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The maximum common edge subgraph problem: A polyhedral investigation

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ABSTRACT

In the Maximum Common Edge Subgraph Problem (MCES), given two graphs G and H with the same number of vertices, one has to find a common subgraph of G and H (not necessarily induced) with the maximum number of edges. This problem arises in parallel programming environments, and was first defined in Bokhari (1981) [2]. This paper presents a new integer programming formulation for the MCES and a polyhedral study of this model. Several classes of valid inequalities are identified, most of which are shown to define facets. These findings were incorporated into a branch&cut algorithm we implemented. Experimental results with this algorithm are reported.

1. Introduction

It is necessary in many applications to compare objects represented as graphs and to determine the degree of the similarity between them. This is often accomplished by formulating the problem as the one involving the maximum common subgraph between the graphs being considered. We investigate here the following version of the maximum common subgraph problem.

Maximum Common Edge Subgraph Problem (MCES):
Given: two connected graphs G and H with $E_G \neq \emptyset$, $E_H \neq \emptyset$ and $|V_G| = |V_H|$.
Find: a common subgraph of G and H, not necessarily an induced one, whose number of *edges* is maximum.

In this paper, graphs are assumed to be simple, finite and undirected. We denote by V_G (resp. E_G) the set of vertices (resp. edges) of a given graph G.

The MCES problem was introduced by Bokhari in [2]. Since the MCES problem is often associated with task assignment issues in parallel programming applications in distributed memory environments, G is usually referred to as the *task interaction graph*, and H as the *processors graph*. Vertices in G represent tasks of a parallel application and its edges join pairs of tasks with communication demands. As for graph H, the vertices represent processors and an edge joining two of these vertices is present in H whenever the corresponding processors are directly connected through a communication channel. We note that two processors directly connected through a communication channel are able to exchange messages without incurring routing overhead. The problem consists of assigning (mapping) each task to one processor in such a way

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that the number of neighboring tasks assigned to connected processors is maximized. It should be noted that each task is assigned to exactly one processor, and that each processor can host only one task. This problem, thus, models the situation where many tasks are simultaneously running, and each one must be attached to one processor, in such a way that the communication costs are minimized. It should be also mentioned that MCES models the task assignment problem under the assumption that the flow of messages is homogeneous among the edges of the task graph (otherwise, some kind of weighted version of the MCES problem would be more appropriate).

Another motivating application of the MCES problem comes from the fact that similarity between the graphs representing molecules plays an important role in many aspects of chemistry and biology. Particularly, the maximum common subgraph problems have become increasingly important in matching 2 and 3-dimensional chemical structures. Raymond and Willett [13], Raymond et al. [14,15] provide a classification and a review of many maximum common subgraph algorithms, both exact and approximate, and make recommendations regarding their applicability to typical chemoinformatic tasks.

The MCES problem is also of particular interest since it trivially generalizes several problems on graphs, including the well-known graph isomorphism problem. Indeed, when G and H have the same number of edges, there exists a common subgraph with $|E_G|$ edges, if and only if, G and H are isomorphic.

Note that if $|V_G| \neq |V_H|$, a suitable number of dummy vertices have to be inserted into the smaller graph in order to obtain an instance of MCES. Besides, to be in accordance with the problem definition which requires the connectivity of the input graphs, we can choose one of the original vertices of the graph and add new edges from this vertex to all the dummy ones. But then, we have to consider again a weighted version of the MCES in which to mappings involving these new edges we assign an appropriate negative weight while to all other mappings we assign unitary weights.

If $|V_G|$ and $|V_H|$ are not required to be equal, we obtain a problem which is APX-hard [6], while the MCES problem is only known to be NP-hard (and it remains NP-hard when restricted to processor graphs that are grids with 4 neighbors per node) [8].

We suppose in this paper that the graphs G and H are connected. More precisely, we only allow trivial components that arise by adding dummy vertices, that is, isolated vertices, to the problem in order to force that G and H have the same number of vertices.

Since MCES is NP-hard and has some important applications, there have been many attempts to devise useful algorithms for MCES. Some of them approximate the solution of the MCES problem, while others give the exact solution for a specialized set of graphs or graphs of moderate size. But most of the approaches to MCES propose heuristic procedures intended for particular architectures [2,4,5,15].

In the present work, integer programming techniques are applied to the MCES problem, aiming at the implementation of a branch&cut (**B**&**C**) algorithm for its resolution. To the best of our knowledge, the only polyhedral study of the MCES problem so far was done by Marenco [8,10,9,11]. We present in Section 2 basic results obtained by this author.

In Section 3, we present a new integer programming formulation for the MCES problem, and in Section 4 some valid inequalities and facets that we identified for the corresponding polytope. Finally, in Section 5 we describe our implementation of the **B**&**C** algorithm for the MCES problem, and the computational results obtained.

Basic definitions and notations. For a given vertex i in a graph G, $N(i)$ denotes the set of all its neighbors and $d_G(i)$ denotes the degree of i in G. For a given subset I of vertices of a graph G, $\delta(I)$ denotes the set of all edges in G that are incident to at least one vertex of I. We say that an edge from $\delta(I)$ is *incident* to I. A *z-cycle* is a cycle with z edges. A *vertex cover* of a graph G is a subset U of its vertices such that each edge has at least one endpoint in U.

2. Previous polyhedral study

Integer programming formulation presented by Marenco [8] for the MCES problem has variables y_{ik}, for $i \in V_G$, $k \in V_H$, which are 1 in a feasible solution if i is mapped to k, and 0 otherwise. Furthermore, his model also has variables x_{ij}, for $ij \in E_G$, which are 1 if there exists $kl \in E_H$ such that i is mapped to k and j to l, and 0 otherwise. We present now the integer programming model proposed by Marenco [8].

$$\max \sum_{ij\in E_G} x_{ij} \tag{1}$$

$$\sum_{k\in V_H} y_{ik} = 1, \quad \forall i \in V_G \tag{2}$$

$$\sum_{i\in V_G} y_{ik} = 1, \quad \forall k \in V_H \tag{3}$$

$$x_{ij} + y_{ik} \leq 1 + \sum_{l\in N(k)} y_{jl}, \quad \forall ij \in E_G, \forall k \in V_H \tag{4}$$

$$y_{ik} \in \{0, 1\}, \quad \forall i \in V_G, \forall k \in V_H \tag{5}$$

$$x_{ij} \in \{0, 1\}, \quad \forall ij \in E_G. \tag{6}$$

In the above formulation, Eq. (2) forces that every vertex of G is mapped to exactly one vertex of H. Eq. (3) forces that for every vertex of H, there is exactly one vertex of G mapped to it.

Consider now inequality (4). Let ij be a fixed edge in G, and k a fixed vertex from H. If $y_{ik} = 0$, then the constraint (4) is trivially satisfied. On the other hand, if $y_{ik} = 1$, then the constraint (4) has the form $x_{ij} \leq \sum_{l \in N(k)} y_{jl}$. Thus, if there is no neighbor l of k such that j is mapped to l, then $x_{ij} = 0$. Note that the variable x_{ij} appears in the objective function (1) with a positive coefficient, and that the x variables are mutually independent. Thus, in the optimum, every x_{ij} which can take value 1 will do that. So, when $y_{ik} = 1, x_{ij} = 1$ whenever $\sum_{l \in N(k)} y_{jl} = 1$, i.e., if j is mapped to a neighbor of k. Then, despite the fact that the formulation allows x_{ij} to be set to zero when $y_{ik} = 1$, we do not need a constraint to eliminate this solution since it will not be optimal.

Define now S as the set of feasible integer solutions of the problem, and let $\text{conv}(S)$ be its convex hull. Marenco [8] showed that $\dim(\text{conv}(S)) = (|V_G| - 1)^2 + |E_G|$. We now present the main results of the polyhedral investigations carried out in [8], that we will refer to later in the text.

The following inequality that involves degrees of vertices is valid for $\text{conv}(S)$.

$$\sum_{j \in N(i)} x_{ij} \leq \sum_{k \in V_H} \min\{d_G(i), d_H(k)\} y_{ik}, \quad \text{for all } i \in V_G. \tag{7}$$

Let U be a vertex cover of graph H. Then, the following inequality is valid for $\text{conv}(S)$ and, furthermore, it defines a facet if U is a minimal vertex cover of H.

$$x_{ij} \leq \sum_{u \in U} (y_{iu} + y_{ju}), \quad \text{for all } ij \in E_G. \tag{8}$$

Let now ij be a fixed edge in G, and k be a fixed vertex from H. Consider inequality

$$x_{ij} \leq \sum_{l \in N(k)} y_{jl}.$$

The above inequality defines a facet of $\text{conv}(S')$, where $S' := S \cap \{(y, x) : y_{ik} = 1\}$, i.e., of the set of feasible integer solutions that satisfy $y_{ik} = 1$. Instead of considering points with restriction $y_{ik} = 1$, one can think of these points as subject to equivalent conditions $y_{i'k} = y_{ik'} = 0$, for $i' \neq i$ and $k' \neq k$. Thus, lifting can be performed on these $2|V_G| - 1$ variables, obtaining the inequality below which defines a facet of $\text{conv}(S)$.

$$x_{ij} \leq \sum_{k' \in N(k)} y_{jk'} + \sum_{i' \neq i} y_{i'k} + \sum_{s \neq k} \psi_s y_{is}. \tag{9}$$

In the above inequality, for k a fixed vertex in H, and all $s \in V_H, s \neq k$, the lifted coefficient ψ_s is defined as follows:

$$\psi_s := \begin{cases} -1 & \text{if } N(s) \subseteq N(k) \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

3. A new integer programming formulation

The main idea of our new model is to create variables that represent the assignment of edges of G to the edges of H. More formally, apart from variables y_{ik} that are defined as mentioned in Section 2, we also include variables c_{ijkl}, for all $ij \in E_G$ and $kl \in E_H$ which are 1 if ij is mapped to kl, and 0 otherwise. With these definitions, we are in a position to present our integer programming model for the MCES problem.

$$\max \sum_{ij \in E_G} \sum_{kl \in E_H} c_{ijkl} \tag{11}$$

$$\sum_{k \in V_H} y_{ik} \leq 1, \quad \forall i \in V_G \tag{12}$$

$$\sum_{i \in V_G} y_{ik} \leq 1, \quad \forall k \in V_H \tag{13}$$

$$\sum_{kl \in E_H} c_{ijkl} \leq \sum_{k \in V_H} y_{ik}, \quad \forall ij \in E_G \tag{14}$$

$$\sum_{ij \in E_G} c_{ijkl} \leq \sum_{i \in V_G} y_{ik}, \quad \forall kl \in E_H \tag{15}$$

$$\sum_{j \in N(i)} c_{ijkl} \leq y_{ik} + y_{il}, \quad \forall i \in V_G, \forall kl \in E_H \tag{16}$$

$$\sum_{l\in N(k)} c_{ijkl} \le y_{ik} + y_{jk}, \quad \forall ij \in E_G, \forall k \in V_H \tag{17}$$

$$c_{ijkl} \in \{0, 1\}, \quad \forall ij \in E_G, \forall kl \in E_H \tag{18}$$

$$y_{ik} \in \{0, 1\}, \quad \forall i \in V_G, \forall k \in V_H. \tag{19}$$

Inequalities (12) and (13) force that every vertex of G is mapped to at most one vertex of H; and that for every vertex of H, there is at most one vertex of G mapped to it. Similar inequalities for edges are in (14) and (15). Inequality (16) forces that for a fixed vertex i from G and a fixed edge kl from H, if some edge incident to i is mapped to kl, then i is mapped either to k or to l (inequality (17) is analogous).

Notice that (12) and (13) are written in the inequality form, which means that we work with a monotonous model. As seen in the next section, the proofs of facet-defining inequalities become substantially easier in this model than in the one given in [8]. This is because the monotone polytope associated with the above formulation can be shown to be full-dimensional. Despite the fact we had loosened these constraints, due to the nature of the objective function, it is not difficult to see that if we switch them to the equality form, the optimum will not change.

Before discussing the dimension of the monotone polytope we introduce a notation used not only in the proof that follows but also in the next section. In the literature, an e-vector on a t-dimensional space usually denotes a vector having one component equals to one and all remaining components equal to zero. Moreover, the vector denoted by e_i is an e-vector for which the i-th component is one. In the context of the MCES, the e-vectors are specified by two or four indices. A two-index e-vector refers to the assignment of a vertex of V_G to a vertex in V_H. Similarly, a four-index e-vector refers to the assignment of an edge in E_G to an edge in E_H. For example, e_{ul} denotes the mapping of vertex u from V_G to vertex l from V_H, and e_{ijkl} denotes the mapping of edge ij from E_G to edge kl from E_H.

Theorem 1. *The monotone polytope P associated with the monotonous formulation (11)–(19) is full-dimensional.*

Proof. To prove this result we show that an $H = \{(c, y) \in \mathbb{R}^{|E_G|\times|E_H|+|V_G|\times|V_H|} : \pi c + \beta y = \beta_0\}$ hyperplane containing P must be of the form $0c + 0y = 0$ (i.e., the only affine space containing P is $\mathbb{R}^{|E_G|\times|E_H|+|V_G|\times|V_H|}$). We do that by plugging some points (c, y) of P into the equation $\pi c + \beta y = \beta_0$ and deriving the values of the components of vectors π and β and that of β_0.

First notice that the null vector belongs to P, which implies that $\beta_0 = 0$. Moreover, the unique assignment of a vertex i in V_G to a vertex k in V_H corresponds to a point $(0, e_{ik})$ which belongs to P. Since P is contained in the hyperplane H, we must have that $(\pi, \beta)(0, e_{ik})^T = \beta_0 = 0$ or, in other words, $\beta_{ik} = 0$. As the vertices i and k were chosen arbitrarily, we conclude that β is the null vector.

Now, the unique assignment of an edge ij in E_G to an edge kl in E_H gives rise to a solution $(e_{ijkl}, e_{ik} + e_{jl})$ belonging to P. Plugging this solution into the equation $\pi c + \beta y = \beta_0$ and, using the fact that $\beta = 0$ and that $\beta_0 = 0$, we end up with $\pi_{ijkl} = 0$. Again, as the edges ij and kl were chosen arbitrarily, we derive that π is null. This completes the proof. □

4. Valid inequalities and facets of the polytope *P*

We present in this section some valid inequalities and facets that we found for the polytope P given by the convex hull of the integer solutions of the integer programming model (11)–(19). The proofs, based on standard techniques from Polyhedral Combinatorics, are sketched in the text. In all of them, we assume the existence of a generic face $\tilde{F}$ of P given by:

$$\tilde{F} := \{(c, y) \in P : \pi c + \beta y = \pi_0\}. \tag{20}$$

Initially, we show two simple facts that we use in the proof of Theorem 11, but that are also interesting for its own sake. Namely, Lemmas 1 and 2 show that inequalities (16) and (17) from the model force that if ij is mapped to kl, then i is mapped to k and j to l, or vice versa.

Lemma 1. *Let ij be an edge in G, and kl an edge in H. If $c_{ijkl} = 1$, then $y_{ik} = 1$ or $y_{il} = 1$.*

Proof. From (12) and (16) we have $1 = c_{ijkl} \le \sum_{j\in N(i)} c_{ijkl} \le y_{ik} + y_{il} \le 1$. □

Lemma 2. *Let ij be an edge in G, and kl an edge in H. If $c_{ijkl} = 1$ and $y_{ik} = 1$, then $y_{jl} = 1$.*

Proof. From (16) we have $1 = c_{ijkl} \le \sum_{i\in N(j)} c_{jikl} \le y_{jk} + y_{jl}$. Now, since $y_{ik} = 1$, from (13) it follows that $y_{jk} = 0$, and thus $y_{jl} = 1$. □

Corollary 2. *Let ij be an edge in G. If $\sum_{pl\in E_H} c_{ijpl} = 1$ and $y_{iw} = 1$ for $w \in V_H$, then $\sum_{w'\in N(w)} y_{jw'} = 1$, i.e., j is mapped to a neighbor of w in H.*

Proof. Let $p'l'$ be the edge such that $c_{ijp'l'} = 1$. Now, using (16), we have $1 = c_{ijp'l'} \le \sum_{j\in N(i)} c_{ijp'l'} \le y_{ip'} + y_{il'}$. Since $y_{iw} = 1$, from (12) we get that $p' = w$ or $l' = w$. Suppose, without loss of generality, that $p' = w$. From Lemma 2 we thus have that $y_{jl'} = 1$. Hence, $\sum_{w'\in N(w)} y_{jw'} = 1$. □

The following two theorems show that inequalities (14)–(17) define facets.

Theorem 3. *Inequalities (14) and (15) from the model are facet-defining.*

Proof. Consider first inequality (14). Let ij be a fixed edge from G. We define $F := \{(c, y) \in P : (c, y)$ satisfies (14) at equality$\}$. Suppose that $F \subseteq \tilde{F}$ with $\tilde{F}$ given as in (20). Then, we have that F defines a facet, if and only if,

$$(\pi c + \beta y \leq \pi_0) = \alpha \left(\sum_{kl \in E_H} c_{ijkl} - \sum_{k \in V_H} y_{ik} \leq 0 \right), \quad \text{for an } \alpha > 0. \tag{21}$$

We first note that $0 \in F$, and thus, $\pi_0 = 0$.

Let $u \in V_G$, $u \neq i$, and $l \in V_H$. Note that the point $(0, e_{ul})$ is feasible, that is, it satisfies (11)–(19). Besides, this point is in F and since $F \subseteq \tilde{F}$, we have that $(0, e_{ul}) \in \tilde{F}$. Thus, $\pi 0 + \beta e_{ul} = \pi_0 = 0$, that is,

$$\beta_{ul} = 0, \quad \text{for all } u \in V_G, u \neq i, \text{ and all } l \in V_H. \tag{22}$$

Let now $kl \in E_H$. Note that the point $(e_{ijkl}, e_{ik} + e_{jl})$ is feasible. Besides, this point is in F and since $F \subseteq \tilde{F}$, we have that $\pi_{ijkl} + \beta_{ik} + \beta_{jl} = 0$. From (22) we have that $\beta_{jl} = 0$. Thus,

$$\pi_{ijkl} + \beta_{ik} = 0. \tag{23}$$

Note that the point $(e_{ijkl}, e_{il} + e_{jk})$ is also feasible and is in F. Similarly as above, using (22) we get

$$\pi_{ijkl} + \beta_{il} = 0. \tag{24}$$

Now, from (23) and (24) we have that $\beta_{ik} = \beta_{il}$. Observe that this equality is valid for every $kl \in E_H$. Since the graph H is connected, we can conclude that the values of β_{ik}, for all $k \in V_H$ are equal. Indeed, we could consider another edge incident to k, say kl', and conclude analogously as above that $\beta_{ik} = \beta_{il'}$. Hence, $\beta_{ik} = \beta_{il} = \beta_{il'}$. Continuing, we would obtain that β_{ik}, for all k in V_H are equal. Hence, from (21) it follows that all those values are equal to $-\alpha$, that is,

$$\beta_{ik} = -\alpha, \quad \text{for all } k \in V_H. \tag{25}$$

We already saw that $\pi_{ijkl} + \beta_{ik} = 0$ for all $kl \in E_H$ (inequality (23)). From (25) we thus have $\pi_{ijkl} = \alpha$, for all $kl \in E_H$.

Let now $uv \in E_G$ be such that uv is not incident to i, and $kl \in E_H$. Note that the point $(e_{uvkl}, e_{uk} + e_{vl})$ is feasible. Besides, this point is in F, and thus, $\pi_{uvkl} + \beta_{uk} + \beta_{vl} = 0$. From (22) we have that $\beta_{vl} = \beta_{uk} = 0$. Thus,

$$\pi_{uvkl} = 0, \quad \text{for all } uv \in E_G \text{ such that } u, v \neq i \text{ and for all } kl \in E_H. \tag{26}$$

Finally, if $d_G(i) > 1$, let $j' \in N(i)$ such that $j' \neq j$. Let furthermore $kl \in E_H$. We can of course suppose that at least one endpoint of edge kl has degree greater than 1 (otherwise, since H is connected, the MCES problem would be trivial). Suppose that $d_H(k) > 1$, and let l' be a neighbor of k in H such that $l' \neq l$. Then the point $(e_{ijkl'} + e_{ij'kl}, e_{ik} + e_{jl'} + e_{j'l})$ is feasible and is in F. Thus, $\pi_{ijkl'} + \pi_{ij'kl} + \beta_{ik} + \beta_{jl'} + \beta_{j'l} = 0$. From (22) we have that $\beta_{jl'} = \beta_{j'l} = 0$. Furthermore, by inequality (23), $\pi_{ijkl} + \beta_{ik} = 0$ for all $kl \in E_H$. In special thus, $\pi_{ijkl'} + \beta_{ik} = 0$. Hence, we have that $\pi_{ij'kl} = 0$. Since j' and kl have been chosen arbitrarily, we conclude that $\pi_{ij'kl} = 0$, for all $kl \in E_H$ and $j' \in N(i)$ such that $j' \neq j$.

The proof that inequality (15) from the model defines a facet is analogous. □

Theorem 4. *Inequalities (16) and (17) from the model are facet-defining.*

Proof. Consider inequality (16). Let i be a fixed vertex from G, and kl a fixed edge from H. We define $F := \{(c, y) \in P : (c, y)$ satisfies (16) at equality$\}$. Suppose that $F \subseteq \tilde{F}$ with $\tilde{F}$ given as in (20). Then, we have that F defines a facet, if and only if,

$$(\pi c + \beta y \leq \pi_0) = \alpha \left(\sum_{j \in N(i)} c_{ijkl} - y_{ik} - y_{il} \leq 0 \right), \quad \text{for an } \alpha > 0. \tag{27}$$

We first note that $0 \in F$, and thus, $\pi_0 = 0$.

Similarly as in the proof of (22) from Theorem 3, we get

$$\beta_{up} = 0, \quad \text{for all } u \in V_G \text{ such that } u \neq i, \text{ and all } p \in V_H. \tag{28}$$

Now let $p \in V_H$, such that $p \neq l$, $p \neq k$. The point $(0, e_{ip})$ is feasible and is in F. Since $F \subseteq \tilde{F}$, we have that $(0, e_{ip}) \in \tilde{F}$. Thus, $\pi 0 + \beta e_{ip} = \pi_0 = 0$, that is,

$$\beta_{ip} = 0, \quad \text{for all } p \in V_H, \text{ such that } p \neq l, k. \tag{29}$$

Let now $j \in N(i)$. The point $(e_{ijkl}, e_{ik} + e_{jl})$ is feasible and is in F. Thus, $\pi_{ijkl} + \beta_{ik} + \beta_{jl} = 0$. From (28), $\beta_{jl} = 0$. Hence,

$$\pi_{ijkl} + \beta_{ik} = 0. \tag{30}$$

Analogously, the point $(e_{ijkl}, e_{il} + e_{jk})$ is feasible and is in F. Again, from (28), $\beta_{jk} = 0$. Hence,

$$\pi_{ijkl} + \beta_{il} = 0. \tag{31}$$

Now, from (30) and (31) we have that $\beta_{ik} = \beta_{il}$. From (27) we conclude that

$$\beta_{ik} = \beta_{il} = -\alpha. \tag{32}$$

Since vertex j has been chosen arbitrarily from $N(i)$, equalities (30) and (32) imply that $\pi_{ijkl} = \alpha$, for all $j \in N(i)$.

Similarly as in the proof of (26) from Theorem 3, we have $\pi_{uvpw} = 0$, for $uv \in E_G$ such that $u, v \neq i$, and all $pw \in E_H$.

Finally, let $j \in N(i)$, and pw an edge from H such that $pw \neq kl$. Then, of course, at least one endpoint of pw is neither k nor l. We suppose, without loss of generality, that $p \neq k, l$. The point $(e_{ijpw}, e_{ip} + e_{jw})$ is feasible and is in F. Thus, $\pi_{ijpw} + \beta_{ip} + \beta_{jw} = 0$. From (29) we have that $\beta_{ip} = 0$ and from (28) we have that $\beta_{jw} = 0$. Hence, $\pi_{ijpw} = 0$, for all $j \in N(i)$, and all $pw \in E_H$ such that $pw \neq kl$.

The proof that inequality (17) from the model defines a facet is analogous. $\square$

We show next that a counterpart of inequality (7) can be strengthened in our model. Inequalities so obtained involve mapping of "stars". That is, for any two fixed vertices $i \in V_G$ and $k \in V_H$, and sets $I \subseteq N(i)$, $K \subseteq N(k)$, we estimate the number of edges ij such that $j \in I$ that can be mapped to edges kl from H such that $l \in K$. Inequalities that we obtained involve the cardinality of sets I and K, and are presented in the next theorem.

Theorem 5. *Let i be a fixed vertex from G, k a fixed vertex from H, $I \subseteq N(i)$ and $K \subseteq N(k)$. Then, the following inequalities are valid.*

$$\sum_{j\in I}\sum_{l\in K} c_{ijkl} \leq \min\{|I|, |K|\}y_{ik} + \sum_{p\in K} y_{ip}, \tag{33}$$

$$\sum_{j\in I}\sum_{l\in K} c_{ijkl} \leq \min\{|I|, |K|\}y_{ik} + \sum_{p\in I} y_{pk}. \tag{34}$$

Furthermore, if $|I| < |K|$ and $|I| \geq 2$, then inequality (33) defines a facet, and if $|I| > |K|$ and $|K| \geq 2$, then inequality (34) defines a facet.

Note: the special case of the above theorem is, of course, when $I = N(i)$ and $K = N(k)$. Inequality (33) for example, then, becomes

$$\sum_{j\in N(i)}\sum_{l\in N(k)} c_{ijkl} \leq d_G(i)y_{ik} + \sum_{p\in N(k)} y_{ip}, \quad \text{if } d_G(i) \leq d_H(k).$$

Proof. We first prove that (33) is valid. Note that, if $c_{ijkl} = 0$ for every $j \in I$ and $l \in K$, the inequality is trivially satisfied, since the right hand side of (33) is always greater or equal to zero. Suppose now that i is mapped to k. Then, the number of edges ij with $j \in I$ that can be mapped to edges kl from H such that $l \in K$ is at most $\min\{|I|, |K|\}$ (see Fig. 1(a)). Hence, $\sum_{j\in I}\sum_{l\in K} c_{ijkl} \leq \min\{|I|, |K|\} \leq \min\{|I|, |K|\}y_{ik} + \sum_{p\in K} y_{ip}$, and inequality (33) is satisfied. If, however, i is mapped to a vertex $k' \in V_H$ such that $k' \neq k$, then the value of $\sum_{j\in I}\sum_{l\in K} c_{ijkl}$ is at most 1. Note, furthermore, that if $\sum_{j\in I}\sum_{l\in K} c_{ijkl} = 1$ then i must be mapped to a vertex from K, that is, $k' \in K$, and some $j \in I$ must be mapped to k (see Fig. 1(b)). Thus, we have that $\sum_{p\in K} y_{ip} = 1$. Hence, $1 = \sum_{j\in I}\sum_{l\in K} c_{ijkl} = \sum_{p\in K} y_{ip} \leq \min\{|I|, |K|\}y_{ik} + \sum_{p\in K} y_{ip}$, and the inequality is again satisfied.

We now prove that inequality (33) defines a facet if $|I| < |K|$. Let $F := \{(c, y) \in P : (c, y) \text{ satisfies (33) at equality}\}$. Suppose that $F \subseteq \tilde{F}$. Again we assume that $\tilde{F}$ is given as in (20). Then, we have that F defines a facet, if and only if,

$$(\pi c + \beta y \leq \pi_0) = \alpha\left(\sum_{j\in I}\sum_{l\in K} c_{ijkl} - |I|y_{ik} - \sum_{p\in K} y_{ip} \leq 0\right), \quad \text{for an } \alpha > 0. \tag{35}$$

We first note that $0 \in F$, and thus, $\pi_0 = 0$. Similarly as in the proof of (22) from Theorem 3, we get

$$\beta_{ul} = 0, \quad \text{for all } u \in V_G \setminus i, \text{ and all } l \in V_H. \tag{36}$$

Furthermore, similarly as in the proof of (26) from Theorem 3, we have $\pi_{uvpl} = 0$, for $uv \in E_G$ such that $u, v \neq i$, and for any $pl \in E_H$.

Now, define $[K]$ to denote $K \cup \{k\}$ and let $k' \in V_H \setminus [K]$. The point $(0, e_{ik'})$ is feasible and is in F. Since $F \subseteq \tilde{F}$, we have that

$$\beta_{ik'} = 0, \quad \text{for } k' \in V_H \setminus [K]. \tag{37}$$

Let $j \in N(i)$, and $pl \in E_H$ such that $p \notin [K]$. The point $(e_{ijpl}, e_{ip} + e_{jl})$ is feasible and is in F. From (37) we have that $\beta_{ip} = 0$, and from (36) we have that $\beta_{jl} = 0$. Hence, $\pi_{ijpl} = 0$, for $j \in N(i)$, $pl \in E_H$ such that $p \notin [K]$.

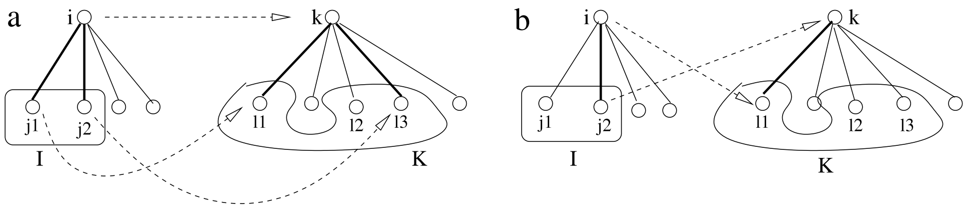

Fig. 1. (a) Case when $y_{ik} = 1$. In this example, edge ij_1 (resp. ij_2) is mapped to kl_1 (resp. kl_3). Note that the number of edges ij for $j \in I$ that can be mapped to edges kl for $l \in K$ is at most $2 = |I|$. (b) Case when i is mapped to a vertex from K (in this case, vertex l_1) and a vertex from I (in this case j_2) is mapped to k.

Since $|I| < |K|$, we can rename vertices in V and H in such a way that $I = \{1, 2, \ldots, p\}$ and $K = \{1', 2', \ldots, p', \ldots, q'\}$, with $q' \geq (p+1)'$. That is, we just rename the vertices in I and K according to an arbitrary order in such a way that the rank in these orders defines a natural one-to-one correspondence between I and an appropriate subset of K. Before we continue, we should mention that despite this renaming of the vertices, i and k are still used in the sequel to denote the vertices cited in the theorem's statement.

If $I \neq N(i)$, then let $j \in N(i) \setminus I$. Observe that by mapping all edges ix to kx', for all $x \in \{1, 2, \ldots, p\}$, and edge ij to $k(p+1)'$ we obtain a point that satisfies (33) at equality. That is, the point $(e_{i1k1'} + \cdots + e_{ipkp'} + e_{ijk(p+1)'}, e_{ik} + e_{11'} + \cdots + e_{pp'} + e_{j(p+1)'})$ is feasible and is in F. Hence,

$$\pi_{i1k1'} + \cdots + \pi_{ipkp'} + \pi_{ijk(p+1)'} + \beta_{ik} + \beta_{11'} + \cdots + \beta_{pp'} + \beta_{j(p+1)'} = 0. \tag{38}$$

But also, mapping all edges as above, except for ij to $k(p+1)'$, results in a point that satisfies (33) at equality. Hence, $(e_{i1k1'} + \cdots + e_{ipkp'}, e_{ik} + e_{11'} + \cdots + e_{pp'})$ is feasible and is in F, that is,

$$\pi_{i1k1'} + \cdots + \pi_{ipkp'} + \beta_{ik} + \beta_{11'} + \cdots + \beta_{pp'} = 0. \tag{39}$$

From (36), $\beta_{j(p+1)'} = 0$, and thus, by subtracting (39) from (38), we obtain that $\pi_{ijk(p+1)'} = 0$. Observe that we could map edges ix, for $x \in \{1, 2, \ldots, p\}$ to different edges that are incident to both k and K. For example, we could map ix to kx', for all $x \in \{1, 2, \ldots, p-1\}$, edge ij to kp', and ip to $k(p+1)'$. Analogously as above we would get that $\pi_{ijkp'} = 0$. We can conclude thus that $\pi_{ijkl} = 0$, for all $j \in N(i) \setminus I$ and $l \in K$.

We now observe that the points $(e_{i1k1'}, e_{i1'} + e_{1k}), (e_{i2k1'}, e_{i1'} + e_{2k}), \ldots, (e_{ipk1'}, e_{i1'} + e_{pk})$ are feasible and are in F. That is, mapping edges ix to $k1'$ (where $x \in \{1, 2, \ldots, p\}$), vertex i to $1'$, and x to k results in a point that satisfies (33) at equality. From (36), $\beta_{1k} = \cdots = \beta_{pk} = 0$. Hence, we obtain that $\pi_{i1k1'} = \cdots = \pi_{ipk1'}$. In an analogous manner, by mapping edges ix to kl (where $x \in \{1, 2, \ldots, p\}$), for different $l \in K$, we conclude that

$$\pi_{i1kl} = \pi_{i2kl} = \cdots = \pi_{ipkl}, \quad \text{for all } l \in K. \tag{40}$$

As we already saw, mapping all edges ix to kx', for all $x \in \{1, 2, \ldots, p\}$ results in a point that satisfies (33) at equality, and this mapping gives origin to (39). But also, $(e_{i1k1'} + \cdots + e_{i(p-1)k(p-1)'} + e_{ipk(p+1)'}, e_{ik} + e_{11'} + \cdots + e_{(p-1)(p-1)'} + e_{p(p+1)'})$ is feasible and is in F, that is,

$$\pi_{i1k1'} + \cdots + \pi_{i(p-1)k(p-1)'} + \pi_{ipk(p+1)'} + \beta_{ik} + \beta_{11'} + \cdots + \beta_{(p-1)(p-1)'} + \beta_{p(p+1)'} = 0. \tag{41}$$

From (36), all the values of β (except for β_{ik}) present in the inequalities (41) and (39) are zero. Thus, by subtracting (41) from (39), we obtain that $\pi_{ipkp'} = \pi_{ipk(p+1)'}$. In an analogous manner, we can obtain

$$\pi_{ijkl} = \pi_{ijks}, \quad \text{for all } j \in I \text{ and } l, s \in K. \tag{42}$$

Using (40) and (42) we now obtain that the values of π_{ijkl} for all $j \in I, l \in K$ are equal. From (35), it follows that they are all equal to α, that is,

$$\pi_{ijkl} = \alpha, \quad \text{for all } j \in I \text{ and } l \in K. \tag{43}$$

Now, for an element $j \in I$ and an element $l \in K$, the point $(e_{ijkl}, e_{jk} + e_{il})$ is feasible and is in F. From (36) we have that $\beta_{jk} = 0$, and from (43) that $\pi_{ijkl} = \alpha$. Since l has been chosen arbitrarily from K, we get, $\beta_{il} = -\alpha$, for all $l \in K$.

Finally, from (36), (39) and (43) we have that $\beta_{ik} = -\alpha|I|$. As for inequality (34), the proof of its validity is analogous to that of inequality (33). The proof that it defines a facet when $|I| > |K|$ is also similar to the one given above for inequality (33) when $|I| < |K|$. However, there are some minor differences between the two, and that is why we give it here. Let $F := \{(c, y) \in P: (c, y) \text{ satisfies (34) at equality}\}$. Suppose that $F \subseteq \tilde{F}$, where $\tilde{F}$ is given by (20). Then, we have that F defines a facet, if and only if,

$$(\pi c + \beta y \leq \pi_0) = \alpha \left(\sum_{j \in I} \sum_{l \in K} c_{ijkl} - |K| y_{ik} - \sum_{p \in I} y_{pk} \leq 0 \right), \quad \text{for an } \alpha > 0. \tag{44}$$

We first note that $0 \in F$, and thus, $\pi_0 = 0$. Similarly as in the proof that (33) defines a facet if $|I| < |K|$, we get

$$\beta_{ul} = 0, \quad \text{for } u \in V_G, u \neq i, \text{ and } l \in V_H, l \neq k. \tag{45}$$

$$\beta_{ik'} = 0, \quad \text{for } k' \in V_H \text{ such that } k' \neq k. \tag{46}$$

$$\beta_{j'k} = 0, \quad \text{for } j' \in V_G, j' \notin I. \tag{47}$$

Let $uv \in E_G$ such that uv is not incident to i, and at least one of u, v is not in I. We can suppose, without loss of generality, that $u \notin I$. Let furthermore $pl \in E_H$. Of course, at least one of p, l is different from k (we suppose here that $l \neq k$). Note that the point $(e_{uvpl}, e_{up} + e_{vl})$ is feasible. Besides, this point is in F and since $F \subseteq \tilde{F}$, we have that $\pi_{uvpl} + \beta_{up} + \beta_{vl} = 0$. From (45) and (47) we have that $\beta_{vl} = \beta_{up} = 0$. Thus, $\pi_{uvpl} = 0$, for all $uv \in E_G$ such that $u, v \neq i$, with at least one of u, v not in I and $pl \in E_H$.

Let $uv \in E_G$, and $pl \in E_H$ such that p and l are different from k. Then $(e_{uvpl}, e_{up} + e_{vl})$ is feasible and is in F. Hence, from (45) and (46) we get $\pi_{uvpl} = 0$, for all $uv \in E_G$ and $pl \in E_H$ such that pl is not incident to k.

Let $uv \in E_G$ such that uv is not incident to i, and both u and v are in I. Let $pl \in E_H$ such that pl is incident to k. Suppose that $p = k$. Let furthermore w' be a vertex from K that satisfies $w' \neq l$ (such a vertex w' exists since $|K| \geq 2$). Then of course, $(e_{iukw'} + e_{uvkl}, e_{iw'} + e_{uk} + e_{vl})$ is feasible and is in F. But also, $(e_{iukw'}, e_{iw'} + e_{uk})$ is feasible and is in F. Since $\beta_{vl} = 0$, we have $\pi_{uvpl} = 0$, for all $uv \in E_G$ such that $u, v \neq i$, both u, v are in I and pl is incident to k.

If $I \neq N(i)$, then let $j \in N(i) \setminus I$, and let pl be an edge incident to k (we suppose here that $p = k$). Observe that the point $(e_{ijpl}, e_{il} + e_{jp})$ is feasible and is in F. From (46) and (47) we thus get $\pi_{ijpl} = 0$. Hence, $\pi_{ijpl} = 0$, for all $j \in N(i) \setminus I$ and pl incident to k.

Now, analogously to what we did in the proof that (33) defines a facet, since $|I| > |K|$, we can rename the vertices in V and H in such a way that $I = \{1, 2, \ldots, p, \ldots, q\}$ and $K = \{1', 2', \ldots, p'\}$, with $p' \geq (q+1)'$. Following a reasoning similar to that for the case $|I| < |K|$, one can obtain that

$$\pi_{ijkl} = \pi_{ijks}, \quad \text{for all } j \in I \text{ and } l, s \in K, \tag{48}$$

and

$$\pi_{i1kl} = \pi_{i2kl} = \cdots = \pi_{iqkl}, \quad \text{for all } l \in K. \tag{49}$$

Using (48) and (49) we now obtain that the values of π_{ijkl} for every $j \in I$, $l \in K$ are all equal. From (44), it follows that they are all equal to α, that is,

$$\pi_{ijkl} = \alpha, \quad \text{for all } j \in I, l \in K. \tag{50}$$

Next, note that for an element $j \in I$ and an element $l \in K$, the point $(e_{ijkl}, e_{jk} + e_{il})$ is feasible and is in F. From (46) and (50) we have $\beta_{jk} = -\alpha$, for all $j \in I$.

Observe that the point $(e_{i1k1'} + \cdots + e_{i(p-1)k(p-1)'} + e_{ipkp'}, e_{ik} + e_{11'} + \cdots + e_{pp'})$ is feasible and is in F, and thus,

$$\pi_{i1k1'} + \cdots + \pi_{i(p-1)k(p-1)'} + \pi_{ipkp'} + \beta_{ik} + \beta_{11'} + \cdots + \beta_{pp'} = 0. \tag{51}$$

But also, the point $(e_{i1k1'} + \cdots + e_{ipkp'} + e_{i(p+1)kl}, e_{ik} + e_{11'} + \cdots + e_{pp'} + e_{(p+1)l})$ where $l \notin [K]$ is feasible and is in F, and thus,

$$\pi_{i1k1'} + \cdots + \pi_{ipkp'} + \pi_{i(p+1)kl} + \beta_{ik} + \beta_{11'} + \cdots + \beta_{pp'} + \beta_{(p+1)l} = 0. \tag{52}$$

From (45), we have that $\beta_{(p+1)l} = 0$. Hence, by substracting (51) from (52), we get $\pi_{i(p+1)kl} = 0$. By similar reasoning, we can conclude that $\pi_{ijkl} = 0$, for all $j \in I$, $l \notin [K]$.

Finally, from (45), (50) and (51) we get $\beta_{ik} = -\alpha|K|$. $\square$

We show next that if the conditions that involve cardinality of sets I and K in Theorem 5 are not satisfied, then corresponding inequalities from that theorem are not facet-defining.

Theorem 6. *Let vertices i, k and sets I, K be as defined in Theorem 5. Then the following inequalities are valid but are not facet-defining.*

$$\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq \min\{|I|, |K|\} y_{ik} + \sum_{p \in K} y_{ip}, \quad \text{if } |I| \geq |K|, \tag{53}$$

$$\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq \min\{|I|, |K|\} y_{ik} + \sum_{p \in I} y_{pk}, \quad \text{if } |I| \leq |K|. \tag{54}$$

Proof. As shown in the proof of Theorem 5, inequalities (53) and (54) are valid.

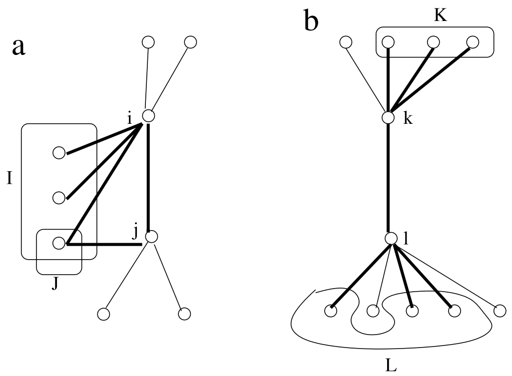

Fig. 2. (a) Highlighted edges are edges in E_{ij}. (b) Highlighted edges are edges in W_{kl}.

Now, let $i \in V_G$, $k \in V_H$, $I \subseteq N(i)$ and $K \subseteq N(k)$ such that $|I| \geq |K|$. Using inequality (16) from the model we have that for each edge kl such that $l \in K$,

$$\sum_{j\in I} c_{ijkl} \leq \sum_{j\in N(i)} c_{ijkl} \leq y_{ik} + y_{il}.$$

By summing above inequalities for each $l \in K$, we get $\sum_{j\in I}\sum_{l\in K} c_{ijkl} \leq |K|y_{ik} + \sum_{p\in K} y_{ip} = \min\{|I|, |K|\}y_{ik} + \sum_{p\in K} y_{ip}$. Hence, inequality (53) does not define a facet.

The proof that (54) does not define a facet is similar (and uses inequality (17) instead of (16)). □

We present now inequalities that generalize results obtained in Theorem 5. Here, given an edge ij in G, and kl in H, sets $I \subseteq N(i) \setminus \{j\}$, $J \subseteq N(j) \setminus \{i\}$, $K \subseteq N(k) \setminus \{l\}$ and $L \subseteq N(l) \setminus \{k\}$, we want to estimate the number of edges from the set $E_{ij} := \{ij\} \cup (\delta(i) \cap \delta(I)) \cup (\delta(j) \cap \delta(J))$ that can be mapped to edges from the set $W_{kl} := \{kl\} \cup (\delta(k) \cap \delta(K)) \cup (\delta(l) \cap \delta(L))$ (see Fig. 2).

Theorem 7. *Let ij be a fixed edge in G, and kl a fixed edge in H. Let furthermore I, J, K, L, E_{ij} and W_{kl} as defined above. Then following inequalities are valid*

$$\sum_{e\in E_{ij}}\sum_{w\in W_{kl}} c_{ew} \leq \min\{|I|, |K|\}y_{ik} + \min\{|I|, |L|\}y_{il} + \min\{|J|, |K|\}y_{jk} + \min\{|J|, |L|\}y_{jl} + c_{ijkl} + \sum_{p\in K\cup L}(y_{ip} + y_{jp}). \tag{55}$$

$$\sum_{e\in E_{ij}}\sum_{w\in W_{kl}} c_{ew} \leq \min\{|I|, |K|\}y_{ik} + \min\{|I|, |L|\}y_{il} + \min\{|J|, |K|\}y_{jk} + \min\{|J|, |L|\}y_{jl} + c_{ijkl} + \sum_{p\in I\cup J}(y_{pk} + y_{pl}). \tag{56}$$

If, in addition, $|I| < |K|$, $|I| < |L|$, $|J| < |K|$, $|J| < |L|$, and $|I| \neq 0$, $|J| \neq 0$, then inequality (55) defines a facet. If, however, $|I| > |K|$, $|I| > |L|$, $|J| > |K|$, $|J| > |L|$, and $|K| \neq 0$, $|L| \neq 0$ then inequality (56) defines a facet.

Note 1: a special case of the above theorem is when $I = N(i) \setminus \{j\}$, $J = N(j) \setminus \{i\}$, $K = N(k) \setminus \{l\}$ and $L = N(l) \setminus \{k\}$. In that case, for given edges ij in G, and kl in H, inequalities from Theorem 7 bound the number of edges in G incident to ij that can be mapped to edges incident to kl in H.

Note 2: we can of course suppose, without loss of generality, that in the above theorem $|J| \leq |I|$ and $|L| \leq |K|$. Observe that for the case when $|J| = |L| = 0$ and $0 \neq |I|, |K|$, inequality (55) is $\sum_{e\in E_{ij}}\sum_{w\in W_{kl}} c_{ew} \leq \min\{|I|, |K|\}y_{ik} + c_{ijkl} + \sum_{p\in K}(y_{ip} + y_{jp})$, and is thus dominated by inequality (33) in Theorem 5 (indeed, using (33) we get $\sum_{e\in E_{ij}}\sum_{w\in W_{kl}} c_{ew} = \sum_{j'\in I}\sum_{l'\in K} c_{ij'kl'} + c_{ijkl} \leq \min\{|I|, |K|\}y_{ik} + \sum_{p\in K} y_{ip} + c_{ijkl}$).

Proof (*Of* Theorem 7)**.** We now prove that (55) is valid. If ij is mapped to kl we suppose first that $y_{ik} = y_{jl} = 1$. In this case, it is clear that $\sum_{e\in\delta(i)\cap\delta(I)}\sum_{w\in\delta(k)\cap\delta(K)} c_{ew} \leq \min\{|I|, |K|\}$ and, analogously, we have that $\sum_{e\in\delta(j)\cap\delta(J)}\sum_{w\in\delta(l)\cap\delta(L)} c_{ew} \leq \min\{|J|, |L|\}$. Hence, $\sum_{e\in E_{ij}}\sum_{w\in W_{kl}} c_{ew} \leq \min\{|I|, |K|\}y_{ik} + \min\{|J|, |L|\}y_{jl} + c_{ijkl}$ (see Fig. 3(a)), and (55) must hold. Similarly, we conclude that (55) is satisfied if $y_{il} = y_{jk} = 1$.

Suppose now that ij is not mapped to kl, but one endpoint of ij is mapped to one endpoint of kl. We suppose that $y_{ik} = 1$ (the proof for the case $y_{il} = 1$ is similar). Then, $\sum_{e\in\delta(i)\cap\delta(I)}\sum_{w\in\delta(k)\cap\delta(K)} c_{ew} \leq \min\{|I|, |K|\}$. Note that since $y_{ik} = 1$, we have

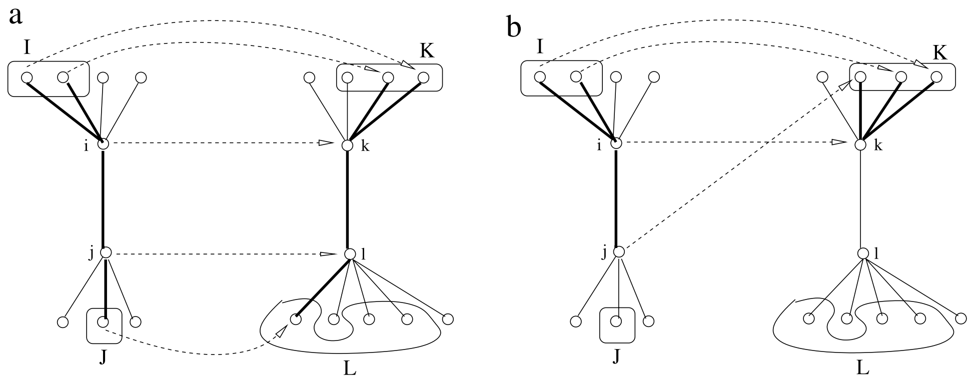

Fig. 3. Edges that are mapped are highlighted. (a) Case when $y_{ik} = y_{jl} = 1$. (b) Case when $y_{ik} = 1$ and $\sum_{p\in K} y_{jp} = 1$.

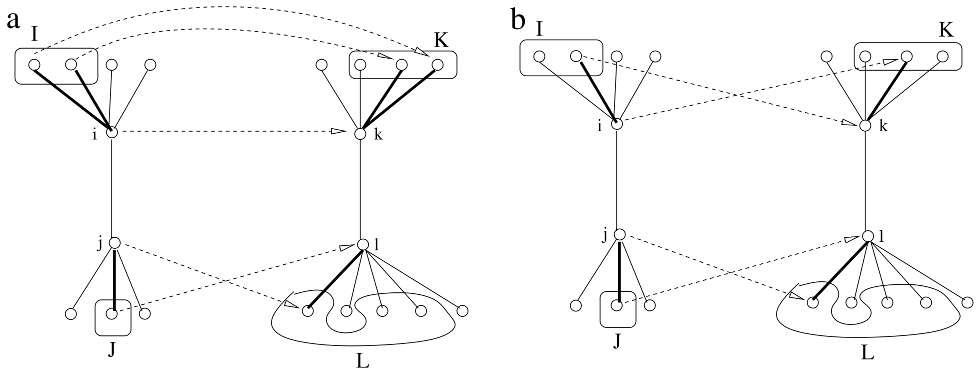

Fig. 4. (a) $y_{ik} = 1$ and $\sum_{p\in L} y_{jp} = 1$. (b) $\sum_{p\in K} y_{ip} = \sum_{v\in I} y_{vk} = 1$ and $\sum_{p\in L} y_{jp} = \sum_{v\in J} y_{vl} = 1$.

that ij can be mapped only to an edge that is incident to k. And if ij is mapped to an edge that is incident to both k and K, then j is mapped to a vertex from K. Hence, $\sum_{e=ij} \sum_{w\in\delta(k)\cap\delta(K)} c_{ew} \le \sum_{p\in K} y_{jp}$ (see Fig. 3(b)). Furthermore, since $y_{ik} = 1$ and j is not mapped to l, at most one edge that is incident to both j and J can be mapped to an edge from W_{kl}. Note that if an edge incident to both j and J is mapped to an edge from W_{kl}, it is mapped to an edge that is incident to both l and L, and in that case, j must be mapped to a vertex from L. That is, $\sum_{e\in\delta(j)\cap\delta(J)} \sum_{w\in\delta(l)\cap\delta(L)} c_{ew} \le \sum_{p\in L} y_{jp}$ (see Fig. 4(a)). Hence, $\sum_{e\in E_{ij}} \sum_{w\in W_{kl}} c_{ew} \le \min\{|I|, |K|\} y_{ik} + \sum_{p\in K\cup L} y_{jp}$, and (55) is satisfied.

Finally, if ij is not mapped to kl and none of endpoint of ij is mapped to endpoint of kl, then at most one edge incident to i (resp. j) is mapped to W_{kl}. Note, furthermore, that if an edge incident to i is mapped to W_{kl}, then $\sum_{p\in K} y_{ip} = \sum_{v\in I} y_{vk} = 1$ or $\sum_{p\in L} y_{ip} = \sum_{v\in I} y_{vl} = 1$. We have analogous equalities if an edge incident to j is mapped to W_{kl} (see Fig. 4(b)). Thus, $\sum_{e\in E_{ij}} \sum_{w\in W_{kl}} c_{ew} \le \sum_{p\in K\cup L} (y_{ip} + y_{jp})$, and again, (55) is satisfied.

The proof that (56) is valid is similar.

The proofs that inequality (55) defines a facet under the assumptions $|I| < |K|$, $|I| < |L|$, $|J| < |K|$, $|J| < |L|$, and $|I| \neq 0$, $|J| \neq 0$, and that inequality (56) defines a facet under the assumptions $|I| > |K|$, $|I| > |L|$, $|J| > |K|$, $|J| > |L|$, and $|K| \neq 0$, $|L| \neq 0$ are similar to the proof that (33) defines a facet. However, the proofs are a bit more extensive and will thus be omitted here. □

In the next theorem we introduce a facet-defining inequality where the benefit of having an extended formulation including the variables c_{ijkl} becomes apparent. More precisely, we are able to express a very simple inequality whose equivalent in the model given in [8] may be hard to find.

Theorem 8. *Let G' be an induced subgraph of G and M a maximal matching in H. If $|V_{G'}| = 2p + 1$ for some $p \ge 1$ and G' has a Hamiltonian cycle, then the inequality*

$$\sum_{ij\in E_{G'}} \sum_{kl\in M} c_{ijkl} \le p \tag{57}$$

is valid. If, furthermore, $|M| \ge p + 1$, then inequality (57) defines a facet.

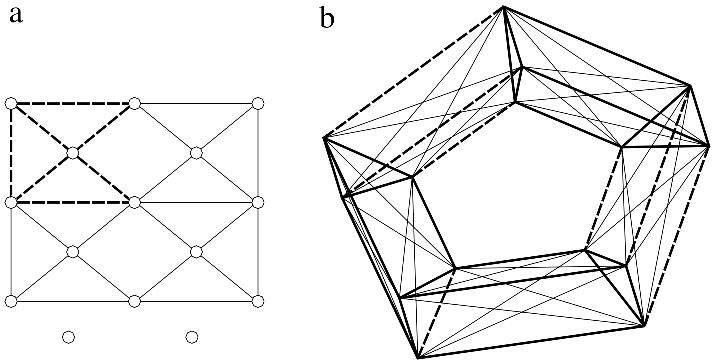

Fig. 5. (a) Dashed lines indicate G'. (b) Dashed lines indicate a maximal matching.

We show on Fig. 5 an example of an instance for which G has a subgraph G' that consists of a 5-cycle together with 2 chords, and H is such that it has a maximal matching with 7 edges. We can thus apply Theorem 8 with $p = 2$.

Proof. Since $|V_{G'}| = 2p + 1$ and G' has a Hamiltonian cycle, there are at most p vertex-disjoint edges in G', and hence, the inequality is trivially satisfied.

Suppose now that $|M| \geq p+1$. We next prove that inequality from the theorem defines a facet. Let $F := \{(c, y) \in P: (c, y)$ satisfies (57) at equality }. Suppose that $F \subseteq \tilde{F}$, where $\tilde{F}$ is given by (20). Then, F defines a facet, if and only if,

$$(\pi c + \beta y \leq \pi_0) = \alpha \left(\sum_{ij \in E_{G'}} \sum_{kl \in M} c_{ijkl} - p \leq 0 \right), \quad \text{for an } \alpha > 0. \tag{58}$$

Let $C = \langle v_1, v_2, \ldots, v_{2p+1} \rangle$ be a Hamiltonian cycle in G'. Let, furthermore, u be any vertex in C. We suppose, without loss of generality, that $u = v_{2p+1}$. Note that $G' - v_{2p+1}$ has a Hamiltonian path $\langle v_1, \ldots, v_{2p} \rangle$, and hence, it has a perfect matching defined by edges $v_1v_2, v_3v_4, \ldots, v_{2p-1}v_{2p}$. Let $w_1w_2, w_3w_4, \ldots, w_{2p-1}w_{2p}, w_{2p+1}w_{2p+2}$ be edges of M (those edges exist since $|M| \geq p + 1$). Then the point $(e_{v_1v_2w_1w_2} + e_{v_3v_4w_3w_4} + \cdots + e_{v_{2p-1}v_{2p}w_{2p-1}w_{2p}}, e_{v_1w_1} + e_{v_2w_2} + \cdots + e_{v_{2p}w_{2p}})$ is feasible and is in F. That is, mapping of edges $v_1v_2, v_3v_4, \ldots, v_{2p-1}v_{2p}$ from G' to edges $w_1w_2, w_3w_4, \ldots, w_{2p-1}w_{2p}$ from M satisfy (57) at equality. Since $F \subseteq \tilde{F}$, we have that

$$\pi_{v_1v_2w_1w_2} + \pi_{v_3v_4w_3w_4} + \cdots + \pi_{v_{2p-1}v_{2p}w_{2p-1}w_{2p}} + \beta_{v_1w_1} + \beta_{v_2w_2} + \cdots + \beta_{v_{2p}w_{2p}} = \pi_0. \tag{59}$$

Now, if apart from mapping of edges $v_1v_2, v_3v_4, \ldots, v_{2p-1}v_{2p}$ to edges $w_1w_2, w_3w_4, \ldots, w_{2p-1}w_{2p}$, we also map u to l (where $l \neq w_1, \ldots, w_{2p}$), the corresponding point satisfies (57) at equality. That is,

$$\pi_{v_1v_2w_1w_2} + \pi_{v_3v_4w_3w_4} + \cdots + \pi_{v_{2p-1}v_{2p}w_{2p-1}w_{2p}} + \beta_{v_1w_1} + \beta_{v_2w_2} + \cdots + \beta_{v_{2p}w_{2p}} + \beta_{ul} = \pi_0. \tag{60}$$

Of course, from (59) and (60) we have that $\beta_{ul} = 0$ (where $u = v_{2p+1}$ and $l \neq w_1, \ldots, w_{2p}$). In fact we could map edges $v_1v_2, v_3v_4, \ldots, v_{2p-1}v_{2p}$ from G' to other edges of M, say $w_3w_4, \ldots, w_{2p+1}w_{2p+2}$. Analogously as above we would obtain that $\beta_{ul} = 0$ (where $u = v_{2p+1}$ and $l \neq w_3, \ldots, w_{2p+2}$). Observe furthermore that u was chosen arbitrarily from V_C. Thus, we can conclude that $\beta_{ul} = 0$, for all $u \in V_C, l \in V_H$.

By reasoning similar as above, it is easy to see that, in fact, inequality (60) is satisfied for all $u \neq v_1, \ldots, v_{2p}$. Hence, more generally, we get

$$\beta_{ul} = 0, \quad \text{for all } u \in V_G, l \in V_H. \tag{61}$$

Let now ij be an edge from G but not in G'. If ij is incident to a vertex from C, we can suppose without loss of generality, that $i \in V_C$ and that $i = v_{2p+1}$ (where $C = \langle v_1, v_2, \ldots, v_{2p+1} \rangle$ is a Hamiltonian cycle in G', as defined above). We remember that (59) is satisfied. Now, if apart from mapping of edges $v_1v_2, v_3v_4, \ldots, v_{2p-1}v_{2p}$ to edges $w_1w_2, w_3w_4, \ldots, w_{2p-1}w_{2p}$, we also map ij to kl (where $kl \neq w_1w_2, \ldots, w_{2p-1}w_{2p}$), the corresponding point satisfies (57) at equality. That is,

$$\pi_{v_1v_2w_1w_2} + \pi_{v_3v_4w_3w_4} + \cdots + \pi_{v_{2p-1}v_{2p}w_{2p-1}w_{2p}} + \pi_{ijkl} + \beta_{v_1w_1} + \beta_{v_2w_2} + \cdots + \beta_{v_{2p}w_{2p}} + \beta_{ik} + \beta_{jl} = \pi_0. \tag{62}$$

From (59), (61) and (62) we have that $\pi_{ijkl} = 0$ (where $kl \neq w_1w_2, \ldots, w_{2p-1}w_{2p}$). Note that we could map edges $v_1v_2, v_3v_4, \ldots, v_{2p-1}v_{2p}$ from G' to other edges of M, say $w_3w_4, \ldots, w_{2p+1}w_{2p+2}$. Analogously as above we would obtain that $\beta_{ijkl} = 0$ (where $kl \neq w_3w_4, \ldots, w_{2p+1}w_{2p+2}$). Observe furthermore that ij was chosen arbitrarily from $E_G \setminus E_{G'}$. Thus, by reasoning similar as above we can conclude that

$$\pi_{ijkl} = 0, \quad \text{for all } ij \in E_G \setminus E_{G'}, kl \in E_H. \tag{63}$$

Let now ij be an edge from G'. We define $G'' := G' - \{i, j\}$. We consider two cases:

- If ij is an edge of the Hamiltonian cycle C in G', then G'' has a Hamiltonian path with $2p - 1$ vertices, and hence, G'' has $p - 1$ disjoint edges.
- If ij is not an edge of the Hamiltonian cycle C in G', then let P (resp. W) be the path from i to j (resp. from j to i) defined by the edges of a Hamiltonian cycle C in G'. Since $|V_C| = 2p + 1$, we have that P has odd number of vertices and W even number of vertices (or vice versa). Note that in both cases G'' has $p - 1$ disjoint edges.

Let, thus, $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ be disjoint edges from G''. Then the point $(e_{x_1x_2w_1w_2} + e_{x_3x_4w_3w_4} + \cdots + e_{x_{2p-3}x_{2p-2}w_{2p-3}w_{2p-2}} + e_{ijw_{2p-1}w_{2p}}, e_{x_1w_1} + e_{x_2w_2} + \cdots + e_{x_{2p-2}w_{2p-2}} + e_{iw_{2p-1}} + e_{jw_{2p}})$ is feasible and is in F. That is, mapping of edges $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ to edges $w_1w_2, w_3w_4, \ldots, w_{2p-3}w_{2p-2}$ from M, and mapping ij to $w_{2p-1}w_{2p}$ satisfy (57) at equality. Since $F \subseteq \tilde{F}$, we have

$$\pi_{x_1x_2w_1w_2} + \cdots + \pi_{x_{2p-3}x_{2p-2}w_{2p-3}w_{2p-2}} + \pi_{ijw_{2p-1}w_{2p}} + \beta_{x_1w_1} + \cdots + \beta_{x_{2p-2}w_{2p-2}} + \beta_{iw_{2p-1}} + \beta_{jw_{2p}} = \pi_0. \tag{64}$$

Similarly, we could map ij to $w_{2p+1}w_{2p+2}$ (instead to $w_{2p-1}w_{2p}$) obtaining

$$\pi_{x_1x_2w_1w_2} + \cdots + \pi_{x_{2p-3}x_{2p-2}w_{2p-3}w_{2p-2}} + \pi_{ijw_{2p+1}w_{2p+2}} + \beta_{x_1w_1} + \cdots + \beta_{x_{2p-2}w_{2p-2}} + \beta_{iw_{2p+1}} + \beta_{jw_{2p+2}} = \pi_0. \tag{65}$$

From (61) and the two inequalities above, we get $\pi_{ijw_{2p-1}w_{2p}} = \pi_{ijw_{2p+1}w_{2p+2}}$. Note that we obtained the above inequality using the hypothesis that edges $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ were mapped to edges $w_1w_2, w_3w_4, \ldots, w_{2p-3}w_{2p-2}$ from M. Analogously, by mapping $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ to another edges from M, and using the same reasoning as above, it is easy to conclude that

$$\pi_{ijkl} = \pi_{ijps}, \quad \text{for an edge } ij \in E_{G'} \text{ and all } kl, ps \in M. \tag{66}$$

Let now i be any vertex of the Hamiltonian cycle C, and let ij, iv be edges of C incident to i. Graph $G'' := G' - \{i, j, v\}$ has a Hamiltonian path with $2p - 2$ vertices, and hence, G'' has $p - 1$ disjoint edges. Let $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ be disjoint edges from G''. Mapping of edges $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ to edges $w_1w_2, w_3w_4, \ldots, w_{2p-3}w_{2p-2}$ from M, and mapping ij to $w_{2p-1}w_{2p}$ leads to a point that satisfies (57) at equality. Since $F \subseteq \tilde{F}$, we have that (64) is valid. Note that we could map edge iv to $w_{2p-1}w_{2p}$ (instead of mapping ij to $w_{2p-1}w_{2p}$). We would obtain

$$\pi_{x_1x_2w_1w_2} + \cdots + \pi_{x_{2p-3}x_{2p-2}w_{2p-3}w_{2p-2}} + \pi_{ivw_{2p-1}w_{2p}} + \beta_{x_1w_1} + \cdots + \beta_{x_{2p-2}w_{2p-2}} + \beta_{iw_{2p-1}} + \beta_{vw_{2p}} = \pi_0. \tag{67}$$

Now, from (61), (64) and (67) we get that $\pi_{ijw_{2p-1}w_{2p}} = \pi_{ivw_{2p-1}w_{2p}}$. Note that we obtained the above inequality using the hypothesis that edges $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ from G'' were mapped to edges $w_1w_2, w_3w_4, \ldots, w_{2p-3}w_{2p-2}$ from M. Observe that by mapping $x_1x_2, x_3x_4, \ldots, x_{2p-3}x_{2p-2}$ from G'' to other edges from M, and using the same reasoning as above, we can get that $\pi_{ijkl} = \pi_{ivkl}$ for all $kl \in M$. Since vertex i has been chosen arbitrarily from V_C, we can conclude that

$$\pi_{ijkl} = \pi_{ivkl}, \quad \text{for all } ij, iv \in E_C, kl \in M. \tag{68}$$

Let now ij be an edge from G' such that ij is not an edge of the Hamiltonian cycle C in G'. Let P (resp. W) be the path from i to j (resp. from j to i) defined by the edges of the Hamiltonian cycle C in G'. Since $|V_C| = 2p + 1$, we have that P has an odd number of vertices and W an even number of vertices (or vice versa). We suppose, without loss of generality, that P has an odd number of vertices. Let $P = \langle i, v, \ldots, j\rangle$ (that is, v is the vertex that follows i on path P). Then, $P - \{i, v, j\}$ and $W - \{i, j\}$ both have an even number of vertices, that is, $G'' := G' - \{i, j, v\}$ has a perfect matching that contains $p - 1$ edges. Mapping those $p - 1$ edges of G'' to edges of M, and mapping ij (resp. iv) to an edge of M, analogously as in the proof of inequality (68), we get

$$\pi_{ijkl} = \pi_{ivkl}, \quad \text{for all } ij \in E_{G'}, ij \notin E_C, iv \in E_C, kl \in M. \tag{69}$$

Since every edge in G' but not in C is incident to an edge from C, using (68) and (69) we can conclude that

$$\pi_{ijkl} = \pi_{twkl}, \quad \text{for all } ij, tw \in E_{G'}, kl \in M. \tag{70}$$

Finally, from (58), (66) and (70) we can conclude that $\pi_{ijkl} = \alpha$, for all $ij \in E_{G'}$, $kl \in M$.

Let now ij be an edge from G' such that it is an edge of the Hamiltonian cycle C in G' (we suppose, without loss of generality that $ij = v_1v_{2p+1}$). Let kl be an edge of H not in M. Since M is maximal, at least one vertex of kl is covered by M. Suppose first that both k and l are covered by M. Suppose, without loss of generality that $k = w_1$ and $l = w_{2p+1}$. Then the point $(e_{ijkl} + e_{iv_2kw_2} + e_{v_3v_4w_3w_4} + \cdots + e_{v_{2p-3}v_{2p-2}w_{2p-3}w_{2p-2}} + e_{v_{2p}jw_{2p+2}l}, e_{ik} + e_{v_2w_2} + \cdots + e_{v_{2p-2}w_{2p-2}} + e_{v_{2p}w_{2p+2}} + e_{jl})$ is feasible and is in F. That is, mapping edges ij to kl, iv_2 to kw_2, v_3v_4 to $w_3w_4, \ldots, v_{2p-3}v_{2p-2}$ to $w_{2p-3}w_{2p-2}$ and $v_{2p}j$ to $w_{2p}l$ results in a point that satisfies (57) at equality. But, mapping all those edges, except for ij to kl also leads to a point that satisfies

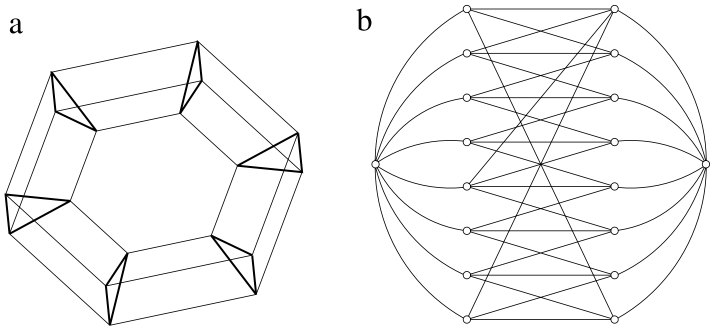

Fig. 6. An instance of the MCES problem. (a) G has 6 edge disjoint triangles (highlighted edges). (b) H has no triangles. Since $|E_G| \leq |E_H|$, considering triangles and applying inequality (71) from Theorem 10 we get $\sum_{ij\in E_G}\sum_{kl\in E_H} c_{ijkl} \leq |E_G| - (z_G - z_H) = 36 - (6 - 0) = 30$. It is not hard to obtain a lower bound of 30 for this instance and, therefore, to show that this is indeed the optimum value.

(57) at equality. Hence, $\pi_{ijkl} = 0$. Suppose next that only k is covered by M (we suppose here that $k = w_1$). Then the point $(e_{ijkl} + e_{iv_2kw_2} + e_{v_3v_4w_3w_4} + \cdots + e_{v_{2p-1}v_{2p}w_{2p-1}w_{2p}}, e_{ik} + e_{v_2w_2} + \cdots + e_{v_{2p}w_{2p}} + e_{jl})$ is feasible and is in F. That is, mapping edges ij to kl, iv_2 to kw_2, v_3v_4 to $w_3w_4, \ldots, v_{2p-1}v_{2p}$ to $w_{2p-1}w_{2p}$ results in a point that satisfies (57) at equality. But also, mapping all those edges, except for ij to kl also results in a point that satisfies (57) at equality. Hence, we again have that $\pi_{ijkl} = 0$. We thus conclude that $\pi_{ijkl} = 0$, for all $ij \in E_{G'}$, ij is an edge of the Hamiltonian cycle C in G and $kl \notin M$.

Observe that in the case when ij is an edge from G' such that it is not an edge of the Hamiltonian cycle C in G', by considering edges of C in G' and by mapping ij to a $kl \notin M$, and some of the edges of the Hamiltonian cycle C to edges of M (similarly as above), we can also conclude that $\pi_{ijkl} = 0$, for all $ij \in E_{G'}$, ij is not an edge of the Hamiltonian cycle C in G and $kl \notin M$. $\square$

We next observe that if the condition that $|M| \geq p + 1$ is not satisfied in Theorem 8 then inequality (57) is not facet-defining.

Theorem 9. *Let G' be an induced subgraph of G and let M be a maximal matching in H. If $|V_{G'}| = 2p + 1$ for some $p \geq 1$, G' has an Hamiltonian cycle, and $|M| \leq p$ then $\sum_{ij\in E_{G'}}\sum_{kl\in M} c_{ijkl} \leq p$ does not define a facet.*

Proof. Using (15) we have that $\sum_{ij\in E_{G'}} c_{ijkl} \leq \sum_{ij\in E_G} c_{ijkl} \leq \sum_{i\in V_G} y_{ik} \leq 1$, for every $kl \in M$. Since $|M| \leq p$, it follows that $\sum_{ij\in E_{G'}}\sum_{kl\in M} c_{ijkl} \leq p$. $\square$

We observed that most of the hardest benchmark instances used in the experiments reported in Section 5 have a highly symmetric structure. For example, task interaction or processors graph of some of the instances are 2-, 4- or 8-regular grids. That is the reason we tried to find some classes of valid inequalities that explore the structure of the task interaction graph and processors graph given as input instances. Indeed, using the following theorem that explores the structure of the input graphs we obtained better upper bounds for some instances.

Theorem 10. *Let z_G be the maximum number of edge disjoint z-cycles in G and let z_H be the maximum number of edge disjoint z-cycles in H. If $z_G \geq z_H$, then the following inequality is valid.*

$$\sum_{ij\in E_G}\sum_{kl\in E_H} c_{ijkl} \leq |E_G| - (z_G - z_H), \quad \text{if } |E_G| \leq |E_H|. \tag{71}$$

Proof. It is clear that the maximum number of z-cycles in G for which we can map all of its z edges to H is equal to z_H. Suppose now that we have mapped z_H edge disjoint z-cycles of G to z_H edge disjoint z-cycles of H. Let $\mathcal{K}_G$ denote the set of those z_H edge disjoint z-cycles of G that we have mapped to z-cycles of H.

Note that for every z-cycle of G not in $\mathcal{K}_G$, we can map at most $z - 1$ of its edges to H, that is, at least one edge of every such z-cycle will not be matched in H. Of course, the number of z-cycles not in $\mathcal{K}_G$ is $z_G - z_H$. Since $|E_G| \leq |E_H|$, the total number of edges mapped from G to H is at most $|E_G| - (z_G - z_H)$. $\square$

We highlight that with inequality (71) we were able to find the optimum for the instance shown in Fig. 6.

We remark that one can write an inequality similar to (71) from Theorem 10 in the case when $z_G \leq z_H$. Note also that Theorem 10 can be generalized in a way that, given any special graph, say $\mathcal{S}$, inequality (71) is valid for numbers z_G and z_H where z_G (resp. z_H) is the maximum number of edge disjoint subgraphs in G (resp. in H), such that each of those subgraphs is isomorphic to $\mathcal{S}$.

We observe next that the inequality that corresponds to inequality (8) (the inequality that involves a minimal vertex cover of H and was obtained by Marenco [8]) does not define a facet in our model, because it is dominated by inequality (17).

Indeed, let ij be a fixed edge from G, and U be a minimal vertex cover of H. We note that by summing inequalities (17) for all $u \in U$ we get

$$\sum_{kl\in E_H} c_{ijkl} \le \sum_{u\in U}\sum_{l\in N(u)} c_{ijul} \le \sum_{u\in U}(y_{iu}+y_{ju}).$$

Let now ij be a fixed edge in G, and k a fixed vertex from H. We note that we can rewrite inequality (9) obtained by Marenco [8] as

$$\begin{aligned} x_{ij} &\le \sum_{k'\in N(k)} y_{jk'} + \left(\sum_{i'\neq i} y_{i'k} + y_{ik}\right) - y_{ik} + \sum_{s\neq k}\psi_s y_{is} \\ &= \sum_{k'\in N(k)} y_{jk'} + \left(\sum_{l\in V_H} y_{il} - y_{ik}\right) + \sum_{s\neq k}\psi_s y_{is} \\ &= \sum_{k'\in N(k)} y_{jk'} + \sum_{l\neq k} y_{il} + \sum_{s\neq k}\psi_s y_{is} \\ &= \sum_{k'\in N(k)} y_{jk'} + \sum_{s\neq k}(1+\psi_s) y_{is}. \end{aligned}$$

We next show that a slight modification of this inequality is valid in our model.

Theorem 11. *Let k be a fixed vertex in H. For all $s \in V_H$, $s \neq k$ let ψ_s as defined in (10). Let furthermore ij be a fixed edge in G. Then the following inequality is valid.*

$$\sum_{pl\in E_H} \gamma c_{ijpl} \le \sum_{k'\in N(k)} y_{jk'} + \sum_{s\neq k}(1+\psi_s) y_{is}, \tag{72}$$

where $\gamma = 2$, if pl is such that both p and l are neighbors of k, otherwise $\gamma = 1$.

Proof. If $\sum_{pl\in E_H}\gamma c_{ijpl} = 0$, then the above inequality is trivially satisfied, since its right hand side is always greater or equal to zero.

Suppose now that $\sum_{pl\in E_H}\gamma c_{ijpl} = 1$ and $y_{ik} = 1$. Then $\sum_{s\neq k} y_{is} = 0$, that is, $\sum_{s\neq k}(1+\psi_s)y_{is} = 0$, and inequality (72) becomes $1 \le \sum_{k'\in N(k)} y_{jk'}$. It thus suffices to show that $\sum_{k'\in N(k)} y_{jk'} = 1$, but this follows directly from Corollary 2.

Suppose next that $\sum_{pl\in E_H}\gamma c_{ijpl} = 1$ and $y_{is} = 1$ for some $s \neq k$. If $N(s) \subseteq N(k)$ then $\psi_s = -1$ and again, inequality (72) becomes $1 \le \sum_{k'\in N(k)} y_{jk'}$. Since $y_{is} = 1$, from Corollary 2 we have $\sum_{k'\in N(s)} y_{jk'} = 1$. But, as $N(s) \subseteq N(k)$, we get $1 = \sum_{k'\in N(s)} y_{jk'} \le \sum_{k'\in N(k)} y_{jk'}$, as desired. If, however, $N(s) \nsubseteq N(k)$ then $\psi_s = 0$, that is, $\sum_{s\neq k}(1+\psi_s)y_{is} = 1$. Since $\sum_{k'\in N(k)} y_{jk'}$ is always greater or equal to zero, we have that (72) is trivially satisfied.

Suppose finally that $\sum_{pl\in E_H}\gamma c_{ijpl} = 2$. Thus, there is an edge $p'l'$ in H such that $c_{ijp'l'} = 1$, and p', l' are both neighbors of k in H. From (16), we have that $y_{ip'} = 1$ or $y_{il'} = 1$. Suppose, without loss of generality, that $y_{ip'} = 1$. Now, Lemma 2 implies that $y_{jl'} = 1$. Furthermore, since p' is neighbor of k, we have that $k \in N(p')$, that is $N(p') \nsubseteq N(k)$, and thus $\psi_{p'} = 0$. It follows that $\sum_{s\neq k}(1+\psi_s)y_{is} = 1$. Since $l' \in N(k)$, we also have $\sum_{k'\in N(k)} y_{jk'} = 1$. Hence, the right hand side of (72) is in this case 2, as desired. □

5. Computational results

The polyhedral investigation described in the previous section was the starting point for the development of a branch-and-bound (**B**&**B**), cut-and-branch (**C**&**B**) and branch-and-cut (**B**&**C**) algorithms that we implemented to assess the strength of our formulation and of the valid inequalities we encountered. In the model used in our experiments, constraints (12) and (13) are given in equality form since preliminary tests indicated that the algorithms perform slightly better in this way. We considered all the valid inequalities discussed in the previous section. However, for some of them, only a few special cases were taken into account. Below we summarize the main aspects of our implementation and discuss our computational results.

Inequalities and separation.

We added *a priori* in the model inequalities (33) and (34) from Theorem 5 for the special case when both $I = N(i)$ and $K = N(k)$. For this particular case, facet-defining inequalities (33) and (34) are indeed easy to implement, since they become

$$\sum_{j\in N(i)}\sum_{l\in N(k)} c_{ijkl} \le d_G(i) y_{ik} + \sum_{p\in N(k)} y_{ip}, \quad \text{if } d_G(i) < d_H(k),$$

$$\sum_{j\in N(i)}\sum_{l\in N(k)} c_{ijkl} \le d_H(k) y_{ik} + \sum_{p\in N(i)} y_{pk}, \quad \text{if } d_G(i) > d_H(k).$$

Furthermore, a fast polynomial time algorithm was designed to separate inequalities (33) and (34) for the case when I may be different from $N(i)$, but $K = N(k)$. The polynomial time algorithm to separate inequalities (33) and (34) in that case works as follows. We define $csol_{ijkl}$, for all $ij \in E_G$ and $kl \in E_H$, to be the real-valued edge mapping variables (calculated during the execution of our program). For each vertex i in G and k in H, the algorithm creates an array $csort$ containing $d_G(i)$ positions, in a way that for every edge ij incident to i we have $csort(ij) := \sum_{l \in N(k)} csol_{ijkl}$. We then sort all edges incident to i in ascending order of their $csort$ value. Furthermore, for every value $p \in \{1, 2, \ldots, d_G(i)\}$ we calculate the left and the right-hand sides of inequality (33) or (34) (depending if $p < d_H(k)$ or $p > d_H(k)$, respectively), by defining the set I as the set of the first p edges incident to i, ordered by their $csort$ value. If the difference between the left and the right-hand side is greater than a pre-established and sufficiently small value ϵ (that is, a tolerance parameter), inequality is considered to be violated and the corresponding cut is found.

We also added *a priori* in the model both inequalities from Theorem 7, but only when $I = N(i) \setminus \{j\}$, $J = N(j) \setminus \{i\}$, $K = N(k) \setminus \{l\}$ and $L = N(l) \setminus \{k\}$. Observe that in this case, it is easy to implement both inequalities (55) and (56). We implemented inequality (55) when $|I| < |K|$, $|I| < |L|$, $|J| < |K|$, $|J| < |L|$, and $|I| \neq 0$, $|J| \neq 0$, since in this case inequality (55) is facet-defining. However, when $|I| > |K|$, $|I| > |L|$, $|J| > |K|$, $|J| > |L|$, and $|K| \neq 0$, $|L| \neq 0$ we implemented inequality (56), since in this particular case, the latter defines a facet.

Besides, a fast polynomial time algorithm was designed for the separation of the maximum matching inequalities (57) from Theorem 8, but only for two specific situations. The first one is when $p = 1$, that is, when G' is a triangle (3-cycle) of G. In this case, the algorithm works as follows. Let T be a triangle of G, and let e_1, e_2, e_3 be edges of T. Then, for every edge $w \in E_H$, we define $SepCostEdge(w) := csol_{e_1 w} + csol_{e_2 w} + csol_{e_3 w}$ (where $csol$ are the real-valued edge variables, as defined above). Finally, we compute a maximum weighted matching in H. It is worth noting that we also separated and used inequalities (57) with the roles of G and H interchanged.

Let z be the weight of the optimal matching computed above. If $z - 1$ is greater than the pre-established sufficiently small value ϵ, then inequality (57) is violated and the corresponding cut is $\sum_{w:u_w=1}(c_{e_1 w} + c_{e_2 w} + c_{e_3 w}) - 1$. We repeat the procedure above for every triangle T of G.

We also separate inequality (57) for when $p = 2$, that is, when G' is an induced subgraph of G with 5 vertices and a Hamiltonian cycle. For that, we proceed as follows. For every subset of 5 vertices from G we first examine whether the subgraph induced by those 5 vertices has a Hamiltonian cycle. If so, we find cuts by using a technique analogous to the one described above for triangles.

As for the implementation of inequalities (71) from Theorem 10, we remark that the following form of these inequalities is also valid. Let G' be an induced subgraph of G. Let, furthermore, $z_{G'}$ be the maximum number of edge disjoint z-cycles in G' and let z_H be the maximum number of edge disjoint z-cycles in H. If $z_{G'} \geq z_H$, then the following inequality is valid.

$$\sum_{ij \in E_{G'}} \sum_{kl \in E_H} c_{ijkl} \leq |E_{G'}| - (z_{G'} - z_H), \quad \text{if } |E_{G'}| \leq |E_H|. \tag{73}$$

We implemented inequality above for two situations. The first one is when $z = 3$, G' is a triangle of G, $z_H = 0$, and $|E_H| \geq 3$. Then, inequality (73) becomes very simple to implement, since it reads

$$\sum_{ij \in E_{G'}} \sum_{kl \in E_H} c_{ijkl} \leq 2.$$

The second case is when $z = 5$, G' is an induced 5-cycle of G, $z_H = 0$, and $|E_H| \geq 5$. For this case, inequality (73) has the following very simple form

$$\sum_{ij \in E_{G'}} \sum_{kl \in E_H} c_{ijkl} \leq 4.$$

For the two particular cases implemented above, there is the requirement that the inequalities only apply when H has no triangles (when $k = 3$) or no 5-cycles (when $k = 5$). To check the existence of a 5-cycle in H, we examine all possible subsets of 5 vertices of H. More precisely, we check the subgraph (denoted by H') induced by every possible subset of 5 vertices of H. If H' has exactly 5 edges, and the degree of every vertex of H' is 2, then H' is a 5-cycle in H. Checking the existence of a 3-cycle in H can be done similarly.

Even though we did not implement inequalities (71) for the general case, as mentioned is Section 4, we did it for the instance depicted in Fig. 6. Before we include this inequality, the duality gap for the corresponding instance was 6.25%.

As a final remark concerning the inequalities we used in our algorithm, it is worth noting that we also added *a priori* in the model the inequalities (72) from Theorem 11.

Now, in theory, mapping G into H, is the same as mapping the other way around. However, in our computational experiments we noticed that when $|E_H| < |E_G|$, even though the number of variables in the IP model stays the same, our algorithm performs better when we map H into G. In principle, this rather simple trick could also be applied to the model given in [8]. In this case, there is a reduction on the number of constraints of the formulation but, apparently, this was unnoticed by the author. In our case, this observation was instrumental to solve 4 additional instances to optimality.

Primal bounds. Another feature of our algorithm was the implementation of a naïve, though efficient, primal heuristic based on the solutions of the linear relaxations computed during the enumeration. Namely, for every $i \in V_G$ and $k \in V_H$, we define $ysol_{ik}$ to be the solution of mapping vertex i to k of the linear relaxation computed during the enumeration. We then sort the values of *ysol* in decreasing order, and assign vertices of G to vertices in H according to the preference suggested by the sorted values. Next, for every edge ij of G, we check if the vertex of H that is assigned to i is a neighbor of the vertex of H assigned to j. That is, we count the number of edges of G that are mapped to edges in H, which is the value returned by our primal heuristic.

Instances. We tested 67 instances also used by Marenco in [8]. Most of those instances come from other papers and archives that deal with the MCES problem. In this set, 16 instances are very small, with the input graphs having less than 10 vertices each; in 19 instances the graphs have from 10 to 19 vertices, in 18 instances they have 20 vertices, in 7 instances they have between 21 and 29 vertices and, finally 7 instances have at least 30 vertices. The largest instance has 36 vertices. All the graphs are quite sparse and present a high degree of symmetry, with most of them being regular grids (see Figs. 5(b) and 6(a) for examples).

The instance set is divided in several groups. The group of *str* instances was proposed by Bokhari [2], all of them having a 8-regular grid as one of the input graphs. Fig. 5 illustrates an example of a *str* instance. Instances of *dc* group have complete binary trees as one of the input graphs and a 4-regular grid as the other one. They are adaptations of instances belonging to the ANDES library for scheduling problems with precedence constraints (cf., [3]). The *df* group is also composed of instances adapted from the ANDES library. An example of such an instance is displayed in Fig. 6. As it can be seen, one of the input graphs has two rows of vertices. Each node in the first row is connected to 3 closest nodes from the second row of vertices, except for the end vertices, which are also connected to the opposite end vertices. There are two more special vertices. The first one is connected to each vertex in the first row of vertices, while the second one is connected to each vertex in the second row of vertices. In addition, there is one more special edge. The other input graph of the *df* instances is a regular grid. Instances in the *wars* group have the graph representing the three-dimensional cube as one of the input graphs. These instances were proposed by Lee and Aggarwal [7] as examples that occur in parallel computer architectures. Instances of the *Gauss* group model situations that appear when solving systems of linear equations using the Gauss method in parallel environments. Instances in the group *prb* are characterized by having small input graphs, with up to 16 vertices. Some of these instances were generated randomly, while others were built by hand to have some special structures (trees, Hamiltonian graphs, etc.). Finally, instances of the group called *memsy*, first presented in [12], have 20 vertices each. They are also meant to represent the situation where one has to assign tasks to processors in a parallel programming environment. The processors graphs have 44 edges each, while the task interaction graphs consist of a pyramidal group of 6 processors, organized into two levels.

Computational environment. We used a Pentium IV, 2.66 GHz, 1 GB of RAM to perform our tests. The XPRESS-MP Optimizer version `v17.01.02` was used as the integer programming solver, and our programs were coded with the XPRESS-MP MOSEL modeling language. Computation times were limited to 3600 s.

Our results. We divide our analysis into two families of instances: those we were able to solve to optimality and those we were not. In this analysis, an attempt is made to compare our results with those reported by Marenco [8]. The two experiments were carried out in very distinct computational environments both in terms of software (e.g., different linear programming solvers were used) and hardware. In this latter aspect, the computer reported in [8] is a Ultra Sparc 1 workstation with 140 MHz processor, with 64 MB of RAM memory and an estimated power of 205 MFlops, whereas our computer has an estimated power of 243 MFlops. Thus, in order to perform a fair comparison between the computational times, we use the rate of 205/243 Mflops as an adjusting factor. We must call the reader's attention to the fact that this factor is a quite rough estimation of the difference between the two machines and, therefore, one has to be very careful before drawing definitive conclusions.

Let us first examine the family of instances for which we found the optimum. We managed to solve to optimality 42 of the 67 instances, compared to the 27 solved by Marenco [8]. In general, for these instances, the optimum is proven quite fast. Indeed, only four instances required more than 10 min to be solved and the execution time in this case never exceeded 16 min.

In Table 1, for each instance we solved to optimality, we list the number of vertices of the respective instance, as well as the number of edges in the graphs G and H. Furthermore, we list the optimum value, and also which strategy among the ones that we implemented, that is, **B&B**, **C&B**, or **B&C** of our model, was the fastest in obtaining that solution. We also present the time needed by each strategy to find the optimal solution, whenever this could be done within the fixed time limit. All execution times in the table are given in seconds and the best time achieved for each instance is detached in bold. The last column of the table gives the time needed in [8] (adjusted by the 205/243 factor as described earlier) to compute the same instances. Fifteen instances of Table 1 could not be solved by Marenco within the one hour computation limit (in the Ultra machine, i.e., without using the correction factor) fixed for his experiments. In these cases we report the percentage gaps obtained by Marenco. In contrast, the **B&B**, **B&C** and **C&B** strategies failed to prove optimality of only, 4, 12 and 2 instances, respectively. Besides, **B&B**, **B&C** and **C&B** computed, respectively, 32, 25 and 31 out of the

Table 1
Solved instances.

Instance	$\|V\|$	$\|E_G\|$	$\|E_H\|$	Opt	IP best strategy	**B&B** time	**B&C** time	**C&B** time	Marenco's besttime
prb1	3	2	3	2	**B&B**	**0.01**	0.04	0.02	0.06
prb2	4	4	4	3	**C&B**	0.02	0.05	**0.01**	0.04
prb3	5	5	6	5	**B&B**	**0.01**	0.05	0.03	0.07
prb4	5	6	6	5	**B&B**	**0.01**	0.15	0.03	0.08
str2	6	15	8	8	**B&B**	**0.01**	0.10	0.02	0.13
prb5	8	10	10	9	**B&B**	**0.04**	1.45	0.62	0.14
prb6	8	13	10	10	**C&B**	0.39	1.33	**0.10**	0.18
prb7b	8	13	12	11	**C&B**	1.66	3.49	0.76	**0.17**
prb8b	8	10	10	6	**B&B**	**0.02**	0.13	0.04	0.14
prb9b	8	13	10	10	**C&B**	0.98	1.96	0.66	**0.21**
wars1	8	10	12	10	**B&B**	**0.03**	1.05	0.41	0.11
wars2	8	9	12	9	**B&B**	**0.04**	0.07	0.06	0.13
wars3	8	13	12	11	**C&B**	1.26	1.89	**0.78**	2.19
wars4	8	12	12	6	**C&B**	0.03	0.06	**0.02**	0.14
wars5	8	13	12	9	**C&B**	2.60	3600.00	1.55	**1.50**
str1	9	36	14	14	**C&B**	0.17	0.11	**0.09**	0.87
prb7	10	16	14	13	**B&B**	3.64	15.73	3.88	**0.45**
prb8	11	23	15	13	**C&B**	8.99	32.60	**3.93**	14.70
prb9	11	17	15	14	**C&B**	7.41	10.70	1.83	**0.72**
df11	12	21	36	18	**B&B**	**66.00**	3600.00	77.06	403.75
df12	12	26	36	23	**B&B**	**101.55**	3600.00	149.86	(gap 4.35%)
df13	12	26	36	23	**B&B**	**106.00**	3600.00	138.00	(gap 8.70%)
df1	12	26	18	18	**C&B**	2.60	4.82	**1.74**	451.17
gauss1	12	16	24	15	**B&B**	**3.00**	73.50	37.96	455.40
dc2	15	14	30	14	**C&B**	1.79	3.12	1.59	**0.55**
str3	15	60	26	26	**C&B**	30.55	50.42	**12.48**	(gap 4.00%)
str4	15	60	26	25	**B&B**	**172.21**	3600.00	232.48	(gap 4.00%)
gauss3	16	25	32	22	**C&B**	127.00	59.86	**48.66**	(gap 4.55%)
prb10	16	26	26	20	**C&B**	303.00	3600.00	**193.75**	(gap 10.53%)
dc1	18	14	36	14	**C&B**	2.63	3.83	2.47	**0.62**
df8	18	41	36	30	Inequality (71)	–	–	–	(gap 6.67%)
gauss2	20	25	40	22	**B&B**	**911.00**	3600.00	1077.37	(gap 4.55%)
memsy3	20	24	44	22	**C&B**	285.00	3600.00	**90.52**	(gap 9.09%)
memsy6	20	24	44	24	**B&B**	**7.01**	104.28	20.25	11.62
memsy8	20	24	44	22	**C&B**	276.00	835.74	**213.77**	(gap 9.09%)
str13	25	100	38	38	**C&B**	628.00	3600.00	**478.18**	(gap 8.57%)
str7	25	100	48	48	**B&B**	**918.00**	3600.00	3600.00	(gap 2.13%)
str9	25	100	37	37	**B&C**	3600.00	601.92	857.19	**152.02**
str17	30	120	54	54	**C&B**	3600.00	1611.20	**426.55**	475.92
str19	30	120	48	48	**C&B**	3600.00	3600.00	**720.88**	(gap 4.34%)
str15	30	120	59	59	**B&B**	**311.38**	1691.74	929.44	(gap 9.26%)
str18	30	120	50	50	**C&B**	674.74	1691.74	**243.59**	(gap 6.38%)

42 instances at least as rapidly as Marenco's algorithm. From the data displayed in Table 1 one can see that the cut-and-branch strategy performs slightly better than the pure branch-and-bound and both are much more efficient than the branch-and-cut one (22, 18 and 1 wins, respectively). We should notice that no strategy was able to solve instance `df8`. However, with the *a priori* addition of inequalities (73), the optimum was found after the computation of the first linear relaxation.

Table 2 exhibits a summary of the results for the family of 25 instances that could not be solved by none of our algorithms. Again, we list the number of vertices of the respective instance, as well as the number of edges in the graphs G and H. Besides, we list the best solution together with the best upper bound we found and the corresponding duality gap. The last column shows the gaps achieved by Marenco in his experiments. For all unsolved instances our best gap was obtained using the **B&C** strategy. Among them, 12 have a duality gap of at most 10%, 11 have a gap between 10% and 20%, and only 2 have a gap greater or equal than 20%. In 22 out of the 25 instances not solved by our algorithms we could generate smaller duality gaps than those reported earlier in the literature. The three other instances belong to group *df* and, for all of them, our duality gap did not surpass the smallest gap known in more than 3%.

6. Concluding remarks

We showed that with our extended integer programming formulation, which includes variables that interlace edges of G with edges of H, we gain on expressiveness with respect to the model given in [8]. We carried out a polyhedral investigation of this new model and presented some valid inequalities and facets. As a result, we developed simple enumeration algorithms that use these inequalities as cutting planes and which were able to prove the optimality of 15 additional instances when compared to the results reported in [8].

Table 2
Unsolved instances.

Instance	$\lvert V\rvert$	$\lvert E_G\rvert$	$\lvert E_H\rvert$	OurBestSol	OurBestBound	OurGap	Marenco'sGap
str10	20	80	37	36	37	**2.70**	2.78
str6	20	80	37	36	37	**2.70**	2.78
dc3	35	30	70	29	30	**3.33**	11.11
df6	16	36	32	28	29	**3.45**	7.41
df5	20	36	40	27	29	**3.57**	11.54
str16	30	120	54	52	54	**3.70**	8.00
memsy7	20	27	44	25	26	**3.85**	8.00
str11	24	96	48	46	48	**4.17**	4.35
gauss4	18	25	36	21	22	**4.55**	9.52
memsy1	20	32	44	28	30	**6.67**	10.71
str12	21	84	37	34	37	**8.11**	8.82
df4	15	31	30	20	24	**9.09**	30.00
memsy5	20	30	44	25	28	**10.71**	16.00
memsy4	20	36	44	29	33	**12.12**	20.69
df7	20	41	40	29	33	12.12	**10.34**
df18	20	46	60	34	40	**12.82**	18.18
df2	30	61	60	38	45	15.56	**12.82**
memsy2	20	40	44	32	38	**15.79**	18.75
df3	18	31	36	21	25	**16.00**	23.81
df16	20	41	60	31	37	**16.22**	20.00
df17	20	41	60	31	37	16.22	**16.13**
df19	24	51	72	36	43	**16.28**	16.67
df20	25	56	75	38	46	**17.39**	18.42
df14	20	31	60	24	30	**20.00**	30.43
df15	20	36	60	27	34	**20.59**	22.22

Despite these promising advances, the MCES remains a very difficult problem to be solved exactly. The graphs we could deal with are limited to less than 40 vertices which is still far from the sizes of the graphs arising in many relevant applications of the problem. A possible research direction that could allow us to handle larger instances would be to deepen the polyhedral investigation of our model in order to obtain new facet-defining inequalities for the associated polytope. In particular, inequalities (12)–(15) indicate that a feasible solution is a stable set of a certain conflict graph in the sense of [1]. A question which remains is to determine the impact of (16)–(17) in the stable set polytope defined by the conflict graph, which would allow writing new facet-defining inequalities and using separation algorithms, in particular the edge projection heuristic [16].

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