On the facial structure of the Common Edge Subgraph polytope

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CTW 2008

Summary

- Common Edge Subgraph problem
  - Definition
  - Applications

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  - New integer programming formulation
  - Valid inequalities and facets of the polytope

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- Our contribution
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  - Valid inequalities and facets of the polytope
- Preliminary computational results

Maximum Common Edge Subgraph Problem

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Given: two graphs with $|V_G| = |V_H|$
Find: a common subgraph of G and H, (not necessary induced) with the maximum number of EDGES.

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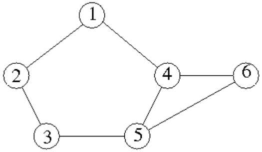

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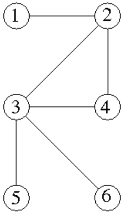
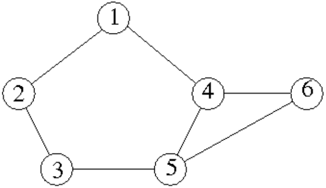


MCES-Example



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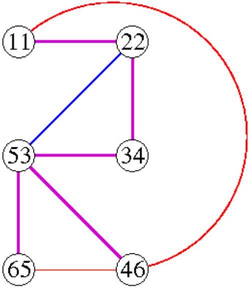

MCES-Application

Application 1: Parallel programming environments

G: task interaction graph (edges join pairs of tasks with communication demands)
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Application 2: Graph isomorphism problem

When $|E_G| = |E_H|$, there exists a common subgraph with $|E_G|$ edges, iff, G and H are isomorphic.

MCES-More applications and complexity

Application 3: Chemistry and biology

Matching $2D$ and $3D$ chemical structures Raymond 02

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Complexity

MCES is $\mathcal{NP}$-hard.

Goal:

Find exact/optimal solution of MCES instances using integer programming (IP) techniques and polyhedral combinatorics.

Previous polyhedral study

- Master's thesis Marenco 99 presented:
  IP formulation for MCES
  some valid inequalities and facets for corresponding polytope
  computational results.

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  some valid inequalities and facets for corresponding polytope
  computational results.
- Subsequent works by Marenco Marenco 06 present new classes of valid inequalities for MCES,
  but no new computational experiments.

IP formulation for MCES

$$y_{ik} := \begin{cases} 1 & \text{if vertex } i \text{ is mapped to vertex } k \\ 0 & \text{otherwise.} \end{cases}$$

$$x_{ij} := \begin{cases} 1 & \text{if exists } kl \in E_H \text{ such that } i \text{ is mapped to } k \text{ and } j \text{ to } l \\ 0 & \text{otherwise.} \end{cases}$$

IP formulation presented by Marenco:

$$\max \sum_{ij \in E_G} x_{ij}$$
$$\sum_{k \in V_H} y_{ik} = 1, \quad \forall i \in V_G$$
$$\sum_{i \in V_G} y_{ik} = 1, \quad \forall k \in V_H$$
$$x_{ij} + y_{ik} \leq 1 + \sum_{l \in N(k)} y_{jl}, \quad \forall ij \in E_G, \forall k \in V_H$$
$$y_{ik} \in \{0,1\}, \quad \forall i \in V_G, \forall k \in V_H; \quad x_{ij} \in \{0,1\}, \quad \forall ij \in E_G$$

IP formulation for MCES

Note:

Consider inequality

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

Let ij be a fixed edge in G, and k a fixed vertex from H.
Then $x_{ij} = 1$ iff j is mapped to a neighbour of k.

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Theorem (Marenco 99):

$\dim(\mathrm{conv}(S)) = (|V_G| - 1)^2 + |E_G|$, where S is the set of feasible integer solutions of the problem, and $\mathrm{conv}(S)$ its convex hull.

New IP formulation

$$c_{ijkl} := \begin{cases} 1 & \text{if } ij \text{ is mapped to } kl \\ 0 & \text{otherwise.} \end{cases}$$

New IP formulation:

$$\max \sum_{ij \in E_G} \sum_{kl \in E_H} c_{ijkl}$$
$$\sum_{k \in V_H} y_{ik} \leq 1, \quad \forall i \in V_G$$
$$\sum_{i \in V_G} y_{ik} \leq 1, \quad \forall k \in V_H$$
$$\sum_{kl \in E_H} c_{ijkl} \leq \sum_{k \in V_H} y_{ik}, \quad \forall ij \in E_G$$
$$\sum_{ij \in E_G} c_{ijkl} \leq \sum_{i \in V_G} y_{ik}, \quad \forall kl \in E_H$$
$$\sum_{j \in N(i)} c_{ijkl} \leq y_{ik} + y_{il}, \quad \forall i \in V_G, \forall kl \in E_H$$
$$\sum_{l \in N(k)} c_{ijkl} \leq y_{ik} + y_{jk}, \quad \forall ij \in E_G, \forall k \in V_H$$
$$c_{ijkl} \in \{0,1\}, \quad \forall ij \in E_G, \forall kl \in E_H$$

New IP formulation

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since the proofs of facet-defining inequalities are easier than in the model given in Marenco 99.

This is because the monotone polytope associated to the above formulation can be easily shown to be full-dimensional.

New IP formulation

- Can be shown that inequalities from our model

$$\begin{array}{ll} \sum_{j \in N(i)} c_{ijkl} \leq y_{ik} + y_{il}, & \forall i \in V_G, \forall kl \in E_H \\ \sum_{l \in N(k)} c_{ijkl} \leq y_{ik} + y_{jk}, & \forall ij \in E_G, \forall k \in V_H \end{array}$$

force that if ij is mapped to kl, then i is mapped to k and j to l, or vice versa.

Our contribution

- We present facets and other valid inequalities for the polytope P given by the convex hull of the integer solutions of the our IP model.

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- We present facets and other valid inequalities for the polytope P given by the convex hull of the integer solutions of the our IP model.
- We present here only the proofs of validity of the corresponding inequalities.

Valid inequalities and facets: inequalities from model

Theorem 1:

Inequalities from model

$$
\begin{aligned}
\sum_{kl \in E_H} c_{ijkl} \leq \sum_{k \in V_H} y_{ik}, &\quad \forall ij \in E_G \\
\sum_{ij \in E_G} c_{ijkl} \leq \sum_{i \in V_G} y_{ik}, &\quad \forall kl \in E_H \\
\sum_{j \in N(i)} c_{ijkl} \leq y_{ik} + y_{il}, &\quad \forall i \in V_G, \forall kl \in E_H \\
\sum_{l \in N(k)} c_{ijkl} \leq y_{ik} + y_{jk}, &\quad \forall ij \in E_G, \forall k \in V_H
\end{aligned}
$$

define facets.

Valid inequalities and facets: inequalities from model

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$$\begin{aligned}\sum_{kl \in E_H} c_{ijkl} \leq \sum_{k \in V_H} y_{ik}, & \quad \forall ij \in E_G \\ \sum_{ij \in E_G} c_{ijkl} \leq \sum_{i \in V_G} y_{ik}, & \quad \forall kl \in E_H \\ \sum_{j \in N(i)} c_{ijkl} \leq y_{ik} + y_{il}, & \quad \forall i \in V_G, \forall kl \in E_H \\ \sum_{l \in N(k)} c_{ijkl} \leq y_{ik} + y_{jk}, & \quad \forall ij \in E_G, \forall k \in V_H\end{aligned}$$

define facets.

Proof:

Using standard techniques from Polyhedral Combinatorics.

Valid inequalities that involve degrees of the vertices

Theorem 2:

Following inequality that involves degrees of the vertices is valid in model given by Marenco 99.

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

Facets that involve degrees of the vertices

Theorem 2*:

Let
i be a fixed vertex from G,
k a fixed vertex from H,
$I \subseteq N(i)$ and
$K \subseteq N(k)$.
Then, following inequalities are valid and define facets in our model.

$$\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |I| y_{ik} + \sum_{p \in K} y_{ip}, \text{ if } |I| < |K|.$$
$$\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |K| y_{ik} + \sum_{p \in I} y_{pk}, \text{ if } |I| > |K|.$$

Facets that involve degrees of the vertices

Proof:

We prove that $\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |I| y_{ik} + \sum_{p \in K} y_{ip}, \text{ if } |I| < |K|$ is valid.

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Proof:

We prove that $\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |I| y_{ik} + \sum_{p \in K} y_{ip}$, if $|I| < |K|$ is valid.

If $c_{ijkl} = 0$ for every $j \in I$ and $l \in K$ then trivial.

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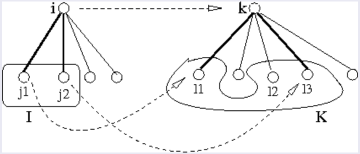
Proof:

We prove that $\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |I| y_{ik} + \sum_{p \in K} y_{ip}$, if $|I| < |K|$ is valid.

If i is mapped to $k \Longrightarrow$

Num. of edges ij s.t. $j \in I$ that can be mapped to edges kl from H s.t. $l \in K$ is at most $\min\{|I|, |K|\} = |I|$.

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



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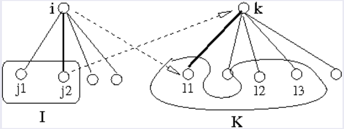
Proof:

We prove that $\sum_{j\in I}\sum_{l\in K} c_{ijkl} \leq |I| y_{ik} + \sum_{p\in K} y_{ip}$, if $|I| < |K|$ is valid.

If i is mapped to a $k' \in V_H$ s.t. $k' \neq k \Longrightarrow$

$\sum_{j\in I}\sum_{l\in K} c_{ijkl} \leq 1$.

If $\sum_{j\in I}\sum_{l\in K} c_{ijkl} = 1$ then i is mapped to a vertex from K (that is, $k' \in K$), and some $j \in I$ must be mapped to k.



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We obtained inequalities that generalize the result of Theorem 2*.

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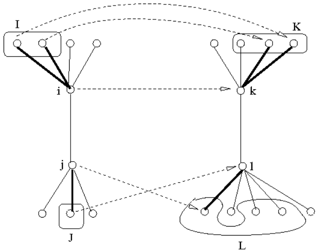
Given an edge ij in G, and kl in H,sets
$I \subseteq N(i) \setminus \{j\}$, $J \subseteq N(j) \setminus \{i\}$, $K \subseteq N(k) \setminus \{l\}$, $L \subseteq N(l) \setminus \{k\}$,
our inequality bounds the number of edges from the set
$E_{ij} := \{ij\} \cup (\delta(i) \cap \delta(I)) \cup (\delta(j) \cap \delta(J))$ that can be mapped to edges from the set $W_{kl} := \{kl\} \cup (\delta(k) \cap \delta(K)) \cup (\delta(l) \cap \delta(L))$.



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Theorem 3:

Let G' be an induced subgraph of G s.t. $|V_{G'}| = 2p + 1$ and G' has an hamiltonian cycle.
Let M be a maximal matching in H.
Then inequality

$$\sum_{ij \in E_{G'}} \sum_{kl \in M} c_{ijkl} \leq p$$

is valid.
If $|M| \geq p + 1$, then the inequality above defines a facet.

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Proof that $\sum_{ij \in E_{G'}} \sum_{kl \in M} c_{ijkl} \leq p$ is valid, where
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Since $|V_{G'}| = 2p + 1$, there are at most p vertex-disjoint edges in G'.

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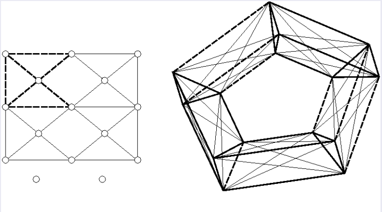

(a) (b)

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That is why, we tried to find valid inequalities that explore the structure of the input graphs, in order to obtain better upper bounds for the problem.

Inequalities that explore the structure of the graphs

Theorem 4

Let
k_G: max. num. of edge disjoint k-cycles in G
k_H: max. num. of edge disjoint k-cycles in H.
If $k_G \geq k_H$, then the following inequality is valid.

$$\sum_{e \in E_G} \sum_{w \in E_H} c_{ew} \quad \leq \quad |E_G| - (k_G - k_H), \text{ if } |E_G| \leq |E_H|.$$

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k_G (resp. k_H): max. num. of edge disjoint k-cycles in G (resp. H)

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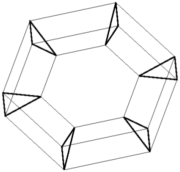

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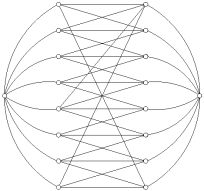

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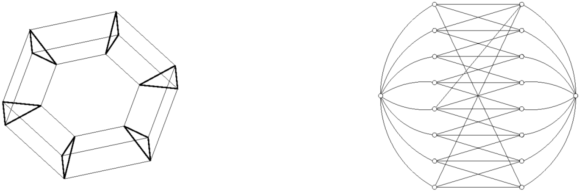

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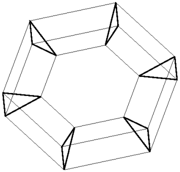

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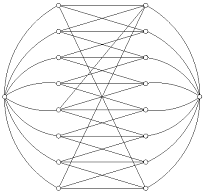

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$\sum_{e \in E_G} \sum_{w \in E_H} c_{ew} \leq |E_G| - (k_G - k_H) = 36 - (6 - 0) = 30.$

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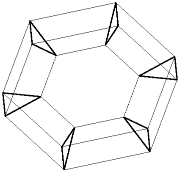

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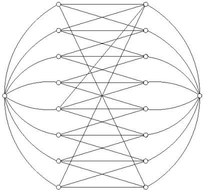

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$\sum_{e \in E_G} \sum_{w \in E_H} c_{ew} \leq |E_G| - (k_G - k_H) = 36 - (6 - 0) = 30.$

Obtained lower bound for this instance is 30 $\implies$ optimal sol. is 30.

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k_G: max. num. of edge disjoint subgraphs in G, s.t. each of those subgraphs is isomorphic to $\mathcal{S}$, and
k_H: max. num. of edge disjoint subgraphs in H, s.t. each of those subgraphs is isomorphic to $\mathcal{S}$.

Other inequalities

By lifting technique, we obtained a few stronger valid inequalities than given in Marenco 99.

Other inequalities

Consider inequality:

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However, this inequality does not define a facet in our model.

It is dominated by inequality from model:

$$\sum_{l \in N(k)} c_{ijkl} \leq y_{ik} + y_{jk}, \quad \forall ij \in E_G, \forall k \in V_H \tag{1}$$

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However, this inequality does not define a facet in our model.

It is dominated by inequality from model:

$$\sum_{l \in N(k)} c_{ijkl} \le y_{ik} + y_{jk}, \quad \forall ij \in E_G, \forall k \in V_H \tag{1}$$

Indeed, let ij be a fixed edge from G, and U be a minimal vertex cover of H.

By summing inequalities (1) for all $u \in U$ we get

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

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Preliminary computational results

- Fast polynomial time algorithm was designed to separate inequalities that involve degrees of vertices:

$$\sum_{j\in I}\sum_{l\in K} c_{ijkl} \leq |I|y_{ik} + \sum_{p\in K} y_{ip}, \text{ if } |I| < |K|.$$
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- Inequalities that explore the structure of the graphs

$$\sum_{e\in E_G}\sum_{w\in E_H} c_{ew} \quad \le \quad |E_G| - (k_G - k_H), \text{ if } |E_G| \le |E_H|$$

were added *a priori* for $k = 3, 4, 5$.

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- Among unsolved instances:
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- Algorithm is quite fast:
  only few instances required more than 10 minutes to be solved and the execution time never exceeded 14 minutes.

Concluding remarks

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- This study led to some advance in obtaining the exact solutions to the MCES problem using IP and **B&C** algorithm.
- Those computational results are preliminary. We will preform more robust test in the future.

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