# Mining Tree Patterns with Partially Injective Homomorphisms

Till Hendrik Schulz, Tamás Horváth, Pascal Welke, and Stefan Wrobel

University of Bonn

# Main Idea

The Two Most Common Pattern Matching Operators in Learning from Structured Data

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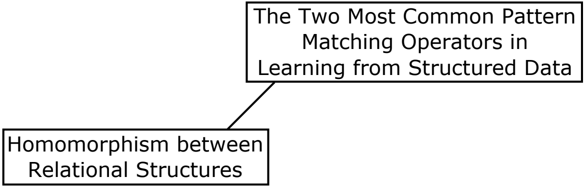

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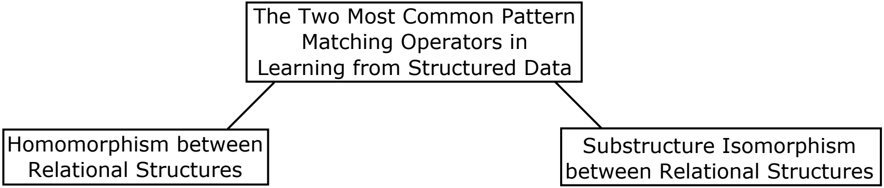

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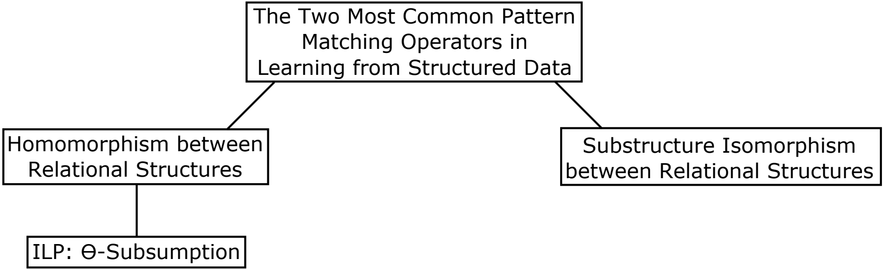

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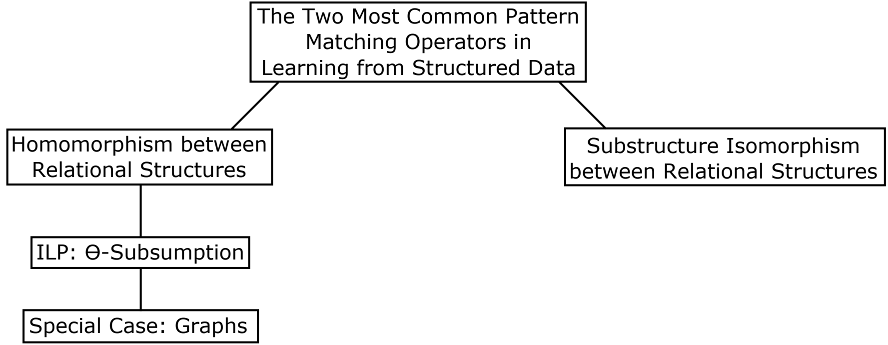

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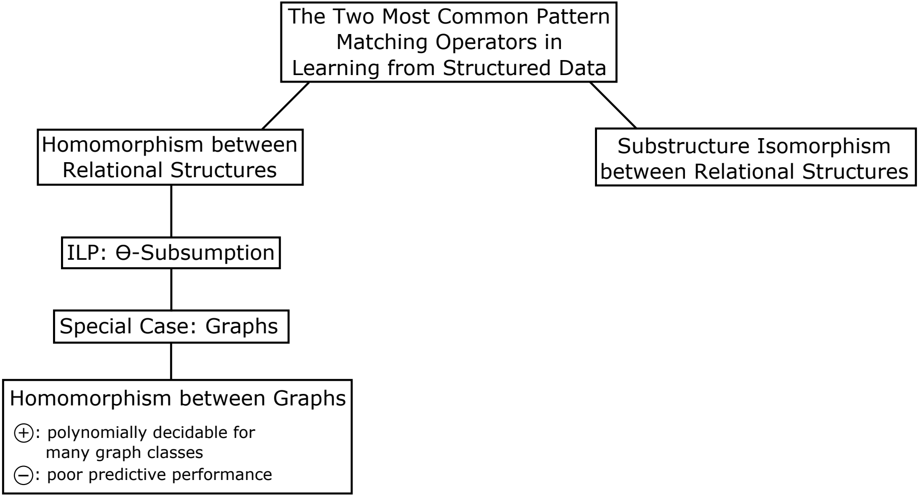

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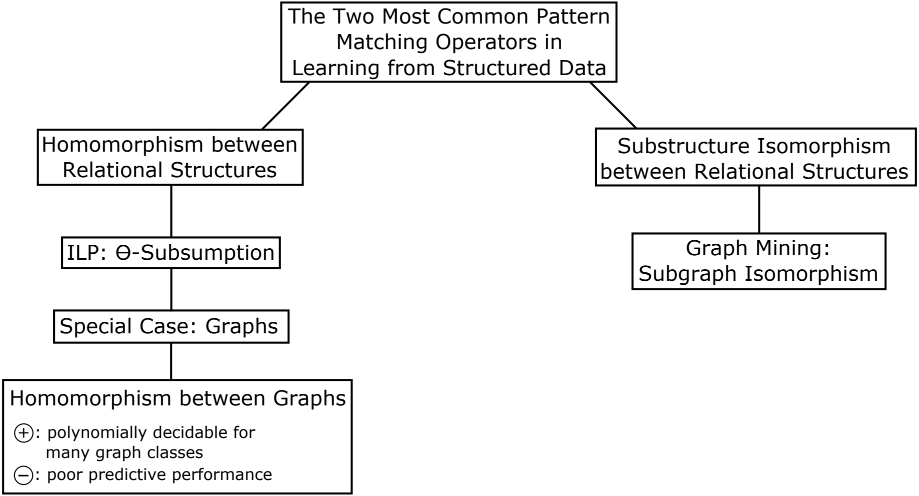

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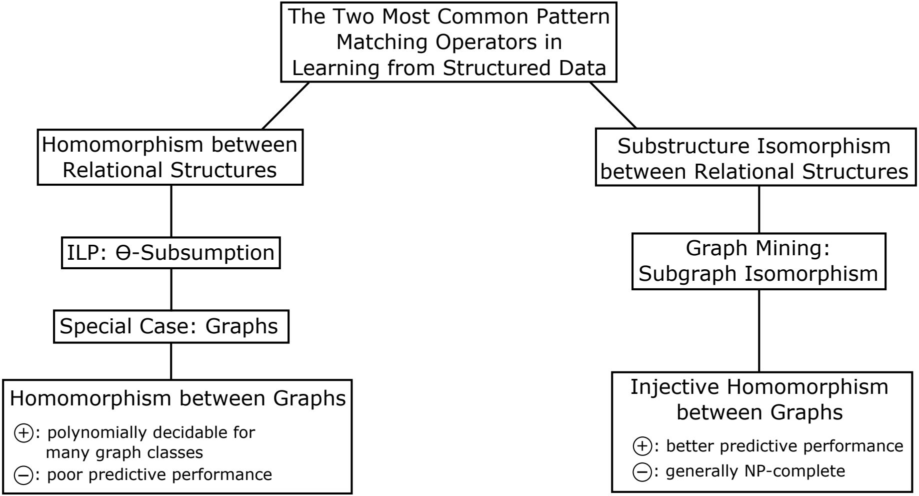

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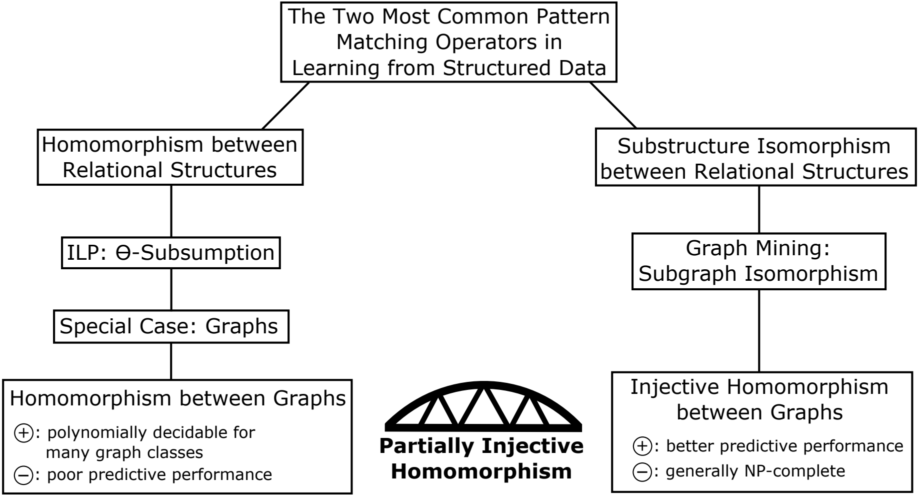

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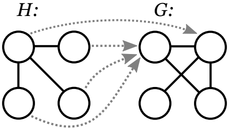

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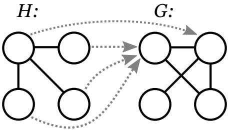

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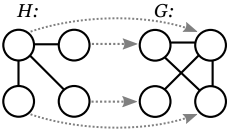

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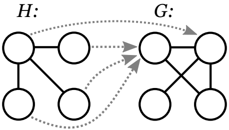

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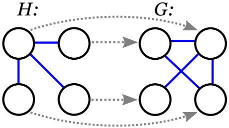

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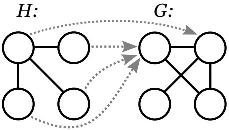

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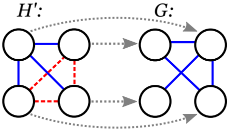

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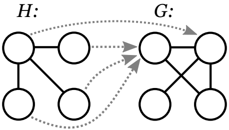

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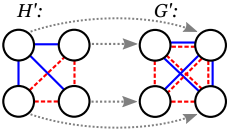

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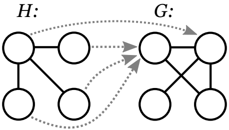

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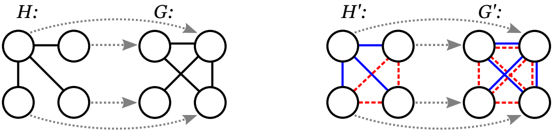

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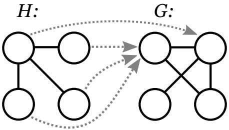

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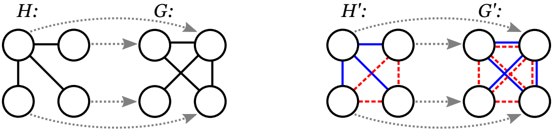

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$\Rightarrow$ **$H$ is subgraph isomorphic to $G$ iff there exists a homomorphism from $H'$ into $G'$**

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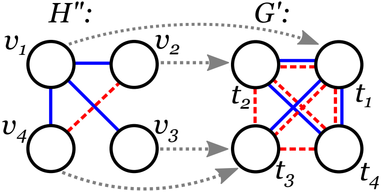

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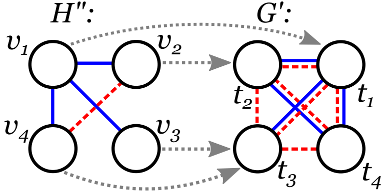

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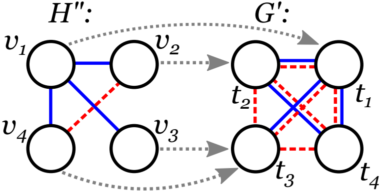

- $v_2$ and $v_4$ of $H''$ must be mapped to distinct vertices in $G'$

☺ **Partially injective homomorphism can be decided in polynomial time if the pattern graph (blue + red edges) has bounded tree width.**

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Generate *frequent trees* w.r.t. partially injective homomorphism

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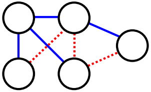

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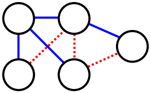

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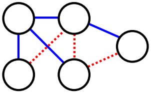

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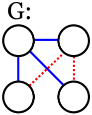

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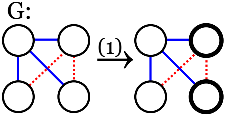

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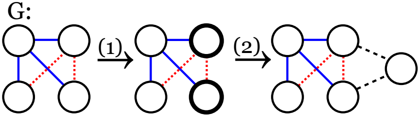

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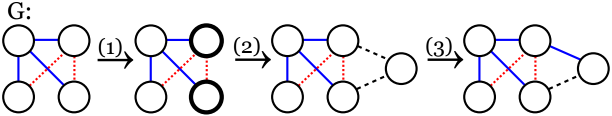

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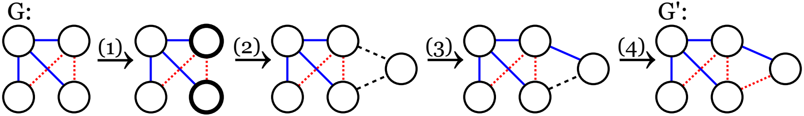

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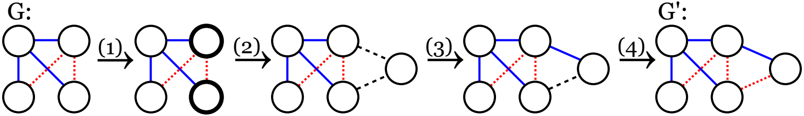

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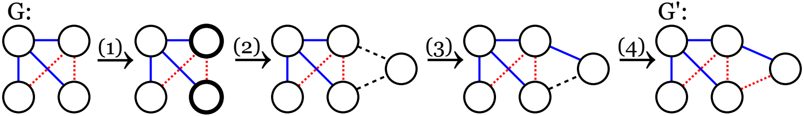

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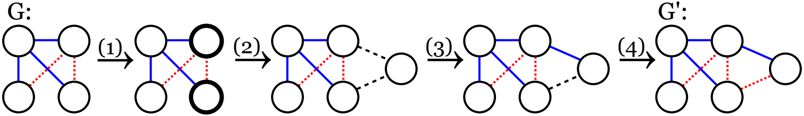

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Properties:

- graphs are *maximally* constrained (i.e. adding another red edge increases the tree-width)
- the embedding decision problem is guaranteed to lie in $P$

# Experiments

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|---|---|---|---|---|---|---|
| NCI1 | s.g.i. graphs | 79.30 | 84.36 | 86.48 | 87.17 | 87.18 |
| | s.g.i. trees | 79.30 | 84.10 | 86.16 | 86.83 | 86.92 |
| | p.i.h. trees ($k = 2$) | 78.94 | 83.18 | 85.02 | 85.41 | 86.07 |
| | p.i.h. trees ($k = 3$) | 80.51 | 84.53 | 85.83 | 86.64 | 86.68 |
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| NCI109 | s.g.i. graphs | 80.04 | 84.64 | 86.50 | 87.04 | 87.29 |
| | s.g.i. trees | 80.04 | 84.51 | 86.39 | 86.79 | 87.09 |
| | p.i.h. trees ($k = 2$) | 79.17 | 83.42 | 85.27 | 85.31 | 85.41 |
| | p.i.h. trees ($k = 3$) | 81.21 | 85.08 | 85.97 | 86.34 | 86.63 |
| | p.i.h. trees ($k = 4$) | 80.04 | 85.18 | 85.89 | 86.27 | 86.28 |
| PTC | s.g.i. graphs | 63.46 | 66.42 | 70.73 | 73.98 | 73.11 |
| | s.g.i. trees | 63.46 | 66.42 | 70.77 | 74.03 | 73.18 |
| | p.i.h. trees ($k = 2$) | 64.12 | 65.54 | 67.45 | 69.60 | 70.66 |
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| | p.i.h. trees ($k = 4$) | 63.50 | 67.67 | 72.56 | 72.68 | 72.14 |
| MUTAG | s.g.i. graphs | 72.71 | 85.28 | 89.27 | 89.89 | 90.29 |
| | s.g.i. trees | 72.71 | 83.05 | 87.23 | 88.50 | 89.49 |
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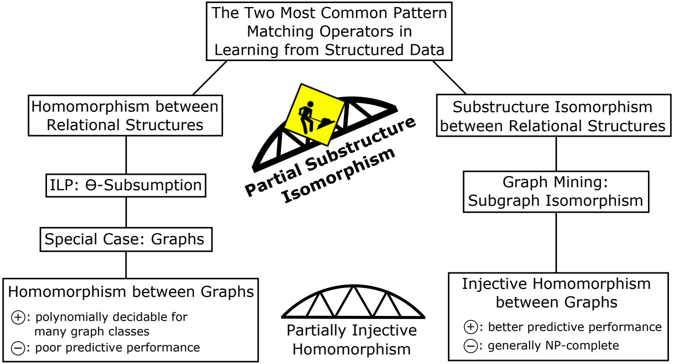

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Partial Substructure Isomorphism

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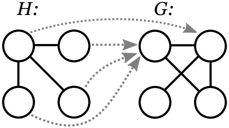
# Appendix

# Homomorphism & Subgraph Isomorphism

A **homomorphism** from a graph $H$ (the *pattern*) into a graph $G$ (the *text*) is a mapping $\varphi : V(H) \to V(G)$ that preserves the edges (i.e., $uv \in E(H)$ implies $\varphi(u)\varphi(v) \in E(G)$ for all $u, v \in V(H)$).

Example:



A **subgraph isomorphism** from $H$ to $G$ is an *injective* homomorphism $\psi : V(H) \to V(G)$ (i.e. $\psi$ is a homomorphism from $H$ into $G$ and for all $u, v \in V(H)$ with $u \neq v$ holds $\psi(u) \neq \psi(v)$).

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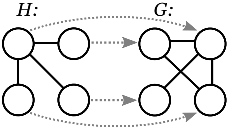


# Tree-width

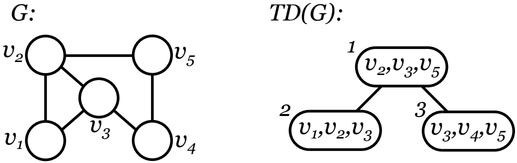
A **tree decomposition** of a graph $G = (V, E)$ is a pair $TD(G) = (T, X)$ where

- $T = (I, F)$ is an unordered tree,
- $X = \{bag(i) : i \in I\}$ is a family of subsets of $V$, s.t.
  - (i) $\bigcup_{i \in I} bag(i) = V$
  - (ii) for every $\{u, v\} \in E$ there is an $i \in I$ with $\{u, v\} \subseteq bag(i)$
  - (iii) for every $v \in V$ the set of nodes $\{i | v \in bag(i)\}$ forms a subtree of $T$

The **width** of $TD(G)$ is $max_i|bag(i)| - 1$

The **tree-width** of $G$ is the minimum width over all tree decompositions of $G$

Example:



$TD(G)$ has a width of 2 which is also the tree-width of $G$.

# k-trees

Algorithmic definition of **k-trees**:

(i) A clique of $k+1$ vertices is a $k$-tree and

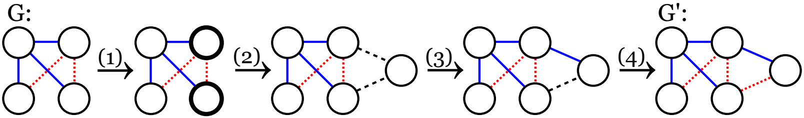
(ii) given a $k$-tree $T_k$ with $n$ vertices, a $k$-tree with $n+1$ vertices is obtained from $T_k$ by adding a new vertex $v$ to $T_k$ and connecting $v$ to all vertices of a $k$-clique of $T_k$.

Properties:

- A $k$-tree has tree-width $k$
- Adding an edge to a $k - tree$ results in a graph of tree-width $k+1$.

# Refinement Operator

**Refinement step**:



(1) select a 2-clique

(2) add a vertex and connect it to the 2-clique

(3) color one edge blue

(4) color all others red

$G'$ is a refinement of $G$. Both graphs are k-trees with $k = 2$.

Properties:

- graphs are *maximally* constrained (i.e. adding another red edge increases the tree-width)
- the embedding decision problem is guaranteed to lie in $P$

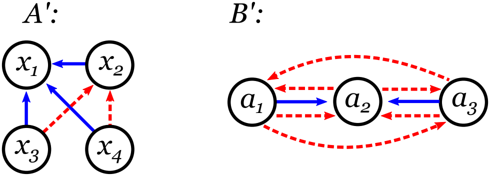
# Partial Substructure Isomorphism

Partially Injective Homomorphisms can be generalized to first-order logic:

Let $A$ and $B$ be function-free first-order clauses. A **partial substructure isomorphism** from $A$ to $B$ satisfying the injectivity constraints in $\mathcal{C} \subseteq [\mathrm{Var}(A)]^2$ is a substitution $\theta$ such that $A\theta \subseteq B$ and for all $xy \in \mathcal{C}$, $x\theta \neq y\theta$.

Example:

$$A = \{P(x_2, x_1), P(x_3, x_1), P(x_4, x_1)\}$$
$$B = \{P(a_1, a_2), P(a_3, a_2)\}$$
$$\mathcal{C} = \{x_3x_2, x_4x_2\}$$



There is a partial substructure isomorphism from $A$ to $B$ w.r.t. constraints $\mathcal{C}$ iff $A'$ subsumes $B'$.