An Application of Graph Products in Rule Inference

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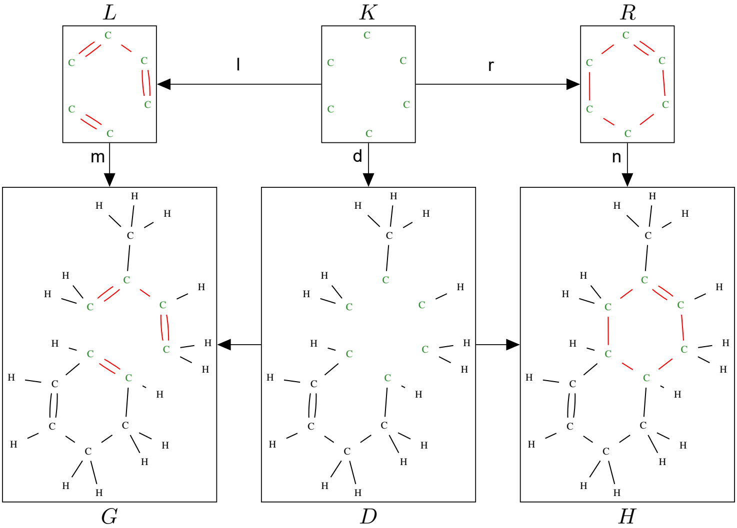
Double Push-Out Approach

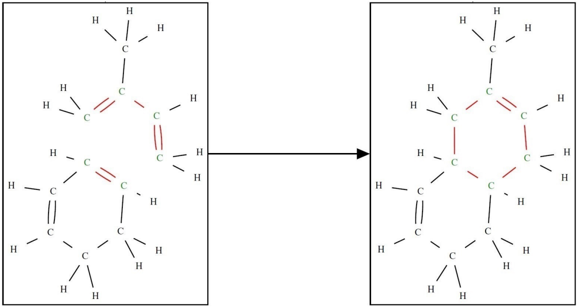


Rule Inference

Our Problem

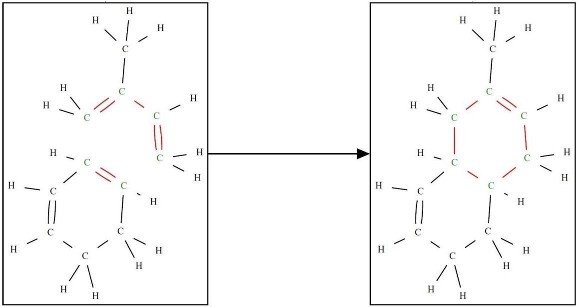
A list of reactions $L := \{R_1, R_2, \ldots, R_n\}$ is given. For every reaction $R_i : G_i \longrightarrow H_i$, an atom map $f_i : G_i \to H_i$ is given, as well. The goal is to find a minimum size list of subrules such that if we apply them on educts, then the result is L.

Combined Graph

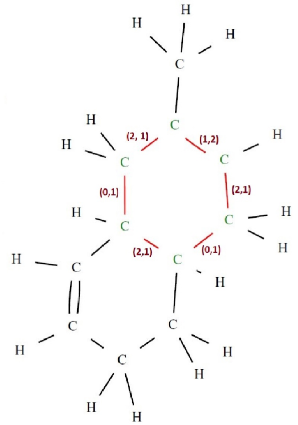


G H

Combined Graph

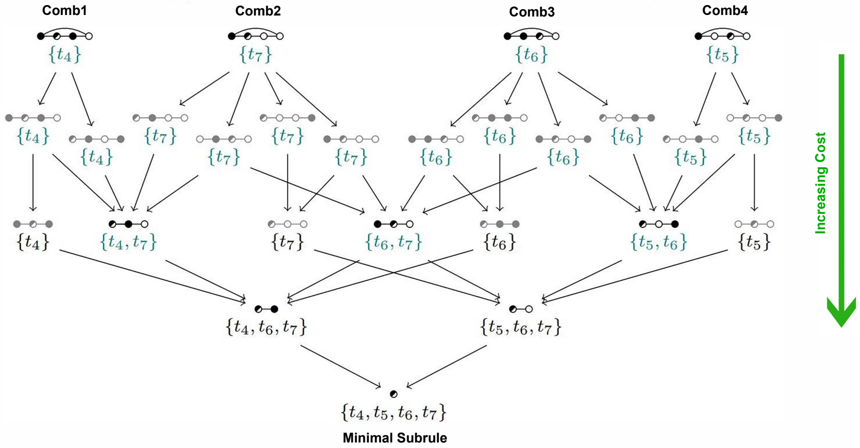


G H



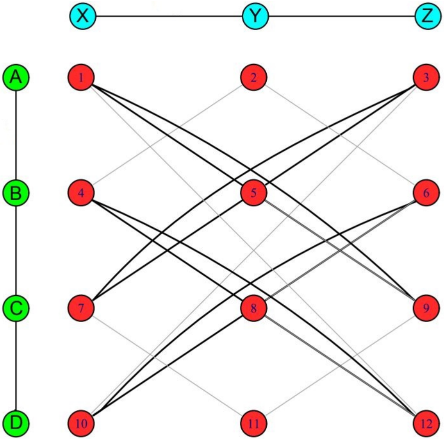
Combined Graph

Maximal Common Subgraph



Definition

The modular product of two graphs $G = (V, E)$ and $G' = (V', E')$ is a graph with vertex set $V \times V'$ and two vertices (u, u') and (v, v') are adjacent iff $(u, v) \in E(G)$ and $(u', v') \in E(G')$ or $(u, v) \notin E(G)$ and $(u', v') \notin E(G')$.



Definitions

Definition (Anchored Subgraph)

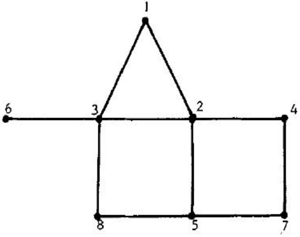
Let $A \subseteq H$. If we can extend this A in H to a copy of G in H, then G is called an anchored subgraph of H to A.

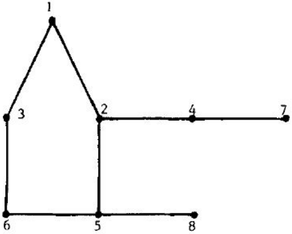
Definition (Maximal Common Subgraph)

Let A be a subgraph of both graphs H_1 and H_2. Then, G is called a maximal common subgraph of graphs H_1 and H_2 with respect to A if

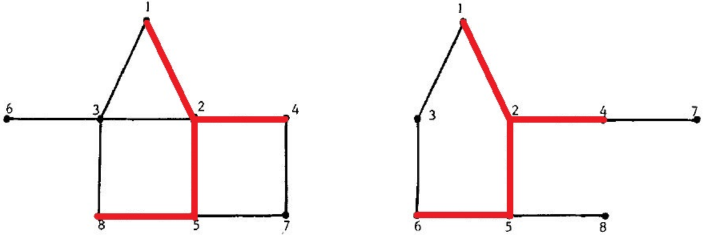
- G is an anchored subgraph of both H_1 and H_2 to A.
- For every graph K, which is an anchored subgraph of H_i's to A, we have $G \not\subseteq K$.

Edge induced and vertex induced subgraphs



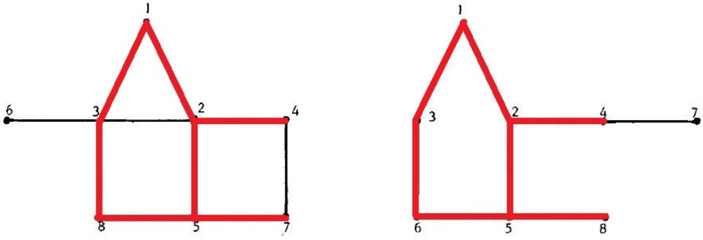


Edge induced and vertex induced subgraphs



Maximum common vertex induced subgraph:
5 vertices and 4 edges

Edge induced and vertex induced subgraphs



Maximum common edge induced subgraph:
7 vertices and 7 edges

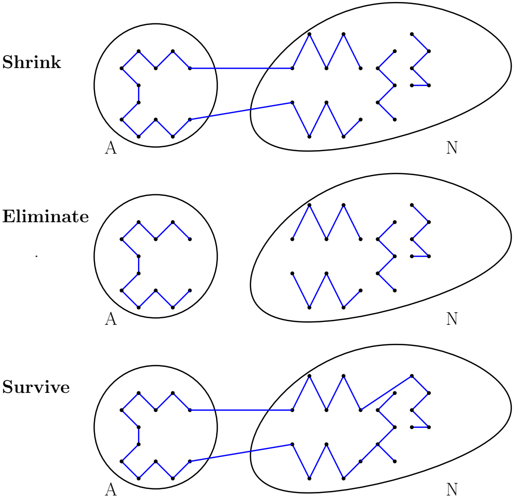
Inputs: $\{H_1, H_2, \ldots, H_t\}$ and A.
Output: Connected MCS of H_i's with respect to anchor A.

$$\overbrace{\underbrace{H_1 \times H_2}_{c_2} \times H_3}^{c_3} \times \cdots \times H_t$$

Step 1 Constructing the labelled modular product of H and H' with two edge types:
$(u, v) \in E(H)$ and $(u', v') \in E(H')$
$(u, v) \notin E(H)$ and $(u', v') \notin E(H')$

Step 2 Obtaining $N := \bigcap_{x \in A} N_{H \times H'}(x)$

Step 3 Removing blue connected components of N which are not connected to A by blue.


Shrink
A
N
Eliminate
A
N
Survive
A
N

MCS(H, H', A)

Inputs: ListN(list of remained blue components) and A
Output: Connected MCS's Anchored in A.

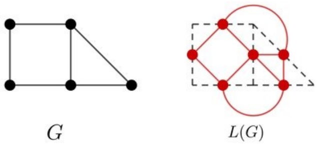
Algorithm 1 (pseudocode)

Answer=$\{\}$
for $N_i \in ListN$ **do**
    L=*MaxCliques*(N_i)
    for $l \in L$ **do**
        if l has no blue edge to A **then**
            Remove l from L
        end if
    end for
    Answer=Answer$\cup\{l \cup A \mid l \in L\}$
end for

Line Graphs

Definition (Line graph)

Let $G = (V, E)$ be a simple graph. The line graph $L(G)$ is another simple graph. Each vertex of $L(G)$ represents an edge of G and two vertices in $L(G)$ are adjacent iff the corresponding edges are adjacent in G.



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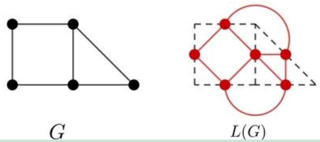
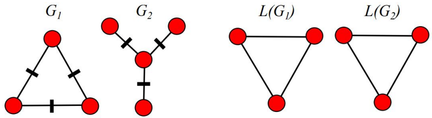


Whitney's Theorem (1932)

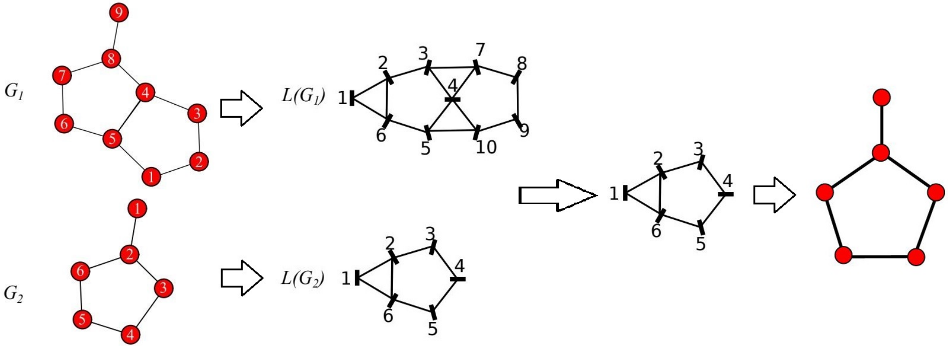
Every graph, except triangle or claw, is uniquely determined by its line graph.



From MCS to MCES

G and $G' \overset{L}{\Longrightarrow} L(G)$ and $L(G') \underset{\text{algorithm}}{\overset{\text{any induced}}{\Longrightarrow}}$ MCS$(L(G), L(G'))$
$\overset{L^{-1}}{\Longrightarrow}$ MCES(G, G')

Example:



Thanks for Your Attention.