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## On approximations, complexity, and applications for copositive programming

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## Chapter 5

# Graph isomorphism and copositive programming

Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two graphs with vertex sets  $V_1$  and  $V_2$ , and edge sets  $E_1$  and  $E_2$  respectively. Furthermore let  $|V_1| = |V_2| = n$ . Then the graph isomorphism problem ( $\mathcal{GIP}$ ) is the problem of deciding whether the two graphs are isomorphic, i.e. whether they are the same after a possible relabeling of the vertices. More formally, recalling that we denote by  $\mathcal{P}_n$  the set of all permutation matrices, we can define the graph isomorphism problem as follows.

**Definition 5.1** (Graph Isomorphism Problem). Given two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  with adjacency matrices  $A$  and  $B$  respectively, the graph isomorphism problem is the problem of deciding whether or not there exists a matrix  $X \in \mathcal{P}_n$  such that  $A = XBX^\top$ . If such a matrix  $X \in \mathcal{P}_n$  exists, we say that  $G_1$  is *isomorphic* to  $G_2$ .

The complexity of the graph isomorphism problem is currently unknown. That is, it is unknown whether or not the problem is solvable in polynomial time or not. Nor is it known if the  $\mathcal{GIP}$  is NP-complete; note that obviously the problem is in NP. This makes the graph isomorphism problem one of the last two problems from the well known list of problems with unknown complexity that was published by Gary and Johnson [GJ79], whose complexity still remains unresolved, the other problem being integer factorization. The problem is generally believed not to be in NP-complete however. Some of the arguments for this belief are the inclusion of  $\mathcal{GIP}$  in the class SPP [AK06], and the fact that the polynomial-time hierarchy collapses to its second level if  $\mathcal{GIP}$  were to be in NP-complete [Sch88]. This makes the  $\mathcal{GIP}$  a possible example of a problem that is neither in P nor NP-complete.

For specific cases the graph isomorphism problem can be solved in polynomial time. Examples include planar graphs [HT71] [HW74], graphs with bounded eigenvalue multiplicity [BGM82] and graphs of bounded degree [Luk82]. For the general case several algorithms have been developed. Some of the most well known are the so called Nauty Algorithm developed by McKay [McK81] and the Weisfeiler-Lehman method [WL68], see [Sch09] for a description of this method in English. The latter is a so called refinement method. It inspects  $k$ -tuples of vertices in an iterative manner and assigns attributes to them based on their neighbors' attributes. When this method was first described in the

1970s it was considered a possible solution to the graph isomorphism problem. However in 1992 a family of graphs was constructed by Cai, Fürer, and Immerman in [CFI92] that the Weisfeiler-Lehman method could not distinguish between. That is, it could not correctly decide that the graphs were not the same. It should be noted that technically the Cai, Fürer, and Immerman constructions are examples for graph isomorphism of so called colored graphs. Define, for some graph  $G = (V, E)$ , the map  $\sigma_P : V \rightarrow V$  as the function induced by a  $P \in \mathcal{P}_n$ , that is  $\sigma_P(i) = j$  if and only if  $P_{ij} = 1$ . Furthermore define the map  $c_G : V \rightarrow U$  that assigns a color to every vertex of  $G$ , where  $U$  is a set of colors. Then the colored graph isomorphism is defined as follows.

**Definition 5.2** (*Colored Graph Isomorphism Problem*). Given two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$ , with adjacency matrices  $A$  and  $B$  respectively, and some coloring of the vertices  $c_{G_1}$  and  $c_{G_2}$ , the colored graph isomorphism problem is the problem of deciding whether or not there exists a matrix  $X \in \mathcal{P}_n$  such that  $A = XB X^T$  while at the same time  $c_{G_1}(v) = c_{G_2}(\sigma_X(v))$  holds for all  $v \in V$ .

It turns out that the graph isomorphism problem and its colored version are actually equivalent in terms of complexity. A polynomial reduction from the colored to the uncolored graph isomorphism can be found in [Sch09]. In essence, this reduction is done by assigning color-specific attributes to every vertex in the form of rooted trees.

Contrary to the Weisfeiler-Lehman method the Nauty algorithm will always work for every possible pair of graphs. The algorithm does, however, have a theoretically exponential running time. Special instances were constructed by Miyazaki [Miy95], based on the constructions by Cai, Fürer, and Immerman, for which it can be shown that the Nauty Algorithm's running time is exponential. Despite the theoretical worst case running time however, the algorithm is reported in [Sch09] to be able to solve moderately large instances in the order of thousands of vertices for random graphs.

Considering the complexity results as well as the state of the art of current  $\mathcal{GIP}$  algorithms, the interest for a copositive formulation comes mostly from the difficult cases, such as the ones constructed by Cai, Fürer and Immerman, rather than the more general case. We will start by defining some of the notation to be used during this chapter. Then we will give a copositive formulation of the  $\mathcal{GIP}$  in Section 5.2. We will then provide an LP formulation of the  $\mathcal{GIP}$  as well in Section 5.3. In Section 5.4 we will discuss approximations for the  $\mathcal{GIP}$ , by using known hierarchies of the copositive cone. Moreover we will show that the use of such approximation techniques is appropriate by showing that an answer to the  $\mathcal{GIP}$  can always be found for some finite level of these hierarchies. In Section 5.5 we will give an alternative formulation of the  $\mathcal{GIP}$

which provides us with a potential approach to establishing polynomial time solvability of the graph isomorphism problem. Finally, during the writing of this chapter we found that another completely positive formulation for the  $\mathcal{GIP}$  has been suggested in [MA13]. They consider the completely positive version of the Lovász  $\vartheta$  function and find that, for any two graphs  $G_1$  and  $G_2$ , this function evaluates to  $n$  if  $G_1$  is isomorphic to  $G_2$  and less than  $n - \frac{1}{4n^4}$  when they are not isomorphic.

## 5.1 Notation

We recall that the (non-symmetric) matrix  $E_n^{ij}$  is defined as an  $n \times n$  matrix made up of all zeros, except for the  $(i, j)$ -th element, which is equal to one. We denote the Kronecker delta as  $\delta_{ij}$ . For any matrix  $A$  we denote its  $i^{\text{th}}$  row and column by  $\mathbf{A}_{i\bullet}$  and  $\mathbf{A}_{\bullet i}$  respectively. Finally, for  $X \in \mathcal{P}_n$  we define  $\mathbf{x} := \text{Vec}(X)$ . During the remainder of this chapter we will slightly abuse this notation by using  $\mathbf{x}$  and  $X$  interchangeably in an effort to make the text more readable. That is, for example, when we write  $\langle D, \mathbf{x}\mathbf{x}^\top \rangle \geq 0$  for all  $X \in \mathcal{P}_n$ , we mean  $\langle D, \mathbf{x}\mathbf{x}^\top \rangle \geq 0$  for every  $\mathbf{x} = \text{Vec}(X)$  with  $X \in \mathcal{P}_n$ . Following the notation used in [PR09], for a matrix  $B \in \mathbb{S}^{n^2}$  we use the block notation

$$B = \begin{pmatrix} B^{11} & \dots & B^{1n} \\ \vdots & \ddots & \vdots \\ B^{n1} & \dots & B^{nn} \end{pmatrix}$$

where  $B^{ij} \in \mathbb{S}^n$  for every  $i, j = 1, \dots, n$ . This notation is not to be confused with  $E_n^{ij}$ , which will be as it was defined above. In particular, note that we will never use  $E$  as anything other than the all ones matrix.

## 5.2 Graph Isomorphism as a Copositive Program

We will now provide a copositive formulation of the  $\mathcal{GIP}$ . In order to do so we shall begin by first rewriting the  $\mathcal{GIP}$  as a quadratic optimization problem. Once we have done that we can use the technique by Povh and Rendl [PR09] to obtain a copositive program.

We can turn the  $\mathcal{GIP}$  into a quadratic optimization problem by rewriting the equality  $A = \mathbf{X}\mathbf{B}\mathbf{X}^\top$ , from Definition 5.1, into a number of linear constraints as follows,

$$\begin{aligned}
 A = XBX^\top &\Leftrightarrow AX = XB \\
 &\Leftrightarrow \mathbf{A}_{i\bullet} \mathbf{X}_{\bullet j} - \mathbf{X}_{i\bullet} \mathbf{B}_{\bullet j} = 0 \quad \forall i, j = 1, \dots, n \\
 &\Leftrightarrow \langle (E_n^{ji} A)^\top, X \rangle - \langle (BE_n^{ji})^\top, X \rangle = 0 \quad \forall i, j = 1, \dots, n. \\
 &\Leftrightarrow \langle (E_n^{ji} A)^\top - (BE_n^{ji})^\top, X \rangle = 0 \quad \forall i, j = 1, \dots, n.
 \end{aligned}$$

Note that the matrix  $E_n^{ij}$  acts as an operator on a matrix  $C \in \mathbb{R}^{n \times n}$  in such a way that  $E_n^{ij} C$  is an all zero matrix apart from the  $i^{\text{th}}$  row, which is identical to the  $j^{\text{th}}$  row of the matrix  $C$ . We can now present the following result

**Lemma 5.3** (*GIP as a Quadratic Program*). *Given two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  with adjacency matrices  $A$  and  $B$  respectively, define for  $i, j = 1, \dots, n$*

$$\mathbf{d}_{ij} = \text{Vec}((E_n^{ji} A)^\top - (BE_n^{ji})^\top) = \text{Vec}(AE_n^{ij} - E_n^{ij} B), \quad (5.1)$$

and let  $D = \sum_{i=1}^n \sum_{j=1}^n \mathbf{d}_{ij} \mathbf{d}_{ij}^\top$ .

Then the graph isomorphism problem as described in Definition 5.1 is equivalent to deciding whether or not the optimal value of the quadratic program

$$\begin{aligned}
 \mathcal{GIP}_{QP} = \min \quad &\langle D, \mathbf{x}\mathbf{x}^\top \rangle \\
 \text{s.t.} \quad &X \in \mathcal{P}_n
 \end{aligned} \quad (5.2)$$

is equal to 0.

*Proof.* From the discussion above, it follows that we can write our equation as follows:

$$\begin{aligned}
 A = XBX^\top &\Leftrightarrow \mathbf{d}_{ij}^\top \mathbf{x} = 0 && \text{for all } i, j = 1, \dots, n \\
 &\Leftrightarrow (\mathbf{d}_{ij}^\top \mathbf{x})^2 = 0 && \text{for all } i, j = 1, \dots, n \\
 &\Leftrightarrow \sum_{i=1}^n \sum_{j=1}^n (\mathbf{d}_{ij}^\top \mathbf{x})^2 = 0 \\
 &\Leftrightarrow \sum_{i=1}^n \sum_{j=1}^n \langle \mathbf{d}_{ij} \mathbf{d}_{ij}^\top, \mathbf{x}\mathbf{x}^\top \rangle = 0 \\
 &\Leftrightarrow \langle D, \mathbf{x}\mathbf{x}^\top \rangle = 0.
 \end{aligned}$$

From Proposition 1.2 it follows that  $D \in \mathcal{S}_+^{n^2}$  and moreover that  $\mathbf{d}_{ij}\mathbf{d}_{ij}^\top \in \mathcal{S}_+^n$  as well. This in turn implies that  $\langle D, \mathbf{xx}^\top \rangle \geq 0$  and  $\langle \mathbf{d}_{ij}\mathbf{d}_{ij}^\top, \mathbf{xx}^\top \rangle \geq 0$  for all  $X \in \mathcal{P}_n$  and all  $i, j = 1, \dots, n$ , and hence  $\langle D, \mathbf{xx}^\top \rangle = 0$  if and only if  $\langle \mathbf{d}_{ij}\mathbf{d}_{ij}^\top, \mathbf{xx}^\top \rangle = 0$  for every  $i, j = 1, \dots, n$ . This proves our claimed result.  $\square$

Using the technique from [PR09], as suggested before, we can now write the  $\mathcal{GIP}$  as a copositive program. In order to do this we first note that we can write the set of permutation matrices as

$$\mathcal{P}_n = \{A \in \mathbb{R}_+^{n \times n} \mid A^\top A = I_n\}.$$

Then redundant equalities can be added to obtain

$$\mathcal{P}_n = \{A \in \mathbb{R}_+^{n \times n} \mid A^\top A = I_n, AA^\top = I_n, (\mathbf{e}^\top A \mathbf{e})^2 = n^2\}.$$

Finally, noting that for any matrices  $X, B, C \in \mathbb{R}^{n \times n}$  we have  $\langle X, BXC \rangle = \langle C^\top \otimes B, \mathbf{xx}^\top \rangle$ ,  $\mathbf{x} = \text{Vec}(X)$ , we obtain the following result using Lagrangian duality, analogue to [PR09]:

$$\begin{aligned} \mathcal{GIP}_{QP} &= \min \left\{ \langle D, \mathbf{xx}^\top \rangle \mid X \in \mathcal{P}_n \right\} \\ &= \min_{X \geq 0} \left\{ \langle D, \mathbf{xx}^\top \rangle + \min_{S, T \in \mathbb{S}^n, v \in \mathbb{R}} \left\{ \langle S, I - XX^\top \rangle + \langle T, I - X^\top X \rangle + v(n^2 - \langle X, EXE \rangle) \right\} \right\} \\ &\geq \max_{S, T \in \mathbb{S}^n, v \in \mathbb{R}} \left\{ \text{Tr}(S) + \text{Tr}(T) + n^2 v + \min_{X \geq 0} \left\{ \mathbf{x}^\top (D - I \otimes S - T \otimes I - vE_{n^2}) \mathbf{x} \right\} \right\} \\ &= \max_{S, T \in \mathbb{S}^n, v \in \mathbb{R}} \left\{ \text{Tr}(S) + \text{Tr}(T) + n^2 v \mid D - I \otimes S - T \otimes I - vE_{n^2} \in \mathcal{COP}^{n^2} \right\} \quad (5.3) \end{aligned}$$

$$= \min_Y \left\{ \langle D, Y \rangle \mid \sum_i Y^{ii} = I, \langle I, Y^{ij} \rangle = \delta_{ij} \quad \forall i, j, \langle E, Y \rangle = n^2, Y \in \mathcal{CP}^{n^2} \right\} \quad (5.4)$$

The copositive formulation (5.3) will be denoted as  $\mathcal{GIP}_{COP}$ . That we have strong duality between (5.3) and (5.4) can be seen by taking  $T = 0$ ,  $v = 0$ , and  $S = -I_n$  in the copositive program (5.3), so that the matrix  $D + I_{n^2}$  is in the interior of  $\mathcal{COP}^{n^2}$ . This result follows from the fact that  $D$  is positive semidefinite, which as noted before follows directly from its definition and Proposition 1.2. From [PR09] we furthermore get the following result with respect to the feasible region of the completely positive program (5.4).

**Theorem 5.4** (Theorem 3, [PR09]). *Let*

$$\mathcal{F} = \left\{ Y \mid \sum_i Y^{ii} = I, \langle I, Y^{ij} \rangle = \delta_{ij} \forall i, j, \langle E, Y \rangle = n^2, Y \in \mathcal{CP}^{n^2} \right\}, \quad (5.5)$$

then

$$\mathcal{F} = \text{conv} \left\{ \mathbf{y}\mathbf{y}^\top \mid \mathbf{y} = \text{Vec}(X), X \in \mathcal{P}_n \right\}. \quad (5.6)$$

Hence we now immediately obtain the following corollary.

**Corollary 5.5.** *The optimal value of  $\mathcal{GIP}_{QP}$  is equal to the optimal value of  $\mathcal{GIP}_{COP}$ .*

In other words, we can solve the  $\mathcal{GIP}$  by solving a copositive program. We summarize this result in the following theorem.

**Theorem 5.6** ( $\mathcal{GIP}$  as a Copositive and Completely Positive Program). *Let there be given two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  with adjacency matrices  $A$  and  $B$  respectively. Let  $D$  be defined as in Lemma 5.3. Then the graph isomorphism as described in Definition 5.1 is equivalent to deciding whether or not the optimal value of the copositive program*

$$\max_{S, T \in \mathbb{S}^n, v \in \mathbb{R}} \left\{ \text{Tr}(S) + \text{Tr}(T) + n^2 v \mid D - I \otimes S - T \otimes I - vE_{n^2} \in \mathcal{COP}^{n^2} \right\} \quad (5.7)$$

is equal to 0, which is the case if and only if  $G_1$  and  $G_2$  are isomorphic. Alternatively, deciding isomorphism can be done by verifying whether the optimal value of the completely positive program

$$\min \left\{ \langle D, Y \rangle \mid \sum_i Y^{ii} = I, \langle I, Y^{ij} \rangle = \delta_{ij} \forall i, j, \langle E, Y \rangle = n^2, Y \in \mathcal{CP}^{n^2} \right\} \quad (5.8)$$

is equal to 0, which again is the case if and only if  $G_1$  is isomorphic to  $G_2$ .

Finally, from Corollary 5.5 we obtain the following lemma that we will need later on in this chapter.

**Lemma 5.7.** *The optimal values of the copositive formulation (5.7) and the completely positive formulation (5.8) of the  $\mathcal{GIP}$  are integer valued.*

*Proof.* This follows directly from Corollary 5.5 and noting that the matrix  $D$  is integer valued.  $\square$



### 5.2.1 Properties of the matrix $D$

We will now explore some of the properties of the matrix  $D$  as defined in Lemma 5.3. We will begin by giving an equivalent definition of  $D$ . This alternative definition of  $D$  will provide us with a better insight into the structure of this particular matrix. We will then use this insight later on in this chapter to rewrite our current copositive reformulation. In order to do so however, we will first have to recall some technical results concerning the Kronecker product, which we will need in order to be able to obtain a new formulation of our matrix  $D$ .

**Lemma 5.8** (Proposition 7.1.6, [Ber09]). *Let  $A \in \mathbb{R}^{n \times m}$ ,  $B \in \mathbb{R}^{l \times k}$ ,  $C \in \mathbb{R}^{m \times q}$ , and  $D \in \mathbb{R}^{k \times p}$ . Then*

$$(A \otimes B)(C \otimes D) = AC \otimes BD. \quad (5.9)$$

**Lemma 5.9** (Proposition 7.1.9, [Ber09]). *Let  $A \in \mathbb{R}^{n \times m}$ ,  $B \in \mathbb{R}^{m \times l}$ , and  $C \in \mathbb{R}^{l \times k}$ . Then*

$$\text{Vec}(ABC) = (C^\top \otimes A) \text{Vec} B. \quad (5.10)$$

Using the above properties, we can now obtain a more convenient form and definition of our matrix  $D$  giving us the following proposition.

**Proposition 5.10.** *Let  $A, B \in \mathbb{S}^n$ , and consider a matrix  $D$ , defined by  $D := \sum_{i=1}^n \sum_{j=1}^n \mathbf{d}_{ij} \mathbf{d}_{ij}^\top$ , with  $\mathbf{d}_{ij} := \text{Vec}(AE_n^{ij} - E_n^{ij} B)$  for every  $i, j = 1, \dots, n$ . Then*

$$D = (I \otimes AA) + (BB \otimes I) - 2(B \otimes A). \quad (5.11)$$

*Proof.* Let  $I$  be the identity matrix of size  $n \times n$  unless otherwise specified. Then we get

$$\begin{aligned} D &:= \sum_{i=1}^n \sum_{j=1}^n \mathbf{d}_{ij} \mathbf{d}_{ij}^\top = \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(AE^{ij} - E^{ij} B) \text{Vec}(AE^{ij} - E^{ij} B)^\top \\ &= \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(AE^{ij}) \text{Vec}(AE^{ij})^\top + \text{Vec}(E^{ij} B) \text{Vec}(E^{ij} B)^\top \\ &\quad - \text{Vec}(AE^{ij}) \text{Vec}(E^{ij} B)^\top - \text{Vec}(E^{ij} B) \text{Vec}(AE^{ij})^\top. \end{aligned}$$

Treating parts of this summation separately, and using Lemmas 5.8 and 5.9, we obtain the following equations:

$$\begin{aligned}
 \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(AE^{ij}) \text{Vec}(AE^{ij})^\top &= \sum_{i=1}^n \sum_{j=1}^n (I \otimes A) \text{Vec}(E^{ij}) \left[ (I \otimes A) \text{Vec}(E^{ij}) \right]^\top \\
 &= (I \otimes A) \left[ \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(E^{ij}) \text{Vec}(E^{ij})^\top \right] (I \otimes A) = (I \otimes A) I_{n^2} (I \otimes A) = (I \otimes AA),
 \end{aligned}$$

and

$$\begin{aligned}
 \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(E^{ij}B) \text{Vec}(E^{ij}B)^\top &= \sum_{i=1}^n \sum_{j=1}^n (B \otimes I) \text{Vec}(E^{ij}) \left[ (B \otimes I) \text{Vec}(E^{ij}) \right]^\top \\
 &= (B \otimes I) \left[ \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(E^{ij}) \text{Vec}(E^{ij})^\top \right] (B \otimes I) = (B \otimes I) I_{n^2} (B \otimes I) = (BB \otimes I),
 \end{aligned}$$

and

$$\begin{aligned}
 \left( \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(E^{ij}B) \text{Vec}(AE^{ij})^\top \right)^\top &= \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(AE^{ij}) \text{Vec}(E^{ij}B)^\top \\
 &= \sum_{i=1}^n \sum_{j=1}^n (I \otimes A) \text{Vec}(E^{ij}) \left[ (B \otimes I) \text{Vec}(E^{ij}) \right]^\top \\
 &= (I \otimes A) \left[ \sum_{i=1}^n \sum_{j=1}^n \text{Vec}(E^{ij}) \text{Vec}(E^{ij})^\top \right] (B \otimes I) \\
 &= (I \otimes A) I_{n^2} (B \otimes I) = (B \otimes A).
 \end{aligned}$$

This proves our statement.  $\square$

Furthermore recall that due to the original definition of the matrix  $D$  we know that it is a sum of semidefinite matrices and hence is itself semidefinite. The fact that  $D \in \mathcal{S}_+^{n^2}$  has a number of consequences. One of them is that it places a restriction on the rank of the matrix. Before we can prove this result, recall that from Lemma 3.3 we know that for  $A \in \mathcal{S}_+^n$  we have  $\mathbf{u}^\top \mathbf{A} \mathbf{u} = 0$  if and only if  $\mathbf{A} \mathbf{u} = \mathbf{0}$ . With the help of this result we can now formulate the following theorem with respect to the rank of  $D$ .

**Theorem 5.11.** *Consider two graphs  $G_1$  and  $G_2$  on  $n$  vertices and let  $A$  and  $B$  be their respective adjacency matrices. Furthermore let*

$$D = (I \otimes AA) + (BB \otimes I) - 2(B \otimes A).$$

*If  $\text{Rank } D = n^2$ , then  $G_1$  is not isomorphic to  $G_2$ .*

*Proof.* Let  $\text{Rank } D = n^2$ , then the dimension of the nullspace of  $D$  is equal to 0, that is  $\text{Null}(D) = \{\mathbf{0}\}$ . Now suppose  $G_1$  and  $G_2$  are isomorphic. From Theorem 5.6 it follows that there exists a completely positive matrix  $Y \neq 0$  (note that  $0 \notin \mathcal{F}$ ) and nonzero vectors  $\mathbf{y}_i \in \mathbb{R}_+^{n^2}$ ,  $i = 1, \dots, k$  for some  $k > 0$ , such that

$$0 = \langle D, Y \rangle = \langle D, \sum_{i=1}^k \mathbf{y}_i \mathbf{y}_i^T \rangle = \sum_{i=1}^k \langle D, \mathbf{y}_i \mathbf{y}_i^T \rangle.$$

Then because  $D \in \mathcal{S}_+^{n^2}$  we know that

$$\langle D, \mathbf{y}_i \mathbf{y}_i^T \rangle \geq 0 \text{ for all } i.$$

So we must have  $\langle D, \mathbf{y}_i \mathbf{y}_i^T \rangle = 0$  for every  $i$ . Then, again because  $D \in \mathcal{S}_+^{n^2}$ , it follows from Lemma 3.3 that  $\mathbf{y}_i^T D \mathbf{y}_i = 0$  if and only if  $D \mathbf{y}_i = 0$ . That is,  $\mathbf{y}_i$  is in the nullspace of  $D$ , which is a contradiction.  $\square$

In fact, because we know that a semidefinite matrix is positive definite if and only if it has full rank, we have the following equivalent corollary.

**Corollary 5.12.** *Consider two graphs  $G_1$  and  $G_2$  on  $n$  vertices, and let  $A$  and  $B$  be their respective adjacency matrices. Furthermore let*

$$D = I \otimes AA + BB \otimes I - 2B \otimes A.$$

*If  $D$  is positive definite, then  $G_1$  is not isomorphic to  $G_2$ .*

The reverse does not hold, the following pair of graphs is a counter example.

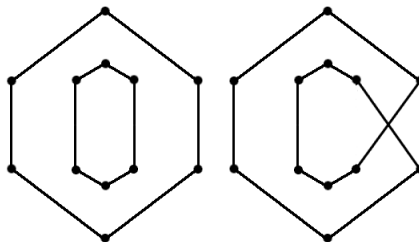


Figure 5.1: *Example of a pair of non-isomorphic graphs created following the construction of Cai, Fürer, and Immerman.*

The resulting matrix  $D$  has a rank of 124 rather than  $12^2 = 144$ . This pair of graphs is an example of the Cai, Fürer, and Immerman constructions

that were mentioned earlier in this chapter. Moreover it is a special case as it does not need a coloring for the two graphs to be non-isomorphic. This means we do not have to add rooted graphs to all the vertices in order to do computations on these graphs in an effort to decide isomorphism. As it turns out, we can already find a certificate for non-isomorphism of these two graphs by replacing the copositive cone  $\mathcal{COP}^n$  by the semidefinite cone  $\mathcal{S}_+^n$  in (5.7). This fact is not necessarily surprising as these graphs are planar graphs, for which we know the  $\mathcal{GIP}$  is decidable in polynomial time from [HT71] [HW74], as mentioned at the start of this chapter.

### 5.3 The Graph Isomorphism Problem as an LP

From Theorem 5.4 we know that we can write our completely positive program (5.8) as follows,

$$\min \{ \langle D, Y \rangle \mid Y \in \text{conv}\{\mathbf{x}\mathbf{x}^\top, \mathbf{x} = \text{Vec}(X), X \in \mathcal{P}_n\} \},$$

or equivalently,

$$\min \{ \langle D, Y \rangle \mid Y = \sum_{X \in \mathcal{P}_n} \lambda_X \text{Vec}(X) \text{Vec}(X)^\top, \text{ for } \lambda_X \geq 0 \text{ and } \sum_{X \in \mathcal{P}_n} \lambda_X = 1 \}.$$

This provides us with a linear programming formulation of the graph isomorphism problem. Note that this does not solve the complexity of the graph isomorphism problem, as we have an exponential number of variables  $\lambda_X$ . By dualizing we obtain an LP with just one variable, but with an exponential number of constraints.

Let  $\mathcal{L}(\lambda_X, \mu)$  be the Lagrangian function belonging to the LP above, then using Lagrangian dualization we get

$$\begin{aligned} \min_{\lambda_X \geq 0} \max_{\mu \in \mathbb{R}} \mathcal{L}(\lambda_X, \mu) &= \min_{\lambda_X \geq 0} \max_{\mu \in \mathbb{R}} \left\{ \left\langle D, \sum_{X \in \mathcal{P}_n} \lambda_X \text{Vec}(X) \text{Vec}(X)^\top \right\rangle + \mu \left( 1 - \sum_{X \in \mathcal{P}_n} \lambda_X \right) \right\} \\ &\geq \max_{\mu \in \mathbb{R}} \min_{\lambda_X \geq 0} \left\{ \mu \left( 1 - \sum_{X \in \mathcal{P}_n} \lambda_X \right) + \left\langle D, \sum_{X \in \mathcal{P}_n} \lambda_X \text{Vec}(X) \text{Vec}(X)^\top \right\rangle \right\} \\ &= \max_{\mu \in \mathbb{R}} \left\{ \mu + \min_{\lambda_X \geq 0} \left\{ \sum_{X \in \mathcal{P}_n} \lambda_X \left( \left\langle D, \text{Vec}(X) \text{Vec}(X)^\top \right\rangle - \mu \right) \right\} \right\} \\ &= \max \left\{ \mu \in \mathbb{R} \mid \left\langle D, \text{Vec}(X) \text{Vec}(X)^\top \right\rangle - \mu \geq 0 \text{ for all } X \in \mathcal{P}_n \right\}. \quad (5.12) \end{aligned}$$

In the case where we have two isomorphic graphs,  $D$  is such that there exists an  $X \in \mathcal{P}_n$  for which  $\langle D, \text{Vec}(X) \text{Vec}(X)^\top \rangle = 0$  by Lemma 5.3, and hence the optimal value for the dual is 0. In the case that our two graphs are not isomorphic we have  $\langle D, \text{Vec}(X) \text{Vec}(X)^\top \rangle > 0$  for every  $X \in \mathcal{P}_n$ . However, due to the fact that  $-2 \leq D_{ij} \leq 2n - 2$  by Proposition 5.10, the inner product  $\langle D, \text{Vec}(X) \text{Vec}(X)^\top \rangle$  must be finite. Hence  $\mu$ , and therefore the optimal value of (5.12) must be finite as well. From duality theory of linear programs it now follows that strong duality holds and so the inequality in the above should in fact be an equality. This then provides us with yet another linear programming formulation for the graph isomorphism problem as claimed. We summarize this result in the following theorem.

**Theorem 5.13** (*GLP as a Linear Program*). *Given two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  with adjacency matrices  $A$  and  $B$  respectively. Let  $D$  be defined as in Lemma 5.3. Then the graph isomorphism problem as described in Definition 5.1 is equivalent to deciding whether or not the optimal value of the linear program*

$$\begin{aligned} & \min \left\{ \langle D, Y \rangle \mid Y = \sum_{X \in \mathcal{P}_n} \lambda_X \text{Vec}(X) \text{Vec}(X)^\top, \text{ for } \lambda_X \geq 0 \text{ and } \sum_{X \in \mathcal{P}_n} \lambda_X = 1 \right\} \\ & = \max \left\{ \mu \in \mathbb{R} \mid \langle D, \text{Vec}(X) \text{Vec}(X)^\top \rangle - \mu \geq 0, \text{ for all } X \in \mathcal{P}_n \right\}. \end{aligned}$$

*is equal to 0, which is the case if and only if  $G_1$  and  $G_2$  are isomorphic.*

## 5.4 Solving the GLP via approximation hierarchies

We will start this section by recalling the definition of the hierarchy of approximations (1.12) as introduced in [dKP02]. That is for  $r \in \mathbb{Z}_+$  and  $n \in \mathbb{N}$

$$C_n^r := \left\{ A \in \mathbb{S}^n \mid \left( \sum_{i=1}^n x_i \right)^r \mathbf{x}^\top A \mathbf{x} \text{ has nonnegative coefficients} \right\}.$$

We then state the following definition.

**Definition 5.14.** For any two graphs  $G_1$  and  $G_2$  with adjacency matrices  $A$  and  $B$ , let

$$D = (I \otimes AA) + (BB \otimes I) - 2(B \otimes A).$$

Then for any  $r \in \mathbb{Z}_+$  we define the following lower bound for (5.7):

$$\eta^r := \max_{S, T \in \mathbb{S}^n, v \in \mathbb{R}} \left\{ \text{Tr}(S) + \text{Tr}(T) + n^2 v \mid D - I \otimes S - T \otimes I - v E_{n^2} \in \mathcal{C}_{n^2}^r \right\}. \quad (5.13)$$

It should be noted that the  $\mathcal{GIP}$  can only have 'yes' and 'no' as answers. Because of this we are not really interested in approximations per sé as they do not necessarily give us any information. Hence we need to know whether the optimum of the copositive formulation (5.7) is obtained by some finite level of the approximation hierarchy. In order to establish that this is indeed the case we will try to obtain an upper bound on  $r$  such that  $\eta^r$  will give us the optimum of (5.7). To this end we present the following known result by de Klerk and Pasechnik [dKP02] which is an adaptation for copositivity of a result by Powers and Reznik [PR01] who constructed a tight upper bound on the value of  $N$  in Theorem 1.13.

**Corollary 5.15** ([dKP02], Corollary 3.5). *Let  $M \in \text{int}(\mathcal{COP}^n)$ , then*

$$P^N(\mathbf{z}) = \left( \sum_{i,j=1}^n M_{ij} z_i z_j \right) \left( \sum_{i=1}^n z_i \right)^N$$

has only nonnegative coefficients if  $N > L/\kappa - 2$  where

$$L = \max_{i,j} |M_{ij}| \quad (5.14)$$

and

$$\kappa = \min_{\mathbf{z} \in \Delta} \mathbf{z}^\top M \mathbf{z} \quad (5.15)$$

where  $\Delta$  denotes the unit simplex.

In particular this corollary is what provides us with a way of obtaining a bound on the number of liftings,  $r$ , needed to obtain an optimal solution for  $\mathcal{GIP}_{CP}$  by solving  $\eta^r$  instead. More importantly, as long as we can show that an optimal solution inside the interior of  $\mathcal{COP}^n$  exists, Corollary 5.15 implies that there exists an  $r$  for which  $\eta^r$  can decide the graph isomorphism problem. For this purpose we have the following proposition.

**Proposition 5.16.** *Given two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$ , let  $D$  be the matrix as defined in Lemma 5.3. Then there exists an  $r \in \mathbb{Z}_+$  such that  $\lceil \eta^{(r)} \rceil$  is equal to the optimal value of  $\mathcal{GIP}_{COP}$ , and hence  $G_1$  is isomorphic to  $G_2$  if and only if  $\eta^{(r)} = 0$ .*

*Proof.* Let  $S^*$ ,  $T^*$  and  $v^*$  be optimal solutions to the copositive program (5.7), and let  $0 < \varepsilon < \frac{1}{n^2}$ . Define the matrix

$$Q_\varepsilon^* = D - I \otimes S^* - T^* \otimes I - (v^* - \varepsilon)E_{n^2}.$$

Due to Theorem 1.13, in order to prove the existence of an  $r \in \mathbb{Z}_+$  for which the  $\mathcal{GIP}$  can be decided by  $\eta^r$ , it suffices to show that  $Q_\varepsilon^* \in \text{int}(\mathcal{COP}^{n^2})$  and that  $Q_\varepsilon^*$  provides an optimal solution.

Obviously  $Q_\varepsilon^* \in \mathcal{COP}^{n^2}$  due to the fact that we can always add nonnegative matrices to any copositive matrix without changing copositivity while we have  $D - I \otimes S^* - T^* \otimes I - v^*E_{n^2} \in \mathcal{COP}^{n^2}$  by definition. In fact, it turns out that we have  $Q_\varepsilon^* \in \text{int}(\mathcal{COP}^{n^2})$  as for  $x \in \mathbb{R}_+^{n^2} \setminus \{0\}$  we have

$$\begin{aligned} & \mathbf{x}^\top (D - I \otimes S^* - T^* \otimes I - (v^* - \varepsilon)E_{n^2}) \mathbf{x} \\ &= \mathbf{x}^\top (D - I \otimes S^* - T^* \otimes I - v^*E_{n^2}) \mathbf{x} + \varepsilon \mathbf{x}^\top E_{n^2} \mathbf{x} \\ &\geq \varepsilon \mathbf{x}^\top E_{n^2} \mathbf{x} > 0. \end{aligned}$$

From Theorem 1.13 it now follows that there exists an  $\bar{r} \in \mathbb{Z}_+$  such that  $Q_\varepsilon^* \in \mathcal{C}_{n^2}^{\bar{r}}$ .

In order to see that  $Q_\varepsilon^*$  provides a solution which gives us the optimal value of  $\mathcal{GIP}_{COP}$ , we consider the objective function of (5.7). First we denote by  $\theta$  the optimal value of  $\mathcal{GIP}_{COP}$ , i.e.  $\theta = \text{Tr}(S^*) + \text{Tr}(T^*) + n^2v^*$ . Furthermore, let

$$\theta_\varepsilon := \text{Tr}(S^*) + \text{Tr}(T^*) + n^2(v^* - \varepsilon).$$

Then, because we know from Lemma 5.7 that  $\theta \in \mathbb{Z}_+$ , we obtain by rounding that

$$\lceil \theta_\varepsilon \rceil = \lceil \text{Tr}(S^*) + \text{Tr}(T^*) + n^2v^* - n^2\varepsilon \rceil = \lceil \theta \rceil - \lceil n^2\varepsilon \rceil = \theta$$

due to the fact that  $0 < \varepsilon < \frac{1}{n^2}$ . Now, because we also know that  $Q_\varepsilon^* \in \mathcal{C}_{n^2}^{\bar{r}}$  it must hold that

$$\lceil \eta^{\bar{r}} \rceil \geq \lceil \theta \rceil.$$

This implies that

$$\theta \geq \lceil \eta^{\bar{r}} \rceil \geq \lceil \theta_\varepsilon \rceil = \theta.$$

Finally, let  $(S, T, v)$  be a feasible solution of (5.13) for some  $r \in \mathbb{Z}_+$  so that  $D - I \otimes S - T \otimes I - vE_{n^2} \in \mathcal{C}_n^r$ . Then the polynomial  $\mathbf{x}^\top (D - I \otimes S - T \otimes I - vE_{n^2}) \mathbf{x}$  has nonnegative coefficients so that for any  $X \in \mathcal{P}_n$  we have

$$0 \leq \langle D - I \otimes S - T \otimes I - vE_{n^2}, \mathbf{xx}^\top \rangle = \langle D, \mathbf{xx}^\top \rangle - (\text{Tr}(S) + \text{Tr}(T) + vn^2).$$

Then because  $\langle D, \mathbf{xx}^\top \rangle \geq 0$  it follows that  $\eta^r \geq \text{Tr}(S) + \text{Tr}(T) + vn^2 \geq 0$  for all  $r \in \mathbb{Z}_+$ . This implies that we do not need to round  $\eta^r$  to verify isomorphism. This proves our statement.  $\square$

In an attempt to obtain an explicit upper bound on  $r \in \mathbb{Z}_+$  so that we can solve the  $\mathcal{GIP}$  by computing  $\eta^r$  instead of  $\mathcal{GIP}_{\text{COP}}$  we now give the following lemma.

**Lemma 5.17.** *Given two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$ , let  $D$  and  $Q_\varepsilon^*$  be the matrices as defined in Proposition 5.16. Then*

$$\kappa := \min_{\mathbf{x} \in \Delta} \mathbf{x}^\top Q_\varepsilon^* \mathbf{x} \geq \frac{1}{n^2}.$$

*Proof.* We have

$$\begin{aligned} \kappa &= \min_{\mathbf{x} \in \Delta} \mathbf{x}^\top (D - I \otimes S^* - T^* \otimes I - (v^* - \varepsilon)E_{n^2}) \mathbf{x} \\ &= \min_{\mathbf{x} \in \Delta} \mathbf{x}^\top (D - I \otimes S^* - T^* \otimes I - v^*E_{n^2}) \mathbf{x} + \varepsilon \mathbf{x}^\top E_{n^2} \mathbf{x} \\ &\geq \min_{\mathbf{x} \in \Delta} \varepsilon \mathbf{x}^\top E_{n^2} \mathbf{x} = \frac{1}{n^2}. \end{aligned}$$

$\square$

In order to apply Corollary 5.15, we would also need an upper bound on  $L = \max_{i,j} |(Q_\varepsilon^*)_{ij}|$ . Unfortunately however we have not been able to find such an upper bound. From computational experiments we found that  $L$  can be quite large. In fact, it would seem that for the general case  $L$  is unbounded as we can always add the positive semidefinite matrix  $nI_{n^2} - E_{n^2}$  to  $Q_\varepsilon^*$  without altering copositivity of  $Q_\varepsilon^*$ , while simultaneously keeping the objective function of (5.7) unchanged. We expect that is possible to bound the problem in some manner to resolve this problem, but it does not look as if there is a straightforward way of doing so. Note, however, that the bound given in Corollary 5.15 is not tight in general. In fact, in many practical cases a much lower level of the hierarchy is sufficient than that given by Corollary 5.15.



## 5.5 Reformulating the copositive formulation

In this section we will reformulate the copositive programming problem (5.7) by investigating its dual, that is the completely positive formulation (5.8). Recall that the feasible set of (5.8), which we denoted as  $\mathcal{F}$ , can be written equivalently as in (5.6). Using this alternative definition for  $\mathcal{F}$ , we will now directly dualize this set, after which we shall substitute this dual for  $\mathcal{COP}^{n^2}$  in our copositive program (5.7). Doing this will allow us to obtain an upper bound for the copositive formulation.

**Proposition 5.18.** *Let  $\mathcal{F}_n = \text{conv} \left\{ \mathbf{y}\mathbf{y}^\top \mid \mathbf{y} = \text{Vec}(X), X \in \mathcal{P}_n \right\}$ . Then its dual cone is the set*

$$\mathcal{F}_n^* = \left\{ A \in \mathbb{S}^{n^2} \mid \langle A, \mathbf{x}\mathbf{x}^\top \rangle \geq 0 \text{ for all } \mathbf{x} = \text{Vec}(X), X \in \mathcal{P}_n \right\}. \quad (5.16)$$

*Proof.* From Definition 1.7 we know that the dual of a set  $\mathcal{F}$  is defined as

$$\mathcal{F}^* = \left\{ A \in \mathbb{S}^{n^2} \mid \langle A, Y \rangle \geq 0 \text{ for all } Y \in \mathcal{F} \right\}.$$

Next, consider the cone

$$\mathcal{H} = \left\{ A \in \mathbb{S}^{n^2} \mid \langle A, \mathbf{x}\mathbf{x}^\top \rangle \geq 0, \text{ for all } \mathbf{x} = \text{Vec}(X), X \in \mathcal{P}_n \right\}.$$

We will prove our proposition by showing that  $\mathcal{F}^* = \mathcal{H}$ . First let  $A \in \mathcal{H}$ . Then for any  $Y \in \mathcal{F}$  we can write  $Y = \sum_{X \in \mathcal{P}_n} \lambda_X \text{Vec}(X) \text{Vec}(X)^\top$  with  $\lambda_X \geq 0$  for all  $X \in \mathcal{P}_n$  and  $\sum_{X \in \mathcal{P}_n} \lambda_X = 1$ . Hence we get

$$\langle A, Y \rangle = \left\langle A, \sum_{X \in \mathcal{P}_n} \lambda_X \text{Vec}(X) \text{Vec}(X)^\top \right\rangle = \sum_{X \in \mathcal{P}_n} \lambda_X \langle A, \text{Vec}(X) \text{Vec}(X)^\top \rangle \geq 0$$

so that  $A \in \mathcal{F}^*$  and consequently  $\mathcal{H} \subseteq \mathcal{F}^*$ .

Next, suppose that  $A \in \mathcal{F}^*$ . Then  $\langle A, Y \rangle \geq 0$  for all  $Y \in \mathcal{F}$ . Observe that for  $X \in \mathcal{P}_n$  we have  $\mathbf{x}\mathbf{x}^\top \in \mathcal{F}$ . Hence

$$\langle A, \mathbf{x}\mathbf{x}^\top \rangle \geq 0 \quad \text{for all } X \in \mathcal{P}_n,$$

which implies that  $A \in \mathcal{H}$  and therefore  $\mathcal{F}^* \subseteq \mathcal{H}$ . Consequently,  $\mathcal{H} = \mathcal{F}^*$ . This completes the proof.  $\square$

Note that clearly we have  $\mathcal{F} \subset \mathcal{CP}$ . So automatically, from duality theory, we get that  $\mathcal{COP} \subset \mathcal{F}^*$ . Hence, simply replacing  $\mathcal{COP}^{n^2}$  by  $\mathcal{F}_n^*$  in (5.7) gives us an upper bound for the particular copositive program. In fact, as it turns out, these two conic optimization problems are in some sense equivalent. By equivalent, in this case, we mean that both problems return nonnegative values while the optimal solution is equal to 0 if and only if the two underlying graphs are isomorphic. We formally state this result in the following theorem.

**Theorem 5.19** (*GLP over  $\mathcal{F}^*$* ). *Consider any two graphs  $G_1$  and  $G_2$  with adjacency matrices  $A$  and  $B$  respectively, and let  $D$  be defined as in Lemma 5.3. Then consider the following problem*

$$\max_{S, T \in \mathbb{S}^n, v \in \mathbb{R}} \left\{ \text{Tr}(S) + \text{Tr}(T) + vn^2 \mid D - I \otimes S - T \otimes I - vE_{n^2} \in \mathcal{F}^* \right\}, \quad (5.17)$$

which we denote as  $\mathcal{GLP}_{\mathcal{P}}$ . Then the optimal value of  $\mathcal{GLP}_{\mathcal{P}}$  is equal to 0 if and only if  $G_1$  is isomorphic to  $G_2$ .

*Proof.* Due to the fact that  $\mathcal{COP}^{n^2} \subseteq \mathcal{F}^*$  the optimal value of  $\mathcal{GLP}_{\mathcal{P}}$  is an upper bound for the optimal value of (5.7) and is therefore nonnegative. Now let  $(S, T, v)$  be a feasible solution of (5.17) and let  $X \in \mathcal{P}_n$ . Then

$$0 \leq \langle D - I \otimes S - T \otimes I - vE_{n^2}, \mathbf{xx}^T \rangle = \langle D, \mathbf{xx}^T \rangle - (\text{Tr}(S) + \text{Tr}(T) + vn^2)$$

or equivalently

$$\langle D, \mathbf{xx}^T \rangle \geq (\text{Tr}(S) + \text{Tr}(T) + vn^2). \quad (5.18)$$

An important observation is that the expression in the right-hand side of (5.18) (which define the feasible set of (5.17)) is also the objective function of (5.17).

Now assume that  $G_1$  is isomorphic to  $G_2$ . From Lemma 5.3 we know that in this case there exists an  $X \in \mathcal{P}_n$  for which  $\langle D, \mathbf{xx}^T \rangle = 0$  so that automatically from (5.18) we know that the optimal value of  $\mathcal{GLP}_{\mathcal{P}}$  is at most 0. Then, because  $S = T = 0$ ,  $v = 0$  defines a feasible solution to (5.17) this must in fact be an optimal solution to (5.17).

Next, assume that  $G_1$  and  $G_2$  are not isomorphic. Then by Lemma 5.3 we know that  $\langle D, \mathbf{xx}^T \rangle > 0$  for every  $X \in \mathcal{P}_n$ . Then  $S = T = 0$  and  $v = \frac{1}{n^2} \min_{X \in \mathcal{P}_n} \langle D, \mathbf{xx}^T \rangle$  is a feasible solution of (5.17) with positive objective value, and hence the optimal value of  $\mathcal{GLP}_{\mathcal{P}}$  is strictly positive. This finishes the proof.  $\square$

Observe that in the proof of Theorem 5.19 explicit feasible solutions are given both when  $G_1$  and  $G_2$  are isomorphic as well when they are non-isomorphic.

Moreover, these solutions are both nonnegative irrespective of  $D$  and  $X \in \mathcal{P}_n$  so that w.l.o.g. we can assume for (5.17) that  $S, T \geq 0$  and  $v \geq 0$ . Finally, because the right-hand side of the inequality (5.18) is independent of both  $X \in \mathcal{P}_n$  as well as  $D$  we can simply substitute  $\text{Tr}(S) + \text{Tr}(T) + vn^2$  by a single nonnegative variable  $\gamma$ , i.e. both  $(\langle I \otimes S - T \otimes I - vE_{n^2}, \mathbf{xx}^\top \rangle)$  in the matrix constraint as well as the objective of (5.17).

More importantly, because  $\mathcal{COP} \subset \mathcal{F}^*$ , Theorem 5.19 implies that we can substitute the copositive cone in (5.7) by any cone  $\mathcal{B} \subseteq \mathbb{R}^{n^2 \times n^2}$  that satisfies  $\mathcal{COP} \subseteq \mathcal{B} \subset \mathcal{F}^*$ . In particular if there exists such a cone that, moreover is tractable, then  $\mathcal{GIP}$  is in P. This presents us with the following interesting open problem.

**Open Problem 5.20.** *Let*

$$\mathcal{F}_n^* = \left\{ A \in \mathbb{S}^{n^2} \mid \langle A, \mathbf{xx}^\top \rangle \geq 0, \text{ for all } \mathbf{x} = \text{Vec}(X), X \in \mathcal{P}_n \right\}.$$

*Does there exist a computationally tractable cone  $\mathcal{B}_n \subseteq \mathbb{R}^{n^2 \times n^2}$  such that  $\mathcal{COP}^{n^2} \subseteq \mathcal{B}_n \subset \mathcal{F}_n^*$ ? If so, this would imply that  $\mathcal{GIP}$  is solvable in polynomial time.*

Note that the inequalities  $\langle A, \mathbf{xx} \rangle \geq 0$ ,  $X \in \mathcal{P}_n$  define supporting hyperplanes for the copositive cone. In other words  $\mathcal{COP}^{n^2}$  and  $\mathcal{F}_n^*$  share parts of their boundaries. In particular, their boundaries touch at an exponential number (in  $n$ ) of points. This seems to suggest that it will be difficult to create a cone  $\mathcal{B}_n$  as suggested in Open Problem 5.20, particularly one for which verifying membership is tractable. However, from Proposition 5.16 we know that there exist finite levels  $\bar{r} \in \mathbb{Z}_+$  for each of the hierarchies  $\mathcal{C}_n^r$ ,  $\mathcal{Q}_n^r$ , and  $\mathcal{K}_n^r$ , that can be used to construct approximations to the copositive formulation (5.7) that are in fact sufficient to decide the graph isomorphism problem. Hence a sufficient certificate for  $\mathcal{GIP}$  to be in P would be a tractable cone  $\mathcal{B}_n$  such that, say  $\mathcal{C}_n^{\bar{r}} \subseteq \mathcal{B}_n \subseteq \mathcal{F}_n^*$ . Whether such a construction is possible seems to depend largely on the upper bound one can obtain for  $\bar{r}$  and the geometry of the cones  $\mathcal{C}_n^r$ ,  $\mathcal{Q}_n^r$ , and  $\mathcal{K}_n^r$ .