Faster Tensor Train Decomposition for Sparse Data

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Abstract

In recent years, the application of tensors has become more widespread in fields that involve data analytics and numerical computation. Due to the explosive growth of data, low-rank tensor decompositions have become a powerful tool to harness the notorious curse of dimensionality. The main forms of tensor decomposition include CP decomposition, Tucker decomposition, tensor train (TT) decomposition, etc. Each of the existing TT decomposition algorithms, including the TT-SVD and randomized TT-SVD, is successful in the field, but neither can both accurately and efficiently decompose large-scale sparse tensors. Based on previous research, this paper proposes a new quasi-best fast TT decomposition algorithm for large-scale sparse tensors with proven correctness and the upper bound of its complexity is derived. In numerical experiments, we verify that the proposed algorithm can decompose sparse tensors faster than the TT-SVD, and have more speed, precision and versatility than randomized TT-SVD, and it can be used to decomposes arbitrary high-dimensional tensor without losing efficiency when the number of non-zero elements is limited. The new algorithm implements a large-scale sparse matrix TT decomposition that was previously unachievable, enabling tensor decomposition based algorithms to be applied in larger-scale scenarios.

Keywords: tensor train decomposition, sparse data, TT-rounding, parallel-vector rounding

1. Introduction

In the fields of physics, data analytics, scientific computing, digital circuit design, machine learning, etc., data are often organized into a matrix or tensor so that various sophisticated data processing techniques can be applied. One example of such a technique is the low-rank matrix decomposition. It is often

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implemented through the well-known singular value decomposition (SVD).

$$A = U\Sigma V^{\top},$$

where $A \in \mathbb{R}^{n \times m}$, $U \in \mathbb{R}^{n \times n}$, $\Sigma \in \mathbb{R}^{n \times m}$, $V \in \mathbb{R}^{m \times m}$. U and V are orthogonal matrices, and Σ is a diagonal matrix whose diagonal elements (a.k.a. singular values) σ_i , $(1 \le i \le \min(m, n))$ are non-negative and non-ascending.

In recent years, tensors, as a high-dimensional extension of matrices, have also been applied as a powerful and universal tool. In order to overcome the curse of dimensionality (the data size of a tensor increases exponentially with the increase of the dimensionality of the tensor), people have extended the notion of a low-rank matrix decomposition to tensors, proposing tensor decompositions such as the CP decomposition [1], the Tucker decomposition [2] and the tensor train (TT) decomposition [3]. Among them, the TT decomposition transforms the storage complexity of an n^d tensor into $O(dnr^2)$, where r is the maximal TT rank, effectively removing the exponential dependence on d. The TT decomposition is advantageous for processing large data sets and has been applied to problems like linear equation solution [4], electronic design automation (EDA) [5, 6, 7], system identification [8], large-scale matrix processing [9, 10, 11], image/video inpainting [12, 13], data mining [14] and machine learning [15, 16, 17].

To realize the TT decomposition, the TT-SVD algorithm [3] was proposed. It involves a sequence of SVD computations on reshaped matrices. For a large-scale sparse tensor, the TT-SVD consumes excessive computing time and memory usage. Another method employs "cross approximation" to perform low-rank TT-approximations [18, 19], but it still needs too many calculations to find a good representation. Recently, a randomized TT-SVD algorithm [20] was proposed, which incorporates the randomized SVD algorithm [21] into the TT-SVD algorithm so as to reduce the runtime for converting a sparse tensor. However, due to the inaccuracy of the randomized SVD, the randomized TT-SVD algorithm usually results in the TT with exaggerated TT ranks or insufficient accuracy. This largely limits its application.

In this work, we propose a fast and effective TT decomposition algorithm specifically for large sparse data tensors. It includes the steps of constructing an exact TT with nonzero fibers, more efficient parallel-vector rounding and revised TT-rounding. The new algorithm, called FastTT, produces the same compact TT representation as the TT-SVD algorithm [3], but exhibits a significant runtime advantage for large sparse data. We have also extended the algorithm to convert a matrix into the "matrix in TT-format", also known as a matrix product operator (MPO). In addition, dynamic approaches are proposed to choose the parameters in the FastTT algorithm. Experiments are carried out on sparse data in problems of image/video inpainting, linear equation solution, and data analysis. The results show that the proposed algorithm without loss of accuracy or an increase of the TT ranks. The speedup ratios are up to 9.6X for the image/video inpainting, 240X for the linear equation

and 35X for the sparse data processing, respectively. The experimental results also reveal the effectiveness of the proposed dynamic approaches for choosing the parameters in the FastTT algorithm, and the advantages of FastTT over TT-cross and the randomized TT-SVD algorithm [20]. For reproducibility, we have shared the C++ codes of the proposed algorithms and experimental data on https://github.com/lljbash/FastTT.

2. Notations and Preliminaries

In this article we use boldface capital calligraphic letters (e.g. \mathcal{A}) to denote tensors, boldface capital letters (e.g. \mathcal{A}) to denote matrices, boldface letters (e.g. \mathcal{A}) to denote vectors, and roman (e.g. \mathcal{A}) or Greek (e.g. α) letters to denote scalars.

2.1. Tensor

Tensors are a high-dimensional generalization of matrices and vectors. A one-dimensional array $\boldsymbol{a} \in \mathbb{R}^n$ is called a vector, and a two-dimensional array $\boldsymbol{A} \in \mathbb{R}^{n_1 \times n_2}$ is called a matrix. When the dimensionality is extended to $d \geq 3$, the d-dimensional array $\boldsymbol{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ is called a d-way tensor. The positive integer d is defined as the **order** of the tensor. (n_1, n_2, \cdots, n_d) are the **dimensions** of the tensor, where each n_k is the dimension of a particular mode. Vectors and matrices can be considered as 1-way and 2-way tensors, respectively.

2.2. Basic Tensor Arithmetic

Definition 1. Vectorization. If we rearrange the entries of $\mathbf{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ into a vector $\mathbf{b} \in \mathbb{R}^{\prod_{k=1}^d n_k}$, where

$$a_{i_1,i_2,\cdots,i_d} = b_{\sum_{k=1}^{d-1} [(i_k-1) \prod_{l=k+1}^d n_l] + i_d},$$

then the vector \boldsymbol{b} is called the vectorization of the tensor $\boldsymbol{\mathcal{A}}$, represented as $\text{vec}(\boldsymbol{\mathcal{A}})$.

Definition 2. Reshaping. Like vectorization, if we rearrange the entries of \mathcal{A} into anther tensor \mathcal{B} satisfying $\text{vec}(\mathcal{A}) = \text{vec}(\mathcal{B})$, then the tensor \mathcal{B} is called the reshaping of \mathcal{A} , represented as reshape(\mathcal{A} , Dims), where Dims denotes the dimensions of \mathcal{B} . In fact, vectorization is a special kind of reshaping.

Definition 3. Unfolding [3]. Unfolding is also a kind of reshaping. If we reshape $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ into a matrix $\mathbf{B} \in \mathbb{R}^{m_1 \times m_2}$ where $m_1 = \prod_{j=1}^k n_j, m_2 = \prod_{j=k+1}^d n_j$, then \mathbf{B} is called the k-unfolding of \mathcal{A} , represented as unfold_k(\mathcal{A}).

Definition 4. Contraction. Contraction is the tensor generalization of matrix product. For two tensors $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_{d_1}}$ and $\mathcal{B} \in \mathbb{R}^{m_1 \times m_2 \times \cdots \times m_{d_2}}$

satisfying $n_{k_1} = m_{k_2}$, their (k_1, k_2) -contraction $\mathcal{C} = \mathcal{A} \circ_{k_1}^{k_2} \mathcal{B}$ is defined as

$$c_{i_1\cdots i_{k_1-1}j_1\cdots j_{k_2-1}j_{k_2+1}\cdots j_{d_2}i_{k_1+1}\cdots i_{d_1}} = \sum_{l=1}^{n_{k_1}} a_{i_1\cdots i_{k_1-1}li_{k_1+1}\cdots i_{d_1}} b_{j_1\cdots j_{k_2-1}lj_{k_2+1}\cdots j_{d_2}},$$

where $C \in \mathbb{R}^{n_1 \times \cdots \times n_{k_1-1} \times m_1 \times \cdots \times m_{k_2-1} \times m_{k_2+1} \times \cdots \times m_{d_2} \times n_{k_1+1} \times \cdots \times n_{d_1}}$. If k_1 and k_2 are not specified, $A \circ B$ means the $(d_1, 1)$ -contraction of A and B.

Definition 5. Tensor-matrix product. The k-product of a tensor \mathcal{A} and a matrix \mathbf{B} can be defined as tensor contraction if the matrix is treated as a 2-way tensor \mathcal{B} .

$$\mathcal{A} \times_k B = \mathcal{A} \circ_k^1 \mathcal{B}.$$

Definition 6. Rank-1 tensor. A rank-1 *d*-way tensor can be written as the outer product

$$\mathbf{A} = \mathbf{u}^{(1)} \circ \mathbf{u}^{(2)} \circ \cdots \circ \mathbf{u}^{(d)},$$

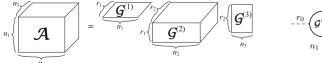
of d column vectors $\boldsymbol{u}^{(1)} \in \mathbb{R}^{n_1}, \dots, \boldsymbol{u}^{(d)} \in \mathbb{R}^{n_d}$. The entries of $\boldsymbol{\mathcal{A}}$ can be computed as $a_{i_1 i_2 \cdots i_d} = u_{i_1}^{(1)} u_{i_2}^{(2)} \cdots u_{i_d}^{(d)}$.

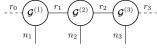
2.3. Tensor Train Decomposition

A tensor train decomposition [3], shown in Figure 1a, represents a d-way tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ with two 2-way tensors and (d-2) 3-way tensors:

$$\mathcal{A} = \mathcal{G}^{(1)} \circ \mathcal{G}^{(2)} \circ \cdots \circ \mathcal{G}^{(d)}$$

where $\mathcal{G}^{(k)} \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ is the k-th core tensor. Per definition, $r_0 = r_d = 1$ such that $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(d)}$ are actually matrices. The dimensions r_0, r_1, \ldots, r_d of the auxiliary indices are called the tensor-train (TT) ranks. When all the TT ranks have the same value, then we can just call it the TT rank.





- (a) A 3-way tensor and its TT decomposition
- (b) TT diagram of a 3-way tensor

Figure 1: Graphical illustrations of the tensor train (TT) decomposition, where a 3-way tensor \mathcal{A} is decomposed into two 2-way tensors $\mathcal{G}^{(1)}$, $\mathcal{G}^{(3)}$ and a 3-way tensor $\mathcal{G}^{(2)}$.

Figure 1b shows a very convenient graphical representation [8] of a tensor train. In this diagram, each circle represents a tensor where each "leg" attached to it denotes a particular mode of the tensor. The connected line between two circles represents the contraction of two tensors. The dimension is labeled besides each "leg". Figure 1b also illustrates a simple tensor network, which is

a collection of tensors that are interconnected through contractions. By fixing the second index of $\mathcal{G}^{(k)}$ to i_k , we obtain a matrix $\mathcal{G}_{i_k}^{(k)}$ (actually a vector if k=1 or k=d). Then the entries of \mathcal{A} can be computed as

$$a_{i_1 i_2 \cdots i_d} = \mathcal{G}_{i_1}^{(1)} \mathcal{G}_{i_2}^{(2)} \cdots \mathcal{G}_{i_d}^{(d)}.$$

The tensor train decomposition can be computed with the TT-SVD algorithm [3], which consists of doing d-1 consecutive reshapings and matrix SVD computations. It is described as Algorithm 1. The expression rank_{δ}(C) denotes the number of remaining singular values after the δ -truncated SVD. An advantage of TT-SVD is that a quasi-optimal approximation can be obtained with a given error bound and an automatic rank determination.

Algorithm 1 TT-SVD [3, p. 2301]

Input: a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times ... \times n_d}$, desired accuracy tolerance ε .

Output: Core tensors $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(d)}$ of the TT-approximation \mathcal{B} to \mathcal{A} with TT

ranks r_k $(k = 0, 1, \dots, d)$ satisfying

$$\|\mathcal{A} - \mathcal{B}\|_F \le \varepsilon \|\mathcal{A}\|_F$$
.

- 1: Compute truncation parameter $\delta = \frac{\varepsilon}{\sqrt{d-1}} \| \mathcal{A} \|_F$.
- 2: $\mathcal{C} := \mathcal{A}, r_0 := 1$.
- 3: **for** k = 1 to d 1 **do**
- $C := \text{reshape}(\mathcal{C}, [r_{k-1}n_k, \prod_{i=k+1}^d n_i]).$ Compute δ -truncated SVD: $C = U\Sigma V^T + E$, $||E||_F \leq \delta$, $r_k :=$ $\operatorname{rank}_{\delta}(\boldsymbol{C}).$
- $\mathcal{G}^{(k)} := \text{reshape}(\boldsymbol{U}, [r_{k-1}, n_k, r_k]).$
- $\mathcal{C}\coloneqq \mathbf{\Sigma} \mathbf{V}^T$.
- 8: end for
- 9: $oldsymbol{\mathcal{G}}^{(d)} := oldsymbol{\mathcal{C}}$
- 10: Return tensor \mathcal{B} in TT-format with cores $\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)}$.

We define the FLOP count of the TT-SVD algorithm as f_{TTSVD} . Then

$$f_{\text{TTSVD}} \approx \sum_{i=1}^{d-1} \left[f_{\text{SVD}} \left(r_{i-1} n_i, \prod_{j=i+1}^{d} n_j \right) \right],$$
 (1)

where $f_{\text{SVD}}(m,n) = C_{\text{SVD}} m n \min(m,n)$ is the FLOP count of performing the economic SVD for an $m \times n$ dense matrix.

A big problem with Algorithm 1 is the large computation cost of δ -truncated SVD on large-scale unfolded matrices when the dimensions grow. A possible solution is to replace SVD with more economic decomposition like pseudo-skeleton decomposition [22]. TT-cross [18, 19] is a multidimensional generalization of the skeleton decomposition to the tensor case. The algorithm uses a sweep strategy and can produce TT-approximates with given accuracy or maximal ranks. The time complexity of TT-cross depends on d linearly.

As for decomposing large-scale sparse tensors, a simple idea is to employ the truncated SVD algorithm based on Krylov subspace iterative method, e.g. the built-in function svds in Matlab. However, svds requests a truncation rank as input, and thus cannot be directly applied here. Moreover, the sparsity can only be taken advantage of at the first iteration step of Algorithm 1. After the first truncated SVD, the tensor becomes dense and thus the computation cannot be reduced.

2.4. Rounding

Sometimes one is given tensor data already in the TT-format but with suboptimal TT-ranks. In order to save storage and speed up the following computation, one can reduce the TT-ranks while maintaining accuracy, through a procedure called *rounding*. It is realized with the TT-rounding algorithm [3] (Algorithm 2). The algorithm is based on the same principle as TT-SVD and also produces quasi-optimal TT-ranks with a given error bound. TT-rounding can be of great use in cases where a large tensor is represented in TT-format.

Algorithm 2 TT-rounding [3, p. 2305]

Input: Cores $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(d)}$ of the TT-format tensor \mathcal{A} with TT-ranks r_1, \ldots, r_{d-1} , desired accuracy tolerance ε .

Output: Cores $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(d)}$ of the TT-approximation \mathcal{B} to \mathcal{A} in the TT-format with TT-ranks r_1, \ldots, r_{d-1} . The computed approximation satisfies

$$||\mathcal{A} - \mathcal{B}||_F \leq \varepsilon ||\mathcal{A}||_F$$
.

```
1: Compute truncation parameter \delta = \frac{\varepsilon}{\sqrt{d-1}} \|\mathcal{A}\|_F.

2: for k = d, \dots, 2 do

3: G \coloneqq \text{unfold}_1^T(\mathcal{G}^{(k)}).

4: Compute economic QR decomposition G = QR, r_{k-1} \coloneqq \text{rank}(G).

5: \mathcal{G}^{(k)} \coloneqq \text{reshape}(Q^T, [r_{k-1}, n_k, r_k]), \mathcal{G}^{(k-1)} \coloneqq \mathcal{G}^{(k-1)} \times_3 R^T.

6: end for

7: for k = 1, \dots, d-1 do

8: G \coloneqq \text{unfold}_2(\mathcal{G}^{(k)}).

9: Compute \delta-truncated SVD: G = U\Sigma V^T + E, \|E\|_F \le \delta, r_k \coloneqq \text{rank}_{\delta}(C).

10: \mathcal{G}^{(k)} \coloneqq \text{reshape}(U, [r_{k-1}, n_k, r_k]), \mathcal{G}^{(k+1)} \coloneqq \mathcal{G}^{(k+1)} \times_1 (\Sigma V^T).

11: end for

12: \mathcal{G}^{(d)} \coloneqq \mathcal{C}

13: Return tensor \mathcal{B} in TT-format with cores \mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)}.
```

Parallel-vector rounding [23] is another rounding method which replaces the truncated SVD with Deparallelisation (Algorithm 3). It removes the paralleled

columns of an $a \times b$ matrix in $O(ab\alpha)$ time, where α is the number of nonparallel columns. Parallel-vector rounding is lossless, runs much faster than TT-rounding and can preserve the sparsity of TT. However, it usually cannot reduce the TT-ranks much; its effectiveness highly depends on the parallelism in TT-cores. Therefore, the parallel-vector rounding is suitable for a constructed sparse TT, rather than the construction of a TT.

Algorithm 3 Deparallelisation [23, Appendix B]

```
Input: Matrix M \in \mathbb{R}^{a \times b}.
Output: Matrix N \in \mathbb{R}^{a \times \beta}, T \in \mathbb{R}^{\beta \times b} s.t. M = \tilde{M} \times T and N has at most as
    many columns as M and no two columns which are parallel to each other.
 1: Let K be the set of kept columns, empty initially.
 2: Let T be the dynamically-resized transfer matrix.
 3: for every column index j \in [1, b] do
       for every kept index i \in [1, |K|] do
 4:
         if the j-th column M_{:j} is parallel to column K_i then
 5:
            Set T_{i,j} to the prefactor between the two columns.
 6:
 7:
            add M_{:j} to K, set T_{|K|,j} = 1.
 8:
         end if
 9:
       end for
10:
11: end for
12: Construct N by horizontally concatenating the columns stored in K.
13: Return N and T.
```

3. Faster tensor train decomposition of sparse tensor

The TT-SVD algorithm does not take advantage of the possible sparsity of data since the δ -truncated SVD is used. In this section, we propose a new algorithm for computing the TT decomposition of a sparse tensor whereby the sparsity is explicitly exploited. The key idea is to rearrange the data in such a way that the desired TT decomposition can be written down explicitly, followed by a parallell-vector rounding step.

3.1. Constructing TT with nonzero p-fibers

For a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ and a given integer p that satisfies $1 \leq p \leq d$, we define a p-fiber of a tensor as a fiber of the tensor in the direction e_p . Figure 2 shows a 1-fiber, a 2-fiber and a 3-fiber of a 3-d tensor. We can specify a p-fiber of \mathcal{A} by fixing the indices except the p-th dimension $i_p = (i_1, \dots, i_{p-1}, i_{p+1}, \dots, i_d)$,

$$\boldsymbol{v}_p(\boldsymbol{i}_p) \coloneqq \boldsymbol{\mathcal{A}}(i_1, \dots, i_{p-1}, :, i_{p+1}, \dots, i_d).$$
 (2)

Then a tensor \mathcal{A}_1 with only one non-zero p-fiber $v_p(i_p)$ can be easily formed as the outer product of the p-fiber and d-1 standard basis vector and is thus a

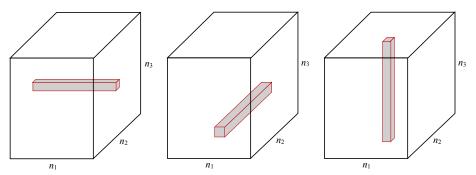


Figure 2: A 1-fiber, a 2-fiber and a 3-fiber of tensor $\mathbf{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$.

rank-1 tensor,

$$\mathcal{A}_1 = e_{i_1} \circ \cdots \circ e_{i_{n-1}} \circ v_p(i_p) \circ e_{i_{n+1}} \circ \cdots \circ e_{i_d}. \tag{3}$$

Suppose we have R nonzero p-fiber of sparse tensor \mathcal{A} with indices $(i_1, \ldots, i_{p-1}, i_{p+1}, \ldots, i_d)$ forming a set S_p with $|S_p| = R$. Then, \mathcal{A} can be represented as the sum of R rank-1 tensors,

$$\mathcal{A} = \sum_{(i_1, \dots, i_{p-1}, i_{p+1}, \dots, i_d) \in S_p} \mathbf{e}_{i_1} \circ \dots \circ \mathbf{e}_{i_{p-1}} \circ \mathbf{v}_{i_1, \dots, i_{p-1}, i_{p+1}, \dots, i_d} \circ \mathbf{e}_{i_{p+1}} \circ \dots \circ \mathbf{e}_{i_d},$$
(4)

where $e_{i_k} \in \mathbb{R}^{n_k}$ is the standard basis vector. Next, we are going to construct a tensor train based on this representation.

Lemma 1. Any rank-1 tensor is equivalent to a tensor train whose TT rank is 1.

$$\mathbf{v}_1 \circ \mathbf{v}_2 \circ \ldots \circ \mathbf{v}_d = \mathbf{\mathcal{V}}^{(1)} \circ \mathbf{\mathcal{V}}^{(2)} \circ \ldots \circ \mathbf{\mathcal{V}}^{(d)},$$
 (5)

where $\mathbf{v}_k \in \mathbb{R}^{n_k}$, $(k = 1, \dots, d)$, $\mathbf{\mathcal{V}}^{(1)} = \operatorname{reshape}(\mathbf{v}_1, [n_1, 1])$, $\mathbf{\mathcal{V}}^{(d)} = \operatorname{reshape}(\mathbf{v}_d, [1, n_d])$, and $\mathbf{\mathcal{V}}^{(k)} = \operatorname{reshape}(\mathbf{v}_k, [1, n_k, 1])$ for 1 < k < d.

Lemma 2. [3, p. 2308] Suppose we have two tensors $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times ... \times n_d}$ and $\mathcal{B} \in \mathbb{R}^{n_1 \times n_2 \times ... \times n_d}$ in the TT format,

$$a_{i_1 i_2 \cdots i_d} = \mathcal{A}_{i_1}^{(1)} \mathcal{A}_{i_2}^{(2)} \cdots \mathcal{A}_{i_d}^{(d)},$$

$$b_{i_1 i_2 \cdots i_d} = \mathcal{B}_{i_1}^{(1)} \mathcal{B}_{i_2}^{(2)} \cdots \mathcal{B}_{i_d}^{(d)}.$$

The TT cores of the sum $\mathcal{C} = \mathcal{A} + \mathcal{B}$ in the TT format then satisfy

$$\mathcal{C}_{i_k}^{(k)} = \begin{bmatrix} \mathcal{A}_{i_k}^{(k)} & \mathbf{O} \\ \mathbf{O} & \mathcal{B}_{i_k}^{(k)} \end{bmatrix}, \ k = 2, \dots, d - 1,$$

$$\mathcal{C}_{i_1}^{(1)} = \begin{bmatrix} \mathcal{A}_{i_1}^{(1)} & \mathcal{B}_{i_1}^{(1)} \end{bmatrix}, \ \mathcal{C}_{i_d}^{(d)} = \begin{bmatrix} \mathcal{A}_{i_d}^{(d)} \\ \mathcal{B}_{i_d}^{(d)} \end{bmatrix},$$
(6)

where O denotes a zero matrix of appropriate dimensions.

The proof of Lemma 1 and 2 can be easily derived from Definition 4 to 6 and the definition of the tensor train decomposition.

Based on (4) and Lemma 1 and 2, we have the following theorem.

Theorem 3. A sparse tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times ... \times n_d}$ can be transformed into an equivalent tensor train with TT rank R, where R is the number of nonzero p-fiber in \mathcal{A} $(1 \leq p \leq d)$. If $p \neq 1$ or d,

$$\mathbf{A} = \mathbf{P}^{(1)} \circ \dots \circ \mathbf{P}^{(p-1)} \circ \mathbf{V} \circ \mathbf{P}^{(p+1)} \circ \dots \circ \mathbf{P}^{(d)}, \tag{7}$$

where $\mathcal{P}^{(k)} \in \{0,1\}^{R \times n_j \times R}$, $(2 \le k \le d, k \ne p)$, $\mathcal{P}^{(1)} \in \{0,1\}^{1 \times n_1 \times R}$, $\mathcal{P}^{(d)} \in \{0,1\}^{R \times n_d \times 1}$, and $\mathcal{V} \in \mathbb{R}^{R \times n_p \times R}$. Similar expressions hold for the situations with p = 1 or d.

The TT cores $\mathcal{P}^{(k)}$ and \mathcal{V} in Theorem 3 are sparse tensors, whose nonzero distributions are illustrated in Figure 3. Each horizontal bar depicted in Figure 3 is a standard basis vector \mathbf{e}_{i_k} for $\mathcal{P}^{(k)}$ or a p-fiber \mathbf{v} for \mathcal{V} . The derived matrices $(\mathcal{P}_{i_k}^{(k)}$ and $\mathcal{V}_{i_p})$ from these TT cores are all diagonal matrices. Furthermore, each of the $\mathcal{P}^{(k)}$ cores is very sparse, as the nonzero elements consist of only R 1's.

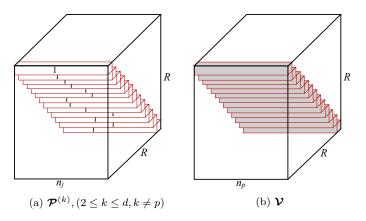


Figure 3: The nonzero distributions of $\mathcal{P}^{(k)}$, $(2 \le k \le d, k \ne p)$ and \mathcal{V} .

3.2. More efficient parallel-vector rounding

From Figure 3, it is obvious that $\mathcal{P}^{(k)}$ are very sparse and the elements are arranged regularly. Hence parallel-vector rounding should be very effective on the TT obtained in Theorem 3. In order to maximize the effect of Deparallelisation, we modify the original algorithm so that the decomposition on the less regular core \mathcal{V} is avoided. By combining this modified algorithm with Theorem 3, we obtain a lossless sparse tensor to TT conversion algorithm, described as Algorithm 4, where Depar refers to the Deparallelisation algorithm.

Algorithm 4 Sparse TT conversion with modified parallel-vector rounding Input: A sparse tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times ... \times n_d}$, an integer p (1 .**Output:** Core tensors $\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)}$ of TT-format tensor \mathcal{B} which is equivalent to \mathcal{A} with TT ranks \tilde{r}_k $(k = 0, 1, \dots, d)$. 1: Initialize empty cores $\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)}$ for TT-format tensor \mathcal{B} . 2: for every $v \in \{\text{all } R \text{ nonzero } p\text{-subvectors of } A\}$ do Determine (d-1) e_i vectors in (4). Construct rank-1 TT \mathcal{T} with \boldsymbol{v} and \boldsymbol{e} vectors as Lemma 1. $\mathcal{B} := \mathcal{B} + \mathcal{T}$, which means $\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)}$ are update with (6). 6: end for 7: $\tilde{r}_0 \coloneqq 1$. 8: **for** k = 1, ..., p - 1 **do** $[N,T] := \overline{\operatorname{Depar}}(\operatorname{unfold}_2(\mathcal{G}^{(k)})), \text{ where } N \in \mathbb{R}^{\tilde{r}_{k-1}n_k \times \tilde{r}_k}, T \in \mathbb{R}^{\tilde{r}_k \times R}.$ $\boldsymbol{\mathcal{G}}^{(k)} \coloneqq \operatorname{reshape}(\boldsymbol{N}, [\tilde{r}_{k-1}, n_k, \tilde{r}_k]).$ $\mathcal{G}^{(k+1)} \coloneqq \mathcal{G}^{(k+1)} \times_1 T^T$. 11: 12: end for 13: $\tilde{r}_d \coloneqq 1$. 14: **for** k = d, ..., p + 1 **do** $[m{N},m{T}]\coloneqq ext{Depar}(ext{unfold}_1^T(m{\mathcal{G}}^{(k)})), ext{ where } m{N}\in\mathbb{R}^{ ilde{r}_kn_k imes ilde{r}_{k-1}},m{T}\in\mathbb{R}^{ ilde{r}_{k-1} imes R}.$ $\mathcal{G}^{(k)} := \operatorname{reshape}(\mathbf{N}^T, [\tilde{r}_{k-1}, n_k, \tilde{r}_k]).$ $\mathcal{G}^{(k-1)} := \mathcal{G}^{(k-1)} \times_3 \mathbf{T}^T.$ 16: 17: 18: end for 19: Return tensor \mathcal{B} in TT-format with cores $\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)}$.

The correctness of Algorithm 4 is due to Theorem 3 and the associative property of matrix multiplications. The graphical representations of the decomposition forms during the algorithm execution are shown in Figure 4 for a 4-way TT.

The original Deparallelisation algorithm (Algorithm 3) dose not consider the special pattern of the core tensors. An important observation from Figure 3 is that each $\mathcal{P}^{(k)}$ obtained by Theorem 3 is consisted of R "diagonally" 2-fiber with only one "1". This means all unfoldings unfold₂($\mathcal{P}^{(k)}$) for k < p and unfold₁ $(\mathcal{P}^{(k)})$ for k > p are so-called quasi-permutation matrices.

Definition 7. Quasi-permutation matrix. If each column of a matrix has only one nonzero element with a value of 1, then the matrix is called a quasi-

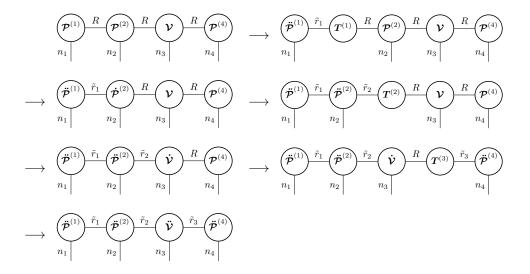


Figure 4: The graphical representations of the decomposition forms during the Algorithm 4 execution for a 4-way TT (p=3)

permutation matrix. A quasi-permutation matrix $\pmb{A} \in \mathbb{R}^{n \times m}$ can be represented as

$$\mathbf{A} = \begin{bmatrix} \mathbf{e}_{i_1} & \mathbf{e}_{i_2} & \cdots & \mathbf{e}_{i_m} \end{bmatrix}, \tag{8}$$

where e_k denotes a standard basis vector in the *n*-dimensional Euclidean space \mathbb{R}^n with a 1 in the *k*th coordinate and 0's elsewhere.

Example 1. Obviously, a permutation or identity matrix belongs to the class of quasi-permutation matrices.

Corollary 4. For Algorithm 3, if the input matrix M is a quasi-permutation matrix, matrix N and the transfer matrix T will also be quasi-permutation matrices.

It turns out that this property of $\mathcal{P}^{(k)}$ is maintained throughout the whole process of parallel-vector rounding, which will enable a more efficient implementation of Deparallelisation.

Theorem 5. In Algorithm 4, each input matrix of the function **Depar** is a quasi-permutation matrix.

Proof. $\mathcal{G}^{(1)}$ is definitely a quasi-permutation matrix according to (5) and (6). For $2 \leq k < p$, $\mathcal{G}^{(k)}$ changes twice during Algorithm 4 — once in iteration k-1 and once in iteration k. Like in Figure 4, we use $\mathcal{P}^{(k)}$, $\dot{\mathcal{P}}^{(k)}$ and $\ddot{\mathcal{P}}^{(k)}$ to denote the three stages of $\mathcal{G}^{(k)}$. The input matrix of *Depar* in iteration k

is unfold₂($\dot{\boldsymbol{\mathcal{P}}}^{(k)}$). $\dot{\boldsymbol{\mathcal{P}}}^{(k)}$ is computed as $\boldsymbol{\mathcal{P}}^{(k)} \times_1 \boldsymbol{T}^T$ in iteration k-1, which is equivalent to

$$\operatorname{unfold}_{1}(\dot{\boldsymbol{\mathcal{P}}}^{(k)}) = \boldsymbol{T} \times \operatorname{unfold}_{1}(\boldsymbol{\mathcal{P}}^{(k)}). \tag{9}$$

We can deduce from Figure 3 that unfold₁($\mathcal{P}^{(k)}$) has the following structure

$$\begin{bmatrix} x_{11} & 0 & \cdots & 0 & x_{12} & 0 & \cdots & 0 & \cdots & x_{1n_k} & 0 & \cdots & 0 \\ 0 & x_{21} & \cdots & 0 & 0 & x_{22} & \cdots & 0 & \cdots & 0 & x_{2n_k} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \dots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_{R1} & 0 & 0 & \cdots & x_{R2} & \cdots & 0 & 0 & \cdots & x_{Rn_k} \end{bmatrix},$$

where $\forall j = 1, 2, ..., R$, vector $[x_{j1} \ x_{j2} \ \cdots \ x_{jn_k}]^T$ is a particular standard basis vector. Let $\mathbf{T} = [\mathbf{e}_{i_1} \ \mathbf{e}_{i_2} \ \cdots \ \mathbf{e}_{i_R}]$ according to Corollary 4. Then unfold₁ $(\dot{\mathbf{P}}^{(k)})$ will have the structure

$$\begin{bmatrix} x_{11}e_{i_1} & x_{21}e_{i_2} & \cdots & x_{R1}e_{i_R} & \cdots & x_{1n_d}e_{i_1} & x_{2n_d}e_{i_2} & \cdots & x_{Rn_k}e_{i_R} \end{bmatrix}$$

and thus the structure of $\operatorname{unfold}_2(\dot{\boldsymbol{\mathcal{P}}}^{(k)})$ will be

$$\begin{bmatrix} x_{11}e_{i_1} & x_{21}e_{i_2} & \cdots & x_{R1}e_{i_R} \\ x_{12}e_{i_1} & x_{22}e_{i_2} & \cdots & x_{R2}e_{i_R} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1n_k}e_{i_1} & x_{2n_k}e_{i_2} & \cdots & x_{Rn_k}e_{i_R} \end{bmatrix}.$$

From this it follows that $\operatorname{unfold}_2(\dot{\mathcal{P}}^{(k)})$ is a quasi-permutation matrix. The same line of reasoning can be used to prove the theorem for k > p.

Now, we consider how to perform Deparallelisation for a quasi-permutation matrix. Our aim is to express a matrix M as the product of two smaller matrices: M = NT. For a quasi-permutation matrix, we need to remove the duplicate columns in M. As shown in Corollary 4, the result T itself is a quasi-permutation matrix. Therefore, N = I and T = M, where I is an identity matrix, can be regarded as the result of performing Deparallelisation on a quasi-permutation matrix, except that the duplicate columns in M have not yet been removed. What remains to be done is the removal of zero rows of T and the corresponding columns in N. This is described as Algorithm 5.

For a quasi-permutation matrix, each column can be represented by the position of 1 in it. Thus, Algorithm 5 has a time complexity of $O(n_1 + n_2)$, where n_1 and n_2 are the dimensions of M. It can be executed much more efficiently than a general Deparallelisation algorithm. From Algorithm 5 we can also observe, that the resulting matrix size β must be no more than n_1 , even if $n_2 \gg n_1$.

According to Theorem 5 and the above analysis, with Algorithm 4 the TT

Algorithm 5 Deparallelisation for a quasi-permutation matrix

```
Input: A quasi-permutation matrix M \in \mathbb{R}^{n_1 \times n_2}.
```

Output: Matrices $N \in \mathbb{R}^{n_1 \times \beta}$, $T \in \mathbb{R}^{\beta \times n_2}$ so that M = NT, and N includes nonduplicate columns of M.

```
1: \beta \coloneqq 0.
```

2: Let $N \in \mathbb{R}^{n_1 \times \beta}$, $T \in \mathbb{R}^{\beta \times n_2}$ be two dynamically resized transfer matrices.

```
3: for i = 1, 2, \dots, n_1 do
```

4: **if** $M_{i,:}$ is not a zero row **then**

5: $\beta := \beta + 1$.

extend matrix N and T

6: $T_{\beta,:} \coloneqq M_{i,:}$

7: Set $N_{i,\beta}$ a zero column except $N_{i,\beta} = 1$.

8: end if

9: end for

10: Return N and T.

ranks will be reduced to \tilde{r} satisfying the following upper bounds

$$\tilde{r}_k \le \bar{r}_k = \begin{cases} \min\left(R, \prod_{i=1}^k n_i\right) & \text{if } 1 \le k < p, \\ \min\left(R, \prod_{i=k+1}^d n_i\right) & \text{if } p \le k < d. \end{cases}$$
(10)

where R is the number of nonzero p-fibers in the original tensor \mathcal{A} .

3.3. More efficient TT-rounding and the FastTT algorithm

Algorithm 4 can already provide rank-reduced TT for sparse tensors while keeping the sparsity and with no precision loss. However, if lower ranks are desired, we can further apply TT-rounding on the TT. This could be useful for applications which do not care about the sparsity. Based on the property of TT obtained in Algorithm 4, we modified the original Algorithm 2 in order to make it more efficient, described as Algorithm 6. Instead of performing a right-to-left QR-sweep and then a left-to-right SVD-sweep, we perform 2 middle-to-edge SVD-sweep from core p. The QR-sweep in our algorithm is proved to be extremely fast due to the orthogonality obtained in Algorithm 4 and former SVD, and that is why our algorithm is more efficient. The truncation parameters in Algorithm 6 satisfy

$$\delta_k := \frac{\varepsilon}{\sqrt{p-1} + \sqrt{d-p}} \| \mathbf{A} \|_F, \ k = 1 \dots d - 1.$$
 (11)

The correctness of Algorithm 6 is explained as follows.

Lemma 6. A quasi-permutation matrix with no duplicate columns is an orthonormal matrix.

Lemma 6 can be easily proved based by the Definition 7 and the definition of an orthonormal matrix.

Algorithm 6 More efficient TT-rounding for the sparse TT conversion

Input: Cores $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(d)}$ of the TT-format tensor \mathcal{A} with TT-ranks r_1, \ldots, r_{d-1} , desired accuracy tolerance ε , an integer p $(1 \le p \le d)$.

Output: Cores $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(d)}$ of the TT-approximation \mathcal{B} to \mathcal{A} in the TT-format with TT-ranks r_1, \ldots, r_{d-1} . The computed approximation satisfies

$$||\mathcal{A} - \mathcal{B}||_F \leq \varepsilon ||\mathcal{A}||_F.$$

```
1: Set truncation parameters according to (11).
  2: (First SVD-sweep)
  3: for k = p, \dots, d-1 do
             G := \operatorname{unfold}_2(\mathcal{G}^{(k)}).
             Compute \delta_k-truncated SVD: G = U\Sigma V^T + E_k, ||E_k||_F \leq \delta_k,
             r_k := \operatorname{rank}_{\delta_k}(\boldsymbol{G}).
             \mathcal{G}^{(k)} \coloneqq \operatorname{reshape}(\boldsymbol{U}, [r_{k-1}, n_k, r_k]).

\mathcal{G}^{(k+1)} \coloneqq \mathcal{G}^{(k+1)} \times_1 (\boldsymbol{V}\boldsymbol{\Sigma}).
  7:
  8: end for
  9: (QR\text{-}sweep)
10: for k = d, \dots, p+1 do
11: \boldsymbol{G} \coloneqq \operatorname{unfold}_{1}^{T}(\boldsymbol{\mathcal{G}}^{(k)}).
              Compute economic QR decomposition: G = QR.
12:
             \boldsymbol{\mathcal{G}}^{(k)} \coloneqq \operatorname{reshape}(\boldsymbol{Q}^T, [r_{k-1}, n_k, r_k]).
13:
             \boldsymbol{\mathcal{G}}^{(k-1)}\coloneqq \boldsymbol{\mathcal{G}}^{(k-1)}\times_{3}\boldsymbol{R}^{T}.
14:
15: end for
        (Second SVD-sweep)
16:
17: for k = p, \dots, 2 do
18: \mathbf{G} \coloneqq \text{unfold}_1^T(\mathbf{G}^{(k)}).
             Compute \delta_{k-1}-truncated SVD: G = U\Sigma V^T + E_{k-1}, ||E_{k-1}||_F < \delta_{k-1},
             r_{k-1} := \operatorname{rank}_{\delta_{k-1}}(\boldsymbol{G}).
             egin{aligned} \mathcal{G}^{(k)} &\coloneqq \operatorname{reshape}(oldsymbol{U}^T, [r_{k-1}, n_k, r_k]). \ \mathcal{G}^{(k-1)} &\coloneqq oldsymbol{\mathcal{G}}^{(k-1)} 	imes_3 (oldsymbol{V}oldsymbol{\Sigma}). \end{aligned}
20:
21:
23: Return \mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)} as cores of \mathcal{B}.
```

In Steps 9 and 15 of Algorithm 4, the duplicate columns in the input quasipermutation matrix (according to Theorem 5) are removed. Then, based on Lemma 6, we have the following statement.

Corollary 7. Supposes the TT cores $\mathcal{G}^{(k)}$ are obtained with Algorithm 4. Then the matrices $\operatorname{unfold}_2(\mathcal{G}^{(k)}), k < p$ and $\operatorname{unfold}_1^T(\mathcal{G}^{(k)}), k > p$ are all orthonormal matrices.

Lemma 8. Suppose $\mathcal{U}^{(i)}$, i = 1, ..., d are the cores of a tensor train. If matrix $\operatorname{unfold}_2(\mathcal{U}^{(i)})$ is an orthonormal matrix for all i = 1, ..., k $(1 \le k \le d)$, then the matrix $\operatorname{unfold}_i(\mathcal{U}^{(1)} \circ \cdots \circ \mathcal{U}^{(j)})$ is an orthonormal matrix for all j = 1, ..., k.

The proof of Lemma 8 can be found in [14, Appendix B]. We can now derive the following theorem.

Theorem 9. (Correctness of Algorithm 6) The approximation \mathcal{B} obtained in Algorithm 6 always satisfies $\|\mathcal{A} - \mathcal{B}\|_F \le \varepsilon \|\mathcal{A}\|_F$.

Proof. For simplicity, we let

- \bullet \mathcal{C} denote the TT-format tensor after first SVD-sweep,
- \mathcal{D} denote the TT-format tensor before second SVD-sweep,
- C_i denote the TT-format tensor after the k = i iteration in first SVD-sweep,
- $\mathcal{A}^{(i...j)}$ denote the contraction of *i*-th to *j*-th core $\mathcal{G}^{(i)} \circ \cdots \circ \mathcal{G}^{(j)}$ of a TT-format tensor \mathcal{A} .

It is obvious that $\mathcal{C} = \mathcal{D}$, hence

$$\|\mathcal{A} - \mathcal{B}\|_F < \|\mathcal{A} - \mathcal{C}\|_F + \|\mathcal{D} - \mathcal{B}\|_F.$$

Based on the observation that $\mathcal{A}^{(1...p-1)} = \mathcal{C}^{(1...p-1)}$, we let $\mathcal{A} = \mathcal{A}^{(1...p-1)} \circ \mathcal{A}^{(p...d)}$ and $\mathcal{C} = \mathcal{A}^{(1...p-1)} \circ \mathcal{C}^{(p...d)}$. According to Corollary 7 and Lemma 8, unfold_{p-1}($\mathcal{A}^{(1...p-1)}$) is an orthonormal matrix. Thus

$$\|\mathcal{A} - \mathcal{C}\|_F = \|\mathcal{A}^{(p...d)} - \mathcal{C}^{(p...d)}\|_F.$$

Let us concentrate on the first iteration (k=p) of first SVD-sweep. The truncated-SVD can be rewritten as $\mathcal{A}^{(p)} = \mathcal{C}_1^{(p)} \times_3 \Sigma V^T + \mathcal{E}_p$, where $\|\mathcal{E}_p\|_F \leq \delta_p$ and $\mathcal{C}_1^{(p)} \circ_3^3 \mathcal{E}_p = \mathbf{0}$. From line 7 we know $\mathcal{C}_1^{(p+1...d)} = \mathcal{A}^{(p+1...d)} \times_1 V \Sigma$. Thus,

$$\begin{split} \| \boldsymbol{\mathcal{A}}^{(p...d)} - \boldsymbol{\mathcal{C}}^{(p...d)} \|_F^2 &= \| \boldsymbol{\mathcal{A}}^{(p)} \circ \boldsymbol{\mathcal{A}}^{(p+1...d)} - \boldsymbol{\mathcal{C}}_1^{(p)} \circ \boldsymbol{\mathcal{C}}^{(p+1...d)} \|_F^2 \\ &= \| (\boldsymbol{\mathcal{C}}_1^{(p)} \times_3 \Sigma \boldsymbol{V}^T + \boldsymbol{\mathcal{E}}_p) \circ \boldsymbol{\mathcal{A}}^{(p+1...d)} - \boldsymbol{\mathcal{C}}_1^{(p)} \circ \boldsymbol{\mathcal{C}}^{(p+1...d)} \|_F^2 \\ &= \| \boldsymbol{\mathcal{C}}_1^{(p)} \circ \boldsymbol{\mathcal{C}}_1^{(p+1...d)} + \boldsymbol{\mathcal{E}}_p \circ \boldsymbol{\mathcal{A}}^{(p+1...d)} - \boldsymbol{\mathcal{C}}_1^{(p)} \circ \boldsymbol{\mathcal{C}}^{(p+1...d)} \|_F^2 \\ &= \| \boldsymbol{\mathcal{E}}_p \circ \boldsymbol{\mathcal{A}}^{(p+1...d)} \|_F^2 + \| \boldsymbol{\mathcal{C}}_1^{(p)} \circ (\boldsymbol{\mathcal{C}}_1^{(p+1...d)} - \boldsymbol{\mathcal{C}}^{(p+1...d)}) \|_F^2 \\ &= \delta_p^2 + \| \boldsymbol{\mathcal{C}}_1^{(p+1...d)} - \boldsymbol{\mathcal{C}}^{(p+1...d)} \|_F^2 \end{split}$$

Proceeding by induction, we have

$$\|\mathcal{A} - \mathcal{C}\|_F^2 = \sum_{k=p}^{d-1} \delta_k^2.$$

Similarly we have

$$\|\mathcal{D} - \mathcal{B}\|_F^2 = \sum_{k=2}^p \delta_{k-1}^2.$$

According to (11),

$$\|\boldsymbol{\mathcal{A}} - \boldsymbol{\mathcal{B}}\|_{F} \le \sqrt{\sum_{k=p}^{d-1} \delta_{k}^{2}} + \sqrt{\sum_{k=2}^{p} \delta_{k-1}^{2}} \le \varepsilon \|\boldsymbol{\mathcal{A}}\|_{F}.$$
 (12)

Now, we are ready to describe the whole algorithm for the conversion of a sparse tensor into a TT, presented as Algorithm 7.

Algorithm 7 Tensor train decomposition of sparse tensor (FastTT)

Input: A sparse tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times ... \times n_d}$, desired accuracy tolerance ε , an integer p $(1 \le p \le d)$.

Output: Cores $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(d)}$ of the TT-approximation \mathcal{B} to \mathcal{A} in the TT-format with TT-ranks r_k . The computed approximation satisfies

$$||\mathcal{A} - \mathcal{B}||_F \leq \varepsilon ||\mathcal{A}||_F.$$

- 1: Obtain \mathcal{B} in the TT-format with cores $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(d)}$ by Algorithm 4, where *Depar* is implemented as Algorithm 3.
- 2: Reduce the TT ranks of \mathcal{B} with Algorithm 6.
- 3: Return the TT-approximation \mathcal{B} .

It should be pointed out that if the accuracy tolerance ε is set to 0^1 , the obtained TT ranks with Algorithm 7 will be maximal and equal to the TT-ranks obtained from the TT-SVD algorithm. We take p=1 as an example to discuss the TT-rank r_1 case. In the TT-SVD algorithm, r_1 is obtained by computing the SVD of $C = \text{unfold}_1(\mathcal{A})$. \mathcal{A} can also represented as the contraction of the TT cores obtained by Algorithm 4.

$$oldsymbol{\mathcal{A}} = oldsymbol{\mathcal{G}}^{(1)} \circ oldsymbol{\mathcal{G}}^{(2)} \circ \cdots \circ oldsymbol{\mathcal{G}}^{(d)}.$$

In practice, ε is usually set to a small value like 10^{-14} due to the inevitable round-off

Thus,

$$C = \text{unfold}_2(\mathcal{G}^{(1)}) \text{ unfold}_1(\mathcal{G}^{(2)} \circ \cdots \circ \mathcal{G}^{(d)}).$$

According to Corollary 7 and Lemma 8, $L = \text{unfold}_1^T(\mathcal{G}^{(2)} \cdots \mathcal{G}^{(d)})$ is an orthonormal matrix, i.e. $L^T L = I$.

$$CC^T = \text{unfold}_2(\mathcal{G}^{(1)})L^TL \text{ unfold}_2^T(\mathcal{G}^{(1)}) = \text{unfold}_2(\mathcal{G}^{(1)}) \text{ unfold}_2^T(\mathcal{G}^{(1)}).$$

This means matrix $\operatorname{unfold}_2(\mathcal{G}^{(1)})$ has the same singular values as C. For Algorithm 1, r_1 equals $\operatorname{rank}_{\delta}(C)$, while the r_1 obtained with Algorithm 7 is $\operatorname{rank}_{\delta_1}(\operatorname{unfold}_2(\mathcal{G}^{(1)}))$ (see lines 4 and 5 of Algorithm 6). These numerical ranks are therefore equal when $\delta = \delta_1$. Similar results for the other TT ranks and for $p \neq 1$ can be derived.

For a sparse tensor the runtime of Algorithm 7 may be smaller than the TT-SVD algorithm, as the SVD is performed on smaller matrices.

3.4. Fixed-rank TT approximations and matrices in TT-format

Sometimes we need a TT approximation of a tensor with given TT-ranks. We can slightly modify Algorithm 6 to fit this scenario. Specifically, the desired accuracy tolerance ε is not needed and thus substituted with the desired TT-ranks. The truncation parameters δ_i will not be computed either. In the truncated SVD computation we simply truncate the matrices with the given ranks instead of truncating them according to the accuracy tolerance. This technique could be useful in applications like tensor completion [13].

Some other applications require matrix-vector multiplications, which are convenient if both the matrix and the vector are in TT-format (as shown in Figure 5). A vector $\mathbf{v} \in \mathbb{R}^N$ can be transformed into TT-format if we first reshape it into a tensor $\mathbf{v} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, where $N = n_1 \cdots n_d$, and then decompose it into a TT. A "matrix in TT-format" [3, pp. 2311-2313], also known as a matrix product operator (MPO), is similar but more complicated. The elements of matrix $\mathbf{M} \in \mathbb{R}^{M \times N}$ are rearranged into a tensor $\mathbf{M} \in \mathbb{R}^{m_1 \times n_1 \times \cdots \times m_d \times n_d}$, where $M = m_1 \cdots m_d$, $N = n_1 \cdots n_d$. The cores $\mathbf{M}^{(i)}(i = 1, \dots, d)$ of the MPO satisfy

$$\mathcal{M}(i_1, j_1, \dots, i_d, j_d) = \mathcal{M}^{(1)}(:, i_1, j_1, :) \cdots \mathcal{M}^{(d)}(:, i_d, j_d, :),$$

where $\mathcal{M}^{(i)} \in \mathbb{R}^{r_{i-1} \times m_i \times n_i \times r_i} (i = 1, \dots, d), r_0 = r_d = 1$. The matrix-to-MPO algorithm is basically computing a TT-decomposition of the d-way tensor $\mathcal{M}' \in \mathbb{R}^{m_1 n_1 \times \dots \times m_d n_d}$, along with a few necessary reshapings, which can also be done with Algorithm 7.

3.5. A dynamic method to choose the truncation parameters

The actual relative error of the truncated SVD is usually not very close to the truncation parameter δ_k , which implies that if the truncation parameters are set statically at the beginning with (11), some of the desired accuracy tolerant ε will be "wasted". The main idea of the dynamic method is to compute the

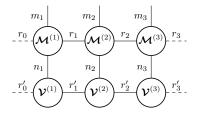


Figure 5: Diagram of matrix-vector-multiplication in the TT-format.

truncation parameters dynamically to make use of those "wastes". One of the possible approaches is shown in Algorithm 8. In each step of the truncated SVD, an expected error is calculated with the current "total error remainder" and used as the truncation parameter. After each truncated SVD, the "total error remainder" is decreased according to the actual error. Such an adaptive approach to setting the truncation parameters can lead to lower TT ranks while keeping the relative error smaller than ε .

Algorithm 8 The revised TT-rounding for the sparse TT conversion

```
Input: (same \ as \ Algorithm \ 6)

Output: (same \ as \ Algorithm \ 6)

1: \delta_{\text{right}} \coloneqq \frac{\sqrt{d-p}}{\sqrt{d-p}+\sqrt{p-1}} \varepsilon \| \mathcal{A} \|_F, \delta_{\text{left}} \coloneqq \frac{\sqrt{p-1}}{\sqrt{d-p}+\sqrt{p-1}} \varepsilon \| \mathcal{A} \|_F.

2: \mathbf{for} \ k = p, \dots, d-1 \ \mathbf{do}

3: \delta_k \coloneqq \frac{\delta_{\text{right}}}{\sqrt{d-k}}.

4: Steps 4-7 of Algorithm 6.

5: \delta_{\text{right}} \coloneqq \sqrt{\delta_{\text{right}}^2 - \| E_k \|_F^2}.

6: \mathbf{end} \ \mathbf{for}

7: Steps 10-15 of Algorithm 6.

8: \mathbf{for} \ k = p, \dots, 2 \ \mathbf{do}

9: \delta_{k-1} \coloneqq \frac{\delta_{\text{left}}}{\sqrt{k-1}}.

10: Steps 18-21 of Algorithm 6.

11: \delta_{\text{left}} \coloneqq \sqrt{\delta_{\text{left}}^2 - \| E_{k-1} \|_F^2}.

12: \mathbf{end} \ \mathbf{for}

13: Return \mathcal{G}^{(1)}, \dots, \mathcal{G}^{(d)} as cores of \mathcal{B}.
```

Theorem 10. (Correctness of Algorithm 8) The approximation \mathcal{B} obtained in Algorithm 8 always satisfies $\|\mathcal{A} - \mathcal{B}\|_F \le \varepsilon \|\mathcal{A}\|_F$.

The proof of Theorem 10 is provided in appendix Appendix A.

3.6. Complexity Analysis

Finding nonzero p-fibers can be accelerated by employing balanced binary search trees or hash tables, while parallel-vector rounding will be efficient if

Depar is implemented as Algorithm 5. Notice that, there is no floating point operation in these procedures. Therefore, the time complexity of Algorithm 7 mainly depends on Algorithm 6, where the cost of SVD is of major concern. The FLOP count $f_{\rm fasttt}$ can thus be estimated as

$$f_{\text{fasttt}} \approx f_{\text{SVD}}(\tilde{r}_{p-1}n_p, \tilde{r}_p) + \sum_{i=p+1}^{d-1} f_{\text{SVD}}(r_{i-1}n_i, \tilde{r}_i) + \sum_{i=2}^{p} f_{\text{SVD}}(\tilde{r}_{i-1}, n_i r_i),$$
(13)

where $\{\tilde{r}_k\}$ and $\{r_k\}$ are the TT-ranks before and after executing Algorithm 6. According to (10), where the upper bound of \tilde{r}_k , i.e., \bar{r}_k , is given, we can estimate the upper bound of the FLOP count before any actual computation. With this estimation, p can be automatically selected as described in Algorithm 9. In line 3, $\{\tilde{r}_k\}$ can be obtained alternatively by actually executing Depar for a more precise estimation since it will not take much time after all.

Algorithm 9 Automatically select p

Input: A sparse tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times ... \times n_d}$.

Output: Selected \bar{p} for best estimated performance in Algorithm 7.

- 1: **for** p = 1, ..., d **do**
- 2: $R := \text{the number of nonzero } p\text{-subvectors of } \mathcal{A}$.
- 3: $\{\tilde{r}_k\} := \{\bar{r}_k\}$ given in (10).
- 4: $\{r_k\} := \{\tilde{r}_k\}$, or specified by users.
- 5: $f_p := \text{the estimated FLOP count in (13)}.$
- 6: end for
- 7: Return $\bar{p} = \underset{p}{\operatorname{argmin}} f_p$.

For a more intuitive view of the time complexity, we analyze the FLOP counts for an example from Section 4.1. Suppose we are computing a fixed rank-10 TT-approximation of a sparse 7-way tensor $\mathcal{A} \in \mathbb{R}^{10 \times 20 \times 20 \times 10 \times 15 \times 20 \times 3}$ with density $\sigma = 0.001$. According to (1), the approximate FLOP count of TT-SVD is

$$f_{\text{TTSVD}} \approx f_{\text{SVD}}(10, 20 \times 20 \times 10 \times 15 \times 20 \times 3) + f_{\text{SVD}}(20r, 20 \times 10 \times 15 \times 20 \times 3) + f_{\text{SVD}}(20r, 10 \times 15 \times 20 \times 3) + \cdots + f_{\text{SVD}}(20r, 3)$$

 $\approx (3.6 \times 10^8 + 7.6r^2 \times 10^7)C_{\text{SVD}}$
 $\approx (8 \times 10^9)C_{\text{SVD}}.$

As for f_{fasttt} , we let p=7. Since the elements of \mathcal{A} are grouped in triples stored in the last dimension, the number of nonzero 7-subvectors R satisfies $R \leq \text{nnz}(\mathcal{A})/3 = 12000$, which means $\{\bar{r}_k\}$ given in (10) is no more than $\{10, 200, 4000, 12000, 12000, 12000, 12000\}$. According to (13), we have

$$f_{\text{fasttt}} \approx f_{\text{SVD}}(3, 12000) + f_{\text{SVD}}(20r, 12000) + f_{\text{SVD}}(15r, 12000)$$

+
$$f_{\text{SVD}}(10r, 4000) + f_{\text{SVD}}(20r, 200)$$

 $\approx (1.08 \times 10^5 + 8r^2 \times 10^6)C_{\text{SVD}}$
 $\approx (8 \times 10^8)C_{\text{SVD}}.$

In this case, Algorithm 7 is about 10X faster than TT-SVD. The actual speedup will be a bit lower due to the uncounted operations such as those in Algorithm 4. If we increase the density σ to 0.01, $f_{\rm TTSVD}$ will remain the same and $f_{\rm fasttt}$ will change into

$$f_{\text{fasttt}} \approx f_{\text{SVD}}(3, 120000) + f_{\text{SVD}}(20r, 120000) + f_{\text{SVD}}(15r, 40000) + f_{\text{SVD}}(10r, 4000) + f_{\text{SVD}}(20r, 200) \approx (1.08 \times 10^6 + 5.7r^2 \times 10^7) C_{\text{SVD}} \approx (5.7 \times 10^9) C_{\text{SVD}},$$

and the speedup drops to 1.4. The actual speedup will be a bit higher because we overestimate $\{\tilde{r}_k\}$ and the uncounted operations become insignificant with the increasing SVD cost. For matrix-to-MPO applications, the main operation is the TT-decomposition of $\mathcal{M}' \in \mathbb{R}^{m_1 n_1 \times \cdots \times m_d n_d}$, hence (13) also works here. We just need to replace n_i with $m_i n_i$.

We now look at the memory cost of the FastTT algorithm. Before the TT-rounding step, all data are stored in a sparse format. Therefore, the extra memory cost occurs in the TT-rounding which is similar to the TT-SVD algorithm and is of similar size to the cores in the obtained TT.

4. Numerical Experiments

In order to provide empirical proof of the performance of the developed FastTT algorithm, we conduct several numerical experiments. Since Algorithm 4 is not friendly to MATLAB, FastTT is implemented in C++ based on the xerus C++ toolbox [24] and with Intel Math Kernel Library². The xerus library also contains implementations of TT-SVD and randomized TT-SVD (rTTSVD) [20]. As no C++ implementation of the TT-cross method [18] is available, we use TT-cross from TT-toolbox³ in MATLAB. All experiments are carried out on a x86-64 Linux server with 32 CPU cores and 512G RAM. The desired accuracy tolerance ε of TT-SVD, TT-cross and our FastTT algorithms is 10^{-14} , unless otherwise stated. The oversampling parameter of rTTSVD algorithm is set to 10. In all experiments, the CPU time is reported.

4.1. Image/video inpainting

Applications like tensor completion [13] require a fixed-rank TT-approximate of the given tensors. The tensors used in this section are a large color image

²https://software.intel.com/en-us/mkl

 $^{^3}$ https://github.com/oseledets/TT-Toolbox

 $Dolphin^4$ which has been reshaped into a $10 \times 20 \times 20 \times 10 \times 15 \times 20 \times 3$ tensor and a color video $Mariano~Rivera~Ultimate~Career~Highlights^5$ which has been reshaped into a $20 \times 18 \times 20 \times 32 \times 12 \times 12 \times 3$ tensor. Most pixels of the image/video are not observed and are regarded as zeros whereas the observed pixels are chosen randomly. The observation ratio σ is the ratio of observed pixels to the total number of pixels. Table 1 shows the results for different specified TT-ranks and observation ratios.

Table 1: Experimental results on an image and a video with different observation ratios and preset $\operatorname{TT-ranks}$.

data	TT-rank	σ		speedup			
dava	11 101111		TT-SVD	TT-cross	rTTSVD	FastTT	Броссир
image	10	0.001	20.2	20.2	24.1	3.43	9.6X
	10	0.005	32.3	22.7	23.9	10.9	3.0X
	10	0.01	32.8	23.7	26.0	14.2	2.3X
	30	0.001	42.7	68.1	38.1	12.2	3.5X
	30	0.005	42.9	70.9	33.8	20.5	2.1X
	100	0.001	67.3	366	91.5	23.7	2.8X
	10	0.001	66.2	24.9	56.0	10.4	6.4X
	10	0.005	66.6	30.3	60.5	26.2	2.5X
video	10	0.01	66.9	31.2	62.7	33.3	2.0X
	30	0.001	103	122	108	26.5	3.9X
	30	0.005	110	140	94.2	47.6	2.3X
	100	0.001	232	1080	221	107	2.2X

It can be seen from Table 1 that our algorithm can greatly speed up the calculation of a TT-approximation when the observation ratio is small. We have also tested the TT-cross algorithm and the rTTSVD algorithm which also speed up the calculation in some cases. However, the speedup of them are not as great as ours, and in cases where the preset TT-rank is high we observe that they are even slower than the TT-SVD algorithm. In addition, the quality of the TT-approximation calculated by the TT-cross/rTTSVD algorithm is not as good as ours. For example, in the image inpainting task where the TT-rank is 100 and the observation ratio σ is 0.001, the mean square error (MSE) of both TT-SVD algorithm and our algorithm is 22.3, while the MSE of TT-cross and rTTSVD is 66.0 and 23.5, correspondingly.

For each of the experiments the integer p is selected automatically by the FLOP estimation in Algorithm 9. Now, we validate this FLOP estimation. For the parameters TT-rank = 100, $\sigma = 0.001$ in the image experiment we run

 $^{^4}$ http://absfreepic.com/absolutely_free_photos/original_photos/dolphin-4000x3000_21859.jpg

⁵https://www.youtube.com/watch?v=UPtDJuJMyhc

Algorithm 7 several times while manually setting different integer p and plot the CPU time for each p along with the estimated FLOP count. The results are shown in Figure 6, where we can see that the trend of the two curves is basically consistent. The integer p selected by Algorithm 9 is p=7, with which the exact CPU time is only slightly more than the best selection at p=6. Although Algorithm 9 does not always produce the best p, it certainly avoids bad values like p=3 in this case.

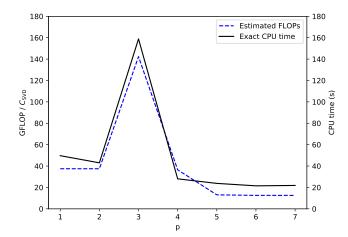


Figure 6: The CPU time and estimated FLOPs with (13) of the FastTT algorithm for different p values.

4.2. Linear equation in finite difference method

The finite difference method (FDM) is widely used for solving partial differential equations, in which finite differences approximate the partial derivatives. With FDM, a linear equation system with sparse coefficient matrix is solved. We consider simulating a three-dimensional rectangular domain with FDM. The resulted linear equation system can be transformed into the matrix TT format (i.e. MPO) and then solved with an alternating least squares (ALS) method [4] or AMEn [25].

For a domain partitioned into $n \times m \times k$ grids, FDM produces a coefficient matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$, where $N = n \times m \times k$. For example, the sparsity pattern of the coefficient matrix \mathbf{A} for FDM with $20 \times 20 \times 20$ grids is shown in Figure 7. Naturally, the \mathbf{A} matrix can be regarded as a 6-way tensor $\mathbf{A} \in \mathbb{R}^{n \times n \times m \times m \times k \times k}$, which is then converted into an MPO. Since the tensor \mathbf{A} is very sparse, replacing the TT-SVD with FastTT will speed up the procedure of computing its TT-decomposition. In this experiment we construct the coefficient matrix with different grid partition, while the coefficients either follow a particular pattern, or are randomly generated. The results for converting the matrix to an MPO are shown in Table 2.

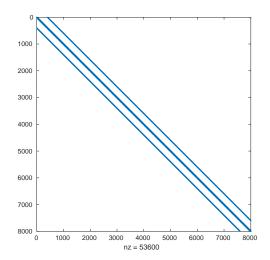


Figure 7: The sparsity pattern of the coefficient matrix for FDM with $20 \times 20 \times 20$ grids.

Table 2: Experimental results on the coefficient matrices for the FDM with $n \times n \times n$ grids.

\overline{n}	coefficients	method	time(s)	speedup	$\varepsilon_{ m actual}^{-1}$	$\mathrm{TT}\text{-}\mathrm{ranks}^2$
20 p		TT-SVD	43.6	_	$4.0\!\times\! 10^{-16}$	r: 2, 2
	nattorn	$\operatorname{TT-cross}$	7.96	5.5X	2.0×10^{-16}	r:2,2
	pattern	${\rm rTTSVD}$	1.29		1.2×10^{-15}	r:2,2
		FastTT	0.788	55X	9.6×10^{-16}	$R:1920; \ \tilde{r}:58,58; \ r:2,2$
30	nattern	TT-SVD	690	_	$2.0\!\times\! 10^{-15}$	r: 2, 2
		$\operatorname{TT-cross}$	26.5	26X	8.8×10^{-16}	r:2,2
		${\rm rTTSVD}$	19.3	36X	1.6×10^{-15}	
		FastTT	2.88	240X	1.1×10^{-15}	$R:4380; \ \tilde{r}:88,88; \ r:2,2$
20 random		TT-SVD	53.4	_	$2.5\!\times\! 10^{-15}$	r: 58, 58
	random	$\operatorname{TT-cross}$	226	0.24X	1.1×10^{-15}	r: 58, 58
		${\rm rTTSVD}$	23.4	2.3X	4.8×10^{-15}	,
		FastTT	1.67	32X	2.4×10^{-15}	$R:1920; \ \tilde{r}:58,58; \ r:58,58$
30 ra		TT-SVD	762	_	3.4×10^{-15}	r: 88, 88
	random	$\operatorname{TT-cross}$	2725	0.28X	6.2×10^{-15}	r: 88, 88
		${\rm rTTSVD}$	67.0	11X	4.2×10^{-15}	r: 88, 88
		FastTT	12.4	61X	3.3×10^{-15}	$R:4380; \ \tilde{r}:88,88; \ r:88,88$
40	random	TT-SVD	NA	_	NA	NA
		$\operatorname{TT-cross}$	NA	_	NA	NA
		${\rm rTTSVD}$	597	_	5.0×10^{-15}	r: 118, 118
		FastTT	57.5	_	2.6×10^{-15}	$R\!:\!7840; \tilde{r}\!:\!118,\!118; r\!:\!118,\!118$

 $[\]varepsilon_{
m actual} = \frac{\| \boldsymbol{\mathcal{A}} - \boldsymbol{\mathcal{B}} \|_F}{\| \boldsymbol{\mathcal{A}} \|_F}$. The same below. ² R is the number of nonzero p-fibers. \tilde{r} is the TT-ranks after parallel-vector rounding. r is the final TT-ranks.

As seen from Table 2, FastTT can convert large sparse matrices much faster than the TT-SVD with up to 240X speedup. These experiments also prove that the *Depar* procedure can greatly reduce the TT-rank and thus simplify the computation of the TT-rounding procedure. Like in the first experiment, the TT-cross algorithm is faster when the TT-ranks are low but gets slower when the ranks grow. The results of rTTSVD are obtained by setting the TT-ranks same as those obtained by TT-SVD and FastTT. From the result we can see the rTTSVD algorithm is not as fast as FastTT even if we know the proper TT-ranks.

If we set n=40 with random coefficients, the TT-SVD/TT-cross algorithm cannot produce any result in a reasonable time, while FastTT finishes in 57.5 seconds with a resulting TT-rank of r=118.

4.3. Data of road network

A directed/undirected graph with N nodes is equivalent to its adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$, which can also be decomposed into an MPO if we properly factorize its order $N = n_1 \times \cdots \times n_d$. This may benefit some data mining applications. In this experiment we use the undirected graph $roadNet\text{-}PA^6$ from SNAP [26]. Since the graph is fairly large, we only take the subgraph of the first N nodes as our data and preprocess its adjacency matrix by performing reverse Cuthill-McKee ordering [27]. Additionally, different desired accuracy tolerances ε and the actual relative error are tested in this experiment. The truncation parameters in Algorithm 6 is either set as $\delta_k = \frac{\varepsilon}{\sqrt{p-1} + \sqrt{d-p}} \|\mathbf{A}\|_F$ or determined by Algorithm 8. The results are shown in Table 3. The TT-cross/rTTSVD algorithm is not tested because both of them require the TT-ranks to be set the same, which is not possible in this experiment.

Again, for sparse graphs our FastTT algorithm is much faster than TT-SVD. Also, the actual relative errors are shown to be less than the given ε . If ε is small enough, the TT-rank obtained by FastTT is the same as those obtained by TT-SVD. Otherwise, Algorithm 8 (used in FastTT⁺) usually produces lower TT-ranks and a little bit higher relative error than Algorithm 6 (used in FastTT) which sets unified truncation parameters.

5. Conclusions

This paper analyzes several state-of-the-art algorithms for the computation of the TT decomposition and proposes a faster TT decomposition algorithm for sparse tensors. We prove the correctness and complexity of the algorithm and demonstrate the advantages and disadvantages of each algorithm.

In the subsequent experiments, we have verified the actual performance of each algorithm and confirmed our theoretical analysis. The experimental results also show that our proposed FastTT algorithm for sparse tensors is indeed

Table 3: Experimental	l results on converting	the data o	f roadNet-PA.

\overline{N}	ε	method^1	time (s)	speedup	TT-ranks	$\varepsilon_{ m actual}$
20^{3}	1×10^{-14}	TT-SVD FastTT	$75.4 \\ 14.1$	- 5.3X	58, 400 58, 400	$3.7 \times 10^{-15} 3.3 \times 10^{-15}$
20^{3}	5×10^{-1}	TT-SVD FastTT FastTT ⁺	62.2 11.8 10.4	- 5.3X 6.0X	31, 281 31, 281 55, 209	4.8×10^{-1} 4.8×10^{-1} 5.0×10^{-1}
10^{4}	1×10^{-14}	TT-SVD FastTT	833 23.3	- 34X	28, 1407, 70 28, 1407, 70	$3.9 \times 10^{-15} 4.3 \times 10^{-15}$
10^4	1×10^{-2}	TT-SVD FastTT FastTT ⁺	839 24.4 24.2	- 34X 35X	28, 1390, 70 28, 1395, 70 28, 1377, 70	5.5×10^{-3} 3.8×10^{-3} 9.8×10^{-3}

¹ FastTT: use Algorithm 6 for TT-rounding; FastTT+: use Algorithm 8 for TT-rounding.

an algorithm with excellent efficiency and versatility. Previous state-of-the-art algorithms are mainly limited by the tensor size whereas our proposed algorithm is mainly limited by the number of non-zero elements. As a result, the TT decomposition can be computed quickly regardless of the number of dimensions. This algorithm therefore is very promising to tackle tensor applications that were previously unimaginable, just like the large-scale use of previous sparse matrix algorithms.

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Appendix A. Proof of Theorem 10

Proof. From the proof of Theorem 9, we know that

$$\|m{\mathcal{A}} - m{\mathcal{B}}\|_F \leq \sqrt{\sum_{k=p}^{d-1} \|m{E}_k\|_F^2} + \sqrt{\sum_{k=2}^p \|m{E}_{k-1}\|_F^2}.$$

Now we are going to use a loop invariant [28, pp. 18-19] to prove the correctness of Algorithm 8. The loop invariant for Loop 2-6 is

$$\delta_{\text{right}}^2 + \sum_{i=p}^{k-1} \|\boldsymbol{E}_i\|_F^2 = \frac{d-p}{\sqrt{d-p} + \sqrt{p-1}} \varepsilon^2 \|\boldsymbol{\mathcal{A}}\|_F^2.$$

Initialization: Before the first iteration k = p, $\sum_{i=p}^{k-1} \|\boldsymbol{E}_i\|_F^2 = 0$ and $\delta_{\text{right}} = \frac{\sqrt{d-p}}{\sqrt{d-p} + \sqrt{p-1}} \varepsilon \|\boldsymbol{\mathcal{A}}\|_F$. Thus the invariant is satisfied.

Maintenance: After each iteration, δ_{right}^2 is decreased by $\|\boldsymbol{E}_k\|_F^2$ and $\sum_{i=p}^{k-1} \|\boldsymbol{E}_i\|_F^2$ is increased by $\|\boldsymbol{E}_k\|_F^2$. Thus the invariant remains satisfied.

Termination: When the loop terminates at k=d. Again the loop invariant is satisfied. This means that

$$\delta_{\text{right}}^{2} + \sum_{i=p}^{d-1} \|\boldsymbol{E}_{i}\|_{F}^{2} = \frac{d-p}{\sqrt{d-p} + \sqrt{p-1}} \varepsilon^{2} \|\boldsymbol{\mathcal{A}}\|_{F}^{2}$$

$$\Rightarrow \sqrt{\sum_{k=p}^{d-1} \|\boldsymbol{E}_{k}\|_{F}^{2}} \leq \frac{\sqrt{d-p}}{\sqrt{d-p} + \sqrt{p-1}} \varepsilon \|\boldsymbol{\mathcal{A}}\|_{F}.$$

Similarly we can prove that

$$\sqrt{\sum_{k=2}^{p} \|\boldsymbol{E}_{k-1}\|_{F}^{2}} \leq \frac{\sqrt{p-1}}{\sqrt{d-p} + \sqrt{p-1}} \varepsilon \|\boldsymbol{\mathcal{A}}\|_{F},$$

is satisfied after Loop 8-12.

Thus

$$\begin{split} \|\boldsymbol{\mathcal{A}} - \boldsymbol{\mathcal{B}}\|_{F} &\leq \sqrt{\sum_{k=p}^{d-1} \|\boldsymbol{E}_{k}\|_{F}^{2}} + \sqrt{\sum_{k=2}^{p} \|\boldsymbol{E}_{k-1}\|_{F}^{2}}. \\ &\leq \frac{\sqrt{d-p}}{\sqrt{d-p} + \sqrt{p-1}} \varepsilon \|\boldsymbol{\mathcal{A}}\|_{F} + \frac{\sqrt{p-1}}{\sqrt{d-p} + \sqrt{p-1}} \varepsilon \|\boldsymbol{\mathcal{A}}\|_{F} \\ &= \varepsilon \|\boldsymbol{\mathcal{A}}\|_{F}. \end{split}$$

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