Fundamental Tensor Operations for Large-Scale Data Analysis in Tensor Train Formats

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Abstract

We review and introduce new representations of tensor train decompositions for large-scale vectors, matrices, or low-order tensors. We provide extended definitions of mathematical multi-linear operations such as Kronecker, Hadamard, and contracted products, with their properties for tensor calculus. Then we introduce an effective low-rank tensor approximation technique called the tensor train (TT) format with a number of mathematical and graphical representations. We also provide a brief review of mathematical properties of the TT format as a low-rank approximation technique. With the aim of breaking the curse-of-dimensionality in large-scale numerical analysis, we describe basic operations on large-scale vectors and matrices in TT format. The suggested representations can be used for describing numerical methods based on the TT format for solving large-scale optimization problems such as the system of linear equations and eigenvalue problems.

KEY WORDS: tensor train; tensor networks; matrix product state; matrix product operator; generalized Tucker model; strong Kronecker product; contracted product; multilinear operator; numerical analysis; tensor calculus

1 Introduction

Multi-dimensional or multi-way data is prevalent nowadays, which can be represented by tensors. An $N$th-order tensor is a multi-way array of size $I_1 \times I_2 \times \cdots \times I_N$, where the $n$th dimension or mode is of size $I_n$. For example, a tensor can be induced by the discretization of a multivariate function [24]. Given a multivariate function $f(x_1, \ldots, x_N)$ defined on a domain $[0, 1]^N$, we can get a tensor with entries containing the function values at grid points. For another example, we can obtain tensors based on observed data [22]. We can collect and integrate measurements from different modalities by neuroimaging technologies such as functional magnetic resonance imaging (fMRI) and electroencephalography (EEG): subjects, time, frequency, electrodes, task conditions, trials, and so on. Furthermore, high-order tensors can be created by a process called tensorization or quantization [23], by which a large-scale vectors and matrices are reshaped into higher-order tensors.

However, it is impossible to store a high-order tensor because the number of entries, $I^N$ when $I = I_1 = I_2 = \cdots = I_N$, grows exponentially as the order $N$ increases. This is called the “curse-of-dimensionality”. Even for $I = 2$, with $N = 50$ we obtain $2^{50} \approx 10^{15}$ entries. Such a huge storage and
computational costs required for high dimensional problems prohibit the use of standard numerical algorithms. To make high dimensional problems tractable, there were developed approximation methods including sparse grids \cite{32,1} and low-rank tensor approximations \cite{14,24,13}. In this paper, we focus on the latter approach, where computational operations are performed on tensor formats, i.e., low-parametric representations of tensors.

In this paper, we consider several tensor formats, especially the tensor train (TT) format, which is one of the simplest tensor networks developed with the aim of overcoming the curse-of-dimensionality. Extensive overviews of the modern low-rank tensor approximation techniques are presented in \cite{24,13}. The TT format is equivalent to the matrix product states (MPS) for open boundary conditions proposed in computational physics, and it has taken a key role in density matrix renormalization group (DMRG) methods for simulating quantum many-body systems \cite{33,31}. It was later re-discovered in numerical analysis community \cite{25,19,18}. The TT-based numerical algorithms can accomplish algorithmic stability and adaptive determination of ranks by employing the singular value decomposition (SVD) \cite{30}. Its scope of application is quickly expanding for addressing high-dimensional problems such as multi-dimensional integrals, stochastic and parametric PDEs, computational finance, and machine learning \cite{13}. On the other hand, a comprehensive survey on traditional low-rank tensor approximation techniques for CP and Tucker formats is presented in \cite{5,22}.

Despite the large interest in high-order tensors in TT format, mathematical representations of the TT tensors are usually limited to the representations based on scalar operations on matrices and vectors, which leads to complex and tedious index notation in the tensor calculus. For example, a TT tensor is defined by each entry represented as products of matrices \cite{30,18}. On the other hand, representations of traditional low-rank tensor formats have been developed based on multilinear operations such as the Kronecker product, Khatri-Rao product, Hadamard product, and mode-$n$ multilinear product \cite{2,22}, which enables coordinate-free notation. Through the utilization of the multilinear operations, the traditional tensor formats expanded the area of application to chemometrics, signal processing, numerical linear algebra, computer vision, data mining, graph analysis, and neuroscience \cite{22}.

In this work, we develop extended definitions of multilinear operations on tensors. Based on the tensor operations, we provide a number of new and useful representations of the TT format. We also provide graphical representations of the TT format, motivated by \cite{18}, which are helpful in understanding the underlying principles and TT-based numerical algorithms. Based on the TT representations of large-scale vectors and matrices, we show that the basic numerical operations such as the addition, contraction, matrix-vector product, and quadratic form are conveniently described by the suggested representations. We demonstrate the usefulness of the proposed tensor operations in tensor calculus by giving a proof of orthonormality of the so-called frame matrices. Moreover, we derive explicit representations of localized linear maps in TT format that have been implicitly presented in matrix forms in the literature in the context of alternating linear scheme (ALS) for solving various optimization problems. The suggested mathematical operations and TT representations can be further applied to describing TT-based numerical methods such as the solutions to large-scale systems of linear equations and eigenvalue problems \cite{18}.

This paper is organized as follows. In Section 2, we introduce notations for tensors and definitions for tensor operations. In Section 3, we provide the mathematical and graphical representations of the TT format. We also review mathematical properties the TT format as a low-rank approximation. In Section 4, we describe basic numerical operations on tensors in TT format such as the addition, Hadamard product, matrix-vector multiplication, and quadratic form in terms of the multilinear
operations and TT representations. Discussion and conclusions are given in Section 5.

2 Notations for tensors and tensor operations

The notations in this paper follow the convention provided by [2, 22]. Table 1 summarizes the notations for tensors. Scalars, vectors, and matrices are denoted by lowercase, lowercase bold, and uppercase bold letters $x$, $\mathbf{x}$, and $\mathbf{X}$, respectively. Tensors are denoted by underlined uppercase bold letters $\mathbf{X}$. The $(i_1, i_2, \ldots, i_N)$th entry of $\mathbf{X}$ of size $I_1 \times I_2 \times \cdots \times I_N$ is denoted by $x_{i_1, i_2, \ldots, i_N}$ or $\mathbf{X}(i_1, i_2, \ldots, i_N)$. A subtensor of $\mathbf{X}$ obtained by fixing the indices $i_3, i_4, \ldots, i_N$ is denoted by $\mathbf{X}_{(i_3, i_4, \ldots, i_N)}$ or $\mathbf{X}(\cdot; i_3, i_4, \ldots, i_N)$. We may omit `;' as $\mathbf{X}_{(i_3, i_4, \ldots, i_N)}$ if the rest of the indices are clear to readers. The mode-$n$ matricization of $\mathbf{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is denoted by $\mathbf{X}_{(n)} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_{n-1} \times I_{n+1} \cdots I_N}$. We denote the mode-$(1,2,\ldots,n)$ matricization of $\mathbf{X}$ by $\mathbf{X}_{([n])} \in \mathbb{R}^{I_1 I_2 \times I_{n-1} I_{n+1} \cdots I_N}$ in the sense that $\mathbf{X}_{([n])}$ is the set of integers from 1 to $n$. In addition, we define the multi-index notation by $i_1 i_2 \cdots i_N \equiv i_N + (i_{N-1} - 1)I_N + \cdots + (i_1 - 1)I_2 I_3 \cdots I_N$ for $i_n = 1, 2, \ldots, I_n, n = 1, \ldots, N$. By using this notation, we can write an entry of a Kronecker product as $(a \otimes b)_{ij} = a_i b_j$. Moreover, it is important to note that in this paper the vectorization and matricization are defined in accordance with the multi-index notation. That is, for $\mathbf{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$, we have

\[
\mathbf{x} = \text{vec} (\mathbf{X}) \in \mathbb{R}^{I_1 I_2 \cdots I_N} \quad \Leftrightarrow \quad \mathbf{x}(i_1 i_2 \cdots i_N) = \mathbf{X}(i_1, i_2, \ldots, i_N), \\
\mathbf{X} = \mathbf{X}_{(n)} \in \mathbb{R}^{I_n \times I_1 \cdots I_{n-1} \times I_{n+1} \cdots I_N} \quad \Leftrightarrow \quad \mathbf{X}(i_n, i_1 \cdots i_{n-1} i_{n+1} \cdots i_N) = \mathbf{X}(i_1, i_2, \ldots, i_N), \\
\mathbf{X} = \mathbf{X}_{([n])} \in \mathbb{R}^{I_1 \cdots I_n \times I_{n+1} \cdots I_N} \quad \Leftrightarrow \quad \mathbf{X}(i_1 \cdots i_n, i_{n+1} \cdots i_N) = \mathbf{X}(i_1, i_2, \ldots, i_N),
\]

for $n = 1, \ldots, N$.

Table 2 summarizes the notations and definitions for tensor operations used in this paper.
Table 2: Notations and definitions for tensor operations

| Notation | Description |
|----------|-------------|
| $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$ | Kronecker product of $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$ and $\mathbf{B} \in \mathbb{R}^{J_1 \times \cdots \times J_N}$ yields a tensor $\mathbf{C}$ of size $I_1 J_1 \times \cdots \times I_N J_N$ with entries $\mathbf{C}(i_1, \ldots, i_N) = \mathbf{A}(i_1, \ldots, i_N) \circ \mathbf{B}(j_1, \ldots, j_N)$ |
| $\mathbf{C} = \mathbf{A} \otimes_n \mathbf{B}$ | mode-$n$ Kronecker product of $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_n \times J \times I_{n+1} \times \cdots \times I_N}$ and $\mathbf{B} \in \mathbb{R}^{I_1 \times \cdots \times I_n \times K \times I_{n+1} \times \cdots \times I_N}$ yields a tensor $\mathbf{C}$ of size $I_1 \times \cdots \times I_{n-1} \times J K \times I_{n+1} \times \cdots \times I_N$ with entries $\mathbf{C}(i_1, \ldots, i_{n-1}, : i_{n+1}, \ldots, : i_N) = \mathbf{A}(i_1, \ldots, i_{n-1}, : i_{n+1}, \ldots, : i_N) \circ \mathbf{B}(j_1, \ldots, j_N)$ |
| $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$ | Hadamard (elementwise) product of $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$ and $\mathbf{B} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$ yields a tensor $\mathbf{C}$ of size $I_1 \times \cdots \times I_N$ with entries $\mathbf{C}(i_1, \ldots, i_N) = \mathbf{A}(i_1, \ldots, i_N) \circ \mathbf{B}(i_1, \ldots, i_N)$ |
| $\mathbf{C} = \mathbf{A} \circ \mathbf{B}$ | outer product of $\mathbf{A} \in \mathbb{R}^{i_1 \times \cdots \times i_M}$ and $\mathbf{B} \in \mathbb{R}^{j_1 \times \cdots \times j_N}$ yields a tensor $\mathbf{C}$ of size $I_1 \times \cdots \times I_M \times J_1 \times \cdots \times J_N$ with entries $\mathbf{C}(i_1, \ldots, i_M, j_1, \ldots, j_N) = \mathbf{A}(i_1, \ldots, i_M) \circ \mathbf{B}(j_1, \ldots, j_N)$ |
| $\mathbf{C} = \mathbf{A} \oplus \mathbf{B}$ | direct sum of $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$ and $\mathbf{B} \in \mathbb{R}^{J_1 \times \cdots \times J_N}$ yields a tensor $\mathbf{C}$ of size $(I_1 + J_1) \times \cdots \times (I_N + J_N)$ with entries $\mathbf{C}(k_1,\ldots,k_N) = \mathbf{A}(k_1,\ldots,k_N)$ if $1 \leq k_n \leq I_n \forall n$, $\mathbf{C}(k_1,\ldots,k_N) = \mathbf{B}(k_1 - I_1,\ldots,k_N - I_N)$ if $I_n < k_n \leq I_n + J_n \forall n$, and $\mathbf{C}(k_1,\ldots,k_N) = 0$ otherwise |
| $\mathbf{C} = \mathbf{A} \oplus \mathbf{B}$ | mode-$n$ direct sum of $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times J \times I_{n+1} \times \cdots \times I_N}$ and $\mathbf{B} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times K \times I_{n+1} \times \cdots \times I_N}$ yields a tensor $\mathbf{C}$ of size $(I_1 + J_1) \times \cdots \times (I_{n-1} + J_{n-1}) \times I_n \times (I_{n+1} + J_{n+1}) \times \cdots \times (I_N + J_N)$ with subtensors $\mathbf{C}(i_1,\ldots,i_{n-1},: i_{n+1},\ldots,: i_N) = \mathbf{A}(i_1,\ldots,i_{n-1},: i_{n+1},\ldots,: i_N) \oplus \mathbf{B}(i_1,\ldots,i_{n-1},: i_{n+1},\ldots,: i_N)$ |
| $\mathbf{C} = \mathbf{A} \times_n \mathbf{B}$ | mode-$n$ product [22] of tensor $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$ and matrix $\mathbf{B} \in \mathbb{R}^{I_n \times \mathbf{B}}$ yields a tensor $\mathbf{C}$ of size $I_1 \times \cdots \times I_{n-1} \times J \times I_{n+1} \times \cdots \times I_N$ with mode-$n$ fibers $\mathbf{C}(i_1,\ldots,i_{n-1},i_n,\ldots,i_N) = \mathbf{A}(i_1,\ldots,i_{n-1},i_n,\ldots,i_N) \times \mathbf{B}(i_n)$ |
| $\mathbf{C} = \mathbf{A} \circ_n \mathbf{B}$ | mode-$n$ (vector) product [22] of tensor $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$ and vector $\mathbf{B} \in \mathbb{R}^{I_n}$ yields a tensor $\mathbf{C}$ of size $I_1 \times \cdots \times I_{n-1} \times I_{n+1} \times \cdots \times I_N$ with entries $\mathbf{C}(i_1,\ldots,i_{n-1},i_{n+1},\ldots,i_N) = \mathbf{B}^\top \mathbf{A}(i_1,\ldots,i_{n-1},i_n,\ldots,i_N)$ |
| $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}$ | (mode-$(M,1)$) contracted product of tensor $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_M}$ and tensor $\mathbf{B} \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}$ yields a tensor $\mathbf{C}$ of size $I_1 \times \cdots \times I_{M-1} \times J_2 \times \cdots \times J_N$ with entries $\mathbf{C}(i_1,\ldots,i_{M-1},j_2,\ldots,j_N) = \sum_{j_1=1}^{J_1} \mathbf{A}(i_1,\ldots,i_{M-1}) \circ \mathbf{B}(j_1,J_2,\ldots,J_N)$ |
| $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$ | Strong Kronecker product of two block matrices $\mathbf{A} = [\mathbf{A}_{r_1,r_2}] \in \mathbb{R}^{R_1 I_1 \times R_2 I_2}$ and $\mathbf{B} = [\mathbf{B}_{r_2,r_3}] \in \mathbb{R}^{R_2 J_1 \times R_3 J_2}$ yields a block matrix $\mathbf{C} = [\mathbf{C}_{r_1,r_2}] \in \mathbb{R}^{R_1 I_1 \times R_2 I_2 \times R_3 J_2}$ with blocks $\mathbf{C}_{r_1,r_2} = \sum_{r_3=1}^{R_3} \mathbf{A}_{r_1,r_2} \otimes \mathbf{B}_{r_2,r_3}$ |
| $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$ | Strong Kronecker product of two block tensors $\mathbf{A} = [\mathbf{A}_{r_1,r_2}] \in \mathbb{R}^{R_1 I_1 \times R_2 I_2 \times I_3}$ and $\mathbf{B} = [\mathbf{B}_{r_2,r_3}] \in \mathbb{R}^{R_2 J_1 \times R_3 J_2 \times J_3}$ yields a block tensor $\mathbf{C} = [\mathbf{C}_{r_1,r_2}] \in \mathbb{R}^{R_1 I_1 \times R_2 I_2 \times R_3 J_2 \times J_3}$ with blocks $\mathbf{C}_{r_1,r_2} = \sum_{r_3=1}^{R_3} \mathbf{A}_{r_1,r_2} \otimes \mathbf{B}_{r_2,r_3}$ |
| $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$ | self-contraction operator $\mathbf{S} : \mathbb{R}^{I_1 I_2 \times \cdots \times I_N \times I_1} \rightarrow \mathbb{R}^{I_2 J_3 \times \cdots \times I_N}$ defined by [23] |

[$\mathbf{G}: \mathbf{A}_{(1)}^{(1)}, \ldots, \mathbf{A}_{(N)}^{(N)}$] Tucker operator defined by [2]
2.1 Kronecker, Hadamard, and outer products

Definitions for traditional matrix-matrix product operations such as the Kronecker, Hadamard, and outer products can be generalized to tensor-tensor products.

Definition 2.1 (Kronecker product). The Kronecker product of \( \mathbf{A} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) and \( \mathbf{B} \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N} \) is defined by
\[
\mathbf{C} = \mathbf{A} \otimes \mathbf{B} \in \mathbb{R}^{I_1J_1 \times I_2J_2 \times \cdots \times I_NJ_N}
\]
with entries
\[
C(i_1, i_2, \ldots, i_N, j_1, j_2, \ldots, j_N) = A(i_1, i_2, \ldots, i_N) B(j_1, j_2, \ldots, j_N).
\]

The mode-\(n\) Kronecker product of \( \mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times I_n \times I_{n+1} \times \cdots \times I_N} \) and \( \mathbf{B} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times K \times I_{n+1} \times \cdots \times I_N} \) is defined by
\[
\mathbf{C} = \mathbf{A} \otimes_n \mathbf{B} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times I_n \times I_{n+1} \times \cdots \times I_N}
\]
with mode-\(n\) fibers
\[
C(i_1, \ldots, i_{n-1}, i_n, i_{n+1}, \ldots, i_N) = A(i_1, \ldots, i_{n-1}, i_n, \ldots, i_N) B(i_1, \ldots, i_{n-1}, i_{n+1}, \ldots, i_N).
\]

Similarly, the mode-\(n\) Kronecker product of \( \mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_N} \) and \( \mathbf{B} \in \mathbb{R}^{J_1 \times \cdots \times J_N} \) with common mode size \( I_n = J_n \) is defined by
\[
\mathbf{C} = \mathbf{A} \otimes_n \mathbf{B} \in \mathbb{R}^{I_1J_1 \times \cdots \times I_{n-1}J_{n-1} \times I_n \times I_{n+1}J_{n+1} \times \cdots \times I_NJ_N}
\]
with subtensors
\[
C((i_1, \ldots, i_n, \ldots, i_N)) = A((i_1, \ldots, i_n, \ldots, i_N)) B((i_1, \ldots, i_n, \ldots, i_N))
\]
for each \( i_n = 1, 2, \ldots, I_n \).

Definition 2.2 (Hadamard product). The Hadamard (elementwise) product of \( \mathbf{A} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) and \( \mathbf{B} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) is defined by
\[
\mathbf{C} = \mathbf{A} \odot \mathbf{B} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}
\]
with entries
\[
C(i_1, i_2, \ldots, i_N) = A(i_1, i_2, \ldots, i_N) B(i_1, i_2, \ldots, i_N).
\]

Definition 2.3 (Outer product). The outer product of \( \mathbf{A} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_M} \) and \( \mathbf{B} \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N} \) is defined by
\[
\mathbf{C} = \mathbf{A} \circ \mathbf{B} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_M \times J_1 \times J_2 \times \cdots \times J_N}
\]
with entries
\[
C(i_1, i_2, \ldots, i_M, j_1, j_2, \ldots, j_N) = A(i_1, i_2, \ldots, i_M) B(j_1, j_2, \ldots, j_N).
\]

Note that an \( N \)th order tensor \( \mathbf{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) is rank-one if it is written as the outer product of \( N \) vectors
\[
\mathbf{X} = \mathbf{v}^{(1)} \circ \mathbf{v}^{(2)} \circ \cdots \circ \mathbf{v}^{(N)}.
\]

In general, \( N \)th order tensor \( \mathbf{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) can be represented as a sum of rank-one tensors, so called CP or PARAFAC [22]
\[
\mathbf{X} = \sum_{r=1}^{R} \mathbf{v}_r^{(1)} \circ \mathbf{v}_r^{(2)} \circ \cdots \circ \mathbf{v}_r^{(N)}.
\]
The smallest number \( R \) of the rank-one tensors that produce \( X \) is called the tensor rank of \( X \). It is possible to define a tensor operation between rank-one tensors and generalize it to sums of rank-one tensors. For example, given two rank-one tensors \( A = a^{(1)} \circ a^{(2)} \circ \ldots \circ a^{(N)} \) and \( B = b^{(1)} \circ b^{(2)} \circ \ldots \circ b^{(N)} \) and Hadamard (elementwise) product of vectors \( a^{(n)} \odot b^{(n)} \),

- the Kronecker product \( A \otimes B \) can be defined by
  \[
  A \otimes B = (a^{(1)} \otimes b^{(1)}) \circ (a^{(2)} \otimes b^{(2)}) \circ \ldots \circ (a^{(N)} \otimes b^{(N)}),
  \]
- the mode-\( n \) Kronecker product by
  \[
  A \otimes_n B = (a^{(1)} \otimes b^{(1)}) \circ (a^{(n-1)} \otimes b^{(n-1)}) \circ (a^{(n)} \otimes b^{(n)}) \circ (a^{(n+1)} \otimes b^{(n+1)}) \circ \ldots \circ (a^{(N)} \otimes b^{(N)}),
  \]
- the mode-\( \bar{n} \) Kronecker product by
  \[
  A \otimes_{\bar{n}} B = (a^{(1)} \otimes b^{(1)}) \circ (a^{(n-1)} \otimes b^{(n-1)}) \circ (a^{(n)} \otimes b^{(n)}) \circ (a^{(n+1)} \otimes b^{(n+1)}) \circ \ldots \circ (a^{(N)} \otimes b^{(N)}),
  \]
- the Hadamard product by
  \[
  A \odot B = (a^{(1)} \odot b^{(1)}) \circ (a^{(2)} \odot b^{(2)}) \circ \ldots \circ (a^{(N)} \odot b^{(N)}),
  \]
- and the outer product by
  \[
  A \circ B = a^{(1)} \circ \ldots \circ a^{(N)} \circ b^{(1)} \circ \ldots \circ b^{(N)}.
  \]

However, the problem of determining the tensor rank of a specific tensor is NP-hard if the order is larger than 2 [10]. So, for practical applications, we will define tensor operations by using index notation and provide examples with rank-one tensors.

### 2.2 Direct sum

The direct sum of matrices \( A \) and \( B \) is defined by

\[
A \oplus B = \text{diag}(A, B) = \begin{bmatrix} A \\ B \end{bmatrix}.
\]

A generalization of the direct sum to tensors is defined as follows.

**Definition 2.4 (Direct sum).** The direct sum of tensors \( A \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) and \( B \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N} \) is defined by

\[
C = A \oplus B \in \mathbb{R}^{(I_1+J_1) \times (I_2+J_2) \times \cdots \times (I_N+J_N)}
\]

with entries

\[
C(k_1, k_2, \ldots, k_N) = \begin{cases} 
A(k_1, k_2, \ldots, k_N) & \text{if } 1 \leq k_n \leq I_n \ \forall n \\
B(k_1 - I_1, k_2 - I_2, \ldots, k_N - I_N) & \text{if } I_n < k_n \leq I_n + J_n \ \forall n \\
0 & \text{otherwise}.
\end{cases}
\]
The mode-$n$ direct sum of $\mathbf{A} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times J \times I_{n+1} \times \cdots \times I_N}$ and $\mathbf{B} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times K \times I_{n+1} \times \cdots \times I_N}$ is defined by

$$\mathbf{C} = \mathbf{A} \oplus_n \mathbf{B} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times (J+K) \times I_{n+1} \times \cdots \times I_N}$$

with mode-$n$ fibers

$$\mathbf{C}(i_1, \ldots, i_{n-1}, ;, i_{n+1}, \ldots, i_N) = \mathbf{A}(i_1, \ldots, ;, i_{n-1}, ;, i_{n+1}, \ldots, i_N) \oplus \mathbf{B}(i_1, \ldots, ;, i_{n-1}, ;, i_{n+1}, \ldots, i_N).$$

The mode-$n$ direct sum of $\mathbf{A} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ and $\mathbf{B} \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}$ with common mode size $I_n = J_n$ is defined by

$$\mathbf{C} = \mathbf{A} \oplus_n \mathbf{B} \in \mathbb{R}^{(I_1+J_1) \times \cdots \times (I_{n-1}+J_{n-1}) \times I_n \times (I_{n+1}+J_{n+1}) \times \cdots \times (I_N+J_N)}$$

with subtensors

$$\mathbf{C}(:, \ldots, ;, i_n, ;, \ldots, :) = \mathbf{A}(:, \ldots, ;, i_n, ;, \ldots, :) \oplus \mathbf{B}(:, \ldots, ;, i_n, ;, \ldots, :)$$

for each $i_n = 1, 2, \ldots, I_n$.

In special cases, the direct sum of vectors $\mathbf{a} \in \mathbb{R}^I$ and $\mathbf{b} \in \mathbb{R}^J$ is the concatenation $\mathbf{a} \oplus \mathbf{b} \in \mathbb{R}^{I+J}$, and the direct sum of matrices $\mathbf{A} \in \mathbb{R}^{I_1 \times J_2}$ and $\mathbf{B} \in \mathbb{R}^{J_1 \times J_2}$ is the block diagonal matrix $\mathbf{A} \oplus \mathbf{B} = \text{diag}(\mathbf{A}, \mathbf{B}) \in \mathbb{R}^{(I_1+J_1) \times (J_2+J_2)}$. We suppose that the direct sum of scalars $a, b \in \mathbb{R}$ is the addition $a \oplus b = a + b \in \mathbb{R}$.

### 2.3 Tucker operator and contracted product

Kolda and Bader [22] further introduced a multilinear operator called the Tucker operator [21] to simplify the expression for the mode-$n$ product. The mode-$n$ product of a tensor $\mathbf{G} \in \mathbb{R}^{R_1 \times R_2 \times \cdots \times R_N}$ and a matrix $\mathbf{A} \in \mathbb{R}^{I_n \times R_n}$ is defined by

$$\mathbf{X} = \mathbf{G} \times_n \mathbf{A} \in \mathbb{R}^{R_1 \times \cdots \times R_{n-1} \times I_n \times R_{n+1} \times \cdots \times R_N}$$

with entries

$$\mathbf{X}(r_1, \ldots, r_{n-1}, i_n, r_{n+1}, \ldots, r_N) = \sum_{r_n=1}^{R_n} \mathbf{G}(r_1, r_2, \ldots, r_N) \mathbf{A}(i_n, r_n),$$

or, in matrix,

$$\mathbf{X}_{(n)} = \mathbf{A} \mathbf{G}_{(n)}.$$

The standard Tucker operator of a tensor $\mathbf{G} \in \mathbb{R}^{R_1 \times R_2 \times \cdots \times R_N}$ and matrices $\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R_n}$, $n = 1, \ldots, N$, is defined by

$$\begin{bmatrix} \mathbf{G}; \mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \ldots, \mathbf{A}^{(N)} \end{bmatrix} = \mathbf{G} \times_1 \mathbf{A}^{(1)} \times_2 \mathbf{A}^{(2)} \times_3 \cdots \times_N \mathbf{A}^{(N)} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}. \quad (1)$$

Here, we generalize this to a multilinear operator between tensors.

**Definition 2.5** (Tucker operator). Let $N \geq 1$ and $M_n \geq 0$ ($n = 1, 2, \ldots, N$). For an $N$th order tensor $\mathbf{G} \in \mathbb{R}^{R_1 \times R_2 \times \cdots \times R_N}$ and $(M_n + 1)$th order tensors $\mathbf{A}^{(n)} \in \mathbb{R}^{I_{n,1} \times I_{n,2} \times \cdots \times I_{n,M_n} \times R_n}$, $n = 1, \ldots, N$,
1, \ldots, N, the Tucker operator is a multilinear operator defined by the \((M_1 + M_2 + \cdots + M_N)\)th order tensor
\[
X = \begin{bmatrix} G; A^{(1)}, \ldots, A^{(N)} \end{bmatrix} \in \mathbb{R}^{I_1 \times \cdots \times I_M \times \cdots \times I_N}
\]
with entries
\[
X(i_1, i_2, \ldots, i_N) = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_N=1}^{R_N} G(r_1, r_2, \ldots, r_N) A^{(1)}(i_1, r_1) A^{(2)}(i_2, r_2) \cdots A^{(N)}(i_N, r_N),
\]
where \(i_n = (i_{n1}, i_{n2}, \ldots, i_{nM_n})\) is the ordered indices.

In a special case, we have the standard Tucker operator \(\mathbb{1}\) if \(A^{(n)}\) are matrices, i.e., \(M_n = 1\). Even in the case of vectors \(a^{(n)} \in \mathbb{R}^{R_n}\), i.e., \(M_n = 0\), we have the scalar
\[
\left[ G; a^{(1)}, a^{(2)}, \ldots, a^{(N)} \right] = G \bar{x}_1 a^{(1)} \bar{x}_2 a^{(2)} \bar{x}_3 \cdots \bar{x}_N a^{(N)} \in \mathbb{R},
\]
where \(\bar{x}_n\) is the mode-\(n\) (vector) product \([22]\).

For example, let \(G = g^{(1)} \circ g^{(2)} \circ g^{(3)} \in \mathbb{R}^{R_1 \times R_2 \times R_3}\) and \(A = a^{(1)} \circ a^{(2)} \circ a^{(3)} \circ a^{(4)} \circ a^{(5)} \in \mathbb{R}^{R_1 \times R_2 \times R_3}\) be rank-one tensors. Then,
\[
\left[ G; I_{R_1}, A, I_{R_3} \right] = \left< g^{(2)}, a^{(5)} \right> \left< g^{(1)} \circ a^{(1)} \circ a^{(2)} \circ a^{(3)} \circ a^{(4)} \circ g^{(3)} \right> \in \mathbb{R}^{R_1 \times R_2 \times R_3},
\]
where \(\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^T \mathbf{w}\) is the inner product of vectors.

In general, we can derive the following properties.

**Proposition 2.6.** Let \(N \geq 1\) and \(M_n \geq 0\) \((n = 1, 2, \ldots, N)\). Let \(G_X\) and \(G_Y\) be \(N\)th order tensors, \(A^{(n)}\) and \(B^{(n)}\) be \((M_n + 1)\)th order tensors, \(n = 1, 2, \ldots, N\), and
\[
X = \begin{bmatrix} G_X; A^{(1)}, \ldots, A^{(N)} \end{bmatrix} \quad \text{and} \quad Y = \begin{bmatrix} G_Y; B^{(1)}, \ldots, B^{(N)} \end{bmatrix}
\]
have the same sizes. Then

(a) \(X \otimes Y = \begin{bmatrix} G_X \otimes G_Y; A^{(1)} \otimes B^{(1)}, \ldots, A^{(N)} \otimes B^{(N)} \end{bmatrix}\),

(b) \(X \circledcirc Y = \begin{bmatrix} G_X \circledcirc G_Y; A^{(1)} \circledcirc M_{i+1} B^{(1)}, \ldots, A^{(N)} \circledcirc M_{N+1} B^{(N)} \end{bmatrix}\),

(c) \(X \oplus Y = \begin{bmatrix} G_X \oplus G_Y; A^{(1)} \oplus B^{(1)}, \ldots, A^{(N)} \oplus B^{(N)} \end{bmatrix}\),

(d) \(X + Y = \begin{bmatrix} G_X \oplus G_Y; A^{(1)} \oplus M_{i+1} B^{(1)}, \ldots, A^{(N)} \oplus M_{N+1} B^{(N)} \end{bmatrix}\).

**Example.** We provide examples where \(A^{(n)}\) and \(B^{(n)}\) are either matrices or vectors.

- Let \(M_n = 1\) \((n = 1, 2, \ldots, N)\), i.e., we have \(X\) and \(Y\) in Tucker format
  \[
  X = \begin{bmatrix} G_X; A^{(1)}, \ldots, A^{(N)} \end{bmatrix} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}
  \]
  \[
  Y = \begin{bmatrix} G_Y; B^{(1)}, \ldots, B^{(N)} \end{bmatrix} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}.
  \]

It follows that the Kronecker product, Hadamard product, direct sum, and addition is also given in the Tucker format.
(a) \(X \otimes Y = [G_X \otimes G_Y; A^{(1)} \otimes B^{(1)}, \ldots, A^{(N)} \otimes B^{(N)}]\),
(b) \(X \otimes Y = [G_X \otimes G_Y; A^{(1)} \otimes_2 B^{(1)}, \ldots, A^{(N)} \otimes_2 B^{(N)}]\),
(c) \(X \oplus Y = [G_X \oplus G_Y; A^{(1)} \oplus B^{(1)}, \ldots, A^{(N)} \oplus B^{(N)}]\),
(d) \(X + Y = [G_X + G_Y; A^{(1)} \oplus_2 B^{(1)}, \ldots, A^{(N)} \oplus_2 B^{(N)}]\).

In the case that \(X\) and \(Y\) are in CP format where the core tensors \(G_X\) and \(G_Y\) are super-diagonal, the results are also given in CP format because the Kronecker product and direct sum of the super-diagonal core tensors are super-diagonal tensors as well.

- Let \(M_n = 0 (n = 1, 2, \ldots, N)\), then we have the scalars

\[
x = [G_X; a^{(1)}, \ldots, a^{(N)}] \in \mathbb{R}
\]

\[
y = [G_Y; b^{(1)}, \ldots, b^{(N)}] \in \mathbb{R}.
\]

The multiplication and addition are given in the form

(a) \(xy = x \otimes y = x \oplus y = [G_X \otimes G_Y; a^{(1)} \otimes b^{(1)}, \ldots, a^{(N)} \otimes b^{(N)}]\),
(b) \(x + y = x \oplus y = [G_X \oplus G_Y; a^{(1)} \oplus b^{(1)}, \ldots, a^{(N)} \oplus b^{(N)}]\).

As a special case, we introduce a tensor-tensor contracted product as follows.

**Definition 2.7** ((Mode-\((M, 1)\)) contracted product). Let \(M \geq 1\) and \(N \geq 1\). The (mode-\((M, 1)\)) contracted product of tensors \(A \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_M}\) and \(B \in \mathbb{R}^{I_M \times I_{M+1} \times \cdots \times I_N}\) is defined by

\[
C = A \cdot B \in \mathbb{R}^{I_1 \times \cdots \times I_{M-1} \times I_{M+1} \times \cdots \times I_N}
\]

with entries

\[
C(i_1, \ldots, i_{M-1}, j_2, \ldots, j_N) = \sum_{i_M=1}^{I_M} A(i_1, \ldots, i_M)B(i_M, j_2, \ldots, j_N).
\]

We note that the tensor-tensor contracted product defined above is a natural generalization of the matrix multiplication as \(AB = A \cdot B\), and the vector innerproduct as \((a, b) = a \cdot b\). Especially, the contracted products between a tensor \(A \in \mathbb{R}^{I_1 \times \cdots \times I_M}\) and vectors \(p \in \mathbb{R}^{I_1}\) and \(q \in \mathbb{R}^{I_M}\) lead to tensors of smaller orders as

\[
p \cdot A \in \mathbb{R}^{I_2 \times \cdots \times I_M},
A \cdot q \in \mathbb{R}^{I_1 \times \cdots \times I_{M-1}}.
\]

The contracted product of rank-one tensors yields

\[
\left(a^{(1)} \circ \cdots \circ a^{(M)}\right) \cdot \left(b^{(1)} \circ \cdots \circ b^{(N)}\right) = \left(a^{(M)} \cdot b^{(1)}\right) \left(a^{(1)} \circ \cdots \circ a^{(M-1)} \circ b^{(2)} \circ \cdots \circ b^{(N)}\right).
\]

In general, we have the following properties:

**Proposition 2.8.** Let \(A \in \mathbb{R}^{I_1 \times \cdots \times I_M}\), \(B \in \mathbb{R}^{I_M \times I_{M+1} \times \cdots \times I_N}\), \(C \in \mathbb{R}^{J_N \times K_{N+1} \times \cdots \times K_L}\), \(G \in \mathbb{R}^{R_1 \times \cdots \times R_N}\), \(P \in \mathbb{R}^{I_1 \times R_1}\), and \(Q \in \mathbb{R}^{R_N \times J}\). Then
\( (a) \ (A \bullet B) \bullet C = A \bullet (B \bullet C). \)

\( (b) \ A \bullet B = [B : A, J_2, \ldots, J_N]. \)

\( (c) \ P \bullet G = G \times_1 P, \)

\( (d) \ G \bullet Q = G \times_N Q^T, \) and

\( (e) \ (A \bullet B)_{\{m\}} = A_{\{m\}} (I_{m+1} \otimes I_{m+2} \otimes \cdots \otimes I_{M-1} \otimes B_{(1)}) \) for \( m = 1, 2, \ldots, M - 1. \)

**Proof of (e).** Note that \( A \bullet B \in \mathbb{R}^{I_1 \times \cdots \times I_{M-1} \times J_1 \cdots J_N}. \) For \( 1 \leq m \leq M - 1, \) we have

\[
(A \bullet B)_{\{m\}} (i_1 \cdots i_m, i_{m+1} \cdots i_{M-1}, j_2, \ldots, j_N) = (A \bullet B) (i_1, \ldots, i_{M-1}, j_2, \ldots, j_N)
\]

\[
= \sum_{i_m = 1}^{I_m} A(i_1, \ldots., i_M) B(i_{M}, j_2, \ldots, j_N) \delta(k_{m+1}, i_{m+1}) \cdots \delta(k_{M-1}, i_{M-1}).
\]

By inserting auxiliary variables \( k_{m+1}, \ldots, k_M, \)

\[
\sum_{i_m = 1}^{I_m} A(i_1, \ldots, i_M) B(i_{M}, j_2, \ldots, j_N) = \sum_{k_{m+1} = 1}^{I_{m+1}} \cdots \sum_{k_{M-1} = 1}^{I_{M-1}} \sum_{i_M = 1}^{I_M} A(i_1, \ldots, i_m, k_{m+1}, \ldots, k_{M-1}, i_M)
\]

\[
B(i_{M}, j_2, \ldots, j_N) \delta(k_{m+1}, i_{m+1}) \cdots \delta(k_{M-1}, i_{M-1}).
\]

We also have

\[
A(i_1, \ldots, i_m, k_{m+1}, \ldots, k_{M-1}, i_M) = A_{\{m\}} (i_1 \cdots i_m, k_{m+1} \cdots k_{M-1} i_M)
\]

and

\[
B(i_{M}, j_2, \ldots, j_N) \delta(k_{m+1}, i_{m+1}) \cdots \delta(k_{M-1}, i_{M-1})
\]

\[
= I_{m+1} (k_{m+1}, i_{m+1}) \cdots I_{M-1} (k_{M-1}, i_{M-1}) B_{(1)} (i_M, j_2 \cdots j_N)
\]

\[
= (I_{m+1} \otimes \cdots \otimes I_{M-1} \otimes B_{(1)}) (k_{m+1} \cdots k_{M-1} i_M, i_{m+1} \cdots i_{M-1} j_2 \cdots j_N).
\]

It follows that \( (A \bullet B)_{\{m\}} = A_{\{m\}} (I_{m+1} \otimes \cdots \otimes I_{M-1} \otimes B_{(1)}). \)

**Proposition 2.9.** Let \( A^{(n)} \) and \( B^{(n)} \) be \( M_n \)th order tensors, \( n = 1, 2, \) and let

\[
X = A^{(1)} \bullet A^{(2)} \quad \text{and} \quad Y = B^{(1)} \bullet B^{(2)}
\]

have the same sizes. Then,

\( (a) \ X \otimes Y = (A^{(1)} \otimes B^{(1)}) \bullet (A^{(2)} \otimes B^{(2)}), \)

\( (b) \ X \oplus Y = (A^{(1)} \oplus M, B^{(1)}) \bullet (A^{(2)} \oplus B^{(2)}), \)

\( (c) \ X \oplus Y = (A^{(1)} \oplus B^{(1)}) \bullet (A^{(2)} \oplus B^{(2)}), \)

\( (d) \ X + Y = (A^{(1)} \oplus M, B^{(1)}) \bullet (A^{(2)} \oplus B^{(2)}) . \)
2.4 Self-contraction operator

We will define a linear operator, $S$, called the self-contraction, which generalizes the trace on matrices to tensors.

**Definition 2.10 (Self-contraction).** The self-contraction, $S : \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N \times I_1} \rightarrow \mathbb{R}^{I_2 \times I_3 \times \cdots \times I_N}$, $N \geq 1$, is a linear operator defined by $Y = S(X)$ with

\[
Y(i_2, i_3, \ldots, i_N) = \sum_{i_1=1}^{I_1} X(i_1, i_2, \ldots, i_N, i_1). \tag{3}
\]

The self-contraction is a generalization of the matrix trace. For a matrix $A \in \mathbb{R}^{I \times I}$,

\[
S(A) = \text{tr}(A) \in \mathbb{R}.
\]

A more formal definition is given by using the contracted product as

\[
S(X) = \sum_{i_1=1}^{I_1} e_{i_1} \bullet X \bullet e_{i_1}, \tag{4}
\]

where $e_{i_1} = [0, \ldots, 1, \ldots, 0]^T \in \mathbb{R}^{I_1}$ is the $i_1$th standard basis vector. The self-contraction of a rank-one tensor is calculated by

\[
S(a(1) \circ a(2) \circ \cdots \circ a(N+1)) = \left\langle a^{(1)} a^{(N+1)} \right\rangle a^{(2)} \circ \cdots \circ a^{(N)},
\]

where $\langle v, w \rangle = v^T w$. For a tensor $X \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N \times I_1}$, the $(i_2, i_3, \ldots, i_N)$th entry of $S(X)$ equals to the matrix trace of the $(i_2, i_3, \ldots, i_N)$th slice as

\[
(S(X))_{i_2, i_3, \ldots, i_N} = \text{tr}(X(:, i_2, i_3, \ldots, i_N, :)).
\]

In addition, let $A \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_{M+1}}$ and $B \in \mathbb{R}^{I_{M+1} \times J_2 \times \cdots \times J_N \times I_1}$. Then

\[
(S(A \bullet B))_{i_2, \ldots, i_{M+1}, j_2, \ldots, j_N} = (S(B \bullet A))_{j_2, \ldots, j_N, i_2, \ldots, i_M}.
\]

As a special case, if $M = N = 2$, then $(S(A \bullet B))^T = S(B \bullet A)$.

2.5 Strong Kronecker product

The strong Kronecker product is an important tool in low-rank TT decompositions of large-scale tensors. We present the definitions of the strong Kronecker product \[27\] and its generalization to tensors.

**Definition 2.11 (Strong Kronecker product).** Let $A$ and $B$ be $R_1 \times R_2$ and $R_2 \times R_3$ block matrices

\[
A = [A_{r_1 r_2}] = \begin{bmatrix}
A_{1,1} & \cdots & A_{1,R_2} \\
\vdots & \ddots & \vdots \\
A_{R_1,1} & \cdots & A_{R_1,R_2}
\end{bmatrix} \in \mathbb{R}^{R_1 I_1 \times R_2 I_2}
\]
\[
B = [B_{r_2,r_3}] = \begin{bmatrix}
B_{1,r_3} & \cdots & B_{1,R_3} \\
\vdots & \ddots & \vdots \\
B_{R_2,1} & \cdots & B_{R_2,R_3}
\end{bmatrix} \in \mathbb{R}^{R_2 \times J_1 \times R_3 \times J_2},
\]
where \(A_{r_1,r_2} \in \mathbb{R}^{I_1 \times I_2}\) and \(B_{r_2,r_3} \in \mathbb{R}^{J_1 \times J_2}\). The strong Kronecker product of \(A\) and \(B\) is defined by the \(R_1 \times R_3\) block matrix
\[
C = [C_{r_1,r_3}] = A \otimes B \in \mathbb{R}^{R_1 \times I_1 \times R_2 \times I_2},
\]
where
\[
C_{r_1,r_3} = \sum_{r_2=1}^{R_2} A_{r_1,r_2} \otimes B_{r_2,r_3} \in \mathbb{R}^{I_1 \times J_1 \times I_2 \times J_2},
\]
for \(r_1 = 1, 2, \ldots, R_1\) and \(r_3 = 1, 2, \ldots, R_3\). More generally, let
\[
A = [A_{r_1,r_2}] \in \mathbb{R}^{R_1 \times I_1 \times R_2 \times I_2},
\]
and
\[
B = [B_{r_2,r_3}] \in \mathbb{R}^{R_2 \times J_1 \times R_3 \times J_3}
\]
be \(R_1 \times R_2\) and \(R_2 \times R_3\) block tensors where \(A_{r_1,r_2} \in \mathbb{R}^{I_1 \times I_2 \times I_3}\) and \(B_{r_2,r_3} \in \mathbb{R}^{J_1 \times J_2 \times J_3}\) are 3rd order tensors. Then the strong Kronecker product of \(A\) and \(B\) is defined by the \(R_1 \times R_3\) block tensor
\[
C = [C_{r_1,r_3}] = A \otimes B \in \mathbb{R}^{R_1 \times I_1 \times R_2 \times I_2 \times I_3}
\]
where
\[
C_{r_1,r_3} = \sum_{r_2=1}^{R_2} A_{r_1,r_2} \otimes B_{r_2,r_3} \in \mathbb{R}^{I_1 \times J_1 \times I_2 \times J_2 \times I_3},
\]
for \(r_1 = 1, 2, \ldots, R_1\) and \(r_3 = 1, 2, \ldots, R_3\).

**Example.** The strong Kronecker product has a similarity with the matrix-matrix multiplication. For example,
\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix} \otimes \begin{bmatrix}
B_{11} & B_{12} \\
B_{21} & B_{22}
\end{bmatrix} = \begin{bmatrix}
A_{11} \otimes B_{11} + A_{12} \otimes B_{21} & A_{11} \otimes B_{12} + A_{12} \otimes B_{22} \\
A_{21} \otimes B_{11} + A_{22} \otimes B_{21} & A_{21} \otimes B_{12} + A_{22} \otimes B_{22}
\end{bmatrix}.
\]

2.6 Graphical representations of tensors

It is quite useful to represent tensors and related operations by graphs of nodes and edges, as was proposed in [18]. Figure II(a), (b), and (c) illustrate the graphs representing a vector, a matrix, and a 3rd order tensor. In each graph, the number of edges connected to a node indicates the order of the tensor, and the mode size can be shown by the label on each edge. Figure II(d) represents the singular value decomposition of a matrix. The orthonormalized matrices are represented by half-filled circles and the diagonal matrix by a circle with slash inside. Figure II(e) represents the mode-3 product, \(A \times_3 B\), for some \(A \in \mathbb{R}^{I_1 \times I_2 \times I_3}\) and \(B \in \mathbb{R}^{J_1 \times J_2}\) \((I_3 = J_2)\). Figure II(f) represents the contracted product, \(A \bullet B\), for some \(A \in \mathbb{R}^{I_1 \times I_2 \times I_3}\) and \(B \in \mathbb{R}^{J_1 \times J_2 \times J_3}\) \((I_3 = J_4)\).
Figure 1: Graphical representations for (a) a vector (b) a matrix, (c) a 3rd order tensor, (d) singular value decomposition of an $I \times J$ matrix, (e) mode-3 product between a 3rd order tensor and a matrix, and (f) contracted product between two 3rd order tensors.

Figure 2: Graphical representation of a 4th order tensor in TT format

3 Tensor train formats

3.1 TT format

In the TT format, a tensor $\mathbf{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is represented as

$$\mathbf{X} = \mathbf{G}^{(1)} \cdot \mathbf{G}^{(2)} \cdot \cdots \cdot \mathbf{G}^{(N-1)} \cdot \mathbf{G}^{(N)},$$

where $\mathbf{G}^{(n)} \in \mathbb{R}^{R_{n-1} \times I_n \times R_n}$, $n = 1, \ldots, N$, are 3rd order tensors called the TT-cores, $R_1, \ldots, R_{N-1}$ are called the TT-ranks, and $R_0 = R_N = 1$. Since $R_0 = R_N = 1$, we consider that the contracted product (5) yields a tensor of order $N$ even if each of the TT-cores are regarded as a 3rd order tensor for notational convenience. Figure 2 illustrates the graphical representation of a 4th order TT tensor.

Alternatively, the TT format is often written entry-wise as

$$x_{i_1,i_2,\ldots,i_N} = G^{(1)}_{i_1} G^{(2)}_{i_2} \cdots G^{(N-1)}_{i_{N-1}} G^{(N)}_{i_N}$$

$$= \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} g^{(1)}_{r_1,i_1,r_1} g^{(2)}_{r_2,i_2,r_2} \cdots g^{(N-1)}_{r_{N-1},i_{N-1},r_{N-1}} g^{(N)}_{r_N,i_N,1},$$

where $G^{(n)}_{i_n} = G^{(n)}(\cdot,i_n,\cdot) \in \mathbb{R}^{R_{n-1} \times R_n}$ is the lateral slice of the $n$th TT-core. Note that $G^{(1)}_{i_1}$ and $G^{(N)}_{i_N}$ are $1 \times R_1$ and $R_{N-1} \times 1$ matrices.
The TT format can also be represented as a sum of outer products. From (3), we have

\[
\mathbf{X} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} \mathbf{g}^{(1)}_{1,r_1} \otimes \mathbf{g}^{(2)}_{r_1,r_2} \otimes \cdots \otimes \mathbf{g}^{(N-1)}_{r_{N-2},r_{N-1}} \otimes \mathbf{g}^{(N)}_{r_{N-1},1},
\]

(7)

where $\mathbf{g}^{(n)}_{r_{n-1},r_n} = \mathbf{G}^{(n)}(r_{n-1}, r_n) \in \mathbb{R}^{I_n}$ is the mode-2 fiber.

A large-scale vector $\mathbf{x}$ of length $I_1 I_2 \cdots I_N$ can be tensorized into $\mathbf{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ and represented in TT format. By vectorizing the TT format (7), we get the TT format for $\mathbf{x}$, represented as a sum of the Kronecker products

\[
\mathbf{x} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} \mathbf{g}^{(1)}_{1,r_1} \otimes \mathbf{g}^{(2)}_{r_1,r_2} \otimes \cdots \otimes \mathbf{g}^{(N-1)}_{r_{N-2},r_{N-1}} \otimes \mathbf{g}^{(N)}_{r_{N-1},1}.
\]

(8)

The above form can be compactly represented as the strong Kronecker products

\[
\mathbf{x} = \mathbf{G}^{(1)} \otimes \mathbf{G}^{(2)} \otimes \cdots \otimes \mathbf{G}^{(N-1)} \otimes \mathbf{G}^{(N)},
\]

(9)

where $\mathbf{G}^{(n)}, n = 1, \ldots, N$, are the $R_{n-1} \times R_n$ block matrices

\[
\mathbf{G}^{(n)} = \begin{bmatrix}
\mathbf{g}^{(n)}_{1,1} & \cdots & \mathbf{g}^{(n)}_{1,R_n} \\
\vdots & \ddots & \vdots \\
\mathbf{g}^{(n)}_{R_{n-1},1} & \cdots & \mathbf{g}^{(n)}_{R_{n-1},R_n}
\end{bmatrix} \in \mathbb{R}^{R_{n-1} \times R_n}
\]

with each block $\mathbf{g}^{(n)}_{r_{n-1},r_n} \in \mathbb{R}^{I_n}$. Table 3 summarizes the alternative representations for the TT format.

In principle, any tensor $\mathbf{X}$ can be represented in TT format through the TT-SVD algorithm [30]. The storage cost for a TT format is $O(NIR^2)$ with $I = \max(I_n)$ and $R = \max(R_n)$. So the storage and computational complexities can be substantially reduced if the TT-ranks are kept small enough.

### 3.2 Recursive representations for TT format

The TT format can be expressed in a recursive manner, which is summarized in Table 4. Given the TT-cores $\mathbf{G}^{(n)}, n = 1, \ldots, N$, we define the partial contracted products $\mathbf{G}^\leq n \in \mathbb{R}^{I_1 \times \cdots \times I_n \times R_n}$ and $\mathbf{G}^\geq n \in \mathbb{R}^{R_n \times I_{n+1} \times \cdots \times I_N}$ as

\[
\mathbf{G}^\leq n = \mathbf{G}^{(1)} \bullet \mathbf{G}^{(2)} \bullet \cdots \bullet \mathbf{G}^{(n)}
\]

(10)

and

\[
\mathbf{G}^\geq n = \mathbf{G}^{(n)} \bullet \mathbf{G}^{(n+1)} \bullet \cdots \bullet \mathbf{G}^{(N)}.
\]

(11)

$\mathbf{G}^\leq n$ and $\mathbf{G}^\geq n$ are defined in the same way. For completeness, we define $\mathbf{G}^\leq 1 = \mathbf{G}^\geq N = 1$. The vectorizations of the partial contracted products yield the following recursive equations

\[
\text{vec} \left( \mathbf{G}^\leq n \right) = \text{vec} \left( \mathbf{G}^{\leq n-1} \times_n \mathbf{G}^{(n)T}_{(1)} \right) = \left( I_{I_1 I_2 \cdots I_{n-1}} \otimes \mathbf{G}^{(n)T}_{(1)} \right) \text{vec} \left( \mathbf{G}^{\leq n-1} \right)
\]

for $n = 2, 3, \ldots, N$, and

\[
\text{vec} \left( \mathbf{G}^\geq n \right) = \text{vec} \left( \mathbf{G}^{\geq n+1} \times_1 \mathbf{G}^{(n)T}_{(3)} \right) = \left( \mathbf{G}^{(n)T}_{(3)} \otimes I_{I_{n+1} I_{n+2} \cdots I_N} \right) \text{vec} \left( \mathbf{G}^{\geq n+1} \right)
\]
Table 3: Various representations for the TT format of a tensor $X$ of size $I_1 \times \cdots \times I_N$

|       | Contracted products                                                                 |
|-------|--------------------------------------------------------------------------------------|
| $X$   | $G^{(1)} \bullet G^{(2)} \cdots \bullet G^{(N-1)} \bullet G^{(N)}$                  |

|       | Matrix products                                                                      |
|-------|--------------------------------------------------------------------------------------|
| $x_{i_1,i_2,\ldots,i_N}$ | $G^{(1)}_{i_1} G^{(2)}_{i_2} \cdots G^{(N-1)}_{i_{N-1}} G^{(N)}_{i_N}$ |

|       | Scalar products                                                                      |
|-------|--------------------------------------------------------------------------------------|
| $x_{i_1,i_2,\ldots,i_N}$ | $\sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} g^{(1)}_{r_1,i_1} g^{(2)}_{r_2,i_2} \cdots g^{(N-1)}_{r_{N-2},i_{N-1}} g^{(N)}_{r_{N-1},i_N,1}$ |

|       | Outer products                                                                       |
|-------|--------------------------------------------------------------------------------------|
| $X$   | $\sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} g^{(1)}_{1,r_1} \circ g^{(2)}_{r_1,r_2} \circ \cdots \circ g^{(N-1)}_{r_{N-2},r_{N-1}} \circ g^{(N)}_{r_{N-1},1}$ |

|       | Strong Kronecker products                                                             |
|-------|--------------------------------------------------------------------------------------|
| $x$   | $\text{vec}(X) = \tilde{G}^{(1)} \otimes \cdots \otimes \tilde{G}^{(N-1)} \otimes \tilde{G}^{(N)}$ |
|       | $\tilde{G}^{(n)} = \left[ g^{(n)}_{r_{n-1},r_n} \right] \in \mathbb{R}^{R_{n-1} \times R_n}$ with each block $g^{(n)}_{r_{n-1},r_n} \in \mathbb{R}^{I_n}$ |

|       | Vectorizations                                                                       |
|-------|--------------------------------------------------------------------------------------|
| $x$   | $\text{vec}(X) = \left( I_{1} \circ I_{2} \cdots \circ I_{N-2} \otimes G^{(N-1)T}_{(1)} \right) \left( I_{1} \circ I_{2} \cdots \circ I_{N-2} \otimes G^{(N-1)T}_{(1)} \right) \cdots \left( I_{1} \circ G^{(2)T}_{(1)} \right) \text{vec} \left( \tilde{G}^{(1)} \right)$ |
|       | $x = \text{vec}(X) = \left( G^{(1)T}_{(3)} \otimes I_{2} \cdots \otimes I_{N} \right) \left( G^{(2)T}_{(3)} \otimes I_{2} \cdots \otimes I_{N} \right) \cdots \left( G^{(N-1)T}_{(3)} \otimes I_{N} \right) \text{vec} \left( \tilde{G}^{(N)} \right)$ |
|       | $x = \text{vec}(X) = \left( G_{(n)}^{<n} \right)^T \otimes I_{n} \otimes \left( G_{(1)}^{>n} \right)^T \text{vec} \left( \tilde{G}^{(n)} \right)$ |
for \( n = 1, 2, \ldots, N - 1 \).

Hence, the vectorization of tensor \( X \) can be expressed as

\[
\text{vec}(X) = \text{vec}(G^{\leq N}) = \left( I_{I_1I_2\ldots I_{N-1}} \otimes G^{(N)}_{(1)} \right) \text{vec}(G^{\leq N-1})
\]

and

\[
\text{vec}(X) = \text{vec}(G^{\geq 1}) = \left( G^{(1)}_{(3)} \otimes I_{I_2I_3\ldots I_N} \right) \text{vec}(G^{\geq 2}).
\]

**Proposition 3.1.** We obtain the following formulas:

\[
\text{vec}(X) = \left( I_{I_1I_2\ldots I_{N-1}} \otimes G^{(N)}_{(1)} \right) \left( I_{I_1I_2\ldots I_{N-2}} \otimes G^{(N-1)}_{(1)} \right) \cdots \left( I_{I_1} \otimes G^{(2)}_{(1)} \right) \text{vec}(G^{(1)})
\]

and

\[
\text{vec}(X) = \left( G^{(1)}_{(3)} \otimes I_{I_2I_3\ldots I_N} \right) \left( G^{(2)}_{(3)} \otimes I_{I_4I_5\ldots I_N} \right) \cdots \left( G^{(N-1)}_{(3)} \otimes I_{N} \right) \text{vec}(G^{(N)}).
\]

### 3.3 Extraction of TT-cores

Using the concept of splitting tensor train to sub-tensor trains, we can obtain an another important expression of the vectorization, in which the \( n \)th core tensor is separated from the others as \([6, 26]\)

\[
\text{vec}(X) = \left( G^{(n)}_{(1)} \times_1 \left( G^{<n}_{(n)} \right)^T \times_3 \left( G^{>n}_{(1)} \right)^T \right)
\]

\[
= \left( \left( G^{<n}_{(n)} \right)^T \otimes I_n \otimes \left( G^{>n}_{(1)} \right)^T \right) \text{vec}(G^{(n)}).
\]

By defining the so-called frame matrix

\[
X^{\neq n} = \left( G^{<n}_{(n)} \right)^T \otimes I_n \otimes \left( G^{>n}_{(1)} \right)^T \in \mathbb{R}^{I_1I_2\ldots I_N \times R_{n-1}I_nR_n}
\]

for \( n = 1, 2, \ldots, N \), we get

\[
\text{vec}(X) = X^{\neq n} \text{vec}(G^{(n)}).
\]

Similarly, we can obtain an expression of the vectorization where two neighboring TT-cores are extracted as \([26]\)

\[
\text{vec}(X) = X^{\neq n,n+1} \text{vec}(G^{(n)} \bullet G^{(n+1)}),
\]

where

\[
X^{\neq n,n+1} = \left( G^{<n}_{(n)} \right)^T \otimes I_n \otimes I_{n+1} \otimes \left( G^{>n+1}_{(1)} \right)^T \in \mathbb{R}^{I_1I_2\ldots I_N \times R_{n-1}I_nI_{n+1}R_{n+1}}
\]

for \( n = 1, 2, \ldots, N - 1 \).
Table 4: Recursive representations for the TT format of a tensor $\mathbf{X}$ of size $I_1 \times \cdots \times I_N$

| $\mathbf{X}$ | $\mathbf{G}^{\leq N}$ with $\mathbf{G}^{\leq n} = \mathbf{G}^{\leq n-1} \cdot \mathbf{G}^{(n)}$, $n = 1, 2, \ldots, N$, $\mathbf{G}^{\leq 0} = 1$ | $\mathbf{G}^{\geq 1}$ with $\mathbf{G}^{\geq n} = \mathbf{G}^{(n)} \cdot \mathbf{G}^{\geq n+1}$, $n = 1, 2, \ldots, N$, $\mathbf{G}^{\geq N+1} = 1$ |
|---|---|---|
| $x_{i_1 \ldots i_N} = \mathbf{G}^{\leq N}_{i_1 \ldots i_N}$ | $\mathbf{G}^{\leq n}_{i_1 \ldots i_n} = \mathbf{G}^{\leq n-1}_{i_1 \ldots i_{n-1}} \mathbf{G}^{(n)}_{i_n}$ | $\mathbf{G}^{\geq 1}_{i_1 \ldots i_N} = \mathbf{G}^{(n)}_{i_n} \mathbf{G}^{\geq n+1}_{i_{n+1} \ldots i_N}$ |
| Matrix products |
| $x_{i_1 \ldots i_N} = \mathbf{G}^{\geq 1}_{i_1 \ldots i_N}$ | $\mathbf{G}^{\geq n}_{i_1 \ldots i_N} = \mathbf{G}^{(n)}_{i_n} \mathbf{G}^{\geq n+1}_{i_{n+1} \ldots i_N}$ | $\mathbf{G}^{\leq n}_{i_1 \ldots i_n} = \sum_{r_{n-1}=1}^{R_n-1} \mathbf{g}^{(n)}_{i_1 \ldots i_{n-1}, r_{n-1}} \mathbf{g}^{\geq n+1}_{r_{n-1}, i_n \ldots i_N}$ |
| Scalar products |
| $x_{i_1 \ldots i_N} = \mathbf{G}^{\leq N}_{i_1 \ldots i_N}$ | $\mathbf{G}^{\leq n}_{i_1 \ldots i_N} = \sum_{r_{n-1}=1}^{R_n-1} \mathbf{g}^{(n)}_{i_1 \ldots i_{n-1}, r_{n-1}} \mathbf{g}^{\leq n-1}_{i_{n-1} \ldots r_{n-1}}$ | $\mathbf{G}^{\geq 1}_{i_1 \ldots i_N} = \sum_{r_{n-1}=1}^{R_n} \mathbf{g}^{\geq n+1}_{r_{n-1}, i_n \ldots i_N} \mathbf{g}^{(n)}_{r_{n-1}, i_{n+1} \ldots i_N}$ |
| Outer products |
| $\mathbf{X} = \mathbf{G}^{\leq N}_{\leq \max \{I_1, \ldots, I_N\}}$ with $\mathbf{G}^{\leq n}_{\leq \max \{I_1, \ldots, I_N\}} = \sum_{r_{n-1}=1}^{R_n-1} \mathbf{G}^{\leq n-1}_{\leq \max \{I_1, \ldots, I_N\}} \mathbf{g}^{(n)}_{\leq \max \{I_1, \ldots, I_N\}}$ | $\mathbf{X} = \mathbf{G}^{\geq 1}_{\geq \max \{I_1, \ldots, I_N\}}$ with $\mathbf{G}^{\geq n}_{\geq \max \{I_1, \ldots, I_N\}} = \sum_{r_{n-1}=1}^{R_n} \mathbf{g}^{\geq n+1}_{\geq \max \{I_1, \ldots, I_N\}} \mathbf{g}^{(n)}_{\leq \max \{I_1, \ldots, I_N\}}$ |
| $\text{vec} \left( \mathbf{X} \right) = \text{vec} \left( \mathbf{G}^{\leq N} \right)$ with $\text{vec} \left( \mathbf{G}^{\leq n} \right) = \left( \mathbf{I}_{I_1} \otimes \cdots \otimes \mathbf{G}^{(n)}_{I_n} \right) \text{vec} \left( \mathbf{G}^{\leq n-1} \right)$ | $\text{vec} \left( \mathbf{X} \right) = \text{vec} \left( \mathbf{G}^{\geq n} \right)$ with $\text{vec} \left( \mathbf{G}^{\geq n} \right) = \left( \mathbf{G}^{(n)}_{I_n} \otimes \mathbf{I}_{I_{n+1} \ldots I_N} \right) \text{vec} \left( \mathbf{G}^{\geq n+1} \right)$ |
| Matricizations |
| $\mathbf{X}(1) = \mathbf{G}^{(1)}_{\{i_1\}} \mathbf{G}^{\geq 1}_{\{i_2\}}$ with $\mathbf{G}^{\geq n+1}_{\{i_1\}} = \mathbf{G}^{(n+1)}_{\{i_1\}}$ | $\mathbf{X}(n) = \mathbf{G}^{(n)}_{\{i_n\}} \mathbf{G}^{\geq n}_{\{i_{n+1}\}}$ with $\mathbf{G}^{\geq n+1}_{\{i_n\}} = \mathbf{G}^{(n+1)}_{\{i_n\}}$ |
3.4 Orthogonalization of core tensors

Orthogonalization of the TT-cores reduces computational costs and guarantees uniqueness of TT-ranks.

**Definition 3.2** (Left- or right-orthogonality, [17]). For $n = 1, 2, \ldots, N$, the $n$th TT-core $G^{(n)}$ is called left-orthogonal if

$$G^{(n)}(3)G^{(n)T}(3) = I_{R_n}, \tag{19}$$

and $G^{(n)}$ is called right-orthogonal if

$$G^{(n)}(1)G^{(n)}T(1) = I_{R_{n-1}}. \tag{20}$$

On the other hand, all orthogonality was defined in the context of Tucker format [4].

**Definition 3.3** (All orthogonality, [4]). A 3rd order tensor $G \in \mathbb{R}^{I_1 \times I_2 \times I_3}$ is called all-orthogonal if

$$G_{(n)}G^{T}_{(n)} = I_{R_n} \text{ for all } n = 1, 2, 3.$$

During iterations in numerical algorithms, the TT-cores are kept either left- or right-orthogonal by SVD or QR decomposition [30, 18]. For a fixed $n$, if all the cores on the left are left-orthogonal, then $G_{< n}^{(n)} \in \mathbb{R}^{R_n \times I_1 \times I_2 \ldots \times I_{n-1}}$ has orthonormal rows. And if all the cores on the right are right-orthogonal, then $G_{> n}^{(1)} \in \mathbb{R}^{R_n \times I_{n+1} \times I_{n+2} \ldots \times R_N}$ has orthonormal rows. Consequently, we can make the frame matrices $X^{\neq n}$ and $X^{\neq n, n+1}$ defined in (15) and (18) have orthonormal columns during iterations. The proof of the orthonormality of $G_{< n}^{(n)}$ and $G_{> n}^{(1)}$ can be given by using the tensor operations described in the previous section as follows.

**Proposition 3.4.** For a fixed $n = 1, 2, \ldots, N$, if $G^{(1)}, G^{(2)}, \ldots, G^{(n-1)}$ are left-orthogonal, then $G_{< n}^{(n)}$ has orthonormal rows. And if $G^{(n+1)}, G^{(n+2)}, \ldots, G^{(N)}$ are right-orthogonal, then $G_{> n}^{(1)}$ has orthonormal rows.

**Proof.** We prove the orthonormality for $G_{< n}^{(n)}$. The orthonormality for $G_{> n}^{(1)}$ follows in a similar way. The left-orthogonality (19) is re-written by the tensor operations as

$$\text{vec} \left( G^{(n)}(3)G^{(n)T}(3) \right) = \left( G^{(n)} \otimes_3 G^{(n)} \right) \overline{x}_1 \mathbf{1}_{R_{n-1}} \overline{x}_2 \mathbf{1}_{I_n} = \text{vec} \left( I_{R_n} \right),$$

where $\overline{x}_n$ is the mode-$n$ (vector) product of a tensor with a vector, and $\mathbf{1}_I = [1, 1, \ldots, 1]^T \in \mathbb{R}^I$ is the vector of ones. We will show that

$$\text{vec} \left( G_{< n}^{(n)} (G_{< n}^{(n)})^T \right) = \text{vec} \left( I_{R_{n-1}} \right), \quad n = 1, 2, \ldots, N. \tag{21}$$

If $n = 1$, then $G_{< n}^{< n} = 1$ and the equality holds. If $n = k > 1$, we assume that the equality holds for $n = 1, \ldots, k-1$. From the recursive representation of the TT format,

$$G_{< k} = G_{< k-1} \cdot G^{(k-1)} \in \mathbb{R}^{I_1 \times \cdots \times I_{k-1} \times R_{k-1}}.$$
The mode-$k$ Kronecker product of $G^{<k}$ with itself is

$$G^{<k} \otimes_k G^{<k} = \left( G^{<k-1} \otimes_{k-1} G^{<k-1} \right) \cdot \left( G^{(k-1)} \otimes_2 G^{(k-1)} \right).$$

The lefthand side of (21) is equivalent to

$$\text{vec} \left( G^{<n} \left( G^{<n} \right)^T \right) = \left( G^{<n} \otimes_n G^{<n} \right) \overline{x}_1 1_I \overline{x}_2 1_I \cdots \overline{x}_{n-1} 1_{I_{n-1}}.$$

Hence, we find that

$$\text{vec} \left( G^{<k} \left( G^{<k} \right)^T \right) = \left( \left( G^{<k-1} \otimes_{k-1} G^{<k-1} \right) \overline{x}_1 1_I \overline{x}_2 1_I \cdots \overline{x}_{k-2} 1_{I_{k-2}} \right) \cdot \left( \left( G^{(k-1)} \otimes_2 G^{(k-1)} \right) \overline{x}_2 1_{I_{k-1}} \right) = \text{vec} \left( \left( G^{(k-1)} \otimes_2 G^{(k-1)} \right) \overline{x}_2 1_{I_{k-1}} \right) = \text{vec} \left( I_{R_{k-2}} \right) \cdot \left( \left( G^{(k-1)} \otimes_2 G^{(k-1)} \right) \overline{x}_2 1_{I_{k-1}} \right) = \left( G^{(k-1)} \otimes_2 G^{(k-1)} \right) \overline{x}_1 1_{R_{k-2}} \overline{x}_2 1_{I_{k-1}} = \text{vec} \left( I_{R_{k-1}} \right).$$

Figure 3(a), (b), and (c) show graphical representations for the TT format of a 4th order tensor. The left-orthogonalized or right-orthogonalized core tensors are represented by half-filled circles. For example, Figure 3(a) shows that the three among the four core tensors have been left-orthogonalized.

### 3.5 Properties of TT format

Mathematical properties of the TT format are closely related to the so-called separation ranks [17]. The $n$th separation rank, $S_n$, of $X$ is defined as the rank of the $n$th canonical unfolding $X_{([n])}$, i.e.,

$$S_n = \text{rank} \left( X_{([n])} \right).$$
A tensor $\mathbf{X}$ of order $N$ is said to be in the TT format with TT-ranks $R_1, \ldots, R_{N-1}$ if it can be expressed in the TT format (5). The TT format (5) is called minimal or fulfilling the full-rank condition [17] if all TT-cores have full left and right ranks, i.e.,

$$R_n = \text{rank} \left( G^{(n)}_{(3)} \right), \quad R_{n-1} = \text{rank} \left( G^{(n)}_{(1)} \right),$$

for all $n = 1, \ldots, N$. By looking at the mode-$n$ matricization of the TT format (5), we can show the following relationship between the separation ranks and the TT-ranks:

$$S_n \leq R_n$$

for $n = 1, \ldots, N-1$. In [30], it is shown that for a tensor $\mathbf{X}$, there exists a TT decomposition with TT-ranks not higher than the separation ranks, i.e.,

$$R_n \leq S_n.$$

Moreover, Holtz et al. [17] proved the uniqueness of the TT-ranks of minimal TT decompositions for a tensor $\mathbf{X}$. That is, if $\mathbf{X}$ admits for a minimal TT decomposition with TT-ranks $R_n$, then it holds that

$$R_n = S_n$$

for $n = 1, \ldots, N-1$. Therefore, the TT-ranks of a tensor $\mathbf{X}$ is defined as the TT-ranks of a minimal TT decomposition of $\mathbf{X}$.

Let $\mathbb{T}_{TT}(R_1, \ldots, R_{N-1})$ denote the set of tensors with TT-ranks bounded by $\{R_n\}$. It has been shown that $\mathbb{T}_{TT}(R_1, \ldots, R_{N-1})$ is closed [14], which implies that there exists a best TT-ranks-$(R_1, \ldots, R_{N-1})$ approximation of any tensor. Oseledets [30] proved that the TT-SVD algorithm returns a quasi-optimal TT approximation. That is, for a tensor $\mathbf{Y}$, the TT-SVD algorithm returns $\hat{\mathbf{X}} \in \mathbb{T}_{TT}(R_1, \ldots, R_{N-1})$ such that

$$\| \mathbf{Y} - \hat{\mathbf{X}} \|_F \leq \sqrt{N-1} \min_{\mathbf{X} \in \mathbb{T}_{TT}(R_1, \ldots, R_{N-1})} \| \mathbf{Y} - \mathbf{X} \|_F,$$

where $\| \cdot \|_F$ is the Frobenius norm.

Moreover, unlike the Tucker format, the TT format requires a storage cost of $O(NIR^2)$, that is linear in $N$. Many algorithms based on the TT format such as the approximation, truncation, contraction, and solution to linear systems, also have computational complexity linear with $N$. Further mathematical properties of TT-based algorithms will be developed in the next section.

### 3.6 Matrix TT format for linear operators

The matrix product operator (MPO), or equivalently the matrix TT format is an extension of the TT format to linear operators and matrices [29]. Various representations, including new ones, for the matrix TT format are summarized in Table 5. Suppose that a linear operator from $\mathbb{R}^{I_1 \times J_2 \times \cdots \times J_N}$ to $\mathbb{R}^{I_1 \times J_2 \times \cdots \times J_N}$ is represented by a tensor $\mathbf{A}$ of size $I_1 \times J_1 \times I_2 \times J_2 \times \cdots \times I_N \times J_N$. The matrix TT format for $\mathbf{A}$ can be represented as outer products

$$\mathbf{A} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} A^{(1)}_{1, r_1} \circ A^{(2)}_{r_1, r_2} \circ \cdots \circ A^{(N-1)}_{r_{N-2}, r_{N-1}} \circ A^{(N)}_{r_{N-1}, 1},$$

where

- $A^{(n)}$ are tensors of size $I_{n-1} \times J_n \times I_n \times J_{n+1}$
- $r_n$ are integers between $1$ and $R_n$

This representation allows for efficient computation and storage of large matrices.
Table 5: Various representations for the matrix TT format of a tensor $\mathbf{A}$ of size $I_1 \times J_1 \times \cdots \times I_N \times J_N$

| Matrix TT format | Contracted products | Matrix products | Scalar products | Strong Kronecker products | Matrix representation |
|------------------|---------------------|----------------|----------------|--------------------------|----------------------|
| $\mathbf{A} = \mathbf{A}^{(1)} \cdot \mathbf{A}^{(2)} \cdot \cdots \cdot \mathbf{A}^{(N-1)} \cdot \mathbf{A}^{(N)}$ | $a_{i_1,j_1,i_2,j_2,\ldots,i_N,j_N} = \mathbf{A}_{i_1,j_1}^{(1)} \mathbf{A}_{i_2,j_2}^{(2)} \cdots \mathbf{A}_{i_{N-1},j_{N-1}}^{(N-1)} \mathbf{A}_{i_{N-1},j_{N-1}}^{(N)}$ | $a_{i_1,j_1,i_2,j_2,\ldots,i_N,j_N} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} a^{(1)}_{1,r_1} a^{(2)}_{r_1,1,r_2} \cdots a^{(N-1)}_{r_{N-2},1,r_{N-1},1} a^{(N)}_{r_{N-1},1}$ | $\mathbf{A} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} \mathbf{A}_{i_1,r_1}^{(1)} \circ \mathbf{A}_{r_1,i_2}^{(2)} \circ \cdots \circ \mathbf{A}_{r_{N-2},r_{N-1},1}^{(N-1)} \circ \mathbf{A}_{r_{N-1},1}^{(N)}$ | $\mathbf{A} = \{ \mathbf{A}^{(1)} \} \otimes \mathbf{I}_{i_2 \ldots i_N} \left( \mathbf{I}_{j_1} \otimes \mathbf{A}^{(2)}_{j_2 \ldots j_N} \right) \cdots \left( \mathbf{I}_{j_1 \ldots j_{N-2}} \otimes \mathbf{A}^{(N-1)}_{j_{N-1}} \otimes \mathbf{I}_{j_N} \right)$ |

where $\mathbf{A}_{i_{n-1},r_n}^{(n)} = \mathbf{A}^{(n)}(r_{n-1}, \ldots, r_n) \in \mathbb{R}^{I_{n-1} \times J_n}$ is a slice of the 4th order core tensor $\mathbf{A}^{(n)} \in \mathbb{R}^{R_{n-1} \times I_n \times J_n \times R_n}$. Note that the matrices $\mathbf{A}_{i_{n-1},r_n}^{(n)}$ are replaced with vectors $\mathbf{g}_{i_{n-1},r_n}^{(n)} \in \mathbb{R}^{I_n}$ in the standard TT/MPS format.

Moreover, the matrix TT format is a representation of a large-scale matrix. The matrix TT format for a matrix $\mathbf{A}$ of size $I_1 I_2 \cdots I_N \times J_1 J_2 \cdots J_N$ can be written as the strong Kronecker products

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

where

$$\mathbf{A}^{(n)} = \begin{bmatrix} \mathbf{A}^{(n)}_{1,1} & \cdots & \mathbf{A}^{(n)}_{1,R_n} \\ \vdots & \ddots & \vdots \\ \mathbf{A}^{(n)}_{R_{n-1},1} & \cdots & \mathbf{A}^{(n)}_{R_{n-1},R_n} \end{bmatrix} \in \mathbb{R}^{R_{n-1} \times I_n \times J_n}.$$

The strong Kronecker product representation is useful, especially for representing large-scale high dimensional operators such as the discrete Laplace operator and Toeplitz matrix [19][20].

With these representations for the matrix TT format, the matrix-vector product and the quadratic form can be conveniently described. See Section 4.3 for such mathematical expressions. Figure 4(a) illustrates a graph for the matrix TT format, (b) represents the matrix-vector multiplication, $\mathbf{A}\mathbf{x}$, in TT format, and (c) represents the quadratic form, $(\mathbf{x}, \mathbf{A}\mathbf{x})$. 

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4 Basic operations with TT format

For numerical operations with tensors in TT format, it is important to perform all the operations in TT format and avoid the explicit calculation of the full tensors. In this section we present basic operations with tensors in TT format, which are represented in simple and very efficient forms by the notations introduced in the previous sections. The basic operations include addition, scalar multiplication, contraction, Hadamard product, matrix-vector product, and quadratic form. We remark that such operations usually increase the TT-ranks, which requires truncation in the following step.

In addition, the matrix-vector product and quadratic form are very important for computational algorithms in optimization problems such as linear equations [7, 8, 9, 18] and eigenvalue problems [6, 25].

Table 6 summarizes the representations for the basic operations on the tensors in TT format.

4.1 Addition and scalar multiplication

Let \( X = X^{(1)} \cdot \cdots \cdot X^{(N)} \) and \( Y = Y^{(1)} \cdot \cdots \cdot Y^{(N)} \) be TT tensors. The sum \( Z = X + Y \) can be expressed in the TT format

\[
Z = (X^{(1)} \oplus_3 Y^{(1)}) \cdot (X^{(2)} \oplus_2 Y^{(2)}) \cdot \cdots \cdot (X^{(N-1)} \oplus_2 Y^{(N-1)}) \cdot (X^{(N)} \oplus_1 Y^{(N)}).
\]

That is, each TT-core of the sum is written as the direct sum of the TT-cores. Alternatively, each entry of \( Z \) can be represented as products of matrices

\[
z_{i_1,i_2,\ldots,i_N} = (X_{i_1}^{(1)} \oplus_2 Y_{i_1}^{(1)}) (X_{i_2}^{(2)} \oplus Y_{i_2}^{(2)}) \cdots (X_{i_{N-1}}^{(N-1)} \oplus Y_{i_{N-1}}^{(N-1)}) (X_{i_N}^{(N)} \oplus Y_{i_N}^{(N)}).
\]

The TT-ranks for \( X + Y \) are the sums, \( \{R_n^X + R_n^Y\} \).

On the other hand, multiplication of \( X \) with a scalar \( c \in \mathbb{R} \) can be obtained by simply multiplying one core, e.g., \( X^{(1)} \), with \( c \) as \( cX^{(1)} \). This does not increase the TT-ranks.

We note that that the set of tensors with TT-ranks bounded by \( \{R_n\} \) is not convex, since a linear combination \( cX + (1-c)Y \) generally increases the TT-ranks, which may exceed \( \{R_n\} \).
Table 6: Representations for basic operations on tensors in TT format

| Operation | Representation | TT-cores |
|-----------|----------------|----------|
| $Z = X + Y$ | Tensors (cores) | $Z^{(1)} = X^{(1)} \oplus Y^{(1)}$ |
|           |                 | $Z^{(n)} = X^{(n)} \oplus Y^{(n)}$ for $n = 2, 3, \ldots, N - 1$ |
|           | Matrices (slices) | $Z_{\ell_1}^{(1)} = X_{\ell_1}^{(1)} \oplus Y_{\ell_1}^{(1)}$ |
|           |                 | $Z_{\ell_1}^{(n)} = X_{\ell_1}^{(n)} \oplus Y_{\ell_1}^{(n)}$ for $n = 2, 3, \ldots, N - 1$ |
|           | Vectors (fibers) | $z_{k_{n-1}, k_n}^{(n)} = \begin{cases} x_{k_{n-1}, k_n}^{(n)} & \text{if } 1 \leq k_n \leq R_n^X \\ Y_{k_{n-1}, k_n}^{(n)} & \text{if } R_n^X < k_n \leq R_n^X + R_n^Y \\ 0 & \text{otherwise} \end{cases}$ |
| $Z = X \otimes Y$ | Tensors (cores) | $Z^{(n)} = X^{(n)} \otimes Y^{(n)}$ |
|           | Matrices (slices) | $Z_{\ell_1}^{(n)} = X_{\ell_1}^{(n)} \otimes Y_{\ell_1}^{(n)}$ |
|           | Vectors (fibers) | $z_{k_{n-1}, k_n}^{(n)} = \left( x_{k_{n-1}, k_n}^{(n)} \otimes Y_{k_{n-1}, k_n}^{(n)} \right)_{C}$ |
| $Z = A(X)$ | Tensors (cores) | $Z^{(n)} = A^{(n)}(X)^{(n)}$ |
|           | Matrices (slices) | $Z_{\ell_1}^{(n)} = \sum_{\ell_n} A_{\ell_1, \ell_n}^{(n)} \otimes X_{\ell_n}^{(n)}$ |
|           | Vectors (fibers) | $z_{k_{n-1}, k_n}^{(n)} = \sum_{j_n} A_{j_n, k_n}^{(n)} \otimes x_{j_n, k_n}^{(n)}$ |
| $z = \langle X, A(X) \rangle$ | Tensors (cores) | $Z^{(n)} = \left( x^{(n)} , A^{(n)}(X)^{(n)} \right)_{C}$ |
|           | Matrices (slices) | $Z_{\ell_1}^{(n)} = \sum_{j_n} \sum_{\ell_n} X_{\ell_n, \ell_n}^{(n)} \otimes A_{j_n, \ell_n}^{(n)} \otimes X_{j_n}^{(n)}$ |
|           | Vectors (fibers) | $z_{k_{n-1}, k_n}^{(n)} = \left( x_{k_{n-1}, k_n}^{(n)} , A_{k_{n-1}, k_n}^{(n)} \otimes x_{k_{n-1}, k_n}^{(n)} \right)_{C}$ |
4.2 Hadamard product and contraction

The Hadamard (elementwise) product \( Z = X \odot Y \) of \( X = X^{(1)} \cdots X^{(N)} \) and \( Y = Y^{(1)} \cdots Y^{(N)} \) can be written in the TT format as

\[
Z = (X^{(1)} \otimes_2 Y^{(1)}) \cdots (X^{(2)} \otimes_2 Y^{(2)}) \cdots (X^{(N-1)} \otimes_2 Y^{(N-1)}) \otimes (X^{(N)} \otimes_2 Y^{(N)}).
\]

That is, each TT-core is written as the mode-2 Kronecker product. As an alternative representation, each entry is written as products of matrices

\[
z_{i_1, i_2, \ldots, i_N} = \left( X^{(1)}_{i_1} \otimes Y^{(1)}_{i_1} \right) \left( X^{(2)}_{i_2} \otimes Y^{(2)}_{i_2} \right) \cdots \left( X^{(N)}_{i_N} \otimes Y^{(N)}_{i_N} \right).
\]

The TT-ranks for the Hadamard product are the multiplications, \( \{ R_X^{(N)} \} \).

The contraction of two tensors \( \mathbf{A} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) and \( \mathbf{B} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N} \) is defined by

\[
\langle \mathbf{A}, \mathbf{B} \rangle = \sum_{i_1=1}^{I_1} \sum_{i_2=1}^{I_2} \cdots \sum_{i_N=1}^{I_N} \mathbf{A}(i_1, i_2, \ldots, i_N) \mathbf{B}(i_1, i_2, \ldots, i_N)
= \langle \text{vec}(\mathbf{A}), \text{vec}(\mathbf{B}) \rangle.
\]

The contraction of a TT tensor \( X = X^{(1)} \cdots X^{(N)} \) with a rank-one tensor \( u^{(1)} \circ \cdots \circ u^{(N)} \) can be simplified as

\[
\langle X, u^{(1)} \circ \cdots \circ u^{(N)} \rangle = \left( X^{(1)} \cdots X^{(N)} \right) \overline{x}_1 u^{(1)} \cdots \overline{x}_N u^{(N)}
= \left( X^{(1)} \overline{x}_1 u^{(1)} \right) \left( X^{(2)} \overline{x}_2 u^{(2)} \right) \cdots \left( X^{(N)} \overline{x}_N u^{(N)} \right).
\]

The contraction of two TT tensors \( X = X^{(1)} \cdots X^{(N)} \in \mathbb{R}^{I_1 \times \cdots \times I_N} \) and \( Y = Y^{(1)} \cdots Y^{(N)} \in \mathbb{R}^{I_1 \times \cdots \times I_N} \) can be calculated by combining the Hadamard product and the contraction with the rank one tensor \( 1_{I_1} \circ \cdots \circ 1_{I_N} \) as

\[
\langle X, Y \rangle = \langle X \odot Y, 1_{I_1} \circ \cdots \circ 1_{I_N} \rangle
= Z^{(1)} Z^{(2)} \cdots Z^{(N)},
\]

where

\[
Z^{(n)} = \left( X^{(n)} \otimes_2 Y^{(n)} \right) \overline{x}_2 1_{I_n}
= \sum_{i_n=1}^{I_n} X^{(n)}_{i_n} \otimes Y^{(n)}_{i_n}
\]

for \( n = 1, \ldots, N \). We remark that \( Z^{(1)} \in \mathbb{R}^{I_1 \times R_X^{(1)} R_Y^{(1)}} \) and \( Z^{(N)} \in \mathbb{R}^{R_X^{(N-1)} R_Y^{(N-1)} \times 1} \) are row and column vectors.

We define a generalized contraction operator of two TT-cores as follows.

**Definition 4.1** (Core contraction). The core contraction of two TT-cores \( X^{(n)} \in \mathbb{R}^{R_X^{(n-1)} I_n \times R_X^{(n)}} \) and \( Y^{(n)} \in \mathbb{R}^{R_Y^{(n-1)} I_n \times R_Y^{(n)}} \) is defined by

\[
\langle X^{(n)}, Y^{(n)} \rangle_C = \sum_{i_n=1}^{I_n} X^{(n)}_{i_n} \otimes Y^{(n)}_{i_n} \in \mathbb{R}^{R_X^{(n-1)} R_Y^{(n-1)} \times R_X^{(n)} R_Y^{(n)}}.
\]
Proposition 4.2. We can express the contraction of two TT-tensors $\mathbf{X} = \mathbf{X}^{(1)} \cdots \mathbf{X}^{(N)}$ and $\mathbf{Y} = \mathbf{Y}^{(1)} \cdots \mathbf{Y}^{(N)}$ by

$$\langle \mathbf{X}, \mathbf{Y} \rangle = \left\langle \mathbf{X}^{(1)}, \mathbf{Y}^{(1)} \right\rangle_C \left\langle \mathbf{X}^{(2)}, \mathbf{Y}^{(2)} \right\rangle_C \cdots \left\langle \mathbf{X}^{(N)}, \mathbf{Y}^{(N)} \right\rangle_C.$$  \hspace{1cm} (24)

The computational cost for calculating the contraction $\langle \mathbf{X}, \mathbf{Y} \rangle$ is $O(NIR^3)$, which is linear in $N$.

4.3 Matrix-vector product

The matrix-vector product, or the linear mapping can also be efficiently represented by the TT format. The computational cost for computing a matrix-vector product in TT format is $O(NIR^3)$.

1. Suppose that a vector $\mathbf{x} \in \mathbb{R}^{J_1 J_2 \cdots J_N}$ is in TT format and a matrix $\mathbf{A} \in \mathbb{R}^{I_1 I_2 \cdots I_N \times J_1 J_2 \cdots J_N}$ is in matrix TT format, and both are represented as Kronecker products

$$\mathbf{x} = \sum_{r_1'=1}^{R_1'} \sum_{r_2'=1}^{R_2'} \cdots \sum_{r_{N-1}'=1}^{R_{N-1}'} \mathbf{x}^{(1)}_{r_1'} \otimes \mathbf{x}^{(2)}_{r_1', r_2'} \otimes \cdots \otimes \mathbf{x}^{(N)}_{r_{N-2}', r_{N-1}'} \otimes \mathbf{x}^{(N)}_{r_{N-1}, 1},$$

and

$$\mathbf{A} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} \mathbf{A}^{(1)}_{r_1, r_2} \otimes \mathbf{A}^{(2)}_{r_1, r_2, r_3} \otimes \cdots \otimes \mathbf{A}^{(N)}_{r_1, r_2, \cdots, r_N}.$$  \hspace{1cm}

Then the matrix-vector product is represented in TT format

$$\mathbf{z} = \mathbf{A} \mathbf{x} = \sum_{k_1=1}^{K_1} \sum_{k_2=1}^{K_2} \cdots \sum_{k_{N-1}=1}^{K_{N-1}} \mathbf{z}^{(1)}_{k_1} \otimes \mathbf{z}^{(2)}_{k_1, k_2} \otimes \cdots \otimes \mathbf{z}^{(N)}_{k_{N-2}, k_{N-1}} \otimes \mathbf{z}^{(N)}_{k_{N-1}, 1},$$

where $K_n = R_n R'_n$ and

$$\mathbf{z}^{(n)}_{k_{n-1}, k_n} = \mathbf{A}^{(n)}_{k_{n-1}, k_n} \mathbf{x}^{(n)}_{k_{n-1}, r_n} \in \mathbb{R}^{J_n}.$$  \hspace{1cm}

We can get the same expression in the case that $\mathbf{X} \in \mathbb{R}^{J_1 \times \cdots \times J_N}$ and $\mathbf{A} \in \mathbb{R}^{I_1 \times J_1 \times \cdots \times I_N \times J_N}$ are represented as outer products.

2. The linear mapping $\mathbf{A}(\mathbf{X}) \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ can also be represented by its entries written as products of matrices. Suppose that $\mathbf{X} \in \mathbb{R}^{J_1 \times \cdots \times J_N}$ and $\mathbf{A} \in \mathbb{R}^{I_1 \times J_1 \times \cdots \times I_N \times J_N}$ are in the TT formats

$$\mathbf{X} = \mathbf{X}^{(1)} \cdots \mathbf{X}^{(N)}$$

and

$$\mathbf{A} = \mathbf{A}^{(1)} \cdots \mathbf{A}^{(N)}.$$  \hspace{1cm}

Then the entries of the linear mapping $\mathbf{Z} = \mathbf{A}(\mathbf{X})$ is calculated by the contraction

$$z_{i_1, \ldots, i_N} = \left\langle \mathbf{A}_{i_1, i_2, \ldots, i_N}, \mathbf{X} \right\rangle$$

$$= \mathbf{Z}^{(1)}_{i_1} \mathbf{Z}^{(2)}_{i_2} \cdots \mathbf{Z}^{(N)}_{i_N},$$

25
where the lateral slices \( Z^{(n)}_{j_n} \) of TT-cores \( Z^{(n)} \) are expressed as

\[
Z^{(n)}_{j_n} = \left( A^{(n)}_{j_n} \otimes X^{(n)} \right) \gamma_{j_n} 1_{J_n} = \sum_{j_n=1}^{J_n} A^{(n)}_{j_n} \otimes X^{(n)}_{j_n}.
\] (25)

Note that \( Z^{(1)}_{i_1} \in \mathbb{R}^{1 \times R_1 R'_1} \) and \( Z^{(N)}_{i_N} \in \mathbb{R}^{R_{N-1} R'_{N-1} \times 1} \) are row and column vectors.

3. We can further simplify the notation (25) by considering the TT-core \( A^{(n)} \in \mathbb{R}^{R_{n-1} \times I_n \times J_n \times R_n} \) as an operator. Let

\[
A^{(n)} : X^{(n)} \in \mathbb{R}^{R'_{n-1} \times J_n \times R'_n} \mapsto A^{(n)}(X^{(n)}) \in \mathbb{R}^{R_{n-1} R'_{n-1} \times I_n \times R_n R'_n}
\]

be a linear map defined by

\[
Z^{(n)} = A^{(n)}(X^{(n)})
\]

with each \( i_n \)th slice

\[
Z^{(n)}_{i_n} = \sum_{j_n=1}^{J_n} A^{(n)}_{i_n j_n} \otimes X^{(n)}_{j_n} = \left( A^{(n)} \cdot X^{(n)} \right)_{i_n}.
\]

We can represent \( A(X) \) in a simplified form as follows.

**Proposition 4.3.** Let \( A = A^{(1)} \cdot \cdots \cdot A^{(N)} : \mathbb{R}^{J_1 \times \cdots \times J_N} \rightarrow \mathbb{R}^{I_1 \times \cdots \times I_N} \) be in matrix TT format and \( X = X^{(1)} \cdot \cdots \cdot X^{(N)} \in \mathbb{R}^{J_1 \times \cdots \times J_N} \) be in TT format. The linear mapping \( A(X) \) is represented by

\[
A(X) = A^{(1)}(X^{(1)}) \cdot \cdots \cdot A^{(N)}(X^{(N)}).
\] (26)

On the other hand, we recall that

\[
x = \text{vec}(X) = X^{\otimes n} x^{(n)},
\]

where \( X^{\otimes n} \) is the frame matrix and \( x^{(n)} = \text{vec}(X^{(n)}) \). A large-scale matrix-vector multiplication reduces to a smaller matrix-vector multiplication as \( Ax = AX^{\otimes n} x^{(n)} = \tilde{A} n x^{(n)} \), where

\[
\tilde{A}_n = AX^{\otimes n} \in \mathbb{R}^{I_1 I_2 \cdots I_N J_n R'_n},
\] (27)

But we cannot calculate \( \tilde{A}_n \) by matrix-matrix multiplication for a large matrix \( A \). However, by using the representation (26), we can show that \( \tilde{A}_n \) can be calculated by recursive core contractions as follows.

**Proposition 4.4.** Let

\[
\tilde{A}_n : \mathbb{R}^{R'_{n-1} \times J_n \times R'_n} \rightarrow \mathbb{R}^{I_1 I_2 \cdots I_N
\]

be a linear map defined by

\[
\tilde{A}_n(W^{(n)}) = A^{(1)}(X^{(1)}) \cdot \cdots \cdot A^{(n-1)}(X^{(n-1)}) \cdot A^{(n)}(W^{(n)}) \cdot A^{(n+1)}(X^{(n+1)}) \cdot \cdots \cdot A^{(N)}(X^{(N)})
\] (28)

for any \( W^{(n)} \in \mathbb{R}^{R'_{n-1} \times J_n \times R'_n} \). Let \( \tilde{A}_n \) be the matrix defined by (27). Then

\[
\tilde{A}_n \text{vec} \left( W^{(n)} \right) = \text{vec} \left( \tilde{A}_n(W^{(n)}) \right)
\]

for any \( W^{(n)} \in \mathbb{R}^{R'_{n-1} \times J_n \times R'_n} \). That is, the matrix-vector product \( \tilde{A}_n w^{(n)} \), where \( w^{(n)} = \text{vec}(W^{(n)}) \), can be computed efficiently via the recursive core contractions in \( \tilde{A}_n(W^{(n)}) \).
Figure 5: Graph for the matrix-vector product $\tilde{A}_n x^{(n)}$ represented by the linear mapping $\tilde{A}_n(x^{(n)})$ \cite{28}, where $x^{(n)} = \text{vec}(X^{(n)})$

Figure 5 illustrates the graph for the linear map $\tilde{A}_n$. For each $k = 1, \ldots, n-1, n+1, \ldots, N$, core tensor $A^{(k)}$ is connected to the core tensor $X^{(k)}$, which is represented as $A^{(k)}(X^{(k)})$ in (28).

4.4 Quadratic form

The quadratic form $\langle x, Ax \rangle$ for a symmetric and very large-scale matrix $A \in \mathbb{R}^{I_1 I_2 \cdots I_N \times I_1 I_2 \cdots I_N}$ can be represented in TT format as follows.

1. Let $A$ and $x$ are represented as Kronecker products

$$x = \sum_{r'_1=1}^{R'_1} \sum_{r'_2=1}^{R'_2} \cdots \sum_{r'_{N-1}=1}^{R'_{N-1}} x^{(1)}_{r'_1} \otimes x^{(2)}_{r'_1 r'_2} \otimes \cdots \otimes x^{(N-1)}_{r'_{N-2} r'_{N-1}} \otimes x^{(N)}_{r'_{N-1} r''_{N}},$$

and

$$A = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_{N-1}=1}^{R_{N-1}} A^{(1)}_{r_1} \otimes A^{(2)}_{r_1 r_2} \otimes \cdots \otimes A^{(N-1)}_{r_{N-2} r_{N-1}} \otimes A^{(N)}_{r_{N-1} r''_{N}},$$

Then the quadratic form is represented as the products

$$z = \langle x, Ax \rangle = \sum_{k_1=1}^{K_1} \sum_{k_2=1}^{K_2} \cdots \sum_{k_{N-1}=1}^{K_{N-1}} z^{(1)}_{k_1 k_2} z^{(2)}_{k_1 k_2} \cdots z^{(N-1)}_{k_{N-2} k_{N-1}} z^{(N)}_{k_{N-1} r''_{N}},$$

where $K_n = R_n (R'_n)^2$ and

$$z^{(n)}_{r_{n-1} r''_{n-1}, r'_{n-1} r''_{n}} = \left< x^{(n)}_{r_{n-1} r''_{n}}, A^{(n)}_{r_{n-1} r''_{n}}, x^{(n)}_{r'_{n-1} r''_{n}} \right>$$

for $r'_n, r''_n = 1, 2, \ldots, R'_n$ and $r_n = 1, 2, \ldots, R_n$ for $n = 1, 2, \ldots, N$. The outer product representation leads to the same expression.

2. Recall that the $n$th core tensor of $W = A(X)$ can be represented by the $i_n$th slices $W_{i_n}^{(n)} = \sum_{j_n} A^{(n)}_{i_n j_n} \otimes X^{(n)}_{j_n}$, $i_n = 1, 2, \ldots, I_n$. The quadratic form $z = \langle X, A(X) \rangle$ is computed by
contraction of the Hadamard product with the rank-one tensor as
\[ z = \langle X \otimes A(x), 1_{I_1} \circ \cdots \circ 1_{I_N} \rangle \]
\[ = Z^{(1)} \cdots Z^{(N)}, \]

where
\[ Z^{(n)} = \sum_{i_n=1}^{I_n} X^{(n)}_{i_n} \otimes W^{(n)}_{i_n} = \sum_{i_n=1}^{I_n} \sum_{j_n=1}^{J_n} X^{(n)}_{i_n} \otimes A^{(n)}_{i_n,j_n} \otimes X^{(n)}_{j_n}, \quad n = 1, 2, \ldots, N. \quad (29) \]

We have \( Z^{(1)} \in \mathbb{R}^{1 \times R_1(R_1)^2} \) and \( Z^{(N)} \in \mathbb{R}^{R_{N-1}(R_{N-1})^2 \times 1}. \)

3. Instead, by using the core contraction defined in (23), we can simplify the expression (29) by
\[ Z^{(n)} = \left\langle X^{(n)}, A^{(n)}(X^{(n)}) \right\rangle_C \in \mathbb{R}^{R_{n-1}(R_{n-1})^2 \times R_n(R_n')^2}, \]

where \( A^{(n)}(X^{(n)}) \in \mathbb{R}^{R_{n-1}R_{n-1}' \times I_n \times R_n R_n'} \) is defined in the previous subsection. Finally, we can express the quadratic form efficiently as
\[ (X, A(X)) = \left\langle X^{(1)}, A^{(1)}(X^{(1)}) \right\rangle_C \cdots \left\langle X^{(N)}, A^{(N)}(X^{(N)}) \right\rangle_C. \quad (30) \]

On the other hand, from
\[ x = \text{vec}(X) = X^{\otimes n} x^{(n)}, \]
the quadratic form \( \langle x, Ax \rangle \) reduces to \( \langle x, A x \rangle = \langle x^{(n)}, (X^{\otimes n})^T A X^{\otimes n} x^{(n)} \rangle \equiv \langle x^{(n)}, \overline{A}_n x^{(n)} \rangle, \)

where
\[ \overline{A}_n = (X^{\otimes n})^T A X^{\otimes n} \in \mathbb{R}^{R_{n-1}I_n R_n R_n'} \quad (31) \]
is a much smaller matrix than \( A \) when TT-ranks \( R_{n-1} \) and \( R_n' \) are moderate. Since \( \overline{A}_n \) cannot be calculated by matrix-matrix multiplication for a large matrix \( A \), we calculate it iteratively by recursive core contractions based on the distributed representation (30) as follows.

**Proposition 4.5.** Let
\[ \Phi_{\overline{A}_n} : \mathbb{R}^{R_{n-1}I_n R_n R_n'} \times \mathbb{R}^{R_{n-1}I_n R_n R_n'} \to \mathbb{R} \]
be a bilinear form defined by
\[ \Phi_{\overline{A}_n} \left( Y^{(n)} , W^{(n)} \right) = \left( X^{(1)}, A^{(1)}(X^{(1)}) \right) C \cdots \left( X^{(n-1)}, A^{(n-1)}(X^{(n-1)}) \right) C \left( Y^{(n)}, A^{(n)}(Y^{(n)}) \right) C \left( X^{(n)}, A^{(n)}(X^{(n)}) \right) C \left( Y^{(n)} , W^{(n)} \right) \]
\[ \left( \text{vec}(Y^{(n)}), \overline{A}_n \text{vec}(W^{(n)}) \right) = \Phi_{\overline{A}_n} \left( Y^{(n)} , W^{(n)} \right) \quad (32) \]

for any \( Y^{(n)}, W^{(n)} \in \mathbb{R}^{R_{n-1}I_n R_n R_n'}. \) Let \( \overline{A}_n \) be the matrix defined by (31). Then
\[ \left( \text{vec}(Y^{(n)}), \overline{A}_n \text{vec}(W^{(n)}) \right) = \Phi_{\overline{A}_n} \left( Y^{(n)} , W^{(n)} \right) \]

for any \( Y^{(n)}, W^{(n)} \in \mathbb{R}^{R_{n-1}I_n R_n R_n'}. \) That is, the bilinear form \( \langle y^{(n)}, \overline{A}_n w^{(n)} \rangle \), where \( y^{(n)} = \text{vec}(Y^{(n)}) \) and \( w^{(n)} = \text{vec}(W^{(n)}) \), can be computed efficiently via the recursive core contractions in \( \Phi_{\overline{A}_n} \left( Y^{(n)} , W^{(n)} \right). \)

Figure 6 illustrates the graph for the bilinear form \( \Phi_{\overline{A}_n} \). It is clear that each core tensor \( \overline{A}^{(k)}_n, k = 1, \ldots, n - 1, n + 1, \ldots, N, \) is connected to the core tensor \( \overline{X}^{(k)} \), which is represented as \( \left( \overline{X}^{(k)} , \overline{A}^{(k)}(X^{(k)}) \right) \) in (32).
5 Discussion and conclusions

In this paper, we proposed several new mathematical operations on tensors and developed novel representations of the TT formats. We generalized the standard matrix-based operations such as the Kronecker product, Hadamard product, and direct sum, and proposed tensor-based operations such as the self-contraction and core contraction. We have shown that the tensor-based operations are able to not only simplify traditional index notation for TT representations but also describe important basic operations which are very useful for computational algorithms. The self-contraction operator can be used for defining the tensor chain (TC) representations, and its properties should be more investigated in the future work. Moreover, the definition of core contraction can also be generalized to any tensor network formats such as hierarchical Tucker (HT) format.

The partial contracted products of either the left or right core tensors are matricized and used as a building block of the frame matrices. We have shown that the suggested tensor operations can be used to prove the orthonormality of the frame matrices, which have been proved only by using index notation in the literature. The developed relationships may also play a key role in the alternating linear scheme (ALS) and modified alternating linear scheme (MALS) algorithms for reducing the large-scale optimizations to iterative smaller scale problems. Recent studies adjust the frame matrices in order to incorporate rank adaptivity and improve convergence for the ALS. In this work, we have derived the explicit representations of the localized linear map $\tilde{A}_n$ and bilinear form $\Phi_{\tilde{A}_n}$ by the proposed tensor operations, which are important for TT-based iterative algorithms for breaking the curse-of-dimensionality. The global convergence of the iterative methods remains as a future work. In addition, it is important to keep the TT-ranks moderate for a feasible computational cost.

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