

NORTH-HOLLAND

The Real Positive Semidefinite Completion Problem for Series-Parallel Graphs

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ABSTRACT

We consider the partial real symmetric matrices X whose diagonal entries are equal to 1 and whose off-diagonal entries are specified only on a subset of the positions. The question is to determine whether X can be completed to a positive semidefinite matrix. Extending a result of Barrett et al. [3], we give a set of necessary conditions for X to be completable and show that these conditions are also sufficient if and only if the graph corresponding to the positions of the specified entries is series-parallel (i.e., has no K_4 -minor). © Elsevier Science Inc., 1997

1. INTRODUCTION

A positive semidefinite matrix whose diagonal entries are all equal to 1 is called a *correlation matrix*. Let $\mathscr{C}_{n \times n}$ denote the set of $n \times n$ correlation matrices, i.e.,

$$\mathscr{E}_{n \times n} \coloneqq \left\{ X = (x_{ij}) \text{ symmetric } n \times n \middle| X \ge 0, x_{ii} = 1 \text{ for all } i = 1, \dots, n \right\}.$$

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The notation $X \ge 0$ means that X is positive semidefinite, i.e., that $x^T X \ge 0$ for all $x \in \mathbb{R}^n$. Let G = (V, E) be a graph, where $V = \{1, \ldots, n\}$. (All the graphs considered here are *simple*, i.e., have no loops or parallel edges.) Then the set $\mathscr{E}(G)$ is defined as the projection of $\mathscr{E}_{n \times n}$ on the subspace \mathbb{R}^E indexed by the edge set of G, i.e.,

$$\mathscr{E}(G) := \left\{ x \in \mathbb{R}^E \middle| \exists A = (a_{ij}) \in \mathscr{E}_{n \times n} \text{ such that } a_{ij} = x_{ij} \text{ for all } ij \in E \right\}.$$

In particular, $\mathscr{C}(K_n)$ consists of the projections of the correlation matrices on their upper triangular part. The convex set $\mathscr{C}_{n \times n}$ and its projection $\mathscr{C}(G)$ are called *elliptopes*. The object of this paper is the description of the elliptope $\mathscr{C}(G)$ for some classes of graphs.

The problem of characterizing the members of the elliptope $\mathscr{C}(G)$ is also known in the literature as the *positive semidefinite completion problem*, which is defined as follows. Consider a partial real symmetric matrix Xwhose entries are specified on the diagonal and on a certain subset E of the off-diagonal positions, while the remaining entries of X are free. The question is to determine whether the free entries can be chosen so as to make X positive semidefinite. If this is the case, we say that X is *completable*.

An easy observation is that it suffices to consider the positive semidefinite completion problem for matrices whose diagonal entries are all equal to 1. (Indeed, if X is completable, then its diagonal entries are nonnegative. Moreover, we can suppose that all diagonal entries are positive, as otherwise the problem reduces to considering the submatrix of X with positive diagonal entries. Finally, if D denotes the diagonal matrix whose *i*th diagonal entry is $1/\sqrt{x_{ii}}$, then the matrix X' := DXD has diagonal entries 1 and is completable if and only if X is completable.)

Suppose X has diagonal entries 1, and let $x := (x_{ij})_{ij \in E} \in \mathbb{R}^E$ denote the vector whose components are the specified entries of X. Moreover, let G denote the graph with edge set E. Then, by definition of the elliptope $\mathscr{E}(G)$, the following equivalence holds:

$$x \in \mathscr{E}(G) \quad \Leftrightarrow \quad X \text{ is completable.}$$

A first obvious necessary condition for X to be completable is that every principal minor of X composed of specified entries is nonnegative. In other words, if $x \in \mathscr{E}(G)$, then x satisfies the following *clique condition*:

For every clique K in G, the projection
$$x_K$$
 of x on the edge set of K belongs to $\mathscr{E}(K)$. (1.1)

Another necessary condition can be formulated in the following way. As every vector $x \in \mathscr{E}(G)$ has all its entries in the interval [-1, 1], we can parametrize it as

$$x_e = \cos \pi a_e$$

where $a_e \in [0, 1]$ for every $e \in E$. Then a necessary condition for $x \in \mathscr{E}(G)$ is that the vector $a := (a_e)_{e \in E}$ satisfies the following cycle condition:

$$\sum_{e \in F} a_e - \sum_{e \in C \setminus F} a_e \le |F| - 1 \quad \text{for } C \text{ a cycle in } G, F \subseteq C \text{ with } |F| \text{ odd};$$
(1.2)

see Section 4 for details.

Hence, a natural question is the characterization of the graphs G for which the clique condition (1.1) and the cycle condition (1.2), taken separately or together, suffice for describing the elliptope $\mathscr{E}(G)$. The graphs for which the clique condition is sufficient have been characterized in [14]; they are the chordal graphs—see Theorem 3.1. The graphs for which the clique condition and the cycle condition taken together suffice for describing the elliptope $\mathscr{E}(G)$ have been characterized in [4, 17]; their result is presented in Theorem 3.2.

The main result of this paper is the characterization of the graphs G for which $\mathscr{E}(G)$ is completely described by the cycle condition (1.2); we show that they are the series-parallel graphs—see Theorem 4.7.

In fact, a much stronger set of necessary conditions for membership in $\mathscr{E}(G)$ (stronger than the cycle condition) is given in Theorem 4.3; it can be derived from a result of [12], presented in Theorem 6.1. It turns out, however, that these conditions are sufficient only for the class of series-parallel graphs—see Theorem 4.7. We show, moreover, that the elliptope $\mathscr{E}(G)$ coincides with the convex hull of its rank-one matrices if and only if the graph G is acyclic—see Theorem 5.1.

The set $\mathscr{E}_{n \times n}$ of correlation matrices has also been studied in [6, 23, 15, 22], where the primary consideration is the question of determining the possible ranks for extreme elements of $\mathscr{E}_{n \times n}$. The set $\mathscr{E}_{n \times n}$ has been recently reintroduced in [24, 19, 12] as a nonlinear relaxation for a hard combinatorial optimization problem, namely, the max-cut problem. Indeed, the rank-one matrices of $\mathscr{E}_{n \times n}$, which are of the form aa^T for $a \in \{-1, 1\}^n$, play a special role in discrete optimization, as they correspond to the cuts of the complete

graph; see Section 2 for more details. A result of [12] shows, moreover, that by optimizing over the elliptope one obtains a very good approximation for the max-cut problem. Several results are given in [19, 20] on the faces of $\mathscr{C}_{n \times n}$. In particular, the vertices of $\mathscr{C}_{n \times n}$ are described in [19]; they are precisely its rank-one matrices. The possible dimensions for the faces (and the polyhedral faces) of $\mathscr{C}_{n \times n}$ are described in [20]. Moreover, a complete description of the faces of the elliptope $\mathscr{C}_{4 \times 4}$ can be found in [20]. Note that, by Theorem 4.7, K_4 is the smallest graph for which the parametric description provided by the cycle condition (1.2) does not apply.

The paper is organized as follows. In Section 2, we introduce some polytopes, related to the elliptope, that we will need in the sequel, and we explain the link with the optimization max-cut problem. In Section 3, we recall the known results relative to the cycle and clique conditions. In Section 4, we present some necessary conditions for membership in the elliptope $\mathscr{E}(G)$ and show that they are sufficient if and only if the graph G is series-parallel. In Section 5, we show that the elliptope $\mathscr{E}(G)$ coincides with the cut polytope (in ± 1 variables) if and only if the graph G is acyclic. We make several additional remarks in Section 6. In particular, we formulate a result of [12] on the inequalities that hold for the pairwise angles between any set of unit vectors.

NOTATION. Let G = (V, E) be a graph. A graph H is said to be a *minor* of G if H can be obtained from G be repeatedly deleting and/or contracting edges. Deleting an edge e in G means simply discarding it from the edge set of G. Contracting an edge e = uv means identifying both end nodes of e and discarding multiple edges if some are created during the identification of the nodes u and v.

Let us call the reverse operation to the contraction operation *splitting*. So, if v is a node in G adjacent to u_1, \ldots, u_p ($p \ge 2$), splitting v means replacing v by two nodes v' and v'' in such a way that v', v'' are adjacent and v' is adjacent to a subset of the neighbors of v, say, to u_1, \ldots, u_q ($1 \le q \le p - 1$) while v'' is adjacent to the remaining neighbors, i.e., to u_{q+1}, \ldots, u_p . Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs such that the set $K := V_1 \cap V_2$ induces a clique (possibly empty) in both G_1 and G_2 and there is no edge between a node of $V_1 \setminus K$ and a node of $V_2 \setminus K$. Then the graph $G := (V_1 \cup V_2, E_1 \cup E_2)$ is called the *clique sum* of G_1 and G_2 . We also say that G is their *clique k-sum if* $|\mathbf{K}| = \mathbf{k}$.

As is customary in graph theory, we call a graph a *cycle* if it can be decomposed as an edge disjoint union of circuits; a *circuit* is a graph with node set $\{v_1, \ldots, v_n\}$ $(n \ge 3)$ and edge set $\{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n, v_1v_n\}$.

2. RELATED POLYTOPES

We introduce here several polytopes related to the elliptope $\mathscr{E}(G)$ and to the max-cut problem.

Let G = (V, E) be a graph with node set $V := \{1, ..., n\}$. For a subset $S \subseteq V$ the cut $\delta_G(S)$ consists of the edges $e \in E$ having one end node in S and the other end node in $V \setminus S$. Given edge weights $w \in \mathbb{R}^E$, the max-cut problem is the problem of finding a cut $\delta_G(S)$ whose weight $\sum_{e \in \delta_G(S)} w_e$ is maximum. This is a hard problem, for which no polynomial algorithm is known in general. (More precisely, the max-cut problem is NP-hard; see [11]. For more information on this problem see, e.g., the survey paper [25].) The cut polytope $CUT^{01}(G)$ is defined as the convex hull of the incidence vectors of the cuts in G, i.e.,

$$\operatorname{CUT}^{01}(G) \coloneqq \operatorname{Conv}(\chi^{\delta_G(S)} | S \subseteq V)$$

(see [2]). Hence, the max-cut problem can be formulated as a linear programming problem over $CUT^{01}(G)$, namely, as

$$\max(w^T x | x \in CUT^{01}(G)).$$

Let MET⁰¹(G) denote the polytope in \mathbb{R}^{E} which consists of the vectors $x \in \mathbb{R}^{E}$ satisfying the inequalities

$$0 \le x_e \le 1 \quad \text{for } e \in E,$$

$$x(F) - x(C \setminus F) \le |F| - 1 \quad \text{for } F \subseteq C, \quad C \text{ a cycle of } G, \quad |F| \text{ odd};$$
(2.1)

MET⁰¹(G) is called the *metric polytope* of G (see [18]). Observe that, in the system (2.1), it suffices to consider the inequalities for all the circuits C of G (instead of the cycles). We have the inclusion

$$\operatorname{CUT}^{01}(G) \subseteq \operatorname{MET}^{01}(G)$$

[as every cut $\delta_G(S)$ has an even intersection with every cycle C of G]. Hence, the metric polytope $MET^{01}(G)$ is a linear relaxation of the cut polytope $CUT^{01}(G)$. It is shown in [2] that

$$\operatorname{CUT}^{01}(G) = \operatorname{MET}^{01}(G) \iff G$$
 has no K_5 -minor. (2.2)

At this point, let us make two remarks: instead of working with 0-1 variables as above, we may work with ± 1 variables; moreover, instead of working in the space \mathbb{R}^E indexed by the edge set of G, we may take as ambient space the space of symmetric $n \times n$ matrices. We give more details, as these various formulations will be used in the paper.

Let $f: \mathbb{R}^E \to \mathbb{R}^E$ denote the linear mapping defined by f(x) = y, where

$$y_e = 1 - 2x_e \quad \text{for} \quad e \in E.$$

Hence, f maps (0, 1) vectors to (1, -1) vectors. Set

$$\operatorname{CUT}^{\pm 1}(G) \coloneqq f(\operatorname{CUT}^{01}(G)), \quad \operatorname{MET}^{\pm 1}(G) \coloneqq f(\operatorname{MET}^{01}(G)).$$

These two polyhedra are again called, respectively, the cut polytope and the metric polytope of G (in the ± 1 variable). Hence,

$$\operatorname{CUT}^{\pm 1}(G) \subseteq \operatorname{MET}^{\pm 1}(G),$$

with equality if and only if G has no K_5 -minor. Moreover, the metric polytope MET $\pm {}^1(G)$ is defined by the following system of linear inequalities:

$$-1 \leq x_e \leq 1 \quad \text{for } e \in E,$$

$$x(F) - x(C \setminus F) \geq 2 - |C| \quad \text{for } F \subseteq C, \quad C \text{ a cycle of } G, \quad |F| \text{ odd.}$$
(2.3)

We also consider the polytopes:

$$\begin{aligned} \text{CUT}_{n \times n}^{\pm 1} &\coloneqq \text{Conv} \big(x x^T \big| \, x \in \{ -1, 1 \}^n \big), \\ \text{MET}_{n \times n}^{\pm 1} &\coloneqq \big\{ X \in \text{SYM}_{n \times n} \big| \, X_{ii} = 1 \text{ for } i = 1, \dots, n, \\ X_{ij} - X_{ik} - X_{jk} \ge -1 \text{ for } 1 \le i, j, k \le n, \\ X_{ij} + X_{ik} + X_{jk} \ge -1 \text{ for } 1 \le i, j, k \le n \big\}, \end{aligned}$$

which are defined in the space of the symmetric $n \times n$ matrices with diagonal entries 1; they are called again the cut and metric polytopes. Let π_E denote the projection from the space $\text{SYM}_{n \times n}$ of the symmetric $n \times n$

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matrices to the subspace \mathbb{R}^{E} indexed by the edge set of G. Then

$$\operatorname{CUT}^{\pm 1}(G) = \pi_E(\operatorname{CUT}_{n \times n}^{\pm 1}),$$

and it follows from a result of [1] that

$$\operatorname{MET}^{\pm 1}(G) = \pi_{E}(\operatorname{MET}_{n \times n}^{\pm 1}).$$

Therefore, MET^{± 1}(G) is the projection of MET^{± 1}(K_n) on the edge set of G; the same holds for the metric polytope in the 0, 1-variable. The vertices of the cut polytope $CUT_{n\times n}^{\pm 1}$ are the matrices xx^T for $x \in \{-1, 1\}^n$; they are called *cut matrices*, as they indeed encode the cuts of K_n (in the ± 1 variable).

Every cut matrix xx^{T} (for $x \in \{\pm 1\}^{n}$) obviously belongs to the elliptope $\mathscr{C}_{n \times n}$. Therefore,

$$\operatorname{CUT}_{n \times n}^{\pm 1} \subseteq \mathscr{E}_{n \times n}, \quad \operatorname{CUT}^{\pm 1}(G) \subseteq \mathscr{E}(G).$$

In other words, the elliptope $\mathscr{E}(G)$ is a (in general, nonpolyhedral) relaxation of the cut polytope $\operatorname{CUT}^{\pm 1}(G)$. This fact (combined with the additional property that one can optimize a linear function over the elliptope in polynomial time) was the essential motivation for considering the elliptope in the papers [24, 19, 12, 21]. We will characterize in Section 5 the graphs G for which the equality $\operatorname{CUT}^{\pm 1}(G) = \mathscr{E}(G)$ holds.

3. RELATED RESULTS

We present here some results from [14], [4], and [17] relative to the clique condition (1.1) and the cycle condition (1.2).

Let G = (V, E) be a graph. Given a circuit C in G, an edge $e \notin C$ is called a *chord* of C if it joins two nodes of C. Then G is said to be *chordal* if every circuit in G of length ≥ 4 has a chord.

As observed in [14], if G is not chordal, then the clique condition (1.1) does not suffice for describing $\mathscr{E}(G)$. Indeed, let C be a circuit of length ≥ 4 in G with no chord. Consider the vector $x \in \mathbb{R}^E$ with value 1 on all edges of C except for -1 on one edge of C, and with value 0 on all remaining edges of G. Then x satisfies (1.1) but $x \notin \mathscr{E}(G)$. The following result from [14] shows that the clique condition characterizes $\mathscr{E}(G)$ if G is chordal; a short proof can be found, e.g., in [16].

THEOREM 3.1 [14]. Let G = (V, E) be a graph. The following assertions are equivalent.

(i) G is chordal.

(ii) $\mathscr{E}(G) = \{x \in \mathbb{R}^E | x_K \in \mathscr{E}(K) \text{ for each clique K of } G\}.$

Following [4], let us call a graph G cycle completable if the conditions (1.1) and (1.2) are sufficient for describing $\mathscr{E}(G)$, i.e., if

$$\mathscr{E}(G) = \left\{ x \in \mathbb{R}^E \middle| x \text{ satisfies (1.1) and } \frac{1}{\pi} \arccos x \text{ satisfies (1.2)} \right\}.$$

Examples of cycle completable graphs include chordal graphs and seriesparallel graphs (this follows from Theorems 3.1 and 4.7) and their clique sums. The equivalence (i) \Leftrightarrow (v) from Theorem 3.2 below shows that all cycle completable graphs arise, in fact, in this way.

Let W_k denote the *wheel* on k nodes, which is composed of a circuit C on k - 1 nodes together with an additional node adjacent to all nodes of C. Hence, $W_4 = K_4$. Note that the wheel W_k for $k \ge 5$ is not cycle completable. (To see it, consider the vector x taking value $-\frac{1}{2}$ on all edges of W_k except for 0 on one edge of the circuit C.) Note, moreover, that W_4 is cycle completable, but not its splittings. The equivalence (i) \Leftrightarrow (ii) from Theorem 3.2 below shows that the wheels W_k ($k \ge 5$) and their splittings (for $k \ge 4$) are, in some sense, the minimal obstructions to cycle completability.

THEOREM 3.2. Let G be a graph. Consider the following assertions.

(i) G is cycle completable.

(ii) No induced subgraph of G is a wheel W_k ($k \ge 5$) or a splitting of a wheel W_k ($k \ge 4$).

(iii) Every induced subgraph of G that has a K_4 -minor also contains a clique of size 4.

(iv) There exists a chordal graph containing G as a subgraph and containing no new clique of size 4.

(v) G can be obtained by means of clique sums from chordal graphs and series parallel graphs.

Then (i) \Leftrightarrow (ii) \Leftrightarrow (iii) \Leftrightarrow (iv) [4], and (i) \Leftrightarrow (v) [17].

4. THE ELLIPTOPE FOR SERIES-PARALLEL GRAPHS

In this section we characterize the graphs G for which the cycle condition (1.2) suffices for describing the elliptope $\mathscr{E}(G)$. As mentioned in the introduction, each vector $x \in \mathscr{E}(G)$ can be parametrized as

$$x_e = \cos \pi a_e$$

where $a_e \in [0, 1]$ for every $e \in E$. For short, we write

$$x = \cos \pi a$$
 or, equivalently, $a = \frac{1}{\pi} \arccos x$,

which means that the relations hold componentwise. This parametrization for the members of the elliptope was introduced in [3].

The elliptope of a circuit has been characterized in [3], using the above parametrization. An equivalent result is given in [10], but the formulation of [3] turns out to be more convenient for our purpose of finding a generalization to a larger class of graphs. The result of [3] basically says that the elliptope of a circuit C is the image of the metric polytope MET⁰¹(C) (scaled by the factor π) of C under the cosine mapping.

THEOREM 4.1 [3]. Let C = (V, E) be a circuit. Then

 $\mathscr{E}(C) = \{ \cos \pi a \, \big| \, a \in \operatorname{MET}^{01}(C) \}.$

An immediate consequence of Theorem 4.1 is:

PROPOSITION 4.2. Let G be a graph. We have the inclusion

$$\mathscr{E}(G) \subseteq \{\cos \pi a | a \in \operatorname{Met}^{01}(G)\}.$$

In other words, the cycle condition (1.2) is necessary for membership in the elliptope $\mathscr{E}(G)$. In fact, the following stronger result can be derived from [12]. We give the proof in Section 6, as it is very simple and beautiful.

THEOREM 4.3. Let G be a graph. We have the inclusion

 $\mathscr{E}(G) \subseteq \{\cos \pi a | a \in \operatorname{CUT}^{01}(G)\}.$

Therefore, we have the following chain of inclusions:

$$\operatorname{CUT}^{\pm 1}(G) \subseteq \mathscr{E}(G) \subseteq \left\{ \cos \pi a \middle| a \in \operatorname{CUT}^{01}(G) \right\} \subseteq \left\{ \cos \pi a \middle| a \in \operatorname{MET}^{01}(G) \right\}.$$

We shall see in Section 5 that equality holds in the leftmost inclusion for acyclic graphs. By (2.2), equality holds in the rightmost inclusion for graphs with no K_5 -minor. Let \mathscr{G}_{met} denote the class of graphs G for which

$$\mathscr{E}(G) = \{ \cos \pi a | a \in \operatorname{MET}^{01}(G) \},\$$

and let \mathscr{G}_{cut} denote the class of graphs for which

$$\mathscr{E}(G) = \{ \cos \pi a | a \in \operatorname{CUT}^{01}(G) \}.$$

Clearly,

$$\mathcal{G}_{\text{met}} \subseteq \mathcal{G}_{\text{cut}}$$

We show below that both classes coincide with the class of graphs having no K_4 -minor.

By Theorem 4.1, we already know that circuits belong to the class \mathscr{G}_{met} ; hence, $K_3 \in \mathscr{G}_{met}$. Note that K_4 does not belong to \mathscr{G}_{cut} . For this, consider the vector $x \in \mathbb{R}^{E(K_4)}$ defined by $x = \cos \pi a = (-\frac{1}{2}, \ldots, -\frac{1}{2})$, where $a = (\frac{2}{3}, \ldots, \frac{2}{3})$. Hence, $a \in \text{MET}^{01}(K_4) = \text{CUT}^{01}(K_4)$. But x does not belong to $\mathscr{E}(K_4)$, as the matrix

$$X := \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix}$$

is not positive semidefinite. [Indeed, $Xe = -\frac{1}{2}e$, where $e = (1, 1, 1, 1)^T$.]

Before proceeding further with the description of the classes \mathscr{G}_{met} and \mathscr{G}_{cut} , we recall the following well-known characterization for graphs with no K_4 -minor (it can be derived from [9]). A graph G has no K_4 -minor if and only if $G = K_3$, or G is a subgraph of a clique k-sum (k = 0, 1, 2) of two smaller (i.e., with less nodes than G) graphs each having no K_4 -minor. Such graphs are also known as the partial 2-trees, or as the (simple) series-parallel graphs. (We stress "simple," as series-parallel graphs are, in general, allowed to have

loops or multiple edges. But here we consider only simple graphs.) (A 2-tree is any graph which can be constructed, starting from K_3 , by taking successive clique 2-sums with K_3 . A partial 2-tree is a subgraph of a 2-tree.)

We show now that the classes \mathscr{G}_{met} and \mathscr{G}_{cut} are composed precisely of the graphs with no K_4 -minor. In view of the above result, the key steps consist of showing that \mathscr{G}_{met} and \mathscr{G}_{cut} are closed under taking minors and clique sums.

PROPOSITION 4.4. Each of the classes \mathscr{G}_{met} and \mathscr{G}_{cut} is closed under taking minors.

Proof. Let G = (V, E) be a graph with n = |V| nodes, let e = uv be an edge of G, and let G' denote the graph obtained from G by deleting or contracting the edge e. We show that $G' \in \mathscr{F}_{met}$ ($G' \in \mathscr{F}_{cut}$) whenever $G \in \mathscr{F}_{met}$ ($G \in \mathscr{F}_{cut}$).

Let us first consider the case when $G' = G \times e$.

We suppose first that $G \in \mathscr{G}_{met}$; we show that $G' \in \mathscr{G}_{met}$. For this, let $a \in MET^{01}(G')$; we show that $\cos \pi a \in \mathscr{E}(G')$. Indeed, let b be a vector of $MET^{01}(G)$ whose projections on the edge set of G' is a. [Such a vector b exists, as the metric polytope of a graph coincides with the projection on its edge set of $MET^{01}(K_n)$. In an elementary way, such b can be explicitly constructed by setting $b_e := \alpha$, where α satisfies $0 \le \alpha \le 1$ and

$$\alpha \ge \max_{(C,F)|e \in C \setminus F} \left[a(F) - a(C \setminus (F \cup \{e\})) - |F| + 1 \right],$$

$$\alpha \le \min_{(C,F)|e \in F} \left[|F| - 1 + a(C \setminus F) - a(F \setminus \{e\}) \right],$$

where the pairs (C, F) consist of a cycle C in G containing e and a subset $F \subseteq C$ of odd cardinality; such an α exists by the assumption that $a \in MET^{01}(G')$.] As $G \in \mathscr{G}_{met}$, we obtain that $\cos \pi b \in \mathscr{E}(G)$. Therefore, its projection $\cos \pi a$ on the edge set of G' belongs to $\mathscr{E}(G')$.

Suppose now that $G \in \mathscr{G}_{cut}$; we show that $G' \in \mathscr{G}_{cut}$. For this, let $a \in CUT^{01}(G')$; we show that $\cos \pi a \in \mathscr{E}(G')$. We can find $b \in CUT^{01}(G)$ whose projection on the edge set of G' is a (as the cut polytope of a graph is the projection on its edge set of the cut polytope of the complete graph). Then, $\cos \pi b \in \mathscr{E}(G)$, which implies that $\cos \pi a \in \mathscr{E}(G')$.

We consider now the case when G' = G/e. Let w denote the node of G' obtained by contraction of the edge e = uv.

We first show that $G' \in \mathscr{G}_{met}$ whenever $G \in \mathscr{G}_{met}$. For this, let $a \in MET^{01}(G')$. We define a vector b on the edge set of G by setting $b_e \coloneqq 0$,

 $b_{iu} := a_{iw}$ if *i* is adjacent to *u* in *G*, $b_{iv} := a_{iw}$ if *i* is adjacent to *v* in *G*, and $b_f := a_f$ for all other edges *f* of *G*. Then, $b \in MET^{01}(G)$, as it satisfies the inequalities (2.1). As $G \in \mathscr{G}_{met}$, we obtain that $\cos \pi b \in \mathscr{E}(G)$. Hence, there exists a matrix $B \in \mathscr{E}_{n \times n}$ whose projection on the edge set of *G* is $\cos \pi b$. Let *A* denote the matrix obtained from *B* by deleting the row and column indexed by *u* (and renaming *v* as *w*). Then, $A \in \mathscr{E}_{(n-1)\times(n-1)}$. Moreover, the projection of *A* on the edge set of *G'* is $\cos \pi a$, which shows that $\cos \pi a \in \mathscr{E}(G')$.

We finally verify that $G' \in \mathscr{G}_{cut}$ whenever $G \in \mathscr{G}_{cut}$. Let $a \in CUT^{01}(G')$, and let b be the vector defined on the edge set of G in the same way as above. Then $b \in CUT^{01}(G)$. [Indeed, as $a \in CUT^{01}(G')$, a can be decomposed as a nonnegative linear combination of cuts in G':

$$a = \sum_{S} \lambda_{S} \chi^{\delta_{C'}(S)},$$

where $\lambda_s \ge 0$ and the sets S are subsets of $V \setminus \{u, v\}$. Then

$$b = \sum_{S} \lambda_{S} \chi^{\delta_{G}(S)},$$

which shows that $b \in CUT^{01}(G)$.] Therefore, $\cos \pi b \in \mathscr{E}(G)$, which implies as above that $\cos \pi a \in \mathscr{E}(G')$.

PROPOSITION 4.5. The class \mathscr{G}_{met} is closed under taking clique sums.

Proof. Let $G_1 = (V_1, E_1)$, $G_2 = (V_2, E_2)$ be two graphs in \mathscr{G}_{met} such that $K \coloneqq V_1 \cap V_2$ induces a clique in both G_1 and G_2 and there are no edges between a node from $V_1 \setminus K$ and a node from $V_2 \setminus K$. Let $G = (V \coloneqq V_1 \cup V_2, E \coloneqq E_1 \cup E_2)$ denote their clique sum. We show that $G \in \mathscr{G}_{met}$. For this, let $a \in MET^{01}(G)$; we show that $\cos \pi a \in \mathscr{E}(G)$. Let a_i denote the projection of a on \mathbb{R}^{E_i} for i = 1, 2. So $a_i \in MET^{01}(G_i)$, which implies that $\cos \pi a_i \in \mathscr{E}(G_i)$. Hence, there exists a matrix $A_i \in \mathscr{G}_{n_i \times n_i}$ $(n_i \coloneqq |V_i|)$ whose entries indexed by the edges $e \in E_i$ are precisely $\cos \pi a_e$. Consider the partial $n \times n$ (n = |V|) matrix M from Figure 1, where the entries (u, v) for $u \in V_1 \setminus K$, $v \in V_2 \setminus K$ remain to be specified.

Let H denote the graph on V whose edges are all pairs contained either in V_1 or in V_2 . So the entries of M are determined on all the edges of the graph H. As H is a chordal graph, we deduce from Theorem 3.1 that M can be completed to a matrix of $\mathscr{C}_{n \times n}$. In other words, values can be found for the unspecified entries of M that make M positive semidefinite. This shows that $\cos \pi a$ belongs to $\mathscr{E}(G)$.



FIC. 1.

THEOREM 4.7. Let G be a graph. The following assertions are equivalent:

(i) $G \in \mathscr{G}_{met}$. (ii) $G \in \mathscr{G}_{cut}$. (iii) G has no K_4 -minor.

Proof. Clearly, (i) \Rightarrow (ii). The implication (ii) \Rightarrow (iii) follows from the fact that \mathscr{G}_{cut} is closed under taking minors and that $K_4 \notin \mathscr{G}_{cut}$. We show (iii) \Rightarrow (i). Suppose G is a graph with no K_4 -minor. We show that $G \in \mathscr{G}_{met}$ by induction on the number of nodes. If $G = K_3$, then $G \in \mathscr{G}_{met}$ by Theorem 4.1. Otherwise, G can be obtained as a subgraph of a clique sum of two smaller graphs G_1 and G_2 having no K_4 -minor. By the induction assumption, G_1 and G_2 belong to \mathscr{G}_{met} . Therefore, $G \in \mathscr{G}_{met}$ by Propositions 4.4 and 4.5.

Note that the implication (iii) \Rightarrow (i) also follows from the implication (v) \Rightarrow (i) in Theorem 3.2 [as (1.1) follows then automatically from (1.2), since all cliques in G have at most three nodes]; however, our proof is direct and much shorter. As an application, we have the following result.

COROLLARY 4.8. Suppose C = (V, E) has no K_4 -minor. Let $x \in \mathbb{R}^E$ such that $x_e = \cos \pi \alpha$ for all $e \in E$, for some $\alpha \in [0, 1]$.

(i) If G is bipartite, then $x \in \mathscr{E}(G)$ for all $\alpha \in [0, 1]$.

(ii) If G is not bipartite and if k denotes the smallest length of an odd cycle in G, then $x \in \mathscr{E}(G)$ if and only if $0 \le \alpha \le (k-1)/k$.

Proof. By Theorem 4.7, $x \in \mathcal{E}(G)$ if and only if α satisfies (2.1), i.e., if

$$\alpha \leq \min\left(\frac{|F|-1}{2|F|-|C|}\middle| F \subseteq C, C \text{ a cycle, } |F| \text{ odd, } 2|F|-|C| > 0\right).$$

The result follows.

5. THE ELLIPTOPE FOR ACYCLIC GRAPHS

As mentioned in Section 2, the elliptope $\mathscr{E}(G)$ is a (in general, nonpolyhedral) relaxation of the cut polytope $\operatorname{CUT}^{\pm 1}(G)$, i.e.,

$$\operatorname{CUT}^{\pm 1}(G) \subseteq \mathscr{E}(G).$$

This inclusion is strict, for instance, for $G = K_3$; indeed, the vector $x := (-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$ belongs to $\mathscr{E}(K_3)$ but not to $\operatorname{CUT}^{\pm 1}(K_3)$. As an illustration, compare the polytope $\operatorname{CUT}^{\pm 1}(K_3)$ (which is a 3-dimensional simplex) and the elliptope $\mathscr{E}(K_3)$ (whose picture can be found in [19]). We show that equality holds in the above inclusion precisely for the acyclic graphs. A graph is *acyclic* if it contains no cycle, i.e., if it is a forest or, equivalently, if it has no K_3 -minor.

THEOREM 5.1. Let G = (V, E) be a graph. Then $\mathscr{E}(G) = \operatorname{CUT}^{\pm 1}(G)$ if and only if G is acyclic, i.e., if G is a forest.

Proof. Suppose that G is acyclic. Then G has no K_4 -minor and thus, by Theorem 4.7, $\mathscr{E}(G) = \{\cos \pi a \mid a \in \text{MET}^{01}(G)\}$. On the other hand, $\text{MET}^{01}(G) = [0, 1]^E$ [by the definition of $\text{MET}^{01}(G)$ in (2.1) and because G has no cycle] and $\text{CUT}^{\pm 1}(G) = \text{MET}^{\pm 1}(G) = [-1, 1]^E$ [using (2.2)]. Therefore,

$$\mathscr{E}(C) = \left\{ \cos \pi a \middle| a \in [0,1]^E \right\} = [-1,1] = \operatorname{CUT}^{\pm 1}(C).$$

Conversely, suppose that $\mathscr{E}(G) = \operatorname{CUT}^{\pm 1}(G)$. We show that G is acyclic. For this, it suffices to show that the property $\mathscr{E}(G) = \operatorname{CUT}^{\pm 1}(G)$ is closed under taking minors, as this will indeed imply that G has no K_3 -minor. So let G be a graph such that $\mathscr{E}(G) = \operatorname{CUT}^{\pm 1}(G)$, and let e be an edge of G. Let us first consider the graph G' obtained from G by deleting the edge e; we show that $\mathscr{E}(G') \subseteq \operatorname{CUT}^{\pm 1}(G')$. For $x \in \mathscr{E}(G')$ there exists a matrix $A \in$ $\mathscr{E}_{n \times n}$ (n = |V|) whose *ij*th entries are x_{ij} for $ij \in E \setminus \{e\}$. Let $y \in \mathbb{R}^{E}$ whose *ij*th coordinate is a_{ij} for $ij \in E$. Hence, $y \in \mathscr{E}(G) = \operatorname{CUT}^{\pm 1}(G)$. This implies that its projection x on $\mathbb{R}^{E \setminus \{e\}}$ belongs to $\operatorname{CUT}^{\pm 1}(G')$. Let now G'denote the graph obtained from G by contracting the edge e; we again show that $\mathscr{E}(G') \subseteq \operatorname{CUT}^{\pm 1}(G')$. Say the end nodes of e are v_{n-1} and v_n and the node set of G' is $V \setminus \{v_n\}$. For $x \in \mathscr{E}(G')$ there exists a matrix $A \in$ $\mathscr{E}_{(n-1)\times(n-1)}$ whose *ij*th entries are x_{ij} for $ij \in E(G')$. Let B denote the $n \times n$ matrix obtained from A by duplicating its last column and its last row and setting the (n, n - 1), and (n, n) entries equal to 1. Clearly, $B \in \mathscr{E}_{n \times n}$. Let $y \in \mathbb{R}^{E}$ whose *ij*th coordinate is b_{ij} for $ij \in E$. Then $y \in \mathscr{E}(G) =$ $\operatorname{CUT}^{\pm 1}(G)$. This implies easily that $x \in \operatorname{CUT}^{\pm 1}(G')$.

6. A GEOMETRICAL RESULT

Let G be a graph. By Theorem 4.3, we know that

$$\left\{\frac{1}{\pi} \arccos x \middle| x \in \mathscr{E}(G)\right\} \subseteq \operatorname{CUT}^{01}(G).$$

Therefore,

$$\operatorname{Conv}\left(\left\{\frac{1}{\pi}\arccos x \middle| x \in \mathscr{E}(G)\right\}\right) \subseteq \operatorname{CUT}^{01}(G).$$

(Here, "Conv" denotes the operation of taking the convex hull.) In fact, equality holds, as every vertex of $\operatorname{CUT}^{01}(G)$ belongs to the convex set on the left-hand side of the above relation. [Indeed, for every cut $\delta_G(S)$ of G, the vector $\cos \pi \chi^{\delta_G(S)}$ belongs to $\mathscr{E}(G)$.] In other words,

$$\operatorname{CUT}^{01}(G) = \operatorname{Conv}\left(\left\{\frac{1}{\pi} \arccos x \middle| x \in \mathscr{E}(G)\right\}\right),$$

i.e., the polytope $CUT^{01}(G)$ is the smallest convex set containing the set

$$\frac{1}{\pi}\arccos \mathscr{E}(G) := \left\{\frac{1}{\pi}\arccos x \middle| x \in \mathscr{E}(G)\right\}.$$

In particular, by Theorem 4.7, the set $(1/\pi) \arccos \mathscr{E}(G)$ is convex if and only if the graph G has no K_4 -minor.

For any graph G, we have the following situation: The elliptope $\mathscr{E}(G)$ contains the cut polytope $\operatorname{CUT}^{\pm 1}(G)$ (in the ± 1 variable) and is contained in the image of the cut polytope $\operatorname{CUT}^{01}(G)$ (in the 0, 1 variable)—scaled by the factor π —under the cosine mapping. Recall that $\operatorname{CUT}^{01}(G)$ is the image of $\operatorname{CUT}^{\pm 1}(G)$ under the mapping $x \mapsto (1-x)/2$. This permits us to conclude that

$$\left\{\cos \pi a \middle| a \in \operatorname{CUT}^{01}(G)\right\} = \left\{\sin\left(\frac{\pi}{2}b\right) \middle| b \in \operatorname{CUT}^{\pm 1}(G)\right\}.$$

Therefore, we have the inclusions

$$\operatorname{CUT}^{\pm 1}(G) \subseteq \mathscr{E}(G) \subseteq \left\{ \sin\left(\frac{\pi}{2}b\right) \middle| b \in \operatorname{CUT}^{\pm 1}(G) \right\},$$

with equality in the rightmost inclusion if and only if G has no K_4 -minor.

We now state a result of geometrical flavor, which shows how to derive valid relations for the pairwise angles between any set of unit vectors.

THEOREM 6.1 [12]. Let v_1, \ldots, v_n be unit vectors in \mathbb{R}^n . Let $a \in \mathbb{R}^{E(K_n)}$, $a_0 \in \mathbb{R}$ such that the inequality $a^T x \leq a_0$ is valid for the cut polytope $\operatorname{CUT}^{01}(K_n)$ (i.e., $a^T x \leq a_0$ holds for all $x \in \operatorname{CUT}^{01}(K_n)$). Then

$$\sum_{1 \leqslant i < j \leqslant n} a_{ij} \frac{\arccos v_i^{\prime} v_j}{\pi} \leqslant a_0.$$

Proof. The proof is based on the following randomized procedure, described in [12]:

- 1. Select a random unit vector $r \in \mathbb{R}^n$.
- 2. Set $S_r := \{1, ..., n\} | v_i^T r \ge 0\}$.

We consider the cut $\delta_{K_n}(S_r)$ in the complete graph K_n , which is constructed by this random procedure. Then, the probability that an edge e := ij of K_n belongs to the cut $\delta_{K_n}(S_r)$ is equal to the probability that $v_i^T r \ge 0$ and $v_j^T r < 0$ or vice versa. In other words, it is equal to the probability that the random hyperplane with normal r separates the vectors v_i and v_j , which in turn is equal to $(\arccos v_i^T v_j)/\pi$. Therefore, the expected weight (with respect to the weights a_{ij}) of the random cut $\delta_{K_r}(S_r)$ is equal to

$$\sum_{1 \leq i < j \leq n} a_{ij} \frac{\arccos v_i^T v_j}{\pi}.$$

But, this expected weight is less than or equal to the maximum weight of a cut, which is less than or equal to a_0 by assumption. This shows that

$$\sum_{\substack{i \le j \le n}} a_{ij} \frac{\arccos v_i^T v_j}{\pi} \le a_0.$$

Theorem 4.3 can now be derived in the following way. Let $x \in \mathscr{C}(G)$. We show that $(1/\pi) \arccos x \in \operatorname{CUT}^{01}(G)$. Let $X \in \mathscr{C}_{n \times n}$ whose projection on \mathbb{R}^E is x. As $X \geq 0$ with diagonal entries 1, it is the Gram matrix of a set of unit vectors $v_1, \ldots, v_n \in \mathbb{R}^n$, i.e., $X_{ij} = v_i^T v_j$ for all $i, j = 1, \ldots, n$. By Theorem 6.1, the vector $((1/\pi) \arccos v_i^T v_j)_{1 \leq i < j \leq n}$ belongs to the cut polytope $\operatorname{CUT}^{01}(K_n)$, as it satisfies all the inequalities that are valid for the polytope $\operatorname{CUT}^{01}(K_n)$.¹ Therefore, its projection $((1/\pi) \arccos v_i^T v_j)_{ij \in E(G)}$ on the edge set of G belongs to the polytope $\operatorname{CUT}^{01}(G)$. This shows that $(1/\pi) \arccos x \in \operatorname{CUT}^{01}(G)$.

Theorem 6.1 contains as a special case the well-known relations

$$\begin{split} \sum_{1 \leq i < j \leq 3} \arccos v_i^T v_j &\leq 2\pi, \\ \arccos v_1^T v_2 &\leq \arccos v_1^T v_3 + \arccos v_2^T v_3, \end{split}$$

which hold for any three unit vectors v_1 , v_2 , v_3 in 3-dimensional space (see [5, Corollary 18.6.10]). They follow from the valid inequalities

$$\sum_{1 \le i < j \le 3} x_{ij} \le 2, \qquad x_{12} \le x_{13} + x_{23}$$

for the polytope $\operatorname{CUT}^{01}(K_3)$. But Theorem 6.1 gives a whole wealth of other inequalities. Indeed, *every* valid inequality for the cut polytope $\operatorname{CUT}^{01}(K_n)$ yields some inequality for the pairwise angles among any set of n vectors in \mathbb{R}^n .

¹ We use here the well-known geometrical fact that every polytope which is given as the convex hull of a finite set of vectors can be alternatively described as the solution set of a system of linear inequalities.

For instance, the inequality

$$\sum_{1 \leq i < j \leq 2k+1} x_{ij} \leq k(k+1)$$

is valid for $CUT^{01}(K_{2k+1})$ $(k \ge 1)$. This implies that

$$\sum_{1 \leq i < j \leq 2k+1} \arccos v_i^T v_j \leq k(k+1)\pi$$

holds for any 2k + 1 unit vectors $v_1, \ldots, v_{2k+1} \in \mathbb{R}^{2k+1}$. Similarly, the inequality

$$\sum_{1 \leq i < j \leq 2k} \arccos v_i^T v_j \leq k^2 \pi$$

holds for any 2k unit vectors in \mathbb{R}^{2k} . As another example, let b_1, \ldots, b_n be integers whose sum $\sigma \coloneqq \sum_{1 \le i \le n} b_i$ is odd. Then the inequality

$$\sum_{1 \le i \le j \le n} b_i b_j x_{ij} \le \frac{\sigma^2 - 1}{4}$$

is valid for $\operatorname{CUT}^{01}(K_n)$. [Indeed, for every cut $\delta_{K_n}(S)$ of K_n ,

$$\sum_{ij\in\delta_{K_n}(S)}b_ib_j=\left(\sum_{i\in S}b_i\right)\left(\sum_{i\notin S}b_i\right)=\sum_{i\in S}b_i\left(\sigma-\sum_{i\in S}b_i\right)\leqslant\frac{\sigma^2-1}{4},$$

as $\sum_{i \in S} b_i$ is an integer.] Therefore,

$$\sum_{1 \le i < j \le n} b_i b_j \arccos v_i^T v_j \le \pi \frac{\sigma^2 - 1}{4}$$

holds for any n unit vectors in \mathbb{R}^n .

Many other inequalities valid for the cut polytope are known; see, e.g., [7, 8]. Most of them have, in fact, a quite complicated form. As a last example, let us mention the following relation (which follows from a valid inequality given in [13]), which holds for any seven unit vectors v_1, \ldots, v_7 in \mathbb{R}^7 :

$$\sum_{1 \leq i < j \leq 4} \arccos v_i^T v_j - 2 \sum_{i \leq i \leq 4} \arccos v_5^T v_i$$

- $\arccos v_1^T v_6 - \arccos v_3^T v_6 - \arccos v_2^T v_7 - \arccos v_4^T v_7$
+ $\arccos v_5^T v_6 + \arccos v_5^T v_7 - \arccos v_6^T v_7 \leq 0.$

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