This approximation step might be improved by employing cross approximation method [36, 1].

The proposed algorithms rely on the optimization of the trace function described in the maximization problem \( \text{(1)} \), so they cannot be applied for computing $K$ smallest singular values directly. In Appendix A, we explained how the $K$ smallest singular values and corresponding singular vectors can be computed by using the EVD-based algorithms. In the future work, we will develop a more efficient method for computing a few smallest singular values and corresponding singular vectors based on TT decompositions.

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A Optimization Problems for Extremal Singular Values

The SVD of a matrix $A \in \mathbb{R}^{P \times Q}$ is closely related to the eigenvalue decomposition (EVD) of the following $(P + Q) \times (P + Q)$ matrix

$$B = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}.$$  

In this section, we show the relationship between the EVD optimization problems of $B$ and the SVD optimization problems of $A$.

A.1 Eigenvalues of $B$

We assume that $P \geq Q$. The SVD of $A \in \mathbb{R}^{P \times Q}$ can be expressed as

$$A = \begin{bmatrix} U_0 & U_0^\perp \end{bmatrix} \begin{bmatrix} \Sigma_0 \\ 0 \end{bmatrix} V_0^T,$$  

where $U_0 \in \mathbb{R}^{P \times Q}$, $U_0^\perp \in \mathbb{R}^{P \times (P - Q)}$, and $V_0 \in \mathbb{R}^{Q \times Q}$ are the matrices of singular vectors and $\Sigma_0 \in \mathbb{R}^{Q \times Q}$ is the diagonal matrix with nonnegative diagonal entries $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_Q$.

Lemma A.1. The EVD of $B$ can be written by

$$B = W_0 \Lambda_0 W_0^T,$$  

where

$$W_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} U_0 & U_0^\perp \sqrt{2}U_0^\perp \\ V_0 & -V_0 & 0 \end{bmatrix} \in \mathbb{R}^{(P + Q) \times (P + Q)},$$

$$\Lambda_0 = \begin{bmatrix} \Sigma_0 \\ -\Sigma_0 \\ 0 \end{bmatrix} \in \mathbb{R}^{(P + Q) \times (P + Q)}.$$

Proof. We can compute that $W_0^T W_0 = I_{P + Q}$. We can show that $BW_0 = W_0 \Lambda_0$. $\square$

We can conclude that the eigenvalues of $B$ consist of $\pm \sigma_1, \pm \sigma_2, \ldots, \pm \sigma_Q$, and an extra zero of multiplicity $P - Q$.  

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A.2 Maximal Singular Values

The $K$ largest eigenvalues of $B$ can be computed by solving the trace maximization problem

$$\maximize_{W} \quad \text{trace} (W^T B W)$$
$$\text{subject to} \quad W^T W = I_K. \quad (47)$$

Instead of building the matrix $B$ explicitly, we solve the equivalent maximization problem described as follows.

**Proposition A.2.** For $K \leq Q$, the maximization problem (47) is equivalent to

$$\maximize_{U,V} \quad \text{trace} (U^T A V)$$
$$\text{subject to} \quad U^T U = V^T V = I_K. \quad (48)$$

**Proof.** Let

$$W = \frac{1}{\sqrt{2}} \begin{bmatrix} U \\ V \end{bmatrix} \in \mathbb{R}^{(P+Q) \times K},$$

then

$$\text{trace} (W^T B W) = \text{trace} (U^T A V).$$

First, we can show that

$$\max_{W^T W = I_K} \text{trace} (W^T B W) \geq \max_{U^T U = V^T V = I_K} \text{trace} (U^T A V).$$

Next, we can show that the maximum value $\sigma_1 + \sigma_2 + \cdots + \sigma_K$ of $\text{trace} (W^T B W)$ is obtained by $\text{trace} (U^T A V)$ when $U$ and $V$ are equal to the first $K$ singular vectors of $U_0$ and $V_0$. \hfill \square

A.3 Minimal Singular Values

Suppose that $P = Q$. The $K$ minimal singular values of $A$ can be obtained by computing $2K$ eigenvalues of $B$ with the smallest magnitudes, that is, $\pm \sigma_Q, \pm \sigma_{Q-1}, \ldots, \pm \sigma_{Q-K+1}$. Computing the $2K$ eigenvalues of $B$ with the smallest magnitudes can be formulated by the following trace minimization problem

$$\minimize_{W} \quad \text{trace} (W^T B^2 W)$$
$$\text{subject to} \quad W^T W = I_{2K}. \quad (49)$$

We can translate the above minimization problem into the equivalent minimization problem without building the matrix $B$ explicitly as follows.

**Proposition A.3.** The minimization problem (49) is equivalent to the following two minimization problems if a permutation ambiguity is allowed:

$$\minimize_{V} \quad \text{trace} (V^T A^T A V)$$
$$\text{subject to} \quad V^T V = I_K \quad (50)$$
and

\[
\begin{align*}
\text{minimize} & \quad \text{trace} \left( U^T A A^T U \right) \\
\text{subject to} & \quad U^T U = I_K.
\end{align*}
\]

(51)

That is, the \( K \) minimal singular values of \( A \) can be calculated by applying the eigenvalue decomposition for \( A^T A \) and \( A A^T \).

**Proof.** Let

\[
W = \frac{1}{\sqrt{2}} \begin{bmatrix}
U & U \\
V & -V
\end{bmatrix} \in \mathbb{R}^{(P+Q) \times 2K},
\]

then we have

\[
\text{trace} \left( W^T B^2 W \right) = \text{trace} \left( U^T A A^T U \right) + \text{trace} \left( V^T A^T A V \right).
\]

By algebraic manipulation, we can derive that the constraint \( W^T W = I_{2K} \) is equivalent to \( U^T U = V^T V = I_K \).

**B  Explicit Tensor Train Representation of Toeplitz Matrix and Hankel Matrix**

Explicit TT representations of Toeplitz matrices are presented in [20]. In this section, we summarize some of the simplest results of [20], and extends them to Hankel matrix and rectangular submatrices.

First, the strong Kronecker product [26] between block matrices are defined as follows. Let \( \tilde{A} = \begin{bmatrix} A_{r_1, r_2} \end{bmatrix} \in \mathbb{R}^{R_1 \times R_2} \) be a \( R_1 \times R_2 \) block matrix with blocks \( A_{r_1, r_2} \in \mathbb{R}^{I_{r_1} \times I_{r_2}} \) and let \( \tilde{B} = \begin{bmatrix} B_{r_2, r_3} \end{bmatrix} \in \mathbb{R}^{R_2 \times R_3} \) be a \( R_2 \times R_3 \) block matrix with blocks \( B_{r_2, r_3} \in \mathbb{R}^{J_{r_2} \times J_{r_3}} \). The strong Kronecker product of \( \tilde{A} \) and \( \tilde{B} \) is defined by a \( R_1 \times R_3 \) block matrix

\[
\tilde{C} = [C_{r_1, r_3}] = \tilde{A} \otimes \tilde{B} \in \mathbb{R}^{R_1 I_{r_1} \times R_3 J_{r_3}},
\]

with blocks

\[
C_{r_1, r_3} = \sum_{r_2=1}^{R_2} A_{r_1, r_2} \otimes B_{r_2, r_3} \in \mathbb{R}^{I_{r_1} J_{r_2} \times J_{r_3} J_{r_3}}.
\]

In the case that the blocks \( A_{r_1, r_2} \) and \( B_{r_2, r_3} \) are scalars, the strong Kronecker product is equivalent to the matrix-by-matrix multiplication. Moreover, the matrix \( A \) in matrix TT format [9] can be rewritten as strong Kronecker products

\[
A = \tilde{A}^{(1)} \otimes \cdots \otimes \tilde{A}^{(N)},
\]

(52)

where \( \tilde{A}^{(n)} \in \mathbb{R}^{R_n \times R_n} \) are \( R_{n-1} \times R_n \) block matrices defined by

\[
\tilde{A}^{(1)} = \begin{bmatrix}
A_{1,1}^{(1)} & \cdots & A_{1,R_n}^{(1)}
\end{bmatrix}, \quad \tilde{A}^{(n)} = \begin{bmatrix}
A_{1,1}^{(n)} & \cdots & A_{1,R_n}^{(n)} \\
\vdots & \ddots & \vdots \\
A_{R_{n-1},1}^{(n)} & \cdots & A_{R_{n-1},R_n}^{(n)}
\end{bmatrix}, \quad \tilde{A}^{(N)} = \begin{bmatrix}
A_{1,1}^{(N)} \\
\vdots \\
A_{R_{n-1},1}^{(N)}
\end{bmatrix}
\]

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Theorem B.1 (An explicit matrix TT representation of Toeplitz matrix, [20]). Let

\[
T = \begin{bmatrix}
0 & s_1 & s_2 & \cdots & s_{2N-2} & s_{2N-1} \\
0 & s_1 & s_2 & \cdots & s_{2N-3} & s_{2N-2} \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\
0 & s_1 & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & \cdots & 0 \\
\end{bmatrix}.
\]

(53)

Similarly, the \(2^N \times 2^N\) upper anti-triangular Hankel matrix generated by \([s_1, s_2, \ldots, s_{2N-1}]^T\) is written by

\[
H = \begin{bmatrix}
s_{2N-1} & s_{2N-2} & \cdots & s_2 & s_1 & 0 \\
s_{2N-2} & s_{2N-3} & \cdots & s_1 & 0 & \vdots \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\
s_1 & 0 & \cdots & 0 & \cdots & 0 \\
0 & \cdots & 0 & \cdots & 0 & \cdots & \cdots \\
\end{bmatrix}.
\]

(54)

The matrix TT representations for the Toeplitz matrix and Hankel matrix are presented in the following theorems.

Theorem B.1 (An explicit matrix TT representation of Toeplitz matrix, [20]). Let

\[
I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad J = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}
\]

be \(2 \times 2\) matrices and let

\[
\bar{L}_1^{(1)} = \begin{bmatrix} I & J \end{bmatrix}, \quad \bar{L}_1^{(2)} = \cdots = \bar{L}_1^{(N-1)} = \begin{bmatrix} I & J \\ 0 & K \end{bmatrix}, \quad \bar{L}_1^{(N)} = \begin{bmatrix} J \\ K \end{bmatrix},
\]
\[
\bar{L}_2^{(1)} = \begin{bmatrix} J & 0 \end{bmatrix}, \quad \bar{L}_2^{(2)} = \cdots = \bar{L}_2^{(N-1)} = \begin{bmatrix} J & 0 \\ K & I \end{bmatrix}, \quad \bar{L}_2^{(N)} = \begin{bmatrix} 0 \\ I \end{bmatrix}
\]

be \(2 \times 2\) block matrices. We denote the \((q_n-1, q_n)\)th block of \(\bar{L}_{k_n}^{(n)}\) by \(L_{k_n}^{(n)}\) for \(q_n-1, q_n = 1, 2\), that is,

\[
\bar{L}_{k_n}^{(n)} = \begin{bmatrix} L_{k_n,1,1}^{(n)} \\ L_{k_n,1,2}^{(n)} \\ L_{k_n,2,1}^{(n)} \\ L_{k_n,2,2}^{(n)} \end{bmatrix}, \quad k_n = 1, 2.
\]

Suppose that \(s = [s_1, s_2, \ldots, s_{2N}]^T\) is represented in TT format as

\[
s_{k_1, k_2, \ldots, k_N} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} s_{1, k_1, r_1} s_{r_1, k_2, r_2} \cdots s_{R_{N-1}, k_N, 1}.
\]

Then, the upper triangular Toeplitz matrix \([53]\) is expressed in matrix TT format as

\[
T = \sum_{t_1=1}^{2R_1} \sum_{t_2=1}^{2R_2} \cdots \sum_{t_{N-1}=1}^{2R_{N-1}} T_{1,t_1}^{(1)} \otimes T_{t_1,t_2}^{(2)} \otimes \cdots \otimes T_{t_{N-1},1}^{(N)},
\]

(56)
where $T_{r_{n-1},t_n}^{(n)} \in \mathbb{R}^{2 \times 2}$ are defined by

$$T_{r_{n-1},q_{n-1},r_n,q_n}^{(n)} = \sum_{k_n=1}^{2} s_{r_{n-1},k_n,r_n}^{(n)} M_{q_{n-1},k_n,q_n}^{(n)}$$

for $r_n = 1, 2, \ldots, R_n$ and $q_n = 1, 2$.

The matrix TT representation for Toeplitz matrices can be extended to Hankel matrices as follows.

**Theorem B.2 (An explicit matrix TT representation of Hankel matrix).** Let

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad R = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

be $2 \times 2$ matrices and let

$$\widetilde{M}_1^{(1)} = \begin{bmatrix} P & Q \end{bmatrix}, \quad \widetilde{M}_1^{(2)} = \cdots = \widetilde{M}_1^{(N-1)} = \begin{bmatrix} P & Q \\ 0 & R \end{bmatrix}, \quad \widetilde{M}_1^{(N)} = \begin{bmatrix} Q \\ R \end{bmatrix}, \quad (58)$$

$$\widetilde{M}_2^{(1)} = \begin{bmatrix} Q & 0 \end{bmatrix}, \quad \widetilde{M}_2^{(2)} = \cdots = \widetilde{M}_2^{(N-1)} = \begin{bmatrix} Q & 0 \\ R & P \end{bmatrix}, \quad \widetilde{M}_2^{(N)} = \begin{bmatrix} 0 \\ P \end{bmatrix}$$

be $2 \times 2$ block matrices. We denote the $(q_{n-1},q_n)$th block of $\widetilde{M}_k^{(n)}$ by $M_{q_{n-1},k_n,q_n}^{(n)}$ for $q_{n-1},q_n = 1, 2$.

Suppose that $s = [s_1, s_2, \ldots, s_{2^N}]^T$ is represented in TT format as

$$s_{k_1,k_2,\ldots,k_N} = \sum_{r_{1,1}=1}^{R_1} \sum_{r_{2,1}=1}^{R_2} \cdots \sum_{r_{N-1,1}=1}^{R_{N-1}} s_{1,k_1,r_1}^{(1)} s_{2,k_2,r_2}^{(2)} \cdots s_{N-1,k_{N-1},r_{N-1}}^{(N-1)} s_{N,k_N}^{(N)},$$

Then, the upper anti-triangular Hankel matrix $[54]$ is expressed in matrix TT format as

$$H = \sum_{t_{1,1}=1}^{2R_1} \sum_{t_{2,1}=1}^{2R_2} \cdots \sum_{t_{N-1,1}=1}^{2R_{N-1}} H_{t_{1,1},t_{2,1}}^{(1)} \otimes H_{t_{1,1},t_{2,1}}^{(2)} \otimes \cdots \otimes H_{t_{N-1,1},t_{N-1,1}}^{(N)}, \quad (59)$$

where $H_{t_{1,1},t_{2,1}}^{(n)} \in \mathbb{R}^{2 \times 2}$ are defined by

$$H_{r_{n-1},q_{n-1},r_n,q_n}^{(n)} = \sum_{k_n=1}^{2} s_{r_{n-1},k_n,r_n}^{(n)} M_{q_{n-1},k_n,q_n}^{(n)}$$

for $r_n = 1, 2, \ldots, R_n$ and $q_n = 1, 2$.

The matrix TT representation of a submatrix of the Hankel matrix $H$ can be derived from the representation of $H$ $[50]$. 

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Corollary B.3. The $2^N \times 2^N - 1$ submatrix $H(:, 1 : 2^N - 1)$ of the Hankel matrix $H$ can be written by

$$H(:, 1 : 2^N - 1) = \sum_{t_1=1}^{2R_1} \sum_{t_2=1}^{2R_2} \cdots \sum_{t_{N-2}=1}^{2R_{N-2}} H^{(1)}_{t_1, t_1} \otimes H^{(2)}_{t_2, t_2} \otimes \cdots \otimes \left( \sum_{t_{N-1}=1}^{2R_{N-1}} H^{(N-1)}_{t_{N-2}, t_{N-1}} \otimes H^{(N)}_{t_{N-1}, 1} (:, 1) \right),$$

where $H^{(N)}_{i_{N-1}, 1} (:, 1)$ is the first column vector of $H^{(N)}_{i_{N-1}, 1}$.

In the same way, we can derive the matrix TT representation of a top-left corner submatrix of the Hankel matrix.

C Explicit Tensor Train Representation of Tridiagonal Matrix

A shift matrix $F \in \mathbb{R}^{P \times P}$ is a banded binary matrix whose nonzero entries are on the first diagonal above the main diagonal. The $(i,j)$th entry of $F$ is $f_{ij} = 1$ if $i + 1 = j$, and $f_{ij} = 0$ otherwise. The following lemma describes a TT representation for the shift matrix.

Lemma C.1 (An explicit matrix TT representation of the shift matrix). Let $	ilde{L}_1^{(n)}$ and $\tilde{M}_1^{(n)}$, $n = 1, 2, \ldots, N$, be the block matrices defined by (55) and (58). The shift matrix $F \in \mathbb{R}^{2^N \times 2^N}$ is represented in TT format [20] by

$$F = \tilde{L}_1^{(1)} \otimes \tilde{L}_1^{(2)} \otimes \cdots \otimes \tilde{L}_1^{(N)}.$$

The transpose of the shift matrix $F$ is represented in TT format by

$$F^T = \tilde{M}_1^{(1)} \otimes \tilde{M}_1^{(2)} \otimes \cdots \otimes \tilde{M}_1^{(N)}.$$

A tridiagonal matrix $A \in \mathbb{R}^{2^N \times 2^N}$ generated by three vectors $a, b, c \in \mathbb{R}^{2^N}$ is written by

$$A = \begin{bmatrix} b_1 & c_2 & 0 & & & & \\ a_1 & b_2 & c_3 & 0 & & & \\ & \ddots & \ddots & \ddots & & & \\ & & 0 & a_{2N-2} & b_{2N-1} & c_{2N} \\ & & & & 0 & a_{2N-1} & b_{2N} \end{bmatrix}.$$

Suppose that the vectors $a, b, c$ are given in vector TT format. Then, by using the basic operations [33], we can compute the tridiagonal matrix $A$ by

$$A = F^T \text{diag}(a) + \text{diag}(b) + F \text{diag}(c).$$