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CP GRAPHS AND SPN GRAPHS

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Dedicated to Prof. Avi Berman on his 80th birthday

Abstract. A graph G is SPN if every copositive matrix realization of it is a sum of a positive semidefinite matrix and a nonnegative one (an SPN matrix). A graph is CP if every doubly nonnegative matrix realization of it is completely positive. This survey describes the current state of the problem of characterizing SPN graphs in comparison to the, by now classical, characterization of CP graphs, which inspired the attempt to define and study SPN graphs.

Keywords. Completely positive matrix; SPN matrix; Doubly nonnegative matrix; Copositive matrix.

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1. Introduction

A real symmetric matrix A is *completely positive* (CP) if $A = BB^T$ for some (entrywise) nonnegative matrix B, not necessarily square. Clearly, a necessary condition for a matrix to be completely positive is that it is both entry-wise nonnegative and positive semidefinite, i.e., it is *doubly nonnegative* (DNN). However, this necessary condition for complete positivity is not sufficient for matrices of order 5 or more. When is the necessary condition also sufficient? Avi Berman addressed, in a series of paper with several co-authors, the combinatorial version of this question: which graphs have the property that every DNN matrix whose zero-nonzero pattern is described by the graph is CP? It began with Hershkowitz in [7], continued with Grone [6] up to the full solution with Kogan in [23, 24][1]. Another version of the solution was given by Ando [1]. See also [3], [4] and [13]. Graphs with this property were named in [24] *completely positive graphs*, later referred to also as *CP graphs*.

A real symmetric matrix is *copositive* (COP) if $\mathbf{x}^T A\mathbf{x} \geq 0$ for every nonnegative vector $\mathbf{x}$ of the right length. Examples of copositive matrices include the real positive semidefinite matrices, and the symmetric nonnegative matrices, and hence also the *SPN matrices*, matrices that are a Sum of a Positive semidefinite matrix and a Nonnegative one. However, the sufficient condition

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[1] The results first appeared in Kogan's Master thesis [23] (in Hebrew).

for copositivity of being SPN is not necessary for matrices of order 5 or more. So, when is this sufficient condition for copositivity also necessary? In view of the characterization of CP graphs, the combinatorial version of this question is: which graphs have the property that every COP matrix whose zero-nonzero pattern is described by the graph is SPN? A graph with this property is called an *SPN graph*. The study of SPN graphs began by this author in [27], followed by a corrigendum [29, 30], a paper with Hogben [22] and one by Drury [15]. A full characterization has not yet been reached.

The problem of characterizing CP graphs seems natural. The equality $A = BB^T$, B nonnegative, is equivalent to $A = \sum \mathbf{b}_i\mathbf{b}_i^T$, where $\mathbf{b}_i$'s are all the columns of the nonnegative B. In this sum of nonnegative rank one matrices there are no cancelations, and the graph of each such rank one summand is therefore a (complete) subgraph of the graph of A, whose edges represent the nonzero entries in A. Thus the graph of A affects the possible CP factorizations of A. In comparison, the problem of characterizing SPN graphs, or associating graphs with copositive matrices, seems less natural, as copositive and SPN matrices may have both nonnegative and negative entries. Yet the SPN graphs characterization problem was inspired by the characterization of CP graphs due to the connections between completely positive matrices and copositive matrices, doubly nonnegative matrices and SPN matrices.

The set of all $n \times n$ completely positive matrices forms a closed convex cone in the space $\mathscr{S}_n$ of $n \times n$ symmetric matrices, denoted by $\mathscr{CP}_n$. The set of all copositive matrices forms a closed convex cone $\mathscr{S}_n$, denoted by $\mathscr{COP}_n$. These cones are dual to each other with respect to the Euclidean inner product in $\mathscr{S}_n$. That is,

$$\mathscr{CP}_n = \{X \in \mathscr{S}_n \mid \operatorname{trace}(XY) \geq 0 \text{ for every } Y \in \mathscr{COP}_n\},$$

and

$$\mathscr{COP}_n = \{X \in \mathscr{S}_n \mid \operatorname{trace}(XY) \geq 0 \text{ for every } Y \in \mathscr{CP}_n\}.$$

The doubly nonnegative matrices and the SPN matrices also form closed convex cones in $\mathscr{S}_n$, denoted by $\mathscr{DNN}_n$ and $\mathscr{SPN}_n$, respectively. These are also dual to each other

$$\mathscr{DNN}_n = \{X \in \mathscr{S}_n \mid \operatorname{trace}(XY) \geq 0 \text{ for every } Y \in \mathscr{SPN}_n\},$$

and

$$\mathscr{SPN}_n = \{X \in \mathscr{S}_n \mid \operatorname{trace}(XY) \geq 0 \text{ for every } Y \in \mathscr{DNN}_n\}.$$

In addition,

$$\mathscr{CP}_n \subseteq \mathscr{DNN}_n \text{ and } \mathscr{SPN}_n \subseteq \mathscr{COP}_n.$$

Equality in these inclusions holds if and only if $n \leq 4$. We omit the subscript n when no ambiguity arises.

It is these duality and inclusion connections that make the problem of characterizing SPN graphs a "natural dual" of the problem of characterizing CP graphs, in spite of the reservations mentioned above. It might seem more reasonable to consider signed graphs in the SPN case. A *signed graph* is a graph together with a function that attaches to each edge a $+$ or a $-$ sign. An *SPN signed graph* may be defined accordingly. However, a characterization of SPN signed graphs does not seem to be a feasible task, as every graph has several sign assignments that make it an SPN signed graph. For example, it turns out that any assignment in which all the edges are negative, except possibly all the edges at ones vertex, yields an SPN signed graph.

It is worth mentioning that the cones of completely positive matrices and copositive matrices are of interest in mathematical optimization. The first uses of these cones in optimization were in the end of the 1990's. The term *copositive optimization* was introduced in [9], where it was shown that the maximum clique problem can be formulated a linear problem over the cone $\mathscr{COP}$, or its dual $\mathscr{CP}$. Since then the field has developed, see the recent survey [16]. Of course, the problems remain difficult, but the difficulty in copositive optimization lies wholly in the cone constraint. Indeed, while it is relatively easy to decide whether a given symmetric matrix is DNN, or whether it is SPN, it is hard to decide whether it is CP, or COP. In complexity terms, it was shown in [12] that determining complete positivity is NP-hard, and in [26] it was shown that determining copositivity is co-NP-compelte. In trying to solve such a difficult optimization problem over $\mathscr{CP}$ or $\mathscr{COP}$, one may start with a relaxation to the tractable cone $\mathscr{DNN}$, respectively $\mathscr{SPN}$, see, e.g., [5]. The study of CP graph and SPN graphs may provide information relevant to the question when does such a relaxation give an exact solution, see, e.g., [17].

This survey is in honor of Avi's contributions to the study of completely positive matrices, and in gratitude for introducing them to me. An introduction that started a collaboration, which produced several papers, a book about completely positive matrices [8] and an updated book about both completely positive matrices and copositive matrices [31]. There one can find an up-to-date exposition of these matrices from a linear algebraic point of view.

In the following section we introduce some notations. In the third section we recall the characterization of CP graphs and the methods used in the proof, and in the fourth section we present the current state of the attempt to characterize SPN graphs, and the steps and methods used. These are described in more detail than in the CP case, still mentioning only some major points. We conclude the fourth section with the remaining open problems.

2. Notation

More terms and notation will be introduced as we proceed, but here are some basic ones.

The standard basis vectors in $\mathbb{R}^n$ are denoted by $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$. The standard basis matrices in $\mathscr{S}_n$ are

$$E_{ij} = \begin{cases} \mathbf{e}_i\mathbf{e}_i^T & \text{if } i = j \\ \mathbf{e}_i\mathbf{e}_j^T + \mathbf{e}_j\mathbf{e}_i^T & \text{if } 1 \le i \ne j \le n \end{cases}.$$

Between matrices and vectors, $\geq$ is used to denote an entry-wise inequality, and $>$ to denote a strict inequality in each entry. For an $n \times n$ matrix A and subsets $\alpha, \beta \subseteq \{1, 2, \dots, n\}$, $A[\alpha|\beta]$ denotes the submatrix of A whose rows are indexed by the elements of α and its columns by those of β. The principal submatrix $A[\alpha|\alpha]$ is denoted also by $A[\alpha]$. The *Schur complement* of $A[\alpha]$, where $A[\alpha]$ is nonsingular, is denoted by $A/A[\alpha]$ and defined by

$$A/A[\alpha] = A[\alpha^c] - A[\alpha^c|\alpha]A[\alpha]^{-1}A[\alpha|\alpha^c].$$

If $\alpha = \{i\}$ the notation will be shortened here to $A/A[i]$. A symmetric matrix A is *irreducible* if it is not a direct sum of smaller matrices. The graph $G(A)$ of a $n \times n$ symmetric matrix A has vertex set $\{1, 2, \dots, n\}$ and $\{i, j\}$ is an edge of G if and only if $a_{ij} \neq 0$. Irreducibility of A is equivalent to $G(A)$ being connected. The matrix A is a *realization* of a graph G if $G(A) = G$. With these terms, we define formally: A graph G is a *CP graph* if every doubly nonnegative matrix realization of G is completely positive. A graph G is an *SPN graph* if every copositive matrix realization of G is SPN.

The graphs we consider are simple (no loops, no multiple edges). We use standard graph terminology. In particular, a graph $H = (V(H), E(H))$ is a *subgraph* of a graph $G = (V(G), E(G))$ if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$, and a *proper subgraph* if any of these inclusions is strict. A *block* is a connected graph with no cut vertex. A *block of a graph* G is a maximal block subgraph of G (not properly contained in any other block subgraph). A block on 3 or more vertices is a 2-*connected* graph, i.e., a connected graph such that a deletion of any one of its vertices together with its incident edges leaves a connected graph with at least one edge.

As usual, the complete graph on n vertices is denoted by K_n, the complete bipartite graph with bipartition sets of sizes m,n by $K_{m,n}$. The cycle graph on n vertices is C_n. Less common notations: T_n is a graph on n vertices consisting of $n-2$ triangles sharing a common base. F_n is the *fan graph* on n vertices: a path on $n-1$ vertices, plus an additional vertex adjacent to all vertices of the path. CD_6 is the *co-domino graph*, a graph with 6 vertices, consisting of a square and two triangles whose bases are two parallel edges of the square. The latter (on the right) and examples of the first two are shown in Figure 1.

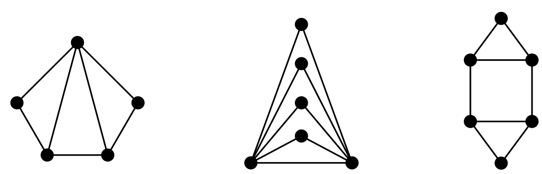

FIGURE 1. F_5, T_6 and CD_6

3. CP GRAPHS

The following theorem is a complete characterization of CP graphs.

Theorem 3.1. *For any graph G the following are equivalent.*

(a) *G is a CP graph,*
(b) *G contains no odd cycle of length 5 or more (a long odd cycle),*
(c) *each block in G is one of these:*
   - *a K_4,*
   - *a bipartite graph,*
   - *a T_n, $n \geq 3$.*

The CP graphs, or NLOC graphs, have also an alternative characterization in terms of line graphs, see [32].

Note that a single edge is a bipartite graph, a triangle is T_3, and K_4 minus one edge is T_4. Together with K_4 these constitute all blocks on 4 vertices or less. The theorem contains two characterizations of CP graphs: in (b) a characterization by a single family of forbidden subgraphs, the long odd cycles, and in (c) a characterization by all the possible blocks. Figure 2 shows a CP graph, with all possible types of blocks. From the left: an edge and a K_4, a triangle K_3 and a T_4, another edge, a bipartite graph and a T_5.

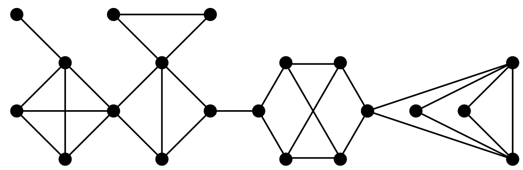

FIGURE 2. A CP graph

Steps and methods in the proof. The fact that DNN matrices of order at most 4 are CP was proved already in 1962 [25]. This implies that every graph on at most 4 vertices is CP. However, the combinatorial point of view first appeared in [7], where it was proved that an acyclic graph is CP and that odd cycles are forbidden subgraphs. The first fact was proved using implicitly the Schur complement. For the latter, a continuity argument was used, based on the fact that the cone $\mathscr{C}\mathscr{P}_n$ is closed. Bipartite graphs were shown to be CP by reducing the question to singular irreducible matrices, and using the spectral properties of nonnegative matrices [6]. Finally, in [23, 24] it was shown that a graph is CP if and only if each of its blocks is CP, that every T_n is CP, and that in 3.1 (b) implies (c). The latter was done by graph theoretic arguments, and some geometric arguments were used in the other proofs. This is due to the observation that a nonnegative Gram matrix of n vectors in $\mathbb{R}^n$ is completely positive if and only if these n vectors may be embedded in the nonnegative orthant of some $\mathbb{R}^k$. This approach to complete positivity study was first used in [18], where such proofs were given for the results of [25]. Different proofs for some of the results of [24] used the Schur complement instead of geometric arguments [1, 14]. The term *NLOC graphs* (No Long Cycle Odd graphs) for these graphs was coined in [13].

4. SPN GRAPHS

The problem of characterizing SPN graphs is still not completely solved. We present here the current state of the study. The existing results aim towards a characterization of these graphs both in terms of forbidden subgraphs, and in terms of the possible blocks of such graphs. For both we need to recall that an *edge subdivision* of G is the graph operation where an edge $\{u, v\}$ is replaced by a path of length 2 whose ends are u and v, and its inner vertex is a new addition to the vertex set of G. A graph is a *subdivision* of G if it is obtained from G by a finite sequence of edge subdivisions, and G is considered to be a subdivision of itself.

The following theorem presents the known forbidden subgraphs for an SPN graph.

Theorem 4.1. *If G is an SPN graph, then G does not contain the following:*

- *any subdivision of K_4 in which more than one of the original edges was subdivided at least once,*
- *any subdivision of the fan F_5,*
- *any subdivision of CD_6,*
- *any subdivision of T_6.*

Figure 3 shows all these forbidden subgraphs. In this figure, each line represents a path of length 1 or more. These are all 2-connected, as any forbidden subgraph has to have a forbidden 2-connected subgraph. Shown, from left to right: two subdivisions of K_4, then subdivisions of F_5, CD_6, T_6.

The next theorem presents the known possible blocks of an SPN graph.

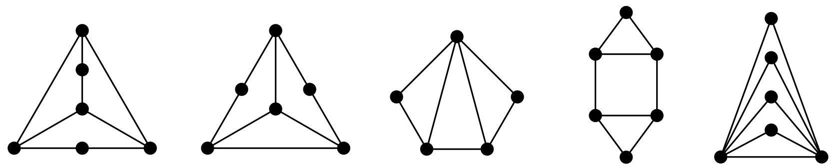

FIGURE 3. Forbidden subgraphs for SPN graphs

Theorem 4.2. *If each block of a graph G is one of the following:*

- *an edge, K_2,*
- *a subdivision of T_n, $n \leq 4$,*
- *a subdivision of K_4 in which at most one of the original edges was subdivided,*
- *a T_5,*
- *a $K_{2,4}$,*

then G is completely positive

Note that the list of possible blocks of an SPN graph includes all blocks on 4 vertices or less, all cycles C_n (subdivisions of the triangle T_3), and all graphs which consist of 3 paths, all sharing the same end vertices and no internal vertices (subdivisions of T_4). A joint descriptions of the graphs T_5 and $K_{2,4}$ is: 4 paths of length at most 2 each, all sharing the same end vertices and no internal vertices.

Figure 4 shows an SPN graph, with blocks of all known allowed kinds. Here each line represents an edge. The blocks from left to right: a cycle C_6, an edge and a K_4, a triangle and a subdivision of T_4, another edge, a $K_{2,4}$ and a T_5.

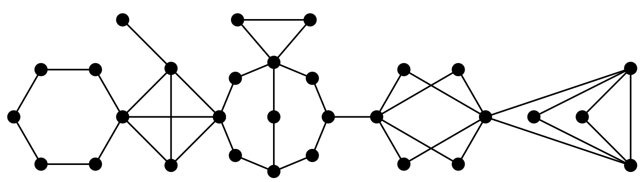

FIGURE 4. An SPN graphs

Steps and methods in the proof. Copositive matrices of order up to 4 were shown to be SPN in [10]. This implies that graphs on at most vertices are SPN. However, the study of the combinatorial version of the problem, of identifying copositive matrices that are SPN matrices by their graph, began only in [27]. There initial results were proved, some methods for approaching the problem were established, and most of the known allowed blocks and forbidden subgraphs were found. It was mistakenly claimed there that every T_n is SPN, corrected in [28, 30] to T_5 is SPN. The fact that the complete subdivision of K_4, where each edge of K_4 was subdivided at least once, is not SPN was proved in [22]. That T_6 is not SPN was proved in [15].

As mentioned in the introduction, graphs may seem less natural in the context of copositive and SPN matrices. Still, a few initial results in [27] give an indication that pursuing the problem of characterizing SPN graphs does make sense. First, it was observed that a direct sum of symmetric matrices is copositive/SPN if and only if each direct summand is copositive/SPN. This allows to consider only connected graphs. Next it was proved that a subgraph of an SPN-graph is also an SPN-graph. As for CP graphs, this was done by using a continuity argument and the fact that $\mathscr{COP}$ is closed. More notable is the following result about a matrix whose graph has a cut vertex. It implies that a graph is SPN if and only if every block of the graph is SPN. As the result may also be of interest of its own right, it is presented here as a theorem.

Theorem 4.3. [27] *Let a copositive matrix A have graph G, where $G = G_1 \cup G_2$ and $G_1 \cap G_2$ is a single vertex. Then there exist copositive matrices A_1 and A_2 such that $G(A_1) = G_1$, $G(A_2) = G_2$ and $A = (A_1 \oplus 0) + (0 \oplus A_2)$.*

With these results in mind, the characterization begins with graphs on up to 4 vertices, which are all SPN, then continues by looking at larger and larger 2-connected graphs. At each step considering graphs all of whose proper subgraphs are SPN. Some of the methods used in the process are pointed out below.

Sign patterns. Though graphs are considered, sign patterns do matter. For example, for each graph G whose proper subgraphs are all SPN, only realizing copositive matrices whose graph of negative entries is connected and spanning need to be considered. The graph $G_-(A)$ of negative entries of an $n \times n$ symmetric A has vertex set $\{1,2,\dots,n\}$ and $\{i,j\}$ is an edge if and only if $a_{ij} < 0$. Also, the ability to use the Schur complement depends also on sign pattern. Specifically, if the i-th row of a symmetric A has only nonpositive off-diagonal elements, then A is copositive/SPN if and only if $A/A[i]$ is copositive/SPN. See [27].

Zeros and minimal zeros. One tool that was extensively used in the study of SPN graphs (including the proof of Theorem 4.3), and has no equivalent in the CP case, is the zeros of copositive matrices. A nonnegative vector $\mathbf{u}$ is a *zero* of a symmetric matrix A, if $\mathbf{u}^T A\mathbf{u} = 0$. A zero is *minimal* if there is no zero of A whose support is a proper subset of the support of $\mathbf{u}$, where $\operatorname{supp}\mathbf{u} = \{i \mid u_i \neq 0\}$. Any copositive matrix has at most a finite number of minimal zeros, up to multiplication by a positive scalar [20]. Zeros may be used to check copositivity: A symmetric matrix A with nonnegative diagonal elements is copositive if and only if $A\mathbf{u} \geq \mathbf{0}$ for every (minimal) zero of A [31, Theorem 2.82]. In some cases they may be used to show that a copositive matrix is SPN: From [2, 19, 11, 20, 27] we have that for a zero $\mathbf{u}$ of an $n \times n$ copositive A,

- $A\mathbf{u} \geq 0$ and $(A\mathbf{u})_i = 0$ whenever $u_i > 0$,
- the principal submatrix $A[\operatorname{supp}\mathbf{u}]$ is positive semidefinite,
- if $|\operatorname{supp}\mathbf{u}| \geq n-1$, then A is SPN,
- if $|\operatorname{supp}\mathbf{u}| \geq n-2$ and $|\{i \mid (A\mathbf{u})_i = 0\}| \geq n-1$, then A is SPN.

Zeros were used to identify copositive matrices that are not SPN, as in the following example.

Example 4.4. [27] The matrix

$$A = \begin{pmatrix} 1 & -1 & 1 & 0 & 0 \\ -1 & 1 & -1 & 1 & 0 \\ 1 & -1 & 1 & -1 & 1 \\ 0 & 1 & -1 & 1 & -1 \\ 0 & 0 & 1 & -1 & 1 \end{pmatrix}$$

is a realization of F_5. The vectors $\mathbf{u}_i = \mathbf{e}_i + \mathbf{e}_{i+1}$, $1 \leq i \leq 4$, are easily seen to be the only minimal zeros of A. The matrix is copositive — either by a characterization of $\{0,\pm 1\}$ copositive matrices [21], or as $A\mathbf{u}_i \geq 0$ for every $1 \leq i \leq 4$. The matrix A cannot be SPN, since if

$A \geq P$, P positive semidefinite, then necessarily the four minimal zeros are also zeros of the positive semidefinite P. Therefore for each i, $(P\mathbf{u})_i = \mathbf{0}$. In particular $(P\mathbf{u}_1)_4 = 0$, which implies $p_{41} = p_{14} = 1$, contradicting the assumption that $A \geq P$. This shows that F_5 is not an SPN graph.

Zeros were also used to prove that certain graphs are SPN, and the next example demonstrates this. It is part of the proof that the graph obtained from K_4 after subdividing one edge once is SPN. For this graph there are two sign patterns of realizing copositive matrices that need to be checked, as copositive matrices with all other sign patterns are easily seen to be SPN by basic results. The sign pattern in the example is one of the two.

Example 4.5. [27] Let A be a copositive matrix whose sign pattern is

$$\begin{pmatrix} + & - & 0 & + & 0 \\ - & + & - & 0 & + \\ 0 & - & + & - & + \\ + & 0 & - & + & - \\ 0 & + & + & - & + \end{pmatrix}$$

Let $B = A - \delta E_{14}$, $\delta \geq 0$, be a $\{1,4\}$-*irreducible* copositive matrix. That is, for any greater δ the matrix B is no longer copositive. If $b_{14} \leq 0$, then $B/B[1]$ is copositive, and SPN as it is 4×4. Hence in this case B is SPN, and so is $A = B + \delta E_{14}$. So consider the case that B has the same sign pattern as A. By [11, Theorem 2.6], $\{1,4\}$-irreducibility implies that there exists a zero $\mathbf{u}$ of B such that $u_1 + u_4 > 0$ and $(B\mathbf{u})_1 = (B\mathbf{u})_4 = 0$. From $(B\mathbf{u})_1 = 0$ and $u_1 + u_4 > 0$ we deduce that $u_2 > 0$, and from $(B\mathbf{u})_4 = 0$ and $u_1 + u_4 > 0$ we deduce that $u_3 + u_5 > 0$. Thus $|\operatorname{supp}\mathbf{u}| \geq 3 = 5 - 2$. As $(B\mathbf{u})_i = 0$ whenever $u_i > 0$, we get by the choice of $\mathbf{u}$ that $|\{i \,|\, (B\mathbf{u})_i = 0\}| \geq 4$. By the final zero property mentioned above, B is SPN and therefore so is A.

Zeros were also used in the proof in [15] that the graph T_6 is not SPN, but the author's way to arrive at the example involved solving a semidefinite programming problem over the cone of 6×6 positive semidefinite matrices with some linear equality and inequality constrains.

Graph transformations. Graphs transformations, such as subdivision, were not needed in the CP graph characterization problem, but in the characterization of SPN graphs some transformations on (signed) graphs were used. For example, subdividing a negative edge in a signed graph several times, replacing it by a path of negative edges, does not change the nature of the signed graph — the resulting signed graph is SPN if and only if the original signed graph was SPN. The same holds for a (non-signed) graph G that has a path P of length 3 or more, whose internal vertices have degree 2 in G, and any graph obtained by subdividing edges in P. For both these results see [27]. Using these results, it is easily seen, by the sign pattern of the copositive matrix realization of T_6 that is not SPN in [15], that any subdivision of T_6 is not SPN. The latter result also shows that to check whether subdividing one edge in G any number of times results in an SPN/non-SPN graph, for a graph G that is known to be SPN/non-SPN, one only needs to check the effect of subdividing that edge once or twice.

Other graph transformations, more specific to this problem, were used in [27] and in [22]. In the latter, a graph transformation was used to show that subdivision of K_4, in which each of the original edges was subdivided once is SPN.

The open gap. It can be shown that if a graph G is 2-connected, and contains none of the known forbidden subgraphs, then G is either a K_4 with at most one edge subdivided at least once, or a subdivision of a T_n [27, Remark 9.11]. With this in mind, Theorems 4.2 and 4.1 imply that following problem remains open.

Open Problem. Which subdivisions of T_5 are SPN, other than T_5 itself and $K_{2,4}$, are allowed blocks, and which are forbidden subgraphs?

A full answer to this problem will conclude the characterization of SPN graphs. If the same line of study is continued, the next graph to consider is a subdivision of T_5 in which a non-base edge is subdivided once.

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