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Completely positive matrices of order 5 with a nearly $\widehat{CP}$-graph

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Abstract. A particular class of graphs, called "nearly $\widehat{CP}$-graphs", extending the class of $\widehat{CP}$-graphs is introduced. From Barioli's characterization of completely positive matrices with a book-graph, two equivalent characterizations of completely positive matrices with a nearly $\widehat{CP}$-graph are deduced. By means of these results, new characterizations of completely positive matrices of order 5 with a book-graph and some alternative demonstrations of known results are derived. A new characterization of completely positive matrices of order 5 with a $\widehat{CP}$-graph and a new elementary proof of the main result obtained by Cedolin-Salce, regarding this particular class of matrices, are shown. It is also attempted to clarify some results obtained by Xu on completely positive matrices of order 5, and it is shown by a counterexample that one of them is incorrect.

Keywords: Completely positive matrices, doubly non-negative matrices, book graphs

MSC 2000 classification: 15A09, 15A18, 15B48, 15B57

1 Introduction

All matrices considered in this paper are real matrices. If A is an n x n matrix, and α, β are sets of indices $\alpha, \beta \subseteq \{1, ..., n\}$, then $A[\alpha|\beta]$ is the submatrix of A with rows indexed by the elements of α and columns indexed by the elements of β (both index sets in increasing order); and $A(\alpha|\beta)$ is the submatrix of A with rows indexed by $\{1, ..., n\} \setminus \alpha$ and columns indexed by $\{1, ..., n\} \setminus \beta$ (both index sets in increasing order). Using these notations we often omit the $\{\cdot\}$ (e.g., we write $A[1, 2|2, 3]$ instead of $A[\{1, 2\} \,|\, \{2, 3\}]$).

A matrix A is called completely positive if it can be written in the form $A = BB^T$, where B is a (not necessarily square) non-negative matrix. A completely positive matrix is necessarily doubly non-negative, i.e., positive semidefinite and non-negative. The classes of completely positive and doubly non-negative matrices of order n are denoted, respectively, by CP_n and DNN_n, therefore $CP_n \subseteq DNN_n$ for every n. It is well known that this inclusion is actually an equality for $n \leq 4$, and that for $n \geq 5$ it is a proper inclusion. Another known fact is that CP_n and DNN_n are closed convex cones in the Euclidean space of all symmetric matrices of order n, where the inner product is given by $\langle A, B\rangle = trace(AB)$ (see, e.g., [2]).

Given a symmetric matrix A of order n, the undirected graph associated with A, $G(A)$, is the graph with n vertices $(1, 2, \ldots, n)$ that contains the edge (i, j), with $i \neq j$, if and only if $a_{ij} \neq 0$.

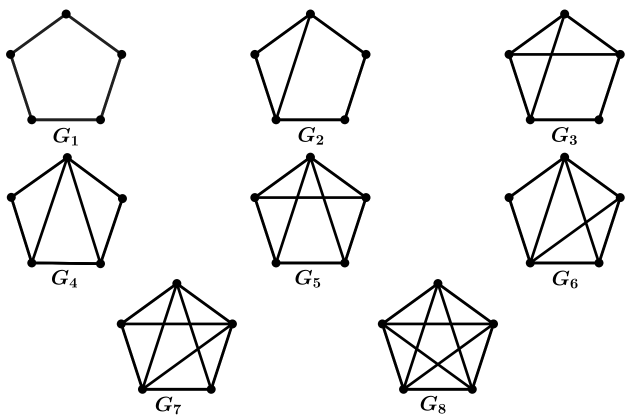
A graph G is called completely positive if every doubly non-negative matrix, whose associated graph is isomorphic to G, is completely positive. In 1993, after contributions by many authors, completely positive graphs were characterized.

Theorem 1 (Kogan-Berman [5]). *A graph G is completely positive if and only if it does not contain cycles of odd length > 3.*

It follows that there are graphs with 5 vertices that are not completely positive, and those are the ones that contain a cycle of length 5, namely Hamiltonian graphs with 5 vertices.

Corollary 1. *Every doubly non-negative matrix of order* 5 *whose graph is not Hamiltonian is completely positive.*

There are, up to isomorphisms, eight different types of Hamiltonian graphs with 5 vertices. We follow the notation in [6], where these graphs are denoted by G_i $(1 \leq i \leq 8)$.



It is clear that G_1, G_2, G_3, G_4, G_6 are book-graphs. Book-graphs were defined by Barioli in [1].

Definition 1 (Barioli [1]). Let G be a graph with set of vertices $V(G)$. We say that G is a *book-graph* with *r completely positive pages* if $V(G)$ is the union of subsets C_1, C_2,..., C_r and:

(1) $\exists u, v \in V(G)$ such that, $\forall i \neq j$, $C_i \cap C_j = \{u, v\}$;

(2) there are no edges connecting vertices in different C_i's, in case except the edge (u, v);

(3) $\forall i$ the induced subgraph generated by C_i is completely positive.

It is also clear that G_1, G_2, G_3 are $\widehat{CP}$-graphs (originally called in [1] excellent graphs), i.e., they are graphs G containing a vertex w, called a hat-vertex, adjacent only to two other vertices u, v which are not each other adjacent, such that $G \setminus \{w\}$ is a completely positive graph. Completely positive matrices with book-graphs and $\widehat{CP}$-graphs were characterized by Barioli in [1].

Completely positive matrices with graphs from G_1 up to G_6 are also studied in [6]. Howewer Cedolin and Salce showed in [3] that Xu's characterizations of completely positive matrices whose graph is G_2 or G_3 are wrong. A doubly non-negative matrix whose graph is G_1, G_2 or G_3 can be assumed without loss of generality to be in the following forms, respectively (it is understood that an entry a_{ij} denotes a positive real number):

$$\begin{bmatrix} 1 & a_{12} & 0 & 0 & a_{15} \\ a_{12} & 1 & a_{23} & 0 & 0 \\ 0 & a_{23} & 1 & a_{34} & 0 \\ 0 & 0 & a_{34} & 1 & a_{45} \\ a_{15} & 0 & 0 & a_{45} & 1 \end{bmatrix}; \quad (1.1) \qquad \begin{bmatrix} 1 & a_{12} & a_{13} & 0 & a_{15} \\ a_{12} & 1 & a_{23} & 0 & 0 \\ a_{13} & a_{23} & 1 & a_{34} & 0 \\ 0 & 0 & a_{34} & 1 & a_{45} \\ a_{15} & 0 & 0 & a_{45} & 1 \end{bmatrix}; \quad (1.2)$$

$$\begin{bmatrix} 1 & a_{12} & a_{13} & 0 & a_{15} \\ a_{12} & 1 & a_{23} & a_{24} & 0 \\ a_{13} & a_{23} & 1 & a_{34} & 0 \\ 0 & a_{24} & a_{34} & 1 & a_{45} \\ a_{15} & 0 & 0 & a_{45} & 1 \end{bmatrix}. \tag{1.3}$$

For completely positive matrices in these forms, Cedolin and Salce obtained the following characterization.

Theorem 2 (Cedolin-Salce [3]). *For a doubly non-negative matrix A whose associated graph is G_1, G_2 or G_3 in the form (1.1), (1.2) or (1.3), the following conditions are equivalent:*

(1) A is completely positive.

(2) $detA \geq 4V_A(5)$.

The quantity $V_A(5)$ in Theorem 2 is the total weight of the hat-vertex 5 in $G(A)$ introduced in [3]; for its definition see next Section 2. We remark that in [3] total weights of hat-vertices are indicated with the letter W. We have decided to change this notation here to avoid misunderstandings, since W in [3] indicates also corrected weights of cycles.

Completely positive matrices of order 5 whose graph is G_4, G_5 or G_6 are studied in [6]. However the characterizations that Xu obtains for these cases are not totally clear. In [6], Xu gives the following definitions:

Definition 2 (Xu [6])**.** Let A be a doubly non-negative matrix, and $C = \{j_1 \to j_2 \to \cdots \to j_k \to j_1\}$ be a cycle in $G(A)$.

- the weight $A_{|C|}$ of the cycle C in $G(A)$ is the following quantity:

$$A_{|C|} := (-1)^{k-1} a_{j_1 j_2} a_{j_2 j_3} \cdots a_{j_{k-1} j_k} a_{j_k j_1};$$

- the quantity $A_{|k|}$ is the algebraic sum of weights of all cycles of length k in $G(A)$.

In the definition above j_1, j_2,..., j_k are distinct vertices.

A doubly non-negative matrix whose graph is G_4, G_5 or G_6 can be assumed without loss of generality to be in the following forms, respectively (it is understood that an entry a_{ij} denotes a positive real number):

$$\begin{bmatrix} 1 & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{12} & 1 & a_{23} & 0 & 0 \\ a_{13} & a_{23} & 1 & a_{34} & 0 \\ a_{14} & 0 & a_{34} & 1 & a_{45} \\ a_{15} & 0 & 0 & a_{45} & 1 \end{bmatrix}; \quad (1.4) \qquad \begin{bmatrix} 1 & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{12} & 1 & a_{23} & 0 & a_{25} \\ a_{13} & a_{23} & 1 & a_{34} & 0 \\ a_{14} & 0 & a_{34} & 1 & a_{45} \\ a_{15} & a_{25} & 0 & a_{45} & 1 \end{bmatrix}; \quad (1.5)$$

$$\begin{bmatrix} 1 & a_{12} & a_{13} & 0 & 0 \\ a_{12} & 1 & a_{23} & a_{24} & a_{25} \\ a_{13} & a_{23} & 1 & a_{34} & a_{35} \\ 0 & a_{24} & a_{34} & 1 & a_{45} \\ 0 & a_{25} & a_{35} & a_{45} & 1 \end{bmatrix}. \tag{1.6}$$

In [6], Xu states the following theorems (where E_{ij} indicates the matrix with all zeroes except the (i, j)-element which is equal to 1, and $\mathbb{I}_n$ denotes the identity matrix of order n).

Theorem 3 ([6])**.** *Let $A \in DNN_5$ in the form (1.4) . Then $A \in CP_5$ if and only if one of the following holds:*

(1) $a_{13} \geq a_{12}a_{23}$*;*

(2) $a_{14} \geq a_{15}a_{45}$*;*

(3) Neither 1. nor 2. holds, but $detA \geq 4A_{|(3,4)|}$.

Theorem 4 ([6])**.** *Let $A \in DNN_5$ in the form (1.5), and*

$$a_{12} = min\left\{\frac{a_{1j}}{a_{2j}} \mid a_{2j} > 0\right\}.$$

Then $A \in CP_5$ if and only if one of the following holds:

(1) $a_{13} \geq a_{12}a_{23} + a_{14}a_{43}$ and $a_{15} \geq a_{12}a_{25} + a_{14}a_{45}$; or

(2) $detA \geq 4\tilde{A}_{|2|}$, where $\tilde{A} = SAS^T$, $S = \mathbb{I}_5 - a_{12}E_{12}$.

Theorem 5 ([6])**.** *Let $A \in DNN_5$ in the form (1.6). Then $A \in CP_5$ if and only if:*

(1) $a_{23} \geq a_{12}a_{13}$; or

(2) $a_{23} < a_{12}a_{13}$ and $detA \geq 4\tilde{A}_{|1|}$, where $\tilde{A} = SAS^T$, $S = \mathbb{I}_5 - \frac{a_{23}}{a_{13}}E_{21}$.

The quantity $A_{|(3,4)|}$ appearing in Theorem 3 is never defined in [6], and the quantity $\tilde{A}_{|1|}$ appearing in Theorem 5 seems to have no meaning, since there are no cycles of length 1.

This paper has several goals. In Section 2 a new characterization of completely positive matrices of order 5 with a $\widehat{CP}$-graph and an elementary proof of Cedolin-Salce's Theorem 2 are given. In Section 3, from Barioli's characterization of completely positive matrices with a book-graph in [1], we deduce two characterizations of completely positive matrices with particular book-graphs, that we will call "nearly $\widehat{CP}$-graphs" (see Section 3 for their precise definition). In Section 4 various characterizations of completely positive matrices of order 5 whose graph is G_4 or G_6 are presented, which are obtained by applying the results of Section 3; it is also attempted to clarify Xu's results for those two cases. In Section 5 it is shown that Xu's Theorem 4 is not correct.

2 Completely positive matrices of order 5 with a $\widehat{CP}$-graph

In this section we are going to show a new characterization of completely positive matrices of order 5 with a $\widehat{CP}$-graph, and also an elementary proof of a Cedolin-Salce's theorem ([3], Theorem 2).

We start recalling the definition of a corrected weight of a cycle, given by Cedolin-Salce in [3]. This definition uses the weight of a cycle in Definition 2.

Definition 3 (Cedolin-Salce [3])**.** Let A be a doubly non-negative matrix. Given a cycle $C = \{j_1 \to j_2 \to \cdots \to j_k \to j_1\}$ in $G(A)$, its *corrected weight* is $W_A(C) = A_{|C|} \cdot \prod_{i \notin C} a_{ii}$.

We remark that, in [3], the weight of a cycle C in $G(A)$ is denoted by $w_A(C)$.

We now give the definition of the weight and the total weight of a set of vertices J. This definition generalizes the one given by Cedolin-Salce in [3] regarding the total weight of a hat-vertex.

Definition 4. Let A be a doubly non-negative matrix, and let J be a set of vertices in $G(A)$.

(1) *The weight* $v_A(J)$ *of* J *in* $G(A)$ is the sum of the weights of all cycles with length > 2 in $G(A)$ that contain the set of vertices J.

(2) *The total weight* $V_A(J)$ *of* J *in* $G(A)$ is the sum of the corrected weights of all cycles with length > 2 in $G(A)$ that contain the set of vertices J.

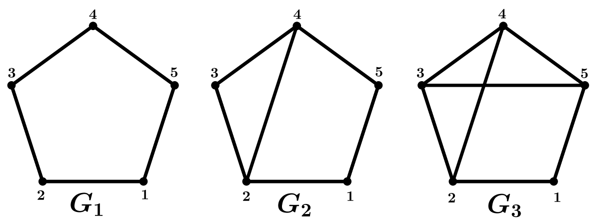
It is important to note that, given any set of vertices J, if all the diagonal elements of A are equal to 1, $V_A(J) = v_A(J)$.

A crucial tool for our purposes is the Cauchy's interlacing theorem for Hermitian matrices.

Theorem 6 (Cauchy)**.** *Let* A *be an Hermitian matrix of order* n*, and let* B *be a principal submatrix of* A *of order* $n-1$*. Let* $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$ *and* $\mu_1 \le \mu_2 \le \cdots \le \mu_{n-1}$ *be, respectively, the eigenvalues of* A *and* B*. Then:*

$$\lambda_1 \le \mu_1 \le \lambda_2 \le \cdots \le \lambda_k \le \mu_k \le \lambda_{k+1} \le \cdots \le \mu_{n-1} \le \lambda_n.$$

We now consider the graphs G_1, G_2, G_3 with the following numeration of vertices:



A doubly non-negative matrix A whose graph is G_1, G_2 or G_3 can be assumed, without loss of generality, to be in the following form:

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & 0 & a_{15} \\ a_{12} & a_{22} & a_{23} & a_{24} & 0 \\ 0 & a_{23} & a_{33} & a_{34} & a_{35} \\ 0 & a_{24} & a_{34} & a_{44} & a_{45} \\ a_{15} & 0 & a_{35} & a_{45} & a_{55} \end{bmatrix}. \tag{2.1}$$

In the case $G(A) = G_3$ all elements a_{ij} in (2.1) are positive, in the case $G(A) = G_2$ we have $a_{35} = a_{53} = 0$, and in the case $G(A) = G_1$ we have $a_{24} = a_{42} = a_{35} = a_{53} = 0$.

Since G_1, G_2, G_3 are $\widehat{CP}$-graphs, we can write:

$$A^- = \begin{bmatrix} a_{11} & a_{12} & 0 & 0 & -a_{15} \\ a_{12} & a_{22} & a_{23} & a_{24} & 0 \\ 0 & a_{23} & a_{33} & a_{34} & a_{35} \\ 0 & a_{24} & a_{34} & a_{44} & a_{45} \\ -a_{15} & 0 & a_{35} & a_{45} & a_{55} \end{bmatrix}. \tag{2.2}$$

The matrix A^- is defined by Barioli in Section 3 of [1].

We can now state the main result of this section.

Theorem 7. *Let $A \in DNN_5$ whose associated graph is G_1, G_2 or G_3 in the form (2.1), and let A^- be the matrix defined by (2.2). Then the following statements are equivalent:*

(1) A is completely positive.

(2) A^- is positive semidefinite.

(3) $detA \geq 4V_A(\{1\})$.

(4) $detA^- \geq 0$.

We remark that the equivalence of statements 1 and 3 of the previous theorem corresponds, after a suitable cogredience, to Cedolin-Salce's Theorem 2. However, in the proof of Theorem 7, we are going to show a new elementary proof that statements 1 and 3 are equivalent.

Proof. The equivalence of statements 1 and 2 derives directly from Barioli's characterization of completely positive matrices with a $\widehat{CP}$-graph ([1], Section 3).

Now we want to show the equivalence of statements 3 and 4. From simple calculations we obtain:

$$\begin{aligned} detA = \; & a_{11}detA\,(1|1) - a_{12}^2 detA\,(1,2|1,2) + 2a_{12}a_{15}detA\,(1,2|1,5) \\ & - a_{15}^2 detA\,(1,5|1,5)\,. \end{aligned}$$

$$\begin{aligned} detA^- = \; & a_{11}detA\,(1|1) - a_{12}^2 detA\,(1,2|1,2) - 2a_{12}a_{15}detA\,(1,2|1,5) \\ & - a_{15}^2 detA\,(1,5|1,5)\,. \end{aligned}$$

So we obtain:

$$detA - detA^{-} = 4a_{12}a_{15}detA\,(1,2|1,5)\,.$$

Another simple calculation shows that the quantity $4a_{12}a_{15}detA\,(1,2|1,5)$ is equal, in all three cases G_1, G_2, G_3, to the quantity $4V_A(\{1\})$, and from that follows the equivalence of statements 3 and 4.

Statement 2 obviously implies statement 4, so the last thing we need to prove is that statement 3 (or 4) implies 1 (or 2). From now on we'll assume that $detA^{-} \geq 0$. We have three cases:

Case 1: $V_A(\{1\}) > 0$. In this case $detA > 0$, A is positive definite and so it is the matrix $A(1|1)$. This last matrix is also a principal submatrix of A^{-}. Now let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_5$ be the eigenvalues of A^{-}, and $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_4$ the eigenvalues of $A(1|1)$. By applying Theorem 6 we obtain: $\lambda_1 \leq \mu_1 \leq \lambda_2 \leq \cdots \leq \mu_4 \leq \lambda_5$. Since $A(1|1)$ is positive definite, $\mu_1 > 0$, so $\lambda_2, \ldots, \lambda_5 > 0$. But $detA^{-} \geq 0$, then $\lambda_1 \geq 0$. Therefore A^{-} is positive semidefinite, and $A \in CP_5$.

Case 2: $V_A(\{1\}) < 0$. In this case we have $detA^{-} = detA - 4V_A(\{1\}) > 0$, since A is by hypothesis doubly non-negative. Using the notations introduced in *Case* 1, by applying Theorem 6 we obtain: $\lambda_1 \leq \mu_1 \leq \lambda_2 \leq \cdots \leq \mu_4 \leq \lambda_5$. The matrix $A(1|1)$ is positive semidefinite because A is, then $\mu_1 \geq 0$. But $detA^{-} > 0$, so $\lambda_2, \ldots, \lambda_5 > 0$. That implies $\lambda_1 > 0$, therefore A^{-} is positive definite and $A \in CP_5$.

Case 3: $V_A(\{1\}) = 0$. Since if $G(A) = G_1$ the quantity $V_A(\{1\})$ is necessarily positive (the only cycle containing vertex 1 is the Hamiltonian cycle), in this case $G(A)$ must be G_2 or G_3, and so $a_{24} > 0$.

For all $d > 0$ we define $A_d := A + d\mathbb{I}_5$ and $A_d^{-} = A^{-} + d\mathbb{I}_5$. For all $d > 0$, A_d is doubly non-negative and $G(A_d) = G(A)$. Simple calculations show:

$$\begin{aligned} detA_d - detA_d^{-} =& 4V_{A_d}(\{1\}) = 4\,(a_{12}a_{23}a_{34}a_{45}a_{15} - a_{12}a_{24}a_{45}a_{15}(a_{33}+d) + \\ & - a_{12}a_{23}a_{35}a_{15}(a_{44}+d) + a_{12}a_{24}a_{43}a_{35}a_{15}) = \\ & = 4V_A(\{1\}) - 4a_{12}a_{15}(a_{45}a_{24} + a_{35}a_{23})d = \\ & = -4a_{12}a_{15}(a_{45}a_{24} + a_{35}a_{23})d. \end{aligned}$$

Since $a_{24} > 0$, we have $detA_d - detA_d^{-} < 0$, for all $d > 0$. It follows that $detA_d^{-} > 0$. For *Case 2* applied to A_d, we obtain that this matrix is completely positive, for all $d > 0$. But CP_5 is a closed convex cone, therefore $\lim_{d \to 0^+} A_d = A$ is completely positive.

QED

We remark that statement 4 of the previous theorem is a new characterization of completely positive matrices of order 5 whose graph is G_2 or G_3. For completely positive matrices whose graph is G_1 the equivalence of statements 1 and 4 was already known (see [1], Section 4).

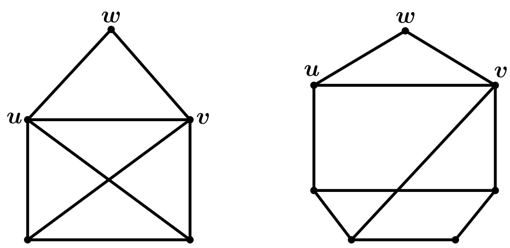
3 Nearly $\widehat{CP}$-graphs

Barioli in [1] obtained a characterization of completely positive matrices whose associated graph is a book-graph, and then simplified this characterization for completely positive matrices with particular book-graphs, namely $\widehat{CP}$-graphs. We recall that a $\widehat{CP}$-graph is a graph G that contains a vertex w, adjacent only to two other vertices u, v which are not each other adjacent, such that $G \setminus \{w\}$ is a completely positive graph.

Using the notations introduced above, we note that the definition of a $\widehat{CP}$-graph requires that the vertex u is not adjacent to the vertex v. In this section we are going to deduce two equivalent characterizations of completely positive matrices whose associated graph is a "nearly" $\widehat{CP}$-graph, meaning that the non-adjacency of u and v it is not specifically required. We start giving a formal definition of these particular graphs.

Definition 5. A graph G is called a *nearly $\widehat{CP}$-graph* if there exists a vertex w of degree 2 such that $G \setminus \{w\}$ is a completely positive graph.

The following are examples of nearly $\widehat{CP}$-graphs:



Note that a $\widehat{CP}$-graph is also a nearly $\widehat{CP}$-graph.

A nearly $\widehat{CP}$-graph is obviously a book-graph, therefore from Barioli's characterization of completely positive matrices with a book-graph we want to deduce a characterization of completely positive matrices with a nearly $\widehat{CP}$-graph.

A doubly non-negative matrix realization A of a nearly $\widehat{CP}$-graph can be written, without loss of generality, in the following form:

$$A = \begin{bmatrix} a & h & x_1 & \mathbf{x}_2^T \\ h & b & y_1 & \mathbf{y}_2^T \\ x_1 & y_1 & a_1 & \mathbf{0}^T \\ \mathbf{x}_2 & \mathbf{y}_2 & \mathbf{0} & A_2 \end{bmatrix}, \tag{3.1}$$

where x_1, y_1 are positive real numbers. Since A is doubly non-negative, we note that also $a_1 > 0$. Sometimes (3.1) will be written in the following more compact form:

$$A = \begin{bmatrix} a & h & \mathbf{x}^T \\ h & b & \mathbf{y}^T \\ \mathbf{x} & \mathbf{y} & \overline{A} \end{bmatrix}, \tag{3.2}$$

where obviously $\mathbf{x}^T = \begin{bmatrix} x_1 & \mathbf{x}_2^T \end{bmatrix}$, $\mathbf{y}^T = \begin{bmatrix} y_1 & \mathbf{y}_2^T \end{bmatrix}$ and $\overline{A} = \begin{bmatrix} a_1 & \mathbf{0}^T \\ \mathbf{0} & A_2 \end{bmatrix}$.

Since a nearly $\widehat{CP}$-graph is a book-graph with two completely positive pages, one on three vertices, we can write Barioli's characterization of completely positive matrices with a book-graph in the following way.

Theorem 8 (Barioli [1])**.** *Let $A \in DNN_n$ whose associated graph is a book-graph in the forms (3.1) and (3.2). Then A is completely positive if and only if:*

(1) $\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 \geq 0$*; or*

(2) $\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 < 0$ *and*

$$\sqrt{a_\perp b_\perp} + h_\perp \geq -2\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2, \tag{3.3}$$

where $\begin{bmatrix} a_\perp & h_\perp \\ h_\perp & b_\perp \end{bmatrix} := A/\overline{A}$, $A/\overline{A}$ is the generalized Schur complement of $\overline{A}$ in A and the symbol $A_2^\dagger$ denotes the Moore-Penrose pseudo-inverse of the matrix A_2. We can now state the main result of this section.

Theorem 9. *Let $A \in DNN_n$ whose associated graph is a nearly $\widehat{CP}$-graph in the forms (3.1) and (3.2). Then the following statements are equivalent:*

(1) A is completely positive.

(2) *a.* $\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 \geq 0$*; or*

b. $\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 < 0$ *and*

$$det\left(A/\overline{A}\right) \geq 4\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 \frac{detA\,[1,3|2,3]}{a_1}.$$

(3) *a.* $detA\,[1,3|2,3] \geq 0$*; or*

b. $detA\,[1,3|2,3] < 0$ *and*

$$det\left(A/\overline{A}\right) \geq 4\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 \frac{detA\,[1,3|2,3]}{a_1}.$$

Proof. We observe that the matrix A is in the canonical forms introduced in Section 2 of [1]. We start by proving the equivalence of statements 1 and 2.

From Theorem 8 we observe that the only thing we need to prove is that, when $\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 < 0$, inequality (3.3) is equivalent to the one stated at point 2, (b) of Theorem 9.

So now we assume $\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 < 0$. Since $A/\overline{A}$ is positive semidefinite, we have:

$$-\sqrt{a_\perp b_\perp} \leq h_\perp \leq \sqrt{a_\perp b_\perp}.$$

From the previous inequality it follows that:

$$-2\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 - h_\perp \geq -\sqrt{a_\perp b_\perp}.$$

Taking also into account inequality (3.3), we obtain:

$$-\sqrt{a_\perp b_\perp} \leq -2\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 - h_\perp \leq \sqrt{a_\perp b_\perp}.$$

That means that inequality (3.3) is satisfied if and only if:

$$a_\perp b_\perp \geq \left(2\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 + h_\perp\right)^2.$$

Since $det\left(A/\overline{A}\right) = a_\perp b_\perp - h_\perp^2$, the previous inequality is equivalent to the following:

$$det\left(A/\overline{A}\right) \geq 4\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 \left(\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 + h_\perp\right).$$

Finally, noticing that $h_\perp = h - x_1 y_1 a_1^{-1} - \mathbf{x}_2^T A_2^\dagger \mathbf{y}_2$, and that $h - x_1 y_1 a_1^{-1} = detA\,[1,3|2,3]\,/a_1$, we obtain that inequality (3.3) is equivalent to:

$$det\left(A/\overline{A}\right) \geq 4\mathbf{x}_2^T A_2^\dagger \mathbf{y}_2 \frac{detA\,[1,3|2,3]}{a_1},$$

and that proves the equivalence of statements 1 and 2.

Now, taking into account that $det\left(A/\overline{A}\right) \geq 0$ always, simple calculations show that also statements 1 and 3 are equivalent.

$\boxed{QED}$

It is important to note that, in case the matrix A_2 is nonsingular, the previous characterizations can be further simplified. In particular, the issue of calculating Schur's complement $A/\overline{A}$ disappears, as stated by the following corollary of Theorem 9.

Corollary 2. *Let $A \in DNN_n$ whose associated graph is a nearly $\widehat{CP}$-graph in the forms (3.1) and (3.2), and let's assume that A_2 is nonsingular. Then the following statements are equivalent:*

(1) A is completely positive.

(2) *a.* $\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 \geq 0$; *or*
b. $\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 < 0$ *and*

$$detA \geq 4\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 \; detA\,[1,3|2,3]\, detA_2.$$

(3) *a.* $detA\,[1,3|2,3] \geq 0$; *or*
b. $detA\,[1,3|2,3] < 0$ *and*

$$detA \geq 4\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 \; detA\,[1,3|2,3]\, detA_2.$$

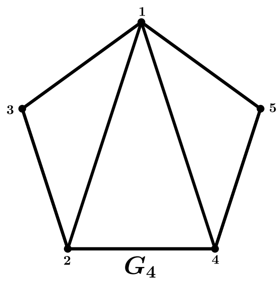
Proof. It follows directly from Theorem 9 and from the formula: $det\left(A/\overline{A}\right) = detA/det\overline{A}$, that is a known property of Schur's complements.

QED

4 Completely positive matrices with G_4, G_6

In this section we are going to deduce, from the results obtained in the previous section, various characterizations of completely positive matrices of order 5 whose graph is G_4 or G_6. We will also try to clarify Xu's Theorems 3, 5, since we have seen in Section 1 that some quantities that appear in those theorems are not defined or don't have meaning.

We start with G_4:



G_4

We observe that G_4 is not a $\widehat{CP}$-graph, but it is a nearly $\widehat{CP}$-graph.

A doubly non-negative matrix realization of G_4 can be assumed, without loss of generality, in the following form:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{12} & a_{22} & a_{23} & a_{24} & 0 \\ a_{13} & a_{23} & a_{33} & 0 & 0 \\ a_{14} & a_{24} & 0 & a_{44} & a_{45} \\ a_{15} & 0 & 0 & a_{45} & a_{55} \end{bmatrix}. \tag{4.1}$$

The main result we obtained for this case is the following.

Theorem 10. *Let $A \in DNN_5$ whose associated graph is G_4 be in the form (4.1). Then the following statements are equivalent:*

(1) A is completely positive.

(2) a. $detA\,[1,5|4,5] \geq 0$; *or*
b. $detA\,[1,5|4,5] < 0$ *and* $detA \geq 4V_A(\{2,4\})$.

(3) a. $detA\,[1,3|2,3] \geq 0$; *or*
b. $detA\,[1,3|2,3] < 0$ *and* $detA \geq 4V_A(\{2,4\})$.

In the proof of this theorem we use the set of notations introduced in Section 3.

Proof. We start observing that the matrix A is in the canonical forms (3.1), (3.2). Since A is positive semidefinite by hypothesis and columns 4 and 5 of A are linearly independent by their sign pattern, the matrix $A_2 = \begin{bmatrix} a_{44} & a_{45} \\ a_{45} & a_{55} \end{bmatrix}$ is necessarily nonsingular.

Now simple calculations show that:

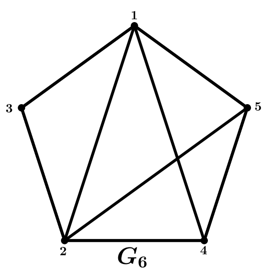
(1) $\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 \geq 0 \iff detA\,[1,5|4,5] \geq 0$;

(2) $\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 \cdot detA\,[1,3|2,3]\, detA_2 = V_A(\{2,4\})$.

At this point the equivalence of statements 1, 2 and 3 follows directly from Corollary 2.

QED

We now focus our attention to G_6:



G_6

Like G_4, the graph G_6 is not a $\widehat{CP}$-graph, but it is a nearly $\widehat{CP}$-graph.

A doubly non-negative matrix realization of G_6 can be assumed, without loss of generality, in the following form:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{12} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{13} & a_{23} & a_{33} & 0 & 0 \\ a_{14} & a_{24} & 0 & a_{44} & a_{45} \\ a_{15} & a_{25} & 0 & a_{45} & a_{55} \end{bmatrix}. \tag{4.2}$$

The main result we obtained for this case is the following.

Theorem 11. *Let $A \in DNN_5$ whose associated graph is G_6 be in the form (4.2). Let $S := \mathbb{I}_5 - \frac{a_{12}}{a_{13}} E_{23}$, and $\tilde{A} := SAS^T$. Then the following statements are equivalent:*

(1) A is completely positive.

(2) a. $detA\,[1,5|4,5] \geq \frac{a_{25}}{a_{24}} \cdot detA\,[1,4|4,5]$; or
b. $detA\,[1,5|4,5] < \frac{a_{25}}{a_{24}} \cdot detA\,[1,4|4,5]$ and $detA \geq 4V_{\tilde{A}}(\{3\})$.

(3) a. $detA\,[1,3|2,3] \geq 0$; or
b. $detA\,[1,3|2,3] < 0$ and $detA \geq 4V_{\tilde{A}}(\{3\})$.

In the proof of this theorem we use the set of notations introduced in Section 3.

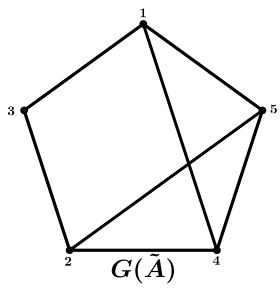
Proof. The matrix A is in the canonical forms (3.1), (3.2). After simple calculations, we obtain that:

$$\tilde{A} = \begin{bmatrix} a_{11} & 0 & a_{13} & a_{14} & a_{15} \\ 0 & a_{22} - 2a_{23}\frac{a_{12}}{a_{13}} + a_{33}\frac{a_{12}^2}{a_{13}^2} & a_{23} - a_{33}\frac{a_{12}}{a_{13}} & a_{24} & a_{25} \\ a_{13} & a_{23} - a_{33}\frac{a_{12}}{a_{13}} & a_{33} & 0 & 0 \\ a_{14} & a_{24} & 0 & a_{44} & a_{45} \\ a_{15} & a_{25} & 0 & a_{45} & a_{55} \end{bmatrix}.$$

The graph associated with $\tilde{A}$ is the following:
One can also check that:

$$\begin{aligned} V_{\tilde{A}}(\{3\}) &= detA\,[1,3|2,3]\,(a_{14}a_{24}a_{55} - a_{15}a_{24}a_{45} + a_{15}a_{25}a_{44} - a_{14}a_{45}a_{25}) = \\ &= detA\,[1,3|2,3]\,(a_{24}detA\,[1,5|4,5] - a_{25}detA\,[1,4|4,5])\,. \end{aligned} \tag{4.3}$$

Now let's assume that $A_2 = \begin{bmatrix} a_{44} & a_{45} \\ a_{45} & a_{55} \end{bmatrix}$ is nonsingular. Simple calculations show that:



$G(\tilde{A})$

(1) $\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 \geq 0 \iff detA\,[1,5|4,5] \geq \frac{a_{25}}{a_{24}} \cdot detA\,[1,4|4,5]$;

(2)

$$\mathbf{x}_2^T A_2^{-1} \mathbf{y}_2 detA\,[1,3|2,3]\, detA_2 = \\ (a_{24} detA\,[1,5|4,5] - a_{25} detA\,[1,4|4,5]) detA\,[1,3|2,3] = V_{\tilde{A}}(\{3\}),$$

by (4.3). In the case A_2 nonsingular, the equivalence of statements 1, 2 and 3 follows from Corollary 2.

Now let's assume A_2 singular. Since a_{44} and a_{55} are positive, A_2 has rank 1. But A is positive semidefinite by hypothesis, therefore column 5 of A is a positive multiple of column 4. Then there exists $\lambda > 0$ such that:

$$A = S^T A' S,$$

where $A' = A\,(5|5)$, $S = \begin{bmatrix} \mathbb{I}_4 & \lambda \mathbf{e}_4 \end{bmatrix}$ and $\mathbf{e}_4$ is the vector in $\mathbb{R}^4$ whose only nonzero entry is the last, which is equal to 1. Since $A' \in DNN_4$ it is completely positive, therefore $A' = BB^T$ with $B \geq 0$. It follows that $A = S^T B (S^T B)^T$ is also completely positive, since $S \geq 0$. Now simple calculations show that

$$detA\,[1,5|4,5] = detA\,[1,4|4,5] = 0,$$

and then $detA\,[1,5|4,5] \geq \frac{a_{25}}{a_{24}} \cdot detA\,[1,4|4,5]$, which proves the equivalence of statements 1 and 2.

Moreover, since in the case A_2 singular $detA = 0$ and $V_{\tilde{A}}(\{3\}) = 0$ by (4.3), $detA \geq 4V_{\tilde{A}}(\{3\})$. Therefore also statements 1 and 3 are equivalent.

QED

Since graphs G_1, G_2, G_3 are $\widehat{CP}$-graphs, they are also nearly $\widehat{CP}$-graphs. Therefore it is possible to characterize completely positive matrices of order 5 with G_1, G_2 or G_3 with Theorem 9 and Corollary 2. Actually one can check that applying the above mentioned results in a similar way to what we did in cases

G_4, G_6, it is possible to obtain an alternative proof of Cedolin-Salce's Theorem 2.

In the last part of this section we are going to try to clarify Xu's results for completely positive matrices with G_4 and G_6 (Theorems 3, 5).

Let's start with Xu's Theorem 3. In this theorem, the quantity $A_{|(3,4)|}$ appears. This quantity, as already explained, has never been defined in [6]. Howewer Xu, in the proof of this theorem, uses the above mentioned quantity like it is the weight $v_A(\{3,4\})$ of the set of vertices $\{3,4\}$ in $G(A)$. To confirm that, look at [6], page 554. Since Xu in [6] studied completely positive matrices with all diagonal elements equal to 1, one can check that, after replacing the quantity $A_{|(3,4)|}$ with $v_A(\{3,4\})$ in Theorem 3, Xu's result follows directly from Theorem 10 (after a suitable cogredience).

Now let's analyze Xu's Theorem 5. In this theorem, the quantity $\tilde{A}_{|1|}$ appears. This quantity doesn't have meaning, since there are no cycles of length 1 in $G(\tilde{A})$. The proof of this theorem is just sketched in [6], and Xu's usage of the quantity $\tilde{A}_{|1|}$ it is not totally clear. However, like we have seen in the case G_4, the quantity $\tilde{A}_{|1|}$ could be interpreted as the weight $v_{\tilde{A}}(\{1\})$ of the vertex 1 in $G(\tilde{A})$. Now if we replace the quantity $\tilde{A}_{|1|}$ with $v_{\tilde{A}}(\{1\})$ in Theorem 5, after a suitable cogredience one can check that Xu's result matches the equivalence between statements 1 and 3 of Theorem 11.

5 Completely positive matrices with G_5

In this section we are going to analyze Xu's Theorem 4. In this theorem, the quantity $\tilde{A}_{|2|}$ appears. This quantity is, by Xu's definition, the algebraic sum of weights of all cycles of length 2 in $G(\tilde{A})$. However, the weight of a cycle of length 2 is always < 0. Therefore $\tilde{A}_{|2|} < 0$, regardless of how $\tilde{A}$ is defined.

Now suppose we have a doubly non-negative matrix A in the form (1.5). Since $detA \geq 0$, we have that $detA \geq 4\tilde{A}_{|2|}$ always. Then by Xu's Theorem 4, we could state that every doubly non-negative matrix in the form (1.5) is completely positive, but this statement is obviously wrong, since G_5 is not a completely positive graph.

In the proof of Theorem 4, Xu's usage of the quantity $\tilde{A}_{|2|}$ is not totally clear. Like we did in cases G_4, G_6, we see that this quantity could be interpreted as the weight $v_{\tilde{A}}(\{2\})$ of the vertex 2 in $G(\tilde{A})$. So now let's replace the quantity $\tilde{A}_{|2|}$ with $v_{\tilde{A}}(\{2\})$ in Theorem 4, and consider the following matrices:

$$B := \begin{bmatrix} 1 & 1 & 1 & 3 & 5 \\ 1 & 6 & 0 & 0 & 0 \\ 0 & 6 & 1 & 0 & 0 \\ 0 & 0 & 6 & 1 & 0 \\ 6 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$$A := \frac{1}{37} BB^T = \frac{1}{37} \begin{bmatrix} 37 & 7 & 7 & 9 & 9 \\ 7 & 37 & 36 & 0 & 6 \\ 7 & 36 & 37 & 6 & 0 \\ 9 & 0 & 6 & 37 & 1 \\ 9 & 6 & 0 & 1 & 37 \end{bmatrix}.$$

The matrix A is completely positive in the form (1.5), and

$$a_{12} = min \left\{ \frac{a_{1j}}{a_{2j}} \mid a_{2j} > 0 \right\}.$$

The matrix $\tilde{A}$, defined in Theorem 4, is:

$$\tilde{A} = \frac{1}{37} \begin{bmatrix} \frac{1320}{37} & 0 & \frac{7}{37} & 9 & \frac{291}{37} \\ 0 & 37 & 36 & 0 & 6 \\ \frac{7}{37} & 36 & 37 & 6 & 0 \\ 9 & 0 & 6 & 37 & 1 \\ \frac{291}{37} & 6 & 0 & 1 & 37 \end{bmatrix}.$$

Now simple calculations show that:

(1) $a_{13} < a_{12}a_{23} + a_{14}a_{43}$;

(2) $detA < 4v_{\tilde{A}}(\{2\})$.

Therefore, even if we replace the quantity $\tilde{A}_{|2|}$ with $v_{\tilde{A}}(\{2\})$, Theorem 4 is not correct.

In the counterexample above note that, since not all the diagonal elements of $\tilde{A}$ are equal to 1 (in particular $\tilde{a}_{11} \neq 1$), the weight $v_{\tilde{A}}(\{2\})$ is not equal to the total weight $V_{\tilde{A}}(\{2\})$.

However in this case one can also check that $detA < 4V_{\tilde{A}}(\{2\})$.

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