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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  - Definition
  - Applications
- **Previous polyhedral study**
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- Our contribution
  - New integer programming formulation
  - Valid inequalities and facets of the polytope
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- **Common Edge Subgraph problem**
  - Definition
  - Applications
- **Previous polyhedral study**
- **Our contribution**
  - New integer programming formulation
  - Valid inequalities and facets of the polytope
- **Preliminary computational results**
Maximum Common Edge Subgraph Problem

Definition (Bokhari 81):

**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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Find: a common subgraph of $G$ and $H$, (not necessary induced) with the maximum number of edges.

We denote this problem by MSEC (Maximum Common Edge Subgraph).
Maximum Common Edge Subgraph Problem

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We denote this problem by MSEC (Maximum Common Edge Subgraph).
MCES-Example

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Common Edge Subgraph polytope
MCES-Application

Application 1: Parallel programming environments

\(G\): task interaction graph (edges join pairs of tasks with communication demands)
\(H\): processors graph (pair of processors being joined by an edge when they are directly connected).

Problem: Find mapping of tasks to processors s.t. number of neighboring tasks assigned onto connected processors is maximized.
MCES-Application

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**Problem:** Find mapping of tasks to processors s.t. number of neighboring tasks assigned onto connected processors is **maximized**.

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**.
Application 3: Chemistry and biology

Matching 2D and 3D chemical structures Raymond 02
MCES-More applications and complexity

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Complexity
MCES is NP-hard.
MCES-More applications and complexity

Application 3: Chemistry and biology
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Complexity
MCES is 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.
Previous polyhedral study

- Master’s thesis Marenco 99 presented:
  IP formulation for MCES
  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:

\[
\begin{align*}
\text{max} & \quad \sum_{ij \in E_G} x_{ij} \\
\sum_{k \in V_H} y_{ik} &= 1, \quad \forall i \in V_G \\
\sum_{i \in V_G} y_{ik} &= 1, \quad \forall k \in V_H \\
x_{ij} + y_{ik} &\leq 1 + \sum_{l \in N(k)} y_{jl}, \quad \forall ij \in E_G, \forall k \in V_H \\
y_{ik} \in \{0, 1\}, \quad \forall i \in V_G, \forall k \in V_H; \quad x_{ij} \in \{0, 1\}, \quad \forall ij \in E_G
\end{align*}
\]
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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\[ x_{ij} + y_{ik} \leq 1 + \sum_{l \in N(k)} y_{jl}, \quad \forall ij \in E_G, \forall k \in V_H. \]

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Theorem (Marenco 99):

\[ \dim(\text{conv}(S)) = (|V_G| - 1)^2 + |E_G|, \] where \( S \) is the set of feasible integer solutions of the problem, and \( \text{conv}(S) \) 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:

\[
\begin{align*}
\max \sum_{ij \in E_G} \sum_{kl \in E_H} c_{ijkl} \\
\sum_{k \in V_H} y_{ik} & \leq 1, \quad \forall i \in V_G \\
\sum_{i \in V_G} y_{ik} & \leq 1, \quad \forall k \in V_H \\
\sum_{kl \in E_H} c_{ijkl} & \leq \sum_{k \in V_H} y_{ik}, \quad \forall ij \in E_G \\
\sum_{ij \in E_G} c_{ijkl} & \leq \sum_{i \in V_G} y_{ik}, \quad \forall kl \in E_H \\
\sum_{j \in N(i)} c_{ijkl} & \leq y_{ik} + y_{il}, \quad \forall i \in V_G, \forall kl \in E_H \\
\sum_{l \in N(k)} c_{ijkl} & \leq y_{ik} + y_{jk}, \quad \forall ij \in E_G, \forall k \in V_H \\
c_{ijkl} & \in \{0, 1\}, \quad \forall ij \in E_G, \forall kl \in E_H
\end{align*}
\]
We decided to work with the monotonous model since the proofs of facet-defining inequalities are easier than in the model given in Marenco 99.
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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

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

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{align*}
\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{align*}
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define facets.
Valid inequalities and facets: inequalities from model

**Theorem 1:**

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

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.

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

\[
\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |I|y_{ik} + \sum_{p \in K} y_{ip}, \quad \text{if } |I| < |K|.
\]

\[
\sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |K|y_{ik} + \sum_{p \in I} y_{pk}, \quad \text{if } |I| > |K|.
\]
Facets that involve degrees of the vertices

**Proof:**

We prove that \( \sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |I|y_{ik} + \sum_{p \in K} y_{ip}, \) if \(|I| < |K|\) is valid.
Facets that involve degrees of the vertices

**Proof:**

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

If \( c_{ijkl} = 0 \) for every \( j \in I \) and \( l \in K \) then trivial.
Facets that involve degrees of the vertices

**Proof:**

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

If \( i \) is mapped to \( k \) \( \implies \)

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, \( \sum_{j \in I} \sum_{l \in K} c_{ijkl} \leq |I| \leq |I| y_{ik} + \sum_{p \in K} y_{ip} \).
Facets that involve degrees of the vertices

**Proof:**

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

If \( i \) is mapped to a \( k' \in V_H \) s.t. \( k' \neq k \)

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

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 \( k \).
We obtained inequalities that generalize the result of Theorem 2*.
Facets that involve degrees of the vertices

We obtained inequalities that generalize the result of Theorem 2*. 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 $W_{kl} := \{kl\} \cup (\delta(k) \cap \delta(K)) \cup (\delta(l) \cap \delta(L))$. 

![Diagram of Common Edge Subgraph polytope](image-url)
Facets that involve maximal matching in $H$

Benefit of having an extended formulation including variables $c_{ijkl}$:
Facets that involve maximal matching in $H$

Benefit of having an *extended formulation* including variables $c_{ijkl}$: We are able to express a simple inequality which cannot be written in the model given by *Marenco 99*. 
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**Theorem 3:**

Let $G'$ be an induced subgraph of $G$ s.t. $|V_{G'}| = 2p + 1$ and $G'$ has a 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.
Facets that involve maximal matching in $H$

Proof:

Proof that $\sum_{ij \in E_{G'}} \sum_{kl \in M} c_{ijkl} \leq p$ is valid, where $G'$ is an induced subgraph of $G$ s.t. $|V_{G'}| = 2p + 1$ and $G'$ has an hamiltonian cycle. $M$ is a maximal matching in $H$. 
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Since $|V_{G'}| = 2p + 1$, there are at most $p$ vertex-disjoint edges in $G'$. 
Facets that involve maximal matching in $H$

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![Diagrams](image_url)
Inequalities that explore the structure of the graphs

Instances that serves to test our implementation of the B&C algorithm present a high degree of symmetry.
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For example, task interaction graph of most of the instances are regular grids.

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
\[ k_G : \text{max. num. of edge disjoint } k\text{-cycles in } G \]
\[ k_H : \text{max. num. of edge disjoint } k\text{-cycles in } H. \]

If \( k_G \geq k_H \), then the following inequality is valid.

\[
\sum_{e \in E_G} \sum_{w \in E_H} c_{ew} \leq |E_G| - (k_G - k_H), \text{ if } |E_G| \leq |E_H|.
\]
Inequalities that explore the structure of the graphs

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

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(a) \( G \) is a 4-regular grid. It has 6 edge disjoint triangles (highlighted edges). (b) \( H \) has no triangles.
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\]

Obtained lower bound for this instance is 30 \( \rightarrow \) optimal sol. is 30.
Inequalities that explore the structure of the graphs

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Note: above inequality can be generalized:
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Note: above inequality can be generalized:
Given any special graph, say \( S \), above inequality is valid for numbers
\( k_G : \text{max. num. of edge disjoint subgraphs in } G, \text{ s.t. each of those subgraphs is isomorphic to } S, \text{ and} \)
\( k_H : \text{max. num. of edge disjoint subgraphs in } H, \text{ s.t. each of those subgraphs is isomorphic to } S. \)
By lifting technique, we obtained a few stronger valid inequalities than given in Manić 99.
Consider inequality:

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

where \( U \) is a vertex cover of graph \( H \).
Other inequalities

Consider inequality:

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Above inequality defines a facet in model given in Marenco 99, if $U$ is a minimal vertex cover of $H$. 
Consider inequality:

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

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Above inequality defines a facet in model given in Marenco 99, if \( U \) is a minimal vertex cover of \( H \).
However, this inequality does not define a facet in our model.
It is dominated by inequality from model:
\[ \sum_{l \in N(k)} c_{ijkl} \leq y_{ik} + y_{jk}, \quad \forall ij \in E_G, \forall k \in V_H \quad (1) \]
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\[ \sum_{l \in N(k)} c_{ijkl} \leq y_{ik} + y_{jk}, \quad \forall ij \in E_G, \forall k \in V_H \quad (1) \]

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

\[ \sum_{kl \in E_H} c_{ijkl} \leq \sum_{u \in U} \sum_{l \in N(u)} c_{ijul} \leq \sum_{u \in U} (y_{iu} + y_{ju}). \]
Preliminary computational results

- Our polyhedral investigation was the starting point of our branch-and-bound (B&B) and branch-and-cut (B&C) algorithms.
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- 16 instances are very small ($|V_G| < 10$),
  19 having 20 vertices each
  9 having at least 30 vertices.
  The largest instance has 36 vertices.
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- We used Xpress-Optimizer v17.01.02 as the IP solver;
- We used MOSEL language to code our programs.
Fast polynomial time algorithm was designed to separate inequalities that involve degrees of vertices:

\[
\begin{align*}
\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|.
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- Inequalities that explore the structure of the graphs

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

were added \textit{a priori} for \(k = 3, 4, 5\).
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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.
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Those computational results are preliminary. We will preform more robust test in the future.

