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A NOTE ON COMPLETELY POSITIVE GRAPHS (II)

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Abstract. A necessary and sufficient condition is given for a doubly nonnegative matrix realization of a cycle to be completely positive. Also some special non-CP graphs are investigated.

1. Introduction

Pioneered by M. Hall Jr. in 1958 [2] and investigated by A. Berman [3, 4, 5] and J. H. Drew, C. R. Johnson and Loewy [7] etc., completely positive matrices have been shown their importance not only in the study of block designs in combinatorial analysis [1], but also in establishing economic models [8].

Recall that an $n\times n$ matrix A is said to be completely positive, denoted by $A\in CP_n$, if there exist m (entrywise) nonnegative column vectors $b_1,\dots,b_m$ such that

$$A=b_1b_1'+\cdots+b_mb_m'$$

where $'$ denotes transpose. The smallest such number m is called the factorization index of A and is denoted by $\phi(A)$. An $n\times n$ nonnegative matrix A is called doubly nonnegative, denoted by $A\in DP_n$, if it is positive semidefinite. It is known that $DP_n=CP_n$ for $n\le 4$; but for $n>4$, CP_n is a proper subset of DP_n (see [1, 3]).

Given an $n\times n$ real matrix A, let $A(l)$ denote the submatrix of A obtained by deleting the lth row and column of A. Let E_{rs} be the square matrix (e_{ij}) given by

$$e_{ij}=\begin{cases}1, & \text{if } (i,j)=(r,s).\\ 0, & \text{otherwise.}\end{cases}$$

For a real symmetric matrix A, the graph $G(A)=(V,E)$ of A is defined by: $V=\{1,\dots,n\}$ and

$$E=\{\{i,j\}:i\ne j,a_{ij}\ne 0,i,j=1,\dots,n\}.$$

For any vertex $l\in V$, let $N(l)$ denote the set of all neighbours of l in G, i.e.

$$N(l)=\{i:\{i,l\}\in E,i\ne l\}.$$

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By a doubly nonnegative realization of a graph G, we mean a matrix $A \in DP_n$ for which $G(A) = G$. The set of all such matrices A is denoted by Λ_G. G is called completely positive (abbrev. CP) if $A \in CP_n$ for any $A \in \Lambda_G$. It is shown in [3, 4, 5] that a graph G is CP if and only if G does not contain an odd cycle of length greater than 4. The following known results will be needed in this paper.

Lemma 1 (Theorem 4.3. of [3]). *Let A be an $n \times n$ nonzero doubly nonnegative matrix whose graph is acyclic (i.e., without a cycle). Then A is completely positive, and $\phi(A) = rank(A) = n - m$, where m is the number of singular components of A.*

Lemma 2 (Theorem 3.5 of [3]). *Let $A = (a_{ij})$ be an $n \times n$ doubly nonnegative matrix whose graph is G. If G has a vertex l which does not lie on a triangle. Then A is completely positive if and only if there exist positive numbers d_j, $j \in N(l)$, such that $a_{ll} \geq \sum_{j \in N(l)} \frac{a_{lj}^2}{d_j}$ and the matrix*

$$H = A(l) - \sum_{j \in N(l)} d_j E_{jj}$$

is completely positive, where the rows and columns of E_{jj} are indexed by $\{1, \ldots, n\} \backslash \{l\}$.

In section 2, we present a necessary and sufficient condition for $A \in \Lambda_G$ to be completely positive when G is an odd cycle of length greater than 4. We also prove that $\phi(A) = n$ for $A \in CP_n \bigcap \lambda_G$.

In section 3, we give the definition of nearly vertex(edge) CP graphs and present the structure characterizations of this type of graphs.

2. A Necessary and Sufficient Condition

Let G be C_{2k+1}, i.e., a cycle with length $2k + 1$ where $k \geq 2$. We know from [3] that not every matrix in Λ_G is completely positive and we would like to determine which matrices are. It is obvious that when $A \in \Lambda_G$, A is permutationally similar to a matrix of the form

$$\begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & 0 & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a_{n-1,n-1} & a_{n-1,n} \\ a_{n1} & 0 & 0 & \cdots & a_{n,n-1} & a_{nn} \end{bmatrix} \tag{1}$$

where $a_{ij} = a_{ji}$ for $1 \leq i, j \leq n$. Henceforth, we may assume that A is of this form.

Theorem 1. *Let $A \in DP_n$ be of the form (1) where $a_{ij} \neq 0$ if and only if $j \equiv i-1, i, i+1 (\mathrm{mod}\, n)$. Then A is in CP_n if and only if there exist two positive numbers a, b such that*

(i) $ab = a_{1n}$.

(ii) $H = A - (a^2E_{11} + b^2E_{nn} + a_{1n}E_{1n} + a_{n1}E_{n1}) \in DP_n$.

Proof. Suppose that there exist $a, b > 0$ satisfying (i) and (ii). Let

$$F = a^2E_{11} + b^2E_{nn} + a_{1n}E_{1n} + a_{n1}E_{n1}.$$

Then $F = \beta\beta'$ where $\beta = (a, 0, \ldots, 0, b)'$ is a nonnegative column vector of dimension n. Since $H \in DP_n$ and the graph of H is acyclic, we have $H \in CP_n$ by Lemma 1. So $H = B_1B_1'$ for some $n \times m$ nonnegative matrix B_1 where $m = \phi(H)$. Put $B = [B_1, \beta]$. Then $BB' = B_1B_1' + \beta\beta' = H + F = A$. Thus A is completely positive.

Conversely, let $A = (a_{ij}) \in CP_n$ be of the form (1). Then there exists an $n \times m$ nonnegative matrix B such that $A = BB'$. Let $B = (b_{ij})$, $\beta_i = (b_{i1}, \ldots, b_{im})'$, $(b_{ij} \geq 0)$, and $S_i = \{k : b_{ik} > 0\}$. Then

$$a_{ij} = (\beta_i, \beta_j), \quad i, j \in \{1, \ldots, n\} \tag{2}$$

where we use (β_i, β_j) to denote the usual inner product of R^m. From (2) and the form of A, we have

$$(\beta_i, \beta_j) = 0 \text{ if and only if } j \not\equiv i-1, i, i+1 (\operatorname{mod} n). \tag{3}$$

Then by (3),

$$S_i \bigcap S_j \neq \phi \text{ if and only if } j \equiv i-1, i, i+1 (\operatorname{mod} n) \tag{4}$$

Permuting the columns of B, if necessary, we may assume that $S_1 \bigcap S_n = \{1, 2, \ldots, p\}$, where $1 \leq p < m$. Now we put

$$a = (\sum_{j=1}^{p} b_{1j}^2)^{\frac{1}{2}}, \qquad b_1 = (\sum_{j=1}^{p} b_{nj}^2)^{\frac{1}{2}}.$$

Since

$$ab_1 = [(\sum_{j=1}^{p} b_{1j}^2)(\sum_{j=1}^{p} b_{nj}^2)]^{\frac{1}{2}} \geq \sum_{j=1}^{p} b_{1j}b_{nj} = (\beta_1, \beta_n) = a_{1n} > 0,$$

there exists a real number b, $0 < b \leq b_1$ such that $ab = a_{1n}$. Next we set $y = \sqrt{b_1^2 - b^2}$, and define $\tilde{\beta}_i \in R^{(m-p+2)}$, $i = 1, \ldots, m$ by

$$\begin{aligned}
\tilde{\beta}_1 &= (0, a, b_{1,p+1}, b_{1,p+2}, \ldots, b_{1m})' \\
\tilde{\beta}_2 &= (0, 0, b_{2,p+1}, \ldots, b_{2m})' \\
&\vdots \\
\tilde{\beta}_{n-1} &= (0, 0, b_{n-1,p+1}, \ldots, b_{n-1,m})' \\
\tilde{\beta}_n &= (y, b, b_{n,p+1}, \ldots, b_{nm})'
\end{aligned}$$

Also let $\tilde{B} = [\tilde{\beta}_1, \ldots, \tilde{\beta}_n]'$. Then we have $A = \tilde{B}\tilde{B}'$, and $H = \hat{B}\hat{B}'$, where $\hat{B}$ is obtained from $\tilde{B}$ by replacing the a in $\tilde{\beta}_1$ and the b in $\tilde{\beta}_n$ both by 0. This completes the proof of the theorem.

Corollary 2. *Let $A \in CP_n$ and suppose that $G(A)$ is an odd cycle of length greater than 4. Then $\phi(A) = n$.*

Proof. We may assume that A is of the form (1). First we use the proof of the converse part of Theorem 1, but with $m = \phi(A)$, to prove $\phi(A) \geq n$: Condition (4) implies that for each $i = 1, 2, \dots, n, S_i \bigcap S_{i-1} \neq \phi$ and $S_i \bigcap S_{i+1} \neq \phi$ (but $S_{i-1} \bigcap S_{i+1} = \phi$), from which inductively it follows that

$$|S_1 \bigcup S_2 \bigcup \cdots \bigcup S_i| \geq i + 1$$

for all $i = 1, \dots, n-1$, where we use $|S|$ to denote the cardinality of a set S; hence we have

$$\phi(A) = m \geq |S_1 \bigcup S_2 \bigcup \cdots \bigcup S_n| \geq n.$$

It suffices to prove $\phi(A) \leq n$. Without loss of generality, we may assume that $a_{11} = \cdots = a_{nn} = 1$. Moreover, denote $a_{i,i+1}$ by a_i, $i = 1, \dots, n$, where $a_{n,n+1} = a_{n1}$. Since $A \in CP_n$, there exist $a, b > 0$ such that both of the following hold:

(I) $1 \geq \frac{a_n^2}{a} + \frac{a_{n-1}^2}{b}$;
(II) $H_1 = A(n) - (aE_{11} + bE_{n-1,n-1}) \in DP_{n-1}$.

If the inequality in (I) is strict, we decrease gradually the value of b while keeping the value of a until the equality occurs in (I). (Note that in doing so, condition (II) still holds.) If the remaining matrix H_1 is positive definite, we increase gradually the value of a while decreasing the value of b to keep the equality in (I) until the matrix H_1 becomes singular. (Note that the process must stop for some $0 < a \leq 1$ since $a_{ii} = 1$ by assumption.) So we may assume that the equality holds in (I), and also that the matrix H_1 is singular. By Lemma 1, $\phi(H_1) = n - 2$. Let $H_1 = B_2B_2'$ be a factorization of H_1 where B_2 is an $(n-1) \times (n-2)$ nonnegative matrix. Set

$$B_1 = [\sqrt{a}e_1, B_2, \sqrt{b}e_{n-1}]$$

where e_i is the i^{th} coordinate vector of R^{n-1}. Then B_1 is a $(n-1) \times n$ nonnegative matrix. Putting

$$x = (\frac{a_n}{\sqrt{a}}, 0, \dots, 0, \frac{a_{n-1}}{\sqrt{b}})$$

where $x \in R_+^n$, and writing

$$B = \begin{bmatrix} B_1 \\ x \end{bmatrix},$$

we have $A = BB'$, from which we can see easily that $\phi(A) \leq n$. The proof is completed.

The following interesting alternative argument for $\phi(A) \leq n$ is based on results in [3] (which is simpler than the above). Since $A \in CP_n$, by Theorem 3.5 of [3] (with $l = 1$), there exist positive numbers d_2, d_n such that both of the following hold:

(a) $1 > \frac{a_{12}^2}{d_2} + \frac{a_{1n}^2}{d_n}$;

(b) $H = A(1) - (d_2E_{22} + d_nE_{n,n}) \in CP_{n-1}$.

If the matrix H is not singular, we increase the value of d_2 gradually (but keeping the value of d_n) until the matrix H becomes singular. Note that in doing so the inequality (a) remains valid. So we may assume that H is singular. Then by Theorem 3.1 of [3] we have $\phi(A) \le \phi(H) + 2 \le (n-2) + 2 = n$ where $\phi(H) \le n-2$ follows from the fact that $G(H)$ is acyclic (and Lemma 1).

3. Nearly CP Graphs

A graph G is called nearly vertex (resp. edge) CP if G is not CP but $G - \{v\}$ (resp. $G - e$) is CP for any $v \in V(G)$ (resp. $e \in E(G)$).

The following facts are obvious.

Proposition 1. *Every nearly vertex CP graph is connected and contains an odd cycle of length greater than* 4.

Proposition 2. *Every connected nearly edge CP graph is nearly vertex CP.*

Proposition 3. *A graph of order* 5 *is nearly vertex CP if and only if it contains a cycle of length* 5.

For graphs of order greater than 5, we have the following result.

Theorem 3. *Let $G = (V, E)$ be a graph with n vertices where $n > 5$. Then G is nearly vertex CP if and only if it is one of the following graphs:*

1. C_{2k+1} *where $k \ge 3$ is an integer;*
2. $C_{2k+1} + e$ *where $k \ge 3$ and e is an edge and lies in a triangle*
3. $C_{2k+1} + e_1 + e_2$ *where $e_1 = \{x_1, x_3\}$, $e_2 = \{x_2, x_4\}$, and $\{x_1, x_2\}$, $\{x_2, x_3\}$, $\{x_3, x_4\}$ are edges of C_{2k+1}.*

Proof. The "if" part can be verified readily. Now we consider the "only if" part. Since G is not CP, G contains an odd cycle C_{2k+1} where $k \ge 2$. If $V(C_{2k+1}) \ne V$, we choose $v \in V \backslash V(C_{2k+1})$. Then $G - \{v\}$ still contains the cycle C_{2k+1}, and so $G - \{v\}$ is not CP, a contradiction. Hence $V = V(C_{2k+1})$.

Since $n = 2k+1 > 5$, we have $k \ge 3$. Suppose G is not the cycle C_{2k+1}. Choose an edge $e \in E \backslash E(C_{2k+1})$. Then the edge e, together with one part of C_{2k+1}, forms an odd cycle, say C_l, where $l \ge 3$ is odd, and e, with the one part of C_{2k+1}, forms an even cycle, say C_{2r} where $2r = 2k+1-l+2 = 2k-1+3$. Choose a vertex $v \in V(C_{2r}) \backslash V(C_l)$. Since G is nearly vertex CP, $G - \{v\}$ is CP. But $G - \{v\}$ contains the odd cycle C_l, so we must have $l = 3$. In other words, e lies in a triangle. If G is an odd cycle plus an edge, then $G = G_{2k+1} + e_1$, and G is of type (2). Suppose G is an odd cycle plus more than one edge. Denote the above edge e by e_1 and let $T_1 = \{u, v, w\}$ be the triangle containing e_1 with $e_1 = \{u, v\}$. Choose an edge e_2 that lies outside $C_{2k+1} + e_1$. From the preceding proof, it is clear that e_2 also lies on a triangle T_2 for which two of its edges belong to the cycle C_{2k+1}, say $T_2 = \{x, y, z\}$ with $e_2 = \{x, z\}$. If T_2 has no common edges with T_1 (but T_2 may have a common vertex with T_1), then the graph $G - \{w\}$ contains the cycle $C_{2k+1} - \{w, y\}$ as its subgraph. But the length of the latter cycle is $2k + 1 - 4 + 2 = 2(k - 1) + 1 \geq 5$. Hence $G - \{w\}$ is not CP, which contradicts the definition of G. Thus T_1 and T_2 must have an edge in common. By a similar argument, we can see that G cannot have any other edges. Therefore, G is type (3). The proof is completed.

We end our discussion by treating nearly edge CP graphs.

Corollary 4. *A connected graph G is nearly edge CP if and only if G is an odd cycle with length greater than* 4.

Proof. The sufficiency of the condition is obvious.

Since G is not CP, G contains an odd cycle C_{2k+1}, where $k \geq 2$. If G has an edge e that does not lie on the cycle C_{2k+1}, then clearly $G - e$ is not CP, a contradiction. So all edges of G lie on C_{2k+1}. Furthermore, all vertices of G belong to C_{2k+1} as G is connected. So we have $G = C_{2k+1}$.

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