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FROM COMPLETELY POSITIVE MATRICES TO COMPLETELY POSITIVE TENSORS

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Dedicated to the 80th birthday of Professor Abraham Berman

Abstract. In this paper, we introduce the doubly nonnegative (dnn) tensor, completely positive (cp) tensor, binary cp tensor and cp pseudograph. Some necessary and sufficient conditions for a tensor to be binary cp are also offered. We also present some conditions for a dnn tensor to be cp by its associated pseudograph.
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1. Introduction

My research experience in the past thirty years mainly concerns the complete positivity of matrices as well as of tensors, partially overlapped with graph theory. The story began with my first meeting with Avi Berman in 1995 when I was a PhD student of the University of Science and Technology of China (abbrev. USTC),which is in Hefei, a city located in the middle of China. Avi was then visiting USTC (I guess this should be Avi's first visit to China). Avi gave a talk and showed us his latest paper on complete positivity[4] where he put forward two basic problems on complete positivity, i.e.,

(1): When is a given $n \times n$ real matrix A completely positive?
(2): How can the cp-rank of A be calculated?

The characterization of completely positive (cp) matrices later turned out to be the title of my PhD thesis, and a permanent topic of my research after my graduation from USTC. Then I visited Technion as a post-doctor hosted by Avi from Oct. 2002 to Nov. 2004. The visit yielded three joint papers with Avi on cp matrices [10, 11, 12].

The cp matrix was investigated since 1960s [13, 20, 18, 9, 40]. It can be applied in many fields such as computer vision [24, 15], exploratory multiway data clustering [24], inequalities [13], quadratic forms [20], combinatorial designs [9] and optimizations[8, 14, 2]. They are also

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applied to statistical models [18]. Kogan and Berman [23] used the graph theory to character the cp matrices [23] in 1993, and Salce and Zanardo [38] use the cp matrix to investigate the positivity of least squares solutions. Later in 1990s Berman etc. initialized a systematical study on cp matrices [9] employing the combinatorial matrix theory, basically utilizing the structure of the associated graph of a doubly nonnegative (dnn) matrix. Actually Berman and Hershkowtz showed in 1991 that a dnn matrix $A \in \mathbb{R}^{n\times n}$ is always cp if its associated graph G contains no long odd cycle (a long odd cycle is a cycle of length $l \geq 5$ with l being an odd number). But we have no idea about the complete positivity of a dnn matrix whose associated graph contains a long odd cycle. In 2004 the author presented a sufficient and necessary condition for a square matrix to be cp without any restriction. An interesting result following this characterization was presented in 2014 by So and Xu [39] where a sufficient condition is offered for a dnn matrix to be cp with its cprank equals its rank. However, it is hard for us to put the condition described in [40] into a practical algorithm to determine the complete positivity of a dnn matrix since it is expressed in the language of cone theory. In 2005 we introduced the concept $(0,1)-cp$ matrices, uniform cp matrices and minimal $(0,1)-cp$ matrices [10, 11, 12]. The applications of cp matrices have been found in pattern recognitions [24, 15] and polynomial optimizations [2, 8, 29] since 2006.

In 2005 Berman and Xu published a joint paper in Linear Algebra and its Applicaitons [11, 12] where they initialized the concept of $(0,1)$-cp matrix, uniform cp matrix and minimal $(0,1)$-cp matrix. The applications of completely positive matrices in pattern recognitions [24, 15] and polynomial optimizations [2, 8, 29] were just addressed in recent twenty years.

Also in 2005 Hazan,Polak and Shashua [19, 36, 37] investigated the third-order tensors and studied the nonnegative symmetric tensor possessing a nonnegative symmetric rank-1 decomposition in the name of multi-way array by where an algorithm was presented to establish a cp decomposition. They the cp factorization of a 3-order cp tensor to image analysis and multi-way clustering. Meanwhile, Qi and Lim independently initialized the eigenvalues of high order tensors in [31, 25]. The high order cp tensors were formally defined by Qi later in [32].

The extension of cp matrices to cp tensors was originated in 2012 when the 10th International Conference on Matrix and its Applications in China (ICMAC) was held in Guiyang, China. Avi was invited as the keynote speaker where he introduced his latest research on cp matrices. During the meeting I also met Professor Liqun Qi who was then chair and professor of Department of Applied Mathematics at the Hong Kong Polytechnic University (HK PolyU) and joined the Hangzhou Dianzi University in 2019. Prof. Qi initialized in 2005 the spectral theory of high order tensors as well as the study on structure tensors. After the meeting, I invited Prof. Qi to visit my university, Suzhou University of Science and Technology (SUST), where we began to talk about the possibility of the generalization of the completely positive matrices to completely positive tensors. I was then invited by Prof. Qi to visit HK Polytechnic University several times from 2013 to 2018. Our frequent communications and cooperations realized our dream: we successfully generalized the cp matrix to cp tensor, and we also extended the concept of cp graph to cp pseudograph, which can be regarded as a kind of multi-hypergraph allowing the repetitions of vertices in some hyper-edges.

For convenience, we denote $[m\ldots n] := \{m, m+1, \ldots, n\}$ for any integers m,n satisfying $0 \leq m \leq n$ and $[n] := [1\ldots n]$, and $|S|$ for the cardinality of set (or multiset) S, $\mathbb{Z}_+^n$ for the set of nonnegative integral vectors of dimension n, and $\mathbb{F}^n$ (resp. $\mathbb{F}^{n\times n}$) the set of all (0,1) vectors of dimension n (matrices of order $n \times n$) with $\mathbb{F} := \{0,1\}$. We also use $\mathbb{R}^n$ to denote the set of real n-dimensional vectors and $\mathbb{R}^n_+$ the set of all nonnegative vectors in $\mathbb{R}^n$. By $\mathtt{supp}(\mathbf{x})$ we mean the support of a vector $\mathbf{x}$, i.e., the index set of nonzero coordinates of $\mathbf{x}$. Following [33], we write

$$S(m,n) := \{\tau = (i_1, i_2, \ldots, i_m) : i_1, i_2, \ldots, i_m \in [n]\}$$

for any positive integer m, n. An element $\sigma \in S(m,n)$ is sometimes identified with an m-tuple or m-multiset or an m-permutation chosen from set $[n]$ with displacement allowed.

A tensor can be regarded as a multi-way array, and a scalar, a vector, and a matrix are respectively a tensor of order 0, 1, and 2. It is recognized that William Hamilton coined the term 200 years ago to describe a mathematical object with some transformation properties. Albert Einstein brought tensors into the spotlight by developing the general relativity entirely in the language of tensors. Nowadays many popular machine learning algorithms e.g. Google's TensorFlow are doubling down on tensors.

We use $\mathscr{T}_{m;n}$ to denote the set of all mth order n-dimensional real tensors . A tensor $\mathscr{A} \in \mathscr{T}_{m;n}$ is called *symmetric* if each of its entries does not alter under any permutation of its subscripts. Denote $\mathbb{S}_{m;n}$ the set of all mth order n-dimensional symmetric tensors , $\mathscr{F}_{m;n}$ the set of all mth order n dimensional (0,1) tensors, and $\mathbb{SF}_{m;n}$ the set of all symmetric tensors in $\mathscr{F}_{m;n}$.

Let $\alpha \in S(m,n)$. The *base* of α, denoted $B(\alpha)$, is the set consisting of all distinct elements in α. For any $\alpha, \beta \in S(m,n)$. We say α is *equivalent* to β, denoted $\alpha \sim \beta$ if $B(\alpha) = B(\beta)$. A tensor $\mathscr{A}$ is called *strong symmetric* if $A_\alpha = A_\beta$ whenever $\alpha \sim \beta, \forall \alpha, \beta \in S(m,n)$. We denote by $\mathscr{ST}_{m;n}$ the set of all mth order n dimensional strong symmetric tensors.

In the next section we introduce the completely positive (cp) matrices before we move onto cp tensors and cp pseudographs. We will also introduce our recent developments on cp tensors and cp pseudographs.

2. CP TENSORS AND BINARY CP TENSORS

A *doubly nonnegative* (dnn) matrix is both entrywise nonnegative and positive semidefinite (psd). We denote the set of all dnn matrices of order n by DNN_n. A matrix $A \in DNN_n$ is called *completely positive* (*cp*) if there exists a nonnegative matrix $W \in \mathbb{R}^{n \times d}$ for some positive integer d such that

$$A = WW^\top, \tag{2.1}$$

where the smallest possible number d, or denoted by $cprank(A)$, is called the *cprank* of A. A is called binary cpif W is a $(0,1)$-matrix. The binary cprank of A is accordingly defined when W is a (0,1) matrix. (2.1) is called a *cp decomposition* of A. It is obvious that $cp_n \subseteq DNN_n$ for all n, and it is shown that $cp_n = DNN_n$ for $n \leq 4$[18, 13]. The inclusion $cp_n \subset DNN_n$ becomes proper when $n \geq 5$[20]. For more detail on *cp* matrices, we refer to [9].

A nonnegative symmetric matrix $A \in \mathbb{R}^{n \times n}_+$ is associated with a (undirected) graph $G(A)$ whose vertex set is $V := [n]$ and the edge set is

$$E := \left\{ \{i,j\} : i,j \in V, a_{ij} \neq 0 \right\}.$$

A matrix $A \in \mathbb{R}^{n \times n}_+$ is called a *realization* of graph G if $G = G(A)$. A is called a *dnn* (resp. *cp, psd* etc.) *realization* of G if A is a dnn (resp. cp and psd, etc.) matrix, and also $G(A) = G$. A graph G is called a *cp graph* if each of its dnn realizations is a cp matrix. Kogan and Berman[23] show that a graph G is cp if and only if G contains no long odd cycle (a cycle with length an odd number greater than 3.). We call a graph with this property a *cp graph*. Thus a graph of size $n \leq 4$ is always a cp graph, and any dnn realization of a cp graph must be cp.

The problem of determining the complete positivity of a given dnn matrix of order large than four still remains open [8, 14, 38, 9], and we employ the associated graphs to classify the matrices in DNN_5 into eight groups and tackled most of them successfully[43]. Also in [11] we establish some practical sufficient conditions by Schur complement of matrices for a dnn matrix to be cp.

In 2006 Shuasha and Hazen[36] present an algorithm for nonnegative tensor factorizations (NTFs) and use it to image analysis. A formal definition for high order cp tensor is introduced by Qi in [32]. A tensor $\mathscr{A}$ is called a *(0,1)-tensor* if each entry of $\mathscr{A}$ is either 1 or 0. $\mathscr{A}$ is an *essential (0,1)-tensor* if each off-diagonal entry of $\mathscr{A}$ is either 1 or 0. Given a tensor $\mathscr{A} = (A_\sigma) \in \mathscr{T}_{m;n}$. A *tensor pattern* $\tilde{\mathscr{A}} = (\tilde{A}_\sigma)$ associated with tensor $\mathscr{A}$ is a (0,1)-tensor satisfying

$$\tilde{A}_\sigma = 1 \Leftrightarrow A_\sigma \neq 0, \quad \forall \sigma \in S(m,n)$$

An mth order n-dimensional real tensor $\mathscr{A} = (A_\sigma) \in \mathscr{T}_{m;n}$ is called a *reducible* tensor if there is a proper subset $\mathscr{I} \subset [1\dots n]$ such that

$$a_{i_1 \dots i_m} = 0,\ \forall i_1 \in \mathscr{I},\ \forall i_2, \dots, i_m \notin \mathscr{I}. \tag{2.2}$$

$\mathscr{A}$ is called *irreducible* if it is not reducible.

We notice that Freidland et al. give an alternative definition of irreducible tensor[17], where a tensor $\mathscr{A} \in \mathscr{T}_{m;n}$ is associated with an m-partite graph $G(\mathscr{A}) = (V,E)$ whose vertex set is partitioned into the disjoint union $V = \cup_{j=1}^m V_j$ with $V_j = [m_j], j \in [d]$, and edge $\mathbf{e} := \{i_k, i_l\} \in E$ ($\mathbf{e} \in V_k \times V_l, k \neq l$) if and only if $A_{i_1 i_2 \dots i_m} > 0$ for some $m-2$ indices $\{i_1, \dots, i_m\} \setminus \{i_k, i_l\}$. Then tensor $\mathscr{A}$ is called irreducible if graph $G(\mathscr{A})$ is connected.

Let $\mathscr{A}, \mathscr{B} \in \mathscr{T}_{m;n}$. We say that $\mathscr{A}$ is *permutational similar* to $\mathscr{B}$, denoted $\mathscr{A} \sim_p \mathscr{B}$, if there exists a permutation matrix $P \in \mathbb{R}^{n \times n}$ such that

$$\mathscr{B} = \mathscr{A} \times_1 P \times_2 P \times_3 \cdots \times_m P,$$

where $\tilde{\mathscr{A}} := \mathscr{A} \times_k P = (\tilde{a}_{i_1 \dots i_m}) \in \mathscr{T}_{m;n}$ is defined as

$$\tilde{a}_{i_1 \dots i_{k-1} i_k i_{k+1} \dots i_m} = \sum_{j=1}^n a_{i_1 \dots i_{k-1} j i_{k+1} \dots i_m} p_{i_k j}$$

An mth order n-dimensional symmetric tensor $\mathscr{A}$ corresponds to an m-degree homogeneous polynomial

$$f_{\mathscr{A}}(\mathbf{x}) \equiv \sum_{j=1} A_{i_1 \dots i_m} x_{i_1} \dots x_{i_m} \tag{2.3}$$

$\mathscr{A}$ is called a *completely positive* or a *cp* tensor if $f_{\mathscr{A}}(\mathbf{x})$ can be written as

$$f_{\mathscr{A}}(\mathbf{x}) = \sum_{j=1}^K (\beta_j^\top \mathbf{x})^m \tag{2.4}$$

with $\beta_j \in \mathbb{R}^n_+$. Write $B = [\beta_1, \dots, \beta_K]$, then (2.4) is equivalent to

$$\mathscr{A} = \sum_{j=1}^K \beta_j^m, \quad \beta_j \in \mathbb{R}^n_+ \tag{2.5}$$

where the smallest possible number K is called the *cp-rank* of $\mathscr{A}$, and is denoted $\texttt{cprank}(\mathscr{A})$. A tensor $\mathscr{A} \in \mathscr{T}_{m;n}$ is called a binary cptensor if $\mathscr{A}$ has a decomposition (2.5) with $\beta_j \in \mathbb{F}^n$, and the corresponding smallest number K is called the *binary cprank* of $\mathscr{A}$, which is denoted $\texttt{cprank}_b(\mathscr{A})$. We call a binary cptensor $\mathscr{A}$ an *r-uniform* for some $r \in [n]$ provided that $\mathscr{A}$ has a decomposition (2.5) with $\left|\texttt{supp}(\alpha_j)\right| = r$ for all $j \in [K]$. A cp(binary cp) tensor is called *minimal cp* (minimal binary cp) if it becomes non-cp (non-binary cp) when any of its diagonal elements is decreased. The minimal cp tensor and uniform cp tensor are generalizations of the matrix case. For more detail on tensors, we refer the reader to [34, 35].

We recall that a *hypergraph* $G(V,E)$ is a generalization of a graph in the sense that each edge (also called a hyper-edge) $\mathbf{e} \in E$ can be any nonempty subset of V (while an edge of a graph is a 2-set of V). A *multi-hypergraph* is a kind of hypergraph $G(V,\mathscr{E})$ each of whose edges can be a multi-subset of its vertex set V, that is, each edge $\mathbf{e} \in \mathscr{E}$ allows repetitions of some vertices within it. We call this kind of graph a *pseudograph*. A pseudograph $G(V,\mathscr{E})$ is called an $m \times n$ pseudograph if $|V| = n$ and each edge of $\mathbf{e}$ is an m-multiset of V. Note that the size of $\mathscr{G}$ is $|\mathscr{E}|$.

A pseudograph $\mathscr{G} = (V,\mathscr{E})$ with $V = [n]$ is associated with an mth order tensor $\mathscr{A}$ in the following way. Let $\mathbf{e} = \{i_1, i_2, \ldots, i_m\} \in S(m,n)$. Then

$$\mathbf{e} \in \mathscr{E} \iff A_{i_1 i_2 \ldots i_m} \neq 0.$$

A (0,1) tensor $\mathscr{A}$ associated with $\mathscr{G}$ is called the *adjacency tensor* of $\mathscr{G}$. $\mathscr{G}$ is called a *cp pseudograph* if its adjacency tensor $\mathscr{A}$ is a cp tensor. We show in [45] that each nonnegative integral diagonal tensor is binary cpwith its binary cprank being the sum of its diagonal elements. Some other special binary cptensors are also investigated there.

3. Gramian Tensors and CP Tensors

For our purpose, we denote for any $\sigma = (i_1, \ldots, i_m) \in S(m,n)$ $(m \in [n])$

$$\gamma_\sigma \equiv \{\alpha_{i_1}, \alpha_{i_2}, \ldots, \alpha_{i_m}\},$$

and define γ_σ as the vector $\alpha_\sigma := \alpha_{i_1} \odot \ldots \odot \alpha_{i_m} \in \mathbb{R}^r$ whose kth coordinate equals $a_{i_1 k} a_{i_2 k} \ldots a_{i_m k}$ for $k \in [r]$ where $\alpha_j = (a_{1j}, \ldots, a_{nj})^\top$. The *m-inner product* of γ_σ, denoted $\Lambda_\sigma = (\alpha_{i_1}, \ldots, \alpha_{i_m})$, is the sum of all coordinates of α_{si}, i.e.,

$$\Lambda_\sigma = \sum_{i=1}^{n} (\prod_{j=1}^{m} a_{ij}) \tag{3.1}$$

(3.1) is called the m-inner product of α when $\alpha = \alpha_{i_1} = \ldots = \alpha_{i_m}$. An m-norm of a vector α is accordingly defined as

$$\| \alpha \|_m := (\alpha, \ldots, \alpha)^{1/m}$$

where $(\alpha, \ldots, \alpha)$ is the m-inner product of α. A tensor $\mathscr{A} \in \mathscr{T}_{m;n}$ is called an m-order *Gramian tensor* generated by vectors $\{\alpha_j\}_{j=1}^{n} \subset \mathbb{R}^d$ if it satisfies

$$A_{i_1 i_2 \ldots i_m} = (\alpha_{i_1}, \ldots, \alpha_{i_m}), \quad \forall \tau := (i_1, i_2, \ldots, i_m) \in S(m,n) \tag{3.2}$$

Denote $B := [\alpha_1, \ldots, \alpha_n]$. Then B is called the associated matrix of $\mathscr{A}$. For a matrix $B \in \mathbb{R}^{d \times n}$ and a positive integer m, we can generate an m-order Gramian tensor by B, and denote it by $\mathscr{A} = \texttt{Gram}^{(m)}(B)$. An 2-order Gramian tensor $\mathscr{A}$ of B is a Gramian matrix $\mathscr{A} = B^\top B$. Moreover, a cp matrix is a Gramian matrix of a nonnegative matrix.

Example 3.1. Let $\mathscr{D} = (D_{i_1 i_2 \dots i_m})$ be a diagonal tensor of m-order n-dimension, i.e.,

$$D_\sigma = \lambda_{\bar{\sigma}} \delta_\sigma, \quad \forall \sigma = (i_1, i_2, \dots, i_m) \in S(m,n)$$

where $\bar{\sigma} = (i_1 + i_2 + \ldots + i_m)/m, \lambda_j \geq 0$ for each $j \in [1 \ldots n]$ and $\delta_{i_1 i_2 \dots i_m}$ is the Kronecker number. Denote $D = diag(d_1, d_2, \dots, d_n)$ with $d_j = \lambda_j^{1/m}$ for $j \in [1 \ldots n]$. Then $\mathscr{D} = \mathtt{Gram}^{(m)}(D)$. Then $\mathscr{D}$ is a completely positive tensor since D is a nonnegative matrix. Note that $\mathtt{cprank}(\mathscr{D})$ is exactly the number of nonzero λ_js.

4. Completely Positive Tensors and binary cpTensors

Let $n > 1$ be an positive integer and $r \in [n]$. An $n \times n$ positive semidefinite (psd) matrix A of rank r can always be written as a Gramian matrix, i.e., $A = \mathtt{Gram}(\alpha_1, \dots, \alpha_n)$ for some linearly independent vectors $\alpha_1, \dots, \alpha_n \in \mathbb{R}^r$. We denote $A = \mathtt{Gram}(B)$ where $B = [\alpha_1, \dots, \alpha_n] \in \mathbb{R}^{r \times n}$ with $\mathtt{rank}(B) = r$. Thus a square matrix is cp if and only if it is a Gramian matrix of some nonnegative vectors. It is known that the complete positivity of a square matrix is equivalent to the double nonnegativity for any $n \in [4]$. However, this is not true for $n \geq 5$.

Given a nonnegative symmetric matrix $A = (a_{ij}) \in \mathbb{R}_+^{n \times n}$. If there exist some nonnegative vectors $\beta_1, \beta_2, \dots, \beta_m \in \mathbb{R}_+^n$ such that

$$A = \beta_1 \beta_1^\top + \beta_2 \beta_2^\top + \ldots + \beta_m \beta_m^\top, \tag{4.1}$$

A is called a *completely positive*(cp) matrix. (4.1) is equivalent to $A = BB^\top$, where $B = [\beta_1, \beta_2, \dots, \beta_m]$ is entrywise nonnegative. The *cprank* of A is defined as the smallest m for (4.1) to hold and is denoted by $cprank(A)$.

A completely positive (cp) tensor is an entrywise nonnegative and symmetric tensor which can be factorized into the sum of some symmetric rank-one tensors [22, 32] where each rank-one tensor is entrywise nonnegative. The determination of a completely positive tensor is a NP-hard question. There are some special cases when feasible algorithms exists [33]. Two kinds of positive(nonnegative) tensors closely related to cp tensors are *doubly nonnegative* or dnn tensors [26] and *copositive* tensors [32], which are respectively analog to the dnn matrices and copositive matrices.

In [27], a cp tensor $\mathscr{A} \in \mathscr{T}_{m,n}$ is associated with a hypergraph $G(V,E)$ where $|V| = n$ and $\sigma := (i_1, \dots, i_m) \in E$ if and only if $B|(\sigma)| = m$. The definition of pseudograph makes possible the correspondence of any symmetric tensor with a graph(pseudograph), as a cp matrix with a graph. Here a pseudograph is defined as a graph whose edge-set allows multi-subsets of its vertex set [44].

Let $\alpha_1, \dots, \alpha_m \in \mathbb{R}_+^n$. By the Hölder inequality, we have [44]

$$(\alpha_1, \dots, \alpha_m)^m \leq \prod_{j=1}^m (\overbrace{\alpha_j, \dots, \alpha_j}^{m}) \tag{4.2}$$

The equality in (4.2) holds if $\mathtt{rank}(\{\alpha_1, \dots, \alpha_m\}) = 1$.

Theorem 4.1. *Let $\mathscr{A} \in \mathscr{T}_{m;n}$ with m an even number. Then*

- **(1):** *$\mathscr{A} \in DNN_n$ if and only if $\mathscr{A}$ is a Gramian tensor, i.e.,$\mathscr{A} = \mathtt{Gram}^{(m)}(\alpha_1, \dots, \alpha_n)$, where $\alpha_j \in \mathbb{R}^K$ for some positive integer.*
- **(2):** *$\mathscr{A}$ is cp if and only if $\mathscr{A} = \mathtt{Gram}^{(m)}(\alpha_1, \dots, \alpha_n)$, where $\alpha_j \in \mathbb{R}_+^K$ for some positive integer.*

The following theorem offers a necessary and sufficient condition for a m-order 2-dimensional tensor to be binary cp.

Theorem 4.2. *Let $\mathscr{A} \in \mathbb{S}_{m;2}$ whose entries are nonnegative integers. Then $\mathscr{A}$ is binary cpiff each off-diagonal element is dominated by the corresponding diagonal element, i.e.,*

$$A_{i_1 i_2 \dots i_m} \le A_{i_k i_k \dots i_k}, \quad \forall k \in [m] \tag{4.3}$$

Furthermore, we have

$$\mathtt{cprank}_b(\mathscr{A}) = A_{11\dots 1} + A_{22\dots 2} - A_{11\dots 12} \tag{4.4}$$

The proof of Theorem 4.1 and that of Theorem 4.2 can be found in [44].

Theorem 4.3. *Let $\mathscr{A} \in \mathbb{S}_{m;2}$ be nonnegative. Then $\mathscr{A}$ is cp if for each $\sigma \in S(m;n)$*

$$A_\sigma \le \min\{A_{ii\dots i} | i \in B(\sigma)\} \tag{4.5}$$

Furthermore, $\mathtt{cprank}(\mathscr{A}) \le 3$, and $\mathtt{cprank}(\mathscr{A}) = 3$ if and only if each diagonal element $A_{ii\dots i}$ is larger than any of off-diagonal elements.

(4.5) is not necessary for a tensor to be cp. This can be illustrated by the following example.

Example 4.4. Consider $m = 2$ and let

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$$

It is easy to check that A is a completely positive tensor (of order-2 dimension-2) since $A = BB^\top$ if we take

$$B = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}$$

However, the inequality (4.5) in Theorem 4.3 is not satisfied since $a_{12} = 2 > 1 = \min\{1, 5\}$.

A *slice* of a tensor $\mathscr{A} \in \mathscr{T}_{m;n}$ is a tensor of order $m-1$ obtained by fixing one of the subscripts. Given a nonempty subset $\mathscr{I} := \{s_1, s_2, \dots, s_r\}$ of $[1\dots n]$, a *principal subtensor* $\mathscr{A}[\mathscr{I}]$ of $\mathscr{A}$ induced by $\mathscr{I}$ is an m-order r-dimensional tensor $\mathscr{B} = (A_{i_1 i_2 \dots i_m})$ whose indices i_ks are all constrained in $\mathscr{I}$. A *zero block* is a principal subtensor whose entries are all zero. An irreducible tensor has no zero slice nor any zero block.

It is pointed out in [44] that all the slices and the induced principal subtensors of a *cp* (binary *cp*) tensor are also *cp* (binary *cp*). By this we present a necessary condition, which is weaker than (4.5), for a tensor to be cp.

Theorem 4.5. *Let $\mathscr{A} \in \mathbb{S}_{m;n}$ be a cp tensor. For any $\tau \in S(m,n)$ with $B(\tau) = \{i, j\}$, we have*

$$A_\tau^2 \le A_{ii\dots i} A_{jj\dots j} \tag{4.6}$$

Proof. Let $\tau := (i_1, i_2, \dots, i_m) \in S(m,n)$ with $B(\tau) = \{i, j\} \subseteq [1\dots n]$. If $i = j$, then inequality (4.6) is obvious. Thus in the following we may assume that $1 \le i < j \le n$, and take $\mathscr{I} = \{i, j\}$. Then the induced subtensor $\mathscr{A}[\mathscr{I}]$ is a 2-dimensional completely positive tensor. We are now confined to $\mathscr{A}_1 := \mathscr{A}[\mathscr{I}]$. Since $\mathscr{A} \in \mathbb{S}_{m;2}$ is completely positive, there exist some nonnegative vectors $\alpha_1, \alpha_2 \in \mathbb{R}_+^N$ ($N = \texttt{cprank}(\mathscr{A}_1)$) such that $\mathscr{A}_1 = \texttt{Gram}(\alpha_1, \alpha_2)$. It follows that $A_\tau = (\alpha_{i_1}, \alpha_{i_2}, \ldots, \alpha_{i_m})$ where $B(\tau) = \mathscr{I}$. By formula (4.2) we get

$$A^m_{i_1 i_2 \ldots i_m} \leq \prod_{k=1}^{m} A_{i_k i_k \ldots i_k} \tag{4.7}$$

where i_k takes value in $\mathscr{I} = \{i, j\}$. Denote $\tau_i = (i, i, \ldots, i, j), \tau_j = (i, j, \ldots, j, j)$. Then we have $A_\tau = A_{\tau_i} = A_{\tau_j}$ since $B(\tau) = B(\tau_i) = B(\tau_j) = \{i, j\}$ and $\mathscr{A}$ is strong symmetric. By (4.7) we have

$$A^m_{ii\ldots ij} \leq A^{m-1}_{ii\ldots ii} A_{jj\ldots jj} \tag{4.8}$$

and

$$A^m_{ij\ldots jj} \leq A_{ii\ldots ii} A^{m-1}_{jj\ldots jj} \tag{4.9}$$

Since $A_{\tau_1} = A_{ii\ldots ij} = A_{ij\ldots jj} = A_{\tau_2}$, we have by (4.8) and (4.9)

$$A^{2m}_\tau = A^m_{\tau_1} A^m_{\tau_2} \leq (A_{ii\ldots ii} A_{jj\ldots jj})^m$$

which implies (4.6) . □

It is not clear yet whether (4.6) is also sufficient for an 2-dimensional nonnegative strong symmetric tensor to be cp.

5. Completely Positive Pseudograph

Let $\mathscr{A} \in \mathbb{S}_{m;n}$ be a k-uniform binary cptensor and let $\mathscr{G}$ be its associated pseudograph. We write $A = [\alpha_1, \ldots, \alpha_r] \in \mathbb{F}^{n\times r}$, where each α_i corresponds to a maximal edge of $\mathscr{G}$. Then $\mathscr{A}$ is the m-power of A in the sense of *Khatri-Rao product* or m-KR power of A[22] ($\odot$ is columnwise Kronecker product), i.e.,

$$A^{\odot m} = \overbrace{A \odot \cdots \odot A}^{m}.$$

$\mathscr{A} = A^{\odot m}$ has r *k-uniform components* α_j^m. $\mathscr{A}$ is sometimes written as $\mathscr{A} = \sum A^{\odot m}$ where

$$\sum A^{\odot m} := \sum_{j=1}^{r} \alpha_j^m$$

and $A \in \mathbb{R}_+^{n\times r}$ is an k-uniform $\{0,1\}$ matrix. The number k is called the *support* of $\mathscr{A}$ and denoted by $\texttt{supp}(\mathscr{A})$.

Theorem 5.1. *Let $\mathscr{A} = \sum(A^{\odot m}) \in \mathscr{T}_{m;n}$ be m-uniform ($2 \leq m \leq n$) and binary cpwith $A = [\alpha_1, \ldots, \alpha_r]$. Let $\mathscr{G} = (V, \mathscr{E})$ be the pseudogrpah associated with $\mathscr{A}$. Then*

(1) If $\mathscr{A}$ is a (0,1) tensor, then $n = mr$ and $\texttt{cprank}(\mathscr{A}) \leq \texttt{cprank}_b(\mathscr{A}) \leq \frac{n}{m}$.
(2) If $\mathscr{A}$ is an essential (0,1) tensor, then $\texttt{cprank}(\mathscr{A}) \leq \texttt{cprank}_b(\mathscr{A}) \leq \lceil \frac{n}{k-1} \rceil$.

Let $\mathscr{G} = \mathscr{G}(\mathscr{A})$ be a pseudograph associated with an essential (0,1) tensor $\mathscr{A} \in \mathbb{S}_{m;n}$, with decomposition (2.5) where each α_j is a (0,1) n-dimensional vector. Denote $\mathscr{A}^*$ as the pattern of $\mathscr{A}$, i.e., $a^*_\sigma = 1$ if $a_\sigma \neq 0$ for any $\sigma \in S(m,n)$. Then $\mathscr{A}$ is permutation similar to a direct sum of some irreducible tensors [44], say,

$$\mathscr{A} \sim_p \mathscr{A}_1 \oplus \mathscr{A}_2 \oplus \ldots \oplus \mathscr{A}_r$$

where $\mathscr{A}_j \in \mathbb{SF}_{m,n_i}$ with $n_1 + \ldots + n_{r+1} = n$.

Here each $\mathscr{A}_i$ corresponds to a complete block. For any nonnegative tensor $\mathscr{A} \in \mathscr{T}_{m;n}$, a pseudograph $\mathscr{G}$ is r-uniform if each of its maximal edges $\mathbf{e}$ satisfies $|\mathbf{e}| = r$. $\mathscr{G}$ is said to have Property R if $\mathscr{D}_\alpha \subseteq \mathscr{E}$ for any $\alpha \in \mathscr{E}$ where

$$\mathscr{D}_\alpha = \{\sigma \in \mathscr{E} : B(\sigma) \subseteq B(\alpha)\} \tag{5.1}$$

Property R implies that $\mathscr{G}$ is uniquely determined by the set of its maximal edges.

Now we consider any nonnegative tensor $\mathscr{A} \in \mathscr{T}_{m;n}$. If $\mathscr{A}$ is binary cp, then $\mathscr{A}$ has a decomposition (2.5) where $\alpha_j \in \mathbb{F}^n$ for each $j \in [r]$. An edge $\sigma = \{i_1, \ldots, i_m\} \in S(m,n)$ is called a *maximal edge* of a pseudograph $\mathscr{G} = (V, \mathscr{E})$ if $\mathscr{G}$ has no edge ε such that $B(\sigma) \subset B(\varepsilon)$. We call a pseudograph $\mathscr{G}$ an r-uniform pseudograph if all its maximal edges have cardinality r. A pseudograph $\mathscr{G} = (V, \mathscr{E})$ is said to have Property R if $\mathscr{D}_\alpha \subseteq \mathscr{E}$ for any $\alpha \in \mathscr{E}$ where

$$\mathscr{D}_\alpha = \{\sigma \in \mathscr{E} : B(\sigma) \subseteq B(\alpha)\} \tag{5.2}$$

Property R, first introduced in [44], implies that $\mathscr{G}$ is uniquely determined by the set of its maximal edges.

A pseudograph $\mathscr{G}$ is called a *cp pseudograph* if its adjacency tensor $\mathscr{A}(\mathscr{G})$ is binary cp. For any m-uniform pseudograph $\mathscr{G}$ of size n, the largest number of the maximum normal edges is $\binom{n}{m}$ among its n^m (multi-)edges. We note that the ratio

$$R(m,n) = \frac{\binom{n}{m}}{n^m},$$

i.e., the number of all m-edges v.s. the number of all possible edges, converges to $R_m := \frac{1}{m!}$ when $n \to \infty$. Now if we consider the ratio of the number of normal m-edges to the number of (multi-)edges, i.e.,

$$R(m,n) := \frac{\binom{n}{m}}{n^m}.$$

$R(m,n)$ converges to $R_m := \frac{1}{m!}$ when $n \to \infty$. This implies that a pseudograph is much more complicated than a hypergraph.

Corollary 5.2. *Let $\mathscr{G} = (V, \mathscr{E})$ be an m-order pseudograph with $V = [n]$. If $\mathscr{G}$ possesses property R and has a unique nonempty maximal edge,then $\mathscr{G}$ is a cp pseudograph .*

The *indicator* of an edge α of $\mathscr{G}$ is defined as vector

$$I_\alpha := (w_1, \ldots, w_n)^\top \in \mathbb{Z}_+^n$$

where w_i denotes the frequency of vertex i in α. An $n \times N$ pseudograph $\mathscr{G}$ is uniquely determined by an $n \times N$ nonnegative integral matrix

$$W = W(\mathscr{G}) := [\mathbf{u}_1, \ldots, \mathbf{u}_N]$$

where $\mathbf{u}_j \in \mathbb{Z}_+^n$ is the indicator of $\alpha_j \in \mathscr{E}$. W is called *the adjacency matrix* of $\mathscr{G}$. Now we form matrix A associated with W by

$$A = WW^\top \tag{5.3}$$

A can be written equivalently as

$$A = \sum_{j=1}^{N} \mathbf{u}_j^2 = \sum_{j=1}^{N} \mathbf{u}_j \mathbf{u}_j^\top$$

which is a binary cpmatrix when each $\mathbf{u}_j$ is a (0,1) vector ([11]). A is called an k-uniform cp matrix if $|\mathrm{supp}(W)| = k$, and $\mathscr{A}$ is called an k-uniform $n\times m$ tensor of rank R if $\mathscr{A}$ has a binary cpdecomposition (2.5).

Now we denote

$$\mathscr{C}_\alpha := \{\beta \in \mathscr{E} : \beta \sim \alpha\}, \quad \text{and } \mathscr{D}_\alpha := \{\beta \in \mathscr{E} : \beta \prec \alpha\}$$

for any edge $\alpha \in \mathscr{E}$. Let $\Gamma_{\mathscr{G}} := \{\alpha_j | j = 1,2,\dots,r\}$ be the set of the maximal edges of $\mathscr{G}$. Then $\{\mathscr{D}_{\alpha_j} : j = 1,2,\dots,r\}$ forms a partition of $\mathscr{E}$. In [44] we show that a (0,1) mth order n-dimensional symmetric tensor $\mathscr{A}$ is binary cpif and only if $\mathscr{P}$ possesses Property R where $\mathscr{P} = \mathscr{P}(\mathscr{A})$. We have shown in [44] that a (0,1) tensor $\mathscr{A}$ is binary cpif and only if $\mathscr{A}$ can be written as the direct sum of some all-ones blocks. This is equivalent to

$$S_i \cap S_j = \emptyset, \forall 1 \le i < j \le r \tag{5.4}$$

where $S_k := \mathrm{supp}(\mathbf{u}_k)$ and r is the smallest number for (2.5) to hold.

Given an $n\times N$ pseudograph $\mathscr{G}$. We let $\mathscr{A}$ denote the tensor generated by the Khartry-Rao product of $W \equiv W(\mathscr{G}) = [\mathbf{u}_1,\dots,\mathbf{u}_N]$, i.e., $\mathscr{A} = \overbrace{W\circ W\circ\dots\circ W}^{m}$, which is defined as (2.5).

It is shown that a (0,1) mth order n-dimensional symmetric tensor $\mathscr{A}$ is binary cpif and only if $\mathscr{P} = \mathscr{P}(\mathscr{A})$ possesses Property R and that a (0,1) tensor is binary cpif and only if it can be written as the direct sum of some all-ones blocks, which is equivalent to $S_i \cap S_j = \emptyset$ for all distinct i, j. By permutation similarity, we can establish some equivalent relations among pseudographs. Let $\mathscr{P}_i = (V_i, \mathscr{E}_i), i = 1,2$ be m-uniform pseudographs associated resp. with tensors $\mathscr{A}$ and $\mathscr{B}$. Then $\mathscr{A} \sim_p \mathscr{B}$ if and only if there exists a bijection ϕ from V_1 to V_2 such that

$$\{i_1,\dots,i_m\} \in \mathscr{E}_1 \mapsto \{\phi(i_1),\dots,\phi(i_m)\} \in \mathscr{E}_2$$

i.e., $\mathscr{P}(\mathscr{B})$ is the pseudograph obtained from $\mathscr{P}(\mathscr{A})$ by vertex reordering, and thus they are isomorphic. Let $\mathscr{A}_i = (a^{(i)}_\sigma) \in \mathscr{T}_{m,n_i}, i = 1,2$ and $n_1 + n_2 = n$. The *direct sum* of $\mathscr{A}_1$ and $\mathscr{A}_2$, denoted $\mathscr{A} = \mathscr{A}_1 \oplus \mathscr{A}_2 = (a_{i_1\dots i_m})$, is defined by

$$a_{i_1\dots i_m} = \begin{cases} a^{(1)}_{i_1\dots i_m} & \text{if} i_1,\dots,i_m \in [n_1], \\ a^{(2)}_{i_1\dots i_m} & \text{if} i_1,\dots,i_m \in n_1 + [n_2], \\ 0 & \text{otherwise.} \end{cases}$$

Here $a + S$ is defined as the translation of set S, i.e., $a + S = \{a + s : s \in S\}$. We are now in a position to describe the decomposition for tensors in the sense of permutation similarity.

Lemma 5.3. *Let $\mathscr{A} \in \mathbb{SF}_{m,n}$, where $m \ge 2, n \ge 1$. Then*

$$\mathscr{A} \sim_p \mathscr{A}_1 \oplus \mathscr{A}_2 \oplus \dots \oplus \mathscr{A}_r \oplus \mathscr{O}_{r+1} \tag{5.5}$$

where $\mathscr{A}_i \in \mathbb{SF}_{m,n_i}$ is irreducible, $\mathscr{O}_{r+1}$ is a zero tensor of order m and dimension n_{r+1}, and $n_1 + \dots + n_{r+1} = n$.

Lemma 5.3 shows that a tensor $\mathscr{A} \in \mathbb{SF}_{m,n}$ can always be decomposed into the direct sum of irreducible tensors, possibly with a zero block. The following lemma offers a necessary and sufficient conditions for an irreducible $(0,1)$ tensor to be binary cp.

Lemma 5.4. *Let $\mathscr{A} \in \mathbb{SF}_{m,n}$ be irreducible. Then the following statements are equivalent:*

(1) $\mathscr{A}$ is binary cp.
(2) $\mathscr{A} = \mathscr{J}$ is an all-1 tensor.
(3) The pseudograph G associated with tensor $\mathscr{A}$ is a complete block.

From Lemma 5.4, we have the following result.

Theorem 5.5. *Let $\mathscr{A} \in \mathbb{SF}_{m,n}$ be associated with pseudograph $G(V,\mathscr{E})$. Then the following are equivalent:*

(1): *$\mathscr{A}$ is binary cptensor.*
(2): *G can be decomposed as the union of some complete blocks G_i of size n_i where $n_1 + \ldots + n_q = n$.*
(3): *$\mathscr{A}$ can be written in form*

$$\mathscr{A} = \sum_{j=1}^{r} \boldsymbol{u}_j^m \tag{5.6}$$

where $\boldsymbol{u}_j \in \mathbb{F}^n$ satisfies $U^T U = diag(n_1, \ldots, n_q)$ for $U = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_q]$.

Proof. To prove $(1) \Leftrightarrow (2)$, we first let $\mathscr{A} \in \mathbb{SF}_{m,n}$ be a binary cptensor. Then by Lemma 5.3 $\mathscr{A}$ can be written in form (5.5) where each $\mathscr{A}_i$ is an irreducible binary cptensor of mth order n_i-dimension (no zero block there since $\mathscr{A}$ has no zero block). By Lemma 5.4, $\mathscr{A}_i$ is associated with a pseudograph $\mathscr{P}_i = (V_i, \mathscr{E}_i)$ where $|V_i| = n_i$ for $i = 1, 2, \ldots, q$, $n_1 + n_2 + \ldots + n_q = n$. For each $i \in [q]$, by Lemma 5.4, $\mathscr{P}_i$ is the complete block of dimension n_i (since $\mathscr{A}_i$ is irreducible and binary cp). Thus $(1) \Rightarrow (2)$ is proved. The proof of $(2) \Rightarrow (1)$ is immediate if we note that the decomposition (5.6) holds by take $\mathtt{supp}(\mathbf{u}_i) = V_i$ for $i = 1, 2, \ldots, q$.

Now we show $(1) \Leftrightarrow (3)$. First we assume that $\mathscr{A} \in \mathbb{SF}_{m,n}$ is binary cp. Then from the proof of Lemma 5.4 there exist some vectors $\mathbf{u}_j \in \mathbb{F}^n$ such that (2.5) holds, and

$$\mathtt{supp}(\mathbf{u}_i) \cap \mathtt{supp}(\mathbf{u}_j) = \emptyset, \forall 1 \le i < j \le q \tag{5.7}$$

It follows that $U^T U = diag(n_1, \ldots, n_q)$ for $U = [\mathbf{u}_1, \ldots, \mathbf{u}_q]$, where n_i is the positive integer described above. Thus $(1) \Rightarrow (3)$ is proved. The other direction can be proved by reversing the above arguments. □

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