Second-order Birkhoff Polytope and the Problem of Graph Isomorphism Detection

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- Several heuristics that perform very well in practice, for e.g., nauty, bliss, traces etc.

The Graph Isomorphism Problem

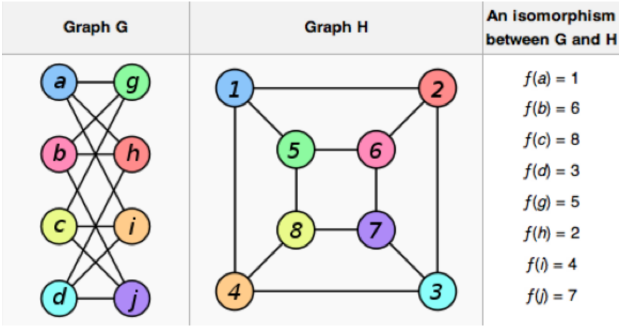

Figure : Isomorphic Graphs

figure taken from http://www.andrew.cmu.edu/user/hgl/2.png

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- Can some re-ordering of the vertices of one graph make it identical to the other?
- Naive algorithm: try all $n!$ permutations

Various Approaches to GI

Graph theoretic

Polynomial time algorithms for planar graphs, graphs of bounded genus, bounded tree width etc.

Group theoretic

Polynomial time algorithms for graphs of bounded degree, graphs with bounded eigenvalue multiplicities etc.; $2^{O(\sqrt{n \log n})}$ time algorithm for general graphs

Combinatorial

General heuristics that are polynomial time for certain classes like interval graphs, graphs with excluded minors etc.; most practical tools use this approach

Linear Programming Approach [Tinhofer 1991]

IP-GI: Find a point $X \in \{0,1\}^{n\times n}$ subject to the following:

$$\sum_k (A_{ik}X_{kj} - X_{ik}B_{kj}) = 0 \ , \ \forall \ i,j \tag{1a}$$

$$\sum_j X_{ij} = 1 \ , \ \forall \ i \tag{1b}$$

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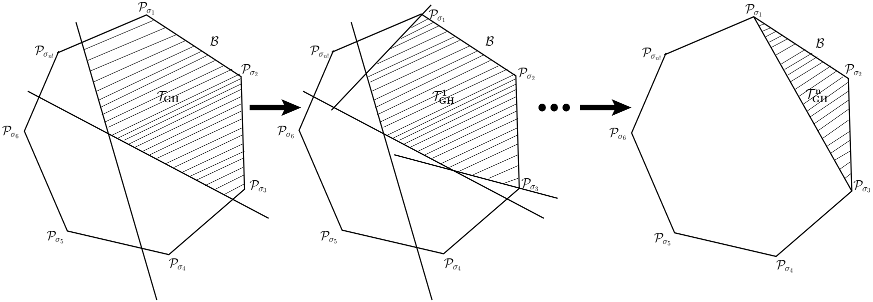
- (1a) corresponds to $P_\sigma^T A P_\sigma = B$

Recent Progress



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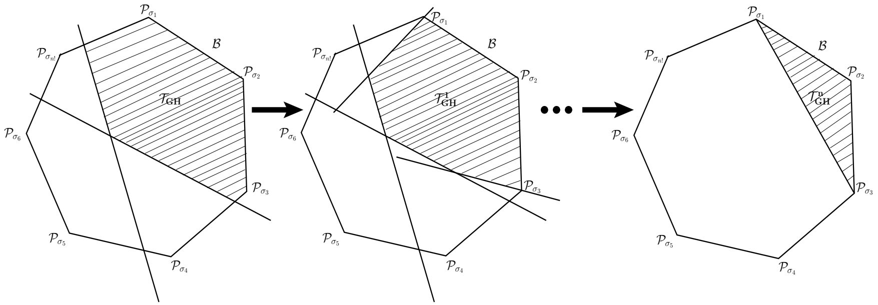

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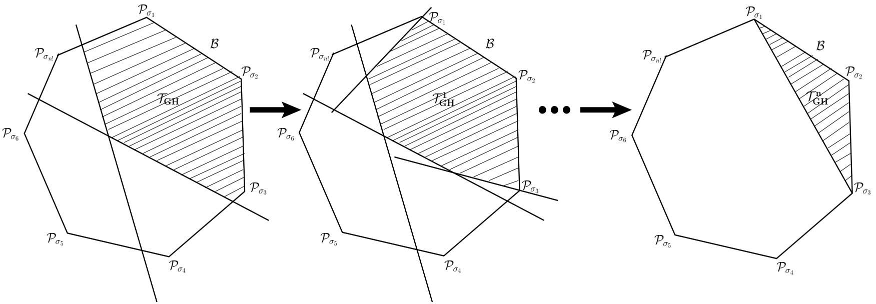

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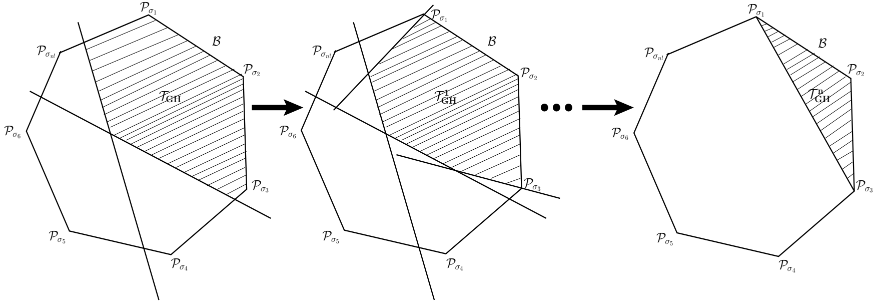

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- Time complexity: $O(n^k)$ for k rounds
- $\Omega(n)$ rounds of SA required for some graphs [Atserias,Maneva 2012; Malkin 2014]

A Second Integer Program

IP-GI: Find a $Y \in \{0,1\}^{n^2 \times n^2}$ that satisfies the following constraints:

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$$Y_{ij,il} = Y_{ji,li} = 0 \ , \ \forall \ i, \forall \ j \neq l \tag{2b}$$

$$\sum_k Y_{ij,kl} = \sum_k Y_{ij,lk} = Y_{ij,ij} \ , \ \forall \ i,j,l \tag{2c}$$

$$\sum_j Y_{ij,ij} = \sum_j Y_{ji,ji} = 1 \ , \ \forall \ i \tag{2d}$$

$$\sum_p A_{kp} \cdot Y_{pl,pl} = \sum_p Y_{kp,kp} \cdot B_{pl} \ , \ \forall \ k,l \tag{2e}$$

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Theorem

Graphs G, H are isomorphic iff IP-GI has a feasible solution

Integer Solutions

- The $n^2 \times n^2$ symmetric matrix $P_\sigma^{[2]}$, with $(P_\sigma^{[2]})_{ij,kl} = (P_\sigma)_{ij}(P_\sigma)_{kl}$

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Theorem

$Y = \mathcal{P}_\sigma^{[2]}$ *is a solution of IP-GI iff* σ *is an isomorphism between* G, H

The Linear Program

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\begin{aligned}
\text{LP-GI:} \quad \text{Find a point} \quad & Y \\
\text{subject to} \quad & 2a\text{-}2f \\
& Y_{ij,kl} \geq 0 \ , \forall \ i,j,k,l \qquad \text{(3a)}
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The feasible region of LP-GI, $\mathcal{P}_{GH}$ corresponds to one lift step of Sherali-Adams starting with the Tinhofer polytope

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Definition

Define $\mathcal{B}^{[2]}_{GH}$ as the integer hull of $\mathcal{P}_{GH}$, for a given G, H, i.e., $\mathcal{B}^{[2]}_{GH} = conv(P^{[2]}_{\sigma} | \ \sigma$ is an isomorphism between $G, H)$

Second-order Birkhoff Polytope, $\mathcal{B}^{[2]}$

Definition

Define polytope $\mathcal{P}$ as $\mathcal{P}_{GH}$ with $G = H = (V, \emptyset)$ or $G = H = K_n$

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The Second-order Birkhoff polytope $\mathcal{B}^{[2]}$ is the integer hull of $\mathcal{P}$ or $\mathcal{B}^{[2]} = conv(P^{[2]}_{\sigma} | \; \sigma \in S_n)$. Clearly, $\mathcal{B}^{[2]} \subseteq \mathcal{P}$

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History of $\mathcal{B}^{[2]}$

Appears in literature as the QAP(Quadratic Assignment Problem)-polytope [Volker Kaibel's PhD Thesis, 1997]

Role of $\mathcal{B}^{[2]}$ in GI

Theorem

Graphs G, H are isomorphic iff $\mathcal{P}_{GH} \cap \mathcal{B}^{[2]} \neq \emptyset$. Moreover, $\mathcal{P}_{GH} \cap \mathcal{B}^{[2]} = \mathcal{B}^{[2]}_{GH}$

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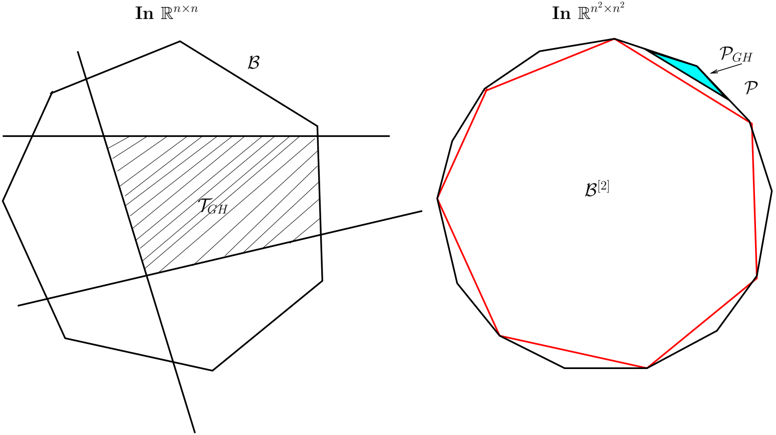
Corollary

For non-isomorphic graphs G, H, $\mathcal{P}_{GH} \subseteq \mathcal{P} \setminus \mathcal{B}^{[2]}$

Motivation

- **Feasible region for Non-Isomorphic Graphs**



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The polytopes $\mathcal{P}$ and $\mathcal{B}^{[2]}$ are full-dimensional in the affine plane P given by (2a)-(2d). Thus a facet plane of $\mathcal{B}^{[2]}$ is a hyperplane in P and hence must split $\mathcal{P}$ into two parts

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Idea

The facet planes of $\mathcal{B}^{[2]}$ separate $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ from $\mathcal{B}^{[2]}$. We can use the knowledge of these facets to eliminate $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ and thus reduce $\mathcal{P}_{GH}$ to its integer hull, $\mathcal{B}^{[2]}_{GH}$

The Trivial Facets of $\mathcal{B}^{[2]}$

Lemma

$Y_{ij,kl} = 0$ for all $i \neq k, j \neq l$, define some of the facets of $\mathcal{B}^{[2]}$. We call them the trivial facets of $\mathcal{B}^{[2]}$

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Theorem

All the vertices of $\mathcal{B}^{[2]}$ are some of the vertices of $\mathcal{P}$ and all the facet planes of $\mathcal{P}$ define some of the facets of $\mathcal{B}^{[2]}$ (its trivial facets)

A Polynomial-Sized Family of Facets

- Let i, i', k be distinct indices

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- $Q_0(k, l, i, i', j, j')$ can be included in LP-GI without affecting its polynomial time complexity

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$$+ \sum_{(ij),(kl)\in P_2\times Q, i<k} Y_{ij,kl} - \sum_{(ij)\in P_1\times Q,(kl)\in P_2\times Q} Y_{ij,kl} + \frac{\beta^2-\beta}{2} \geq 0$$

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$$+ \sum_{(ij),(kl) \in P_2 \times Q, i<k} Y_{ij,kl} - \sum_{(ij) \in P_1 \times Q, (kl) \in P_2 \times Q} Y_{ij,kl} + \frac{\beta^2 - \beta}{2} \geq 0$$

- $Q_3(P_1, P_2, Q, \beta)$ defines a family of facets under certain restrictions on the parameters

Facial Structure of $\mathcal{B}^{[2]}$

A General Inequality

All the known facets of $\mathcal{B}^{[2]}$ are special instances of a general inequality

$$\sum_{ijkl} n_{ij} n_{kl} Y_{ij,kl} + (\beta - 1/2)^2 \geq (2\beta - 1) \sum_{ij} n_{ij} Y_{ij,ij} + 1/4$$

where $\beta \in \mathbb{Z}$ and $n_{ij} \in \mathbb{Z}$ for all (ij)

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There are more Facets

Theorem

There exists at least one facet of $\mathcal{B}^{[2]}$ which is not an instance of the above inequality

Limitations

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- Our analysis will be limited to the situation when $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is separated from $\mathcal{B}^{[2]}$ by facets of type Q_1, Q_2 and Q_3

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- There must exist an inequality $Z \in Q_i$ such that Y violates Z but does not violate any other inequality $I \in Q_i$ s.t. $I \prec Z$

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Consequently

- Let $Y \in \mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ violates an inequality in Q_i for $i \in \{1, 2, 3\}$
- There must exist an inequality $Z \in Q_i$ such that Y violates Z but does not violate any other inequality $I \in Q_i$ s.t. $I \prec Z$
- We call Z a *minimal violated inequality* for point Y

Partial Ordering on the Exponential-Sized Family Q_1

- Let $i_1, \ldots, i_m, k$ be $m+1$ distinct indices
- Similarly let $j_1, \ldots, j_m, l$ be distinct indices
- Let $A = \{(i_1, j_1), \ldots, (i_m, j_m)\}$
- Then the inequality $Q_1(k, l, A)$ is given by

$$\sum_{(i,j)\in A} Y_{ij,kl} \leq Y_{kl,kl} + \sum_{(i,j)\neq(i',j')\in A} Y_{ij,i'j'}$$

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- The facets corresponding to $m = 3$ are polynomial in size

Zero-One Reducibility

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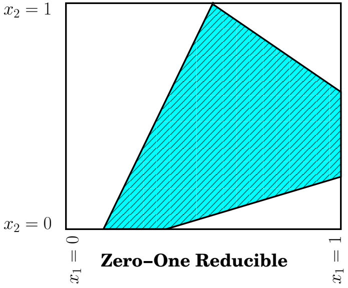
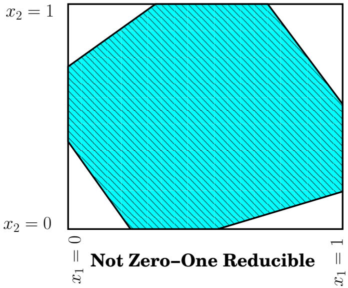
$R|_{x_1=\bar{1}} = \emptyset$, $R|_{x_1=1,x_2=\bar{0}} = \emptyset$; $R|_{x_1=1,x_2=0} = \emptyset$

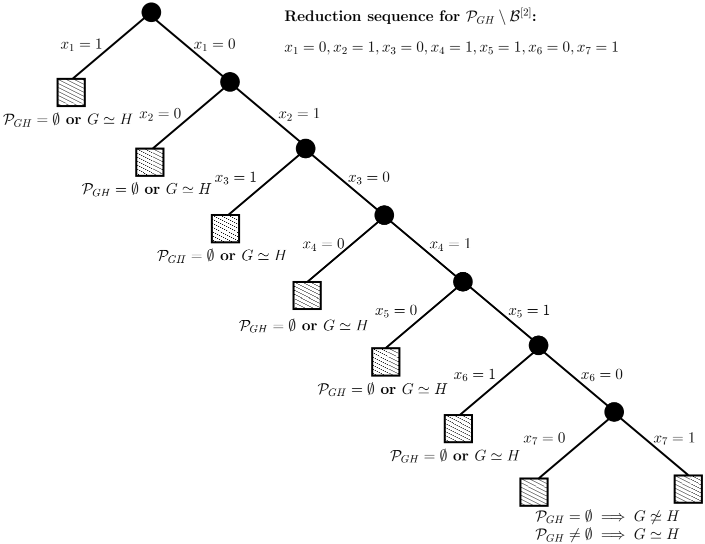


Zero–One Reducible



Not Zero–One Reducible

Solving GI When $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is Zero-One Reducible



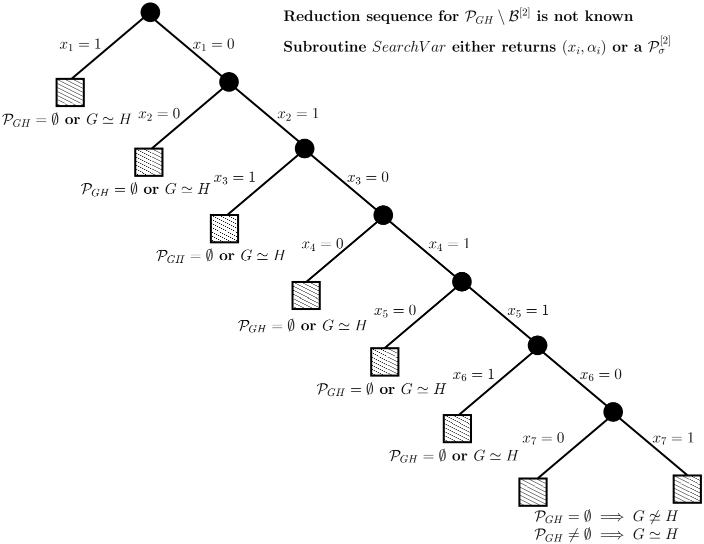
Reduction sequence for $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$:

$x_1 = 0, x_2 = 1, x_3 = 0, x_4 = 1, x_5 = 1, x_6 = 0, x_7 = 1$

Solving GI When $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is Zero-One Reducible

Reduction sequence for $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is not known

Subroutine $SearchVar$ either returns (x_i, α_i) or a $\mathcal{P}_{\sigma}^{[2]}$



Case of Common Minimal Violated Inequality

Lemma

If $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ *is zero-one reducible then there exists a polynomial time procedure for GI*

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If all points in $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ have a common minimal violated inequality from Q_1, Q_2 or Q_3, then $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is zero-one reducible

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Remark

If $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is zero-one reducible then only one round of any of the lift-and-project methods would suffice. For e.g., $LS^1(\mathcal{P}_{GH}) = \mathcal{B}^{[2]}_{GH}$

The General Case

- In general, it may not be true that all points in $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ have a common minimal violated inequality

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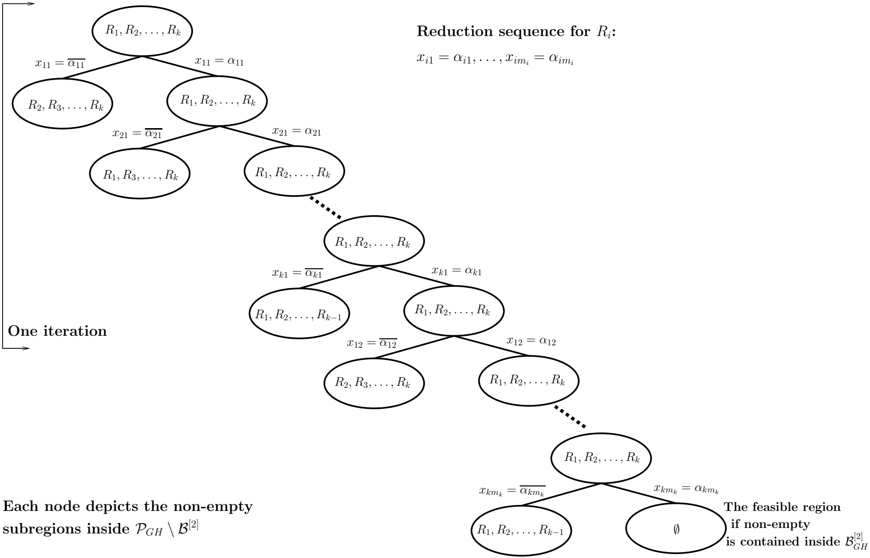
- We will use the fact that each R_j is zero-one reducible to design an efficient procedure for GI

Solving GI When $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]} = \cup_j R_j$, Each R_j is ZOR



Reduction sequence for R_i:

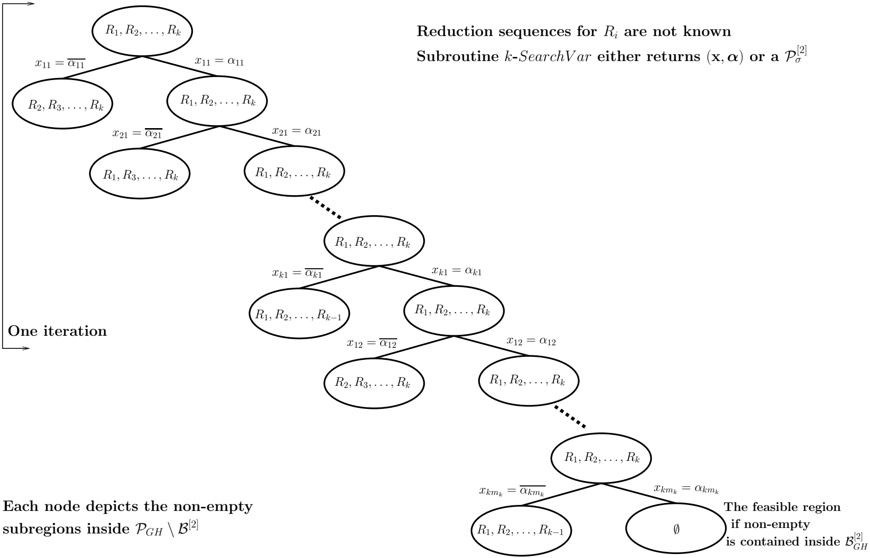
$x_{i1} = \alpha_{i1}, \ldots, x_{im_i} = \alpha_{im_i}$

Each node depicts the non-empty subregions inside $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$

Solving GI When $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]} = \cup_j R_j$, Each R_j is ZOR

Reduction sequences for R_i are not known

Subroutine k-$SearchVar$ either returns $(\mathbf{x}, \boldsymbol{\alpha})$ or a $\mathcal{P}_\sigma^{[2]}$



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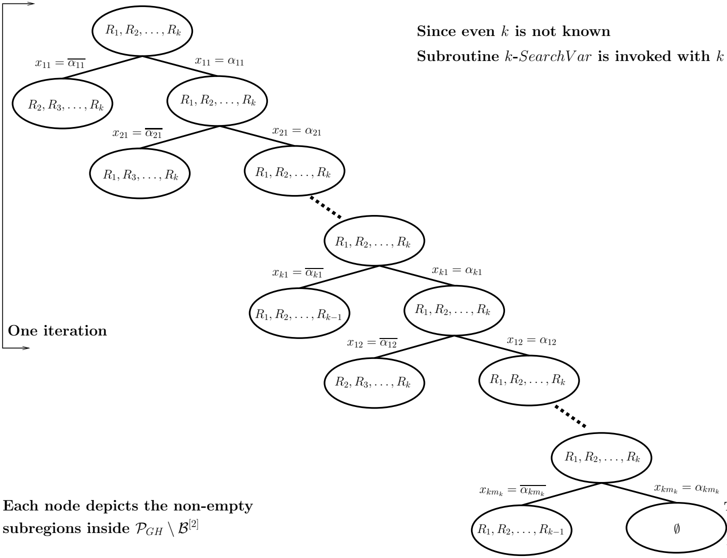
Solving GI When $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]} = \cup_j R_j$, Each R_j is ZOR

Since even k is not known

Subroutine k-$SearchVar$ is invoked with $k = 1, 2, \ldots$



The feasible region if non-empty is contained inside $\mathcal{B}^{[2]}_{GH}$

Each node depicts the non-empty subregions inside $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$

Analysis

The following recurrence sums up the performance of the Algorithm:

$$T(k) \leq N \cdot T(k-1) + \binom{N}{k} 2^k + \binom{N-k}{k} 2^k + \ldots + \binom{k}{k} 2^k$$
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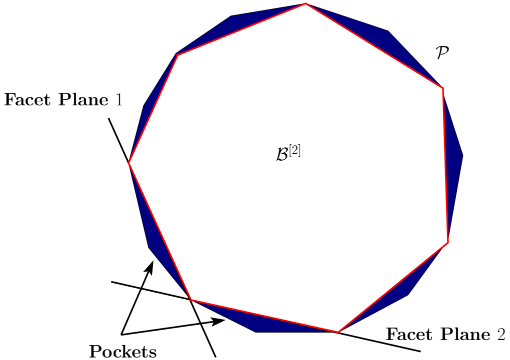
Theorem

The Algorithm solves the graph isomorphism problem in $O(k \cdot 2^k \cdot N^{k+c})$ time where $N = O(n^4)$ is the number of variables in LP-GI and k is the number of subregions into which $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is divided such that each subregion has a common minimal violated inequality of type Q_1, Q_2 or Q_3. Here $O(N^c)$ denotes the cost of solving LP-GI

Bounding the value of k

Pocket

Region of $\mathcal{P} \setminus \mathcal{B}^{[2]}$ on the non-$\mathcal{B}^{[2]}$ side of a facet plane of $\mathcal{B}^{[2]}$



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Theorem

If $\mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$ is confined to a pocket of $\mathcal{P}$ due to a facet in Q_1, then k is bounded by $\sqrt{n}$, leading to a $2^{O(\sqrt{n}\log n)}$ time algorithm for GI

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Experiments

Objective

To determine the value of k for pairs of non-isomorphic graphs taken from families considered hard for GI

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Strongly Regular Graphs

A d-regular n vertex graph is said to be (n, d, λ, μ)-strongly regular if all adjacent pairs of vertices have λ common neighbors and all non-adjacent pairs of vertices have μ common neighbors. Believed to be hard for GI, though not known to be GI-complete

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Results

We found the feasible region to be zero-one reducible ($k = 1$), in all the cases

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Lemma

Let $G = (V \setminus S, E)$ be a graph with the property that $\{u, v\} \in E$ iff $u - v \in LS(S)$. If G is connected, then S is a facet

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Lemma

Let $\Sigma = \{\sigma_1, \ldots, \sigma_6, \sigma'_1, \ldots, \sigma'_6\}$*. Then* $\sum_{\sigma \in \Sigma} sign(\sigma) P_\sigma^{[2]} \equiv \mathbf{0}$

Polytopes $\mathcal{P}, \mathcal{B}^{[2]}$ are Full-Dimensional in Plane P

- Let A be the $\frac{n^4+n^2}{2} \times n!$ matrix given below:

$$A = \begin{bmatrix} | & | & & | \\ symvec(P^{[2]}_{\sigma_1}) & symvec(P^{[2]}_{\sigma_2}) & \dots & symvec(P^{[2]}_{\sigma_{n!}}) \\ | & | & & | \end{bmatrix}$$

$$p = \begin{bmatrix} a & b & c & d \\ b & e & f & g \\ c & f & h & i \\ d & g & i & j \end{bmatrix}$$

$$symvec(p) = \begin{bmatrix} a & b & e & c & f & h & d & g & i & j \end{bmatrix}^T$$

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- Define the $\frac{n^4+n^2}{2} \times \frac{n^4+n^2}{2}$ psd matrix $B = AA^T$

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Table : Eigenvalues of matrix B with the corresponding multiplicities

Eigenvalue	Multiplicity
$(3/2)n!$	1
$n(n-3)!$	$\binom{n-1}{2}^2$
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$$rank(A) = rank(B) = 1 + \binom{n-1}{2}^2 + (\binom{n-1}{2}-1)^2 + (n-1)^2$$

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Corollary

Since $\mathcal{B}^{[2]} \subseteq \mathcal{P}$ *and* $\mathcal{P}$ *is contained in plane P,* $\mathcal{P}$ *is also a full-dimensional polytope in P*

Zero-One Reducibility of a Subregion R_i Due to Q_1

Lemma

Let $Q_1(k, l, A)$ be a minimal violated inequality for region $R_i \subseteq \mathcal{P}_{GH} \setminus \mathcal{B}^{[2]}$. Then R_i is zero-one reducible

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Proof Sketch

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- Reduction sequence: $Y_{i_1 j_1, kl} = 1, Y_{i_2 j_2, kl} = 1, Y_{i_3 j_3, kl} = 1$

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- $GI \in co\text{-}NP$?: can a minimal set of facet planes act as a certificate that can be verified in poly-time using say, the ellipsoid method?
- Can we use the geometry to differentiate faces of $\mathcal{P}$ that touch $\mathcal{B}^{[2]}$ at only a single vertex (the identity permutation) from those that touch at several vertices?

Thank you!
Questions?