Mining Tree Patterns with Partially Injective Homomorphisms

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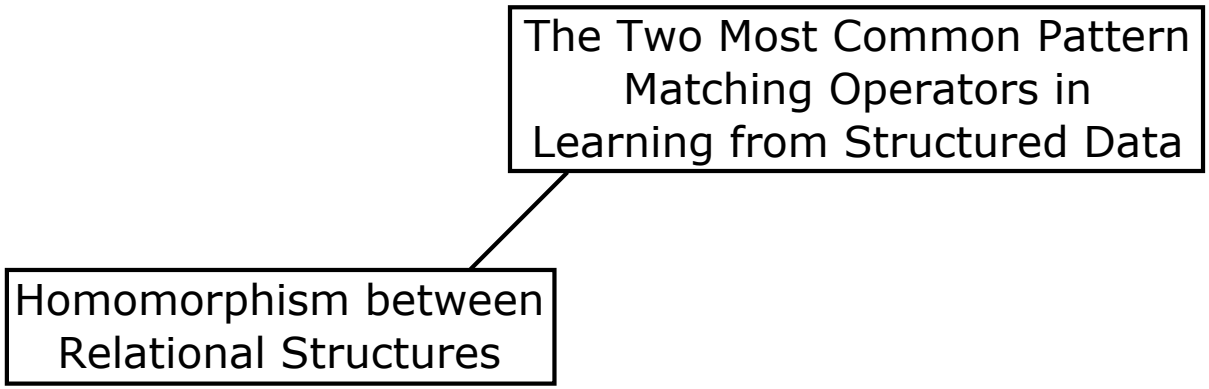
Learning from Structured Data

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

Learning from Structured Data



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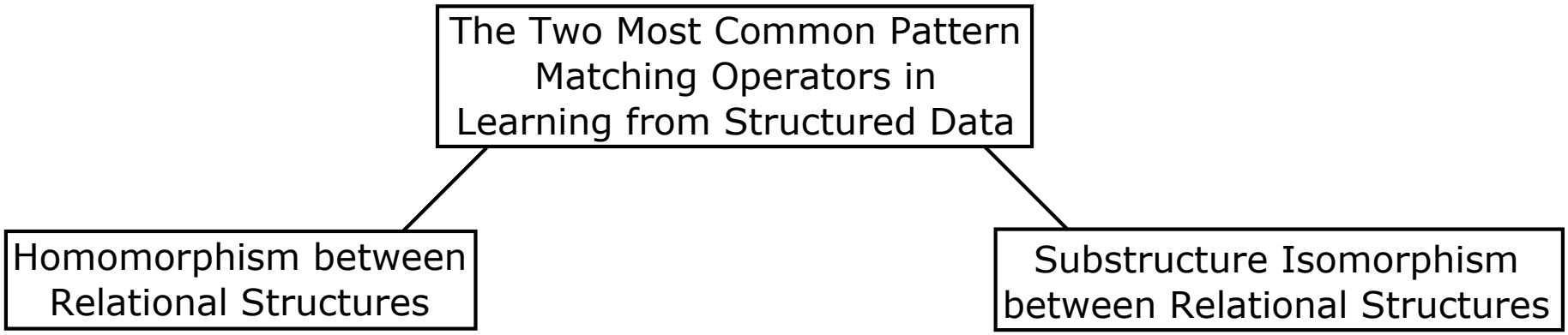

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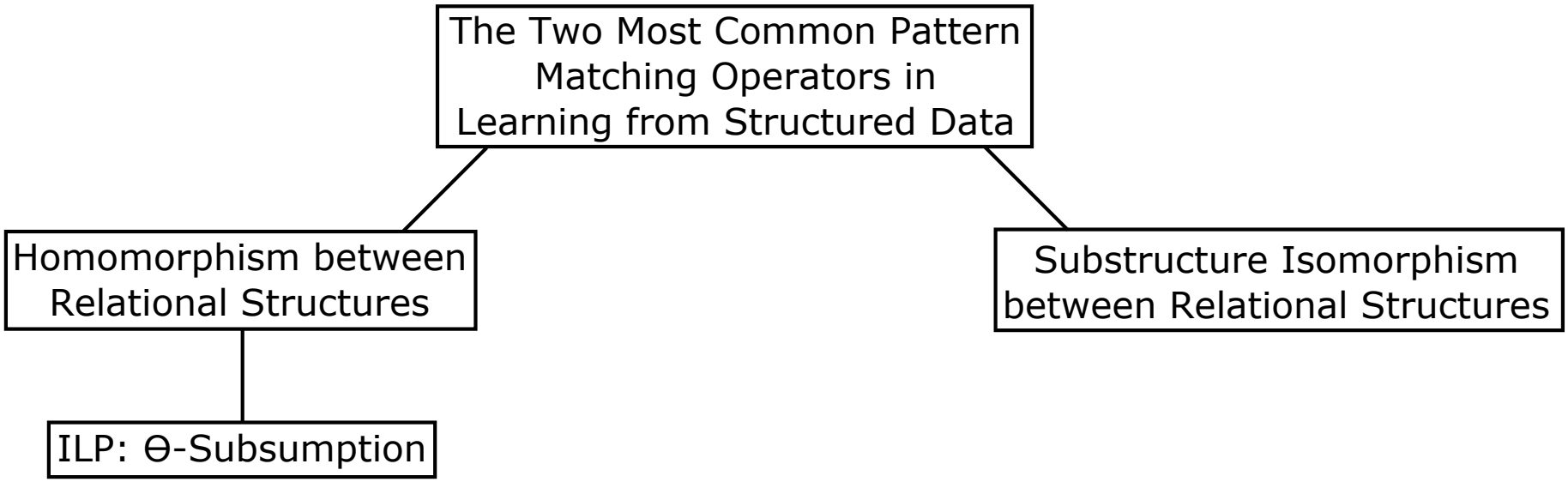

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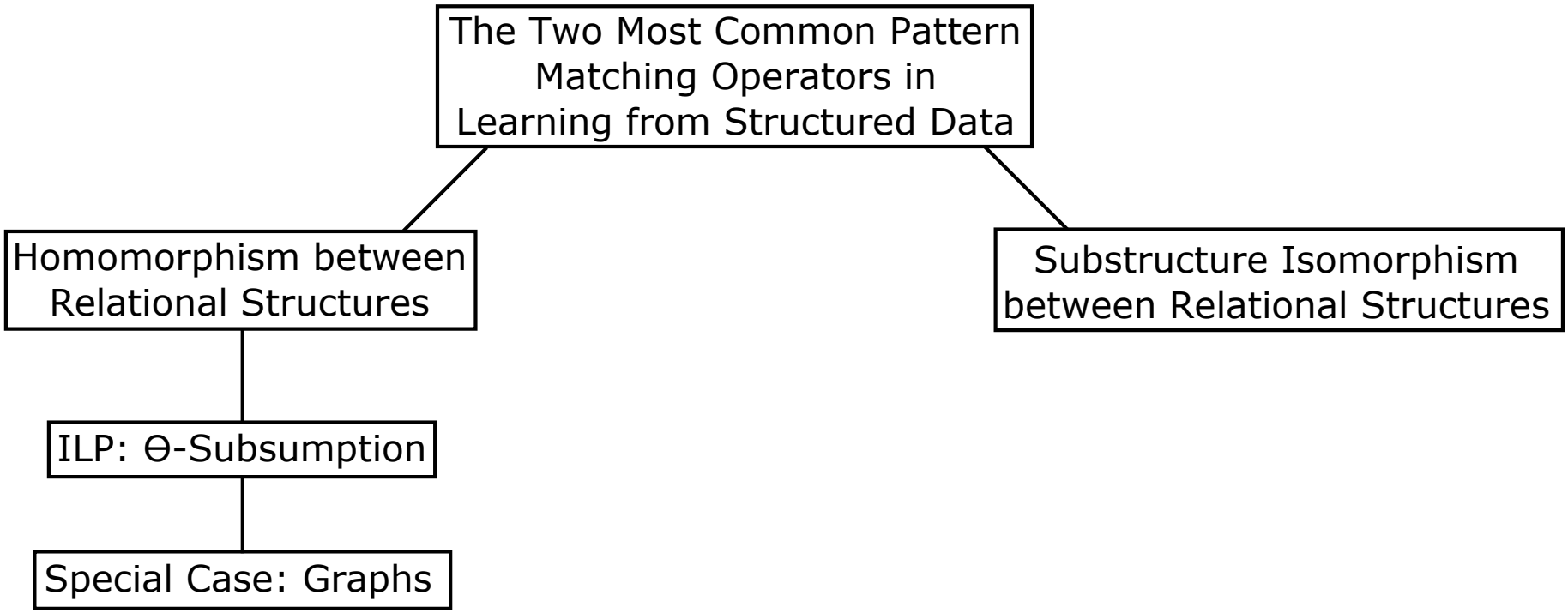

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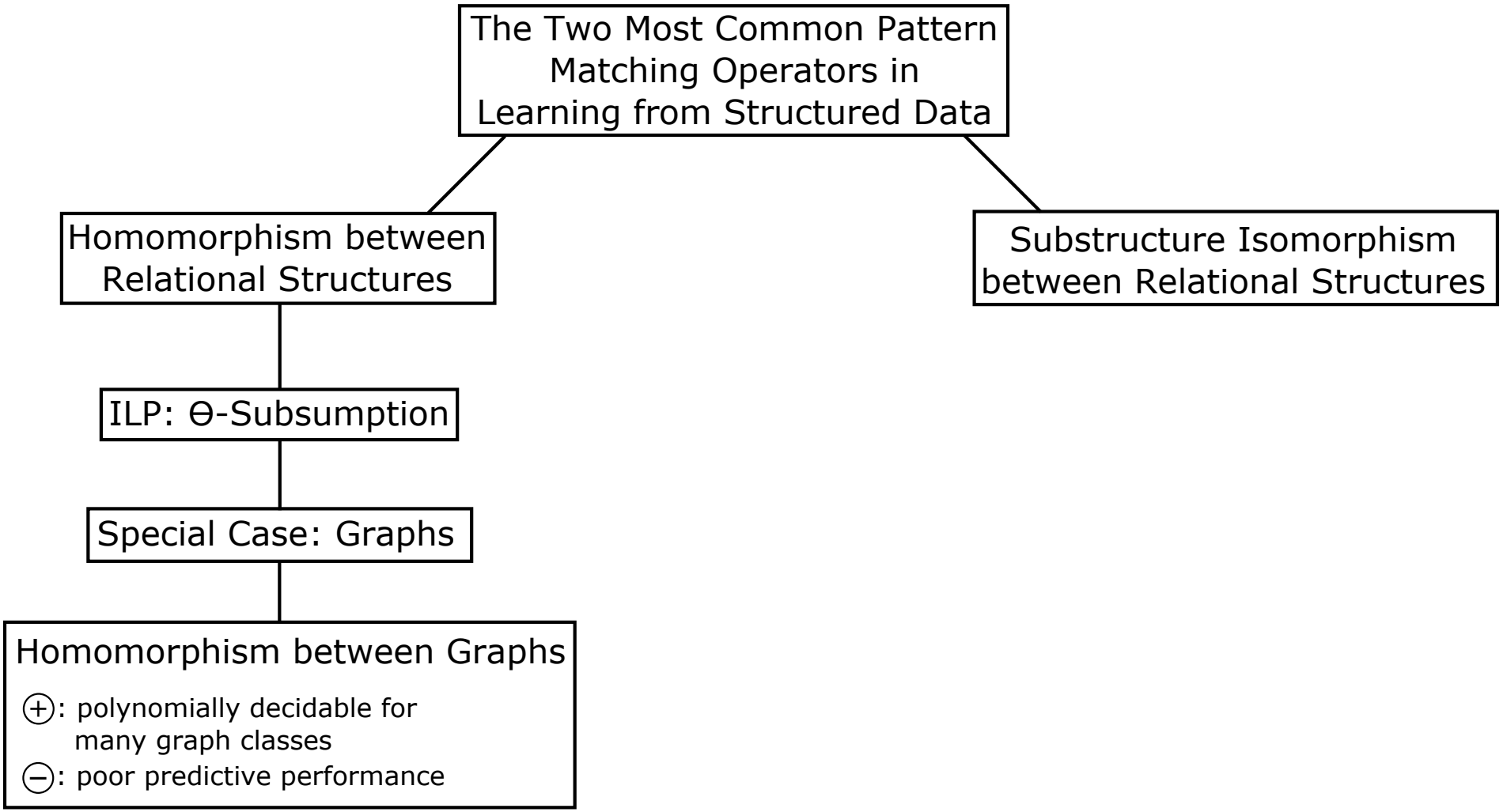

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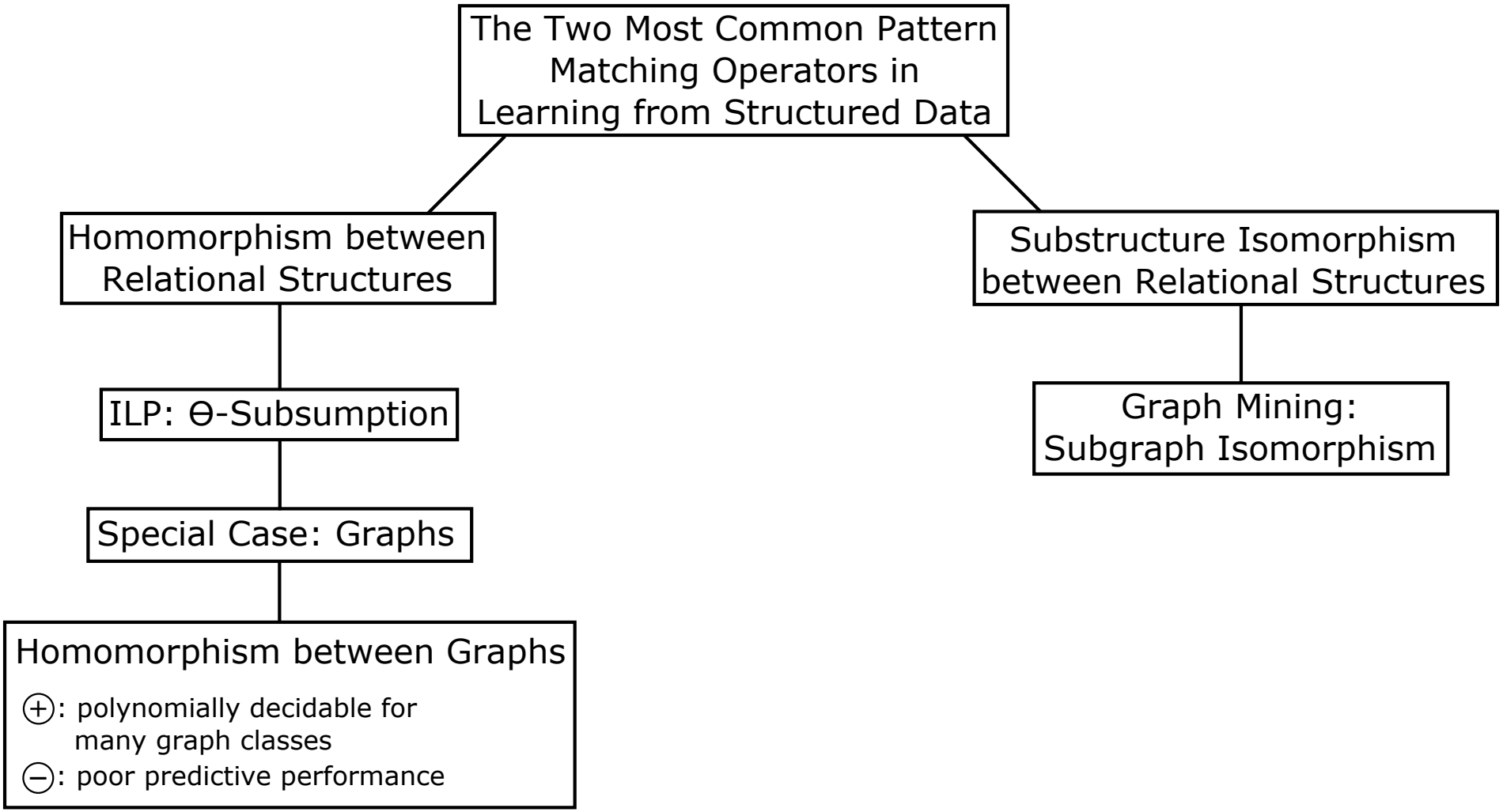

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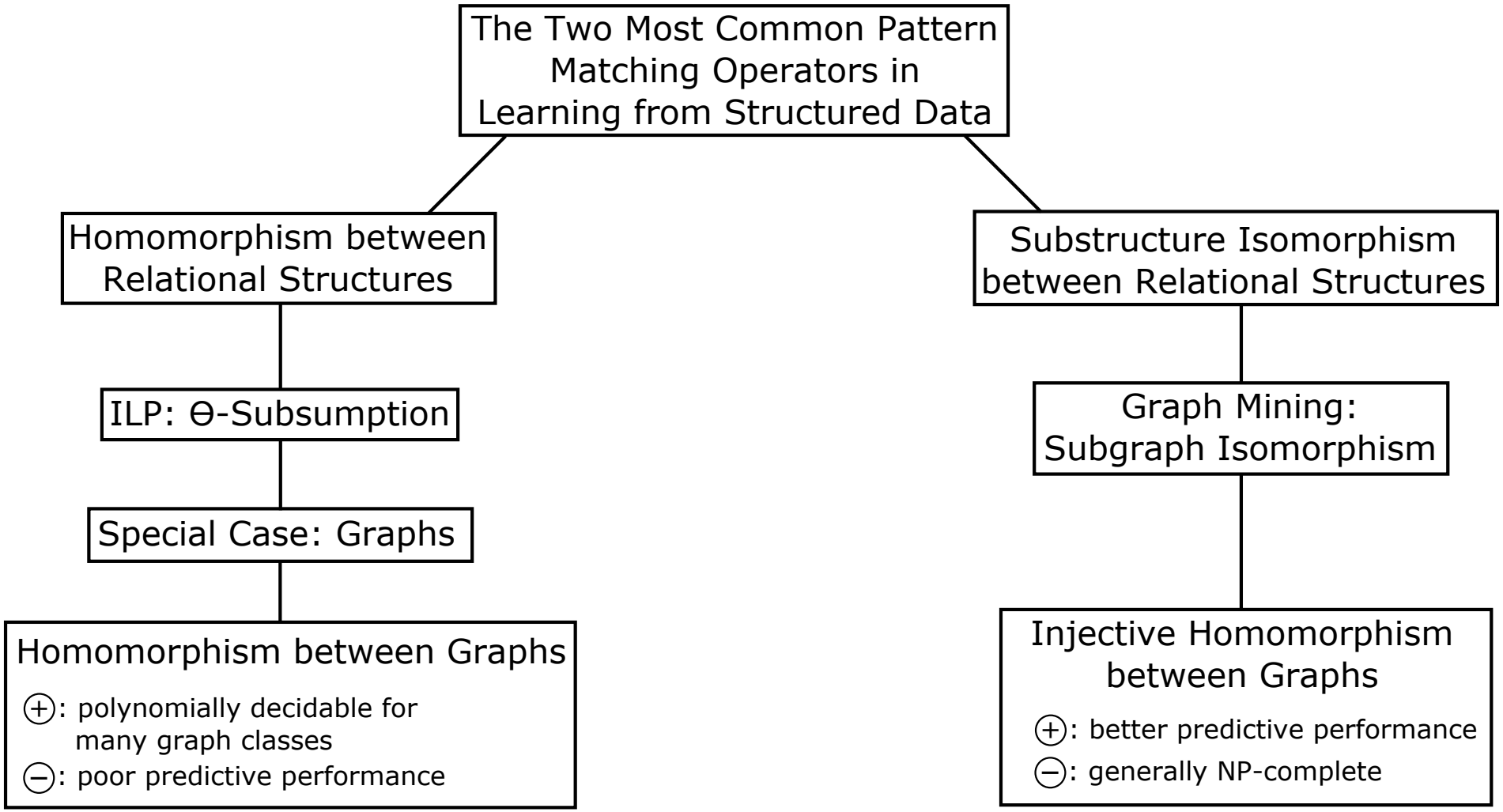


Learning from Structured Data

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

Homomorphism between Relational Structures

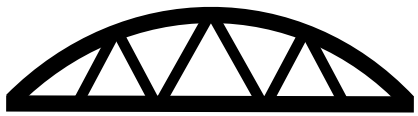
ILP: Θ-Subsumption

Special Case: Graphs

Homomorphism between Graphs

⊕: polynomially decidable for many graph classes

⊖: poor predictive performance



Partially Injective Homomorphism

Substructure Isomorphism between Relational Structures

Graph Mining: Subgraph Isomorphism

Injective Homomorphism between Graphs

⊕: better predictive performance

⊖: generally NP-complete

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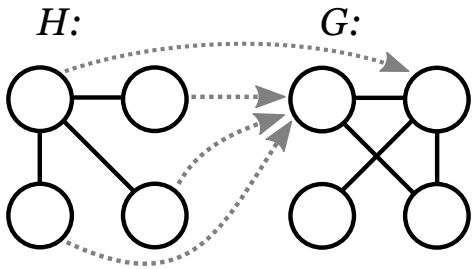
Solution: Bridge the gap by requiring only partial injectivity

Injective Homomorphism

Graph homomorphism:



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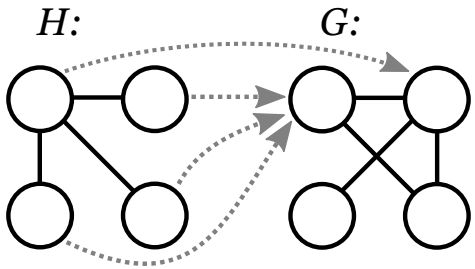

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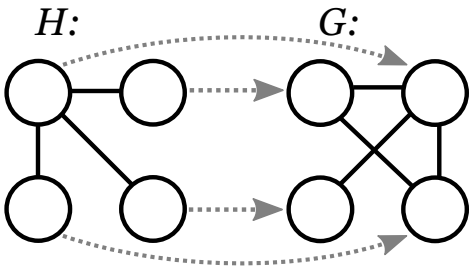

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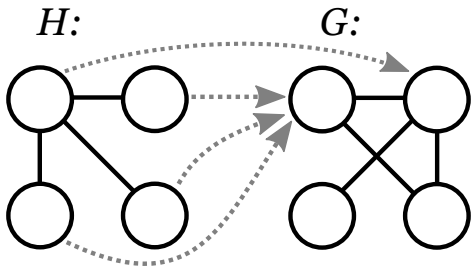

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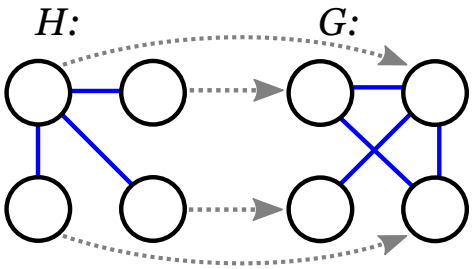

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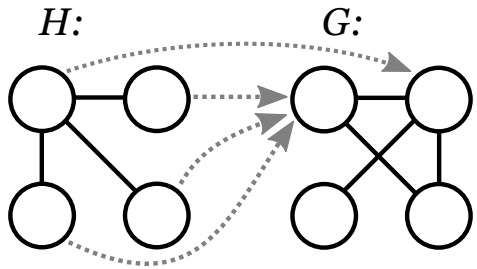

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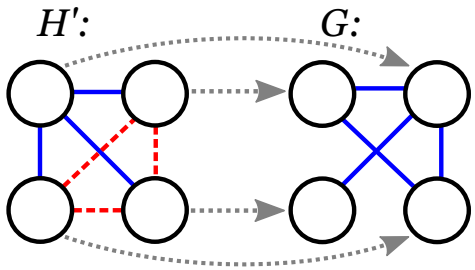

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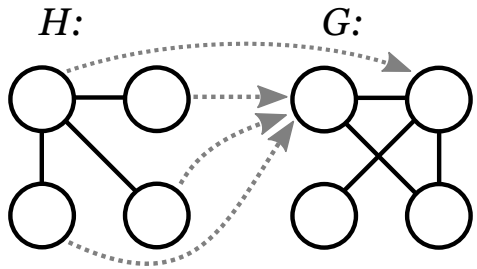

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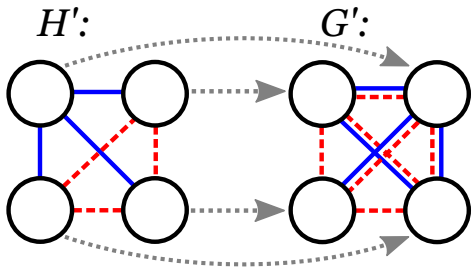

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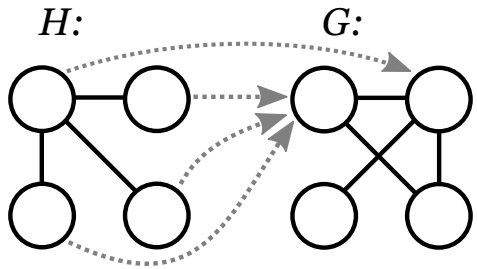

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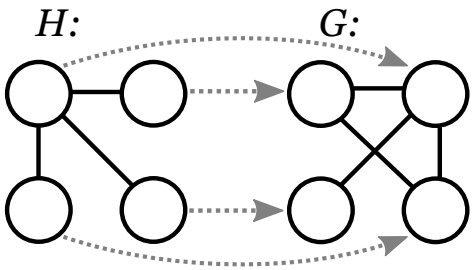

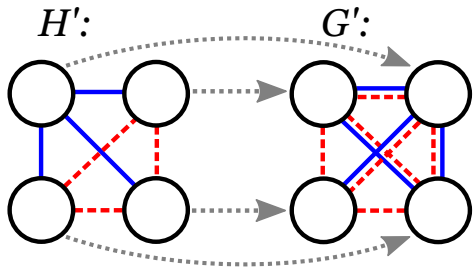

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H is subgraph isomorphic to G iff there exists a homomorphism from H' into G'

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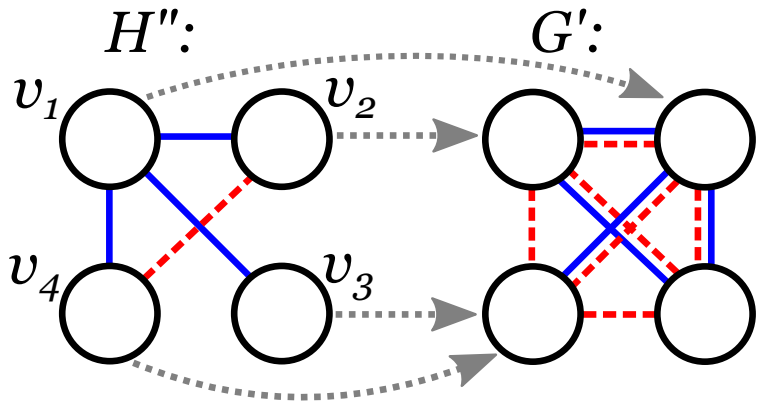

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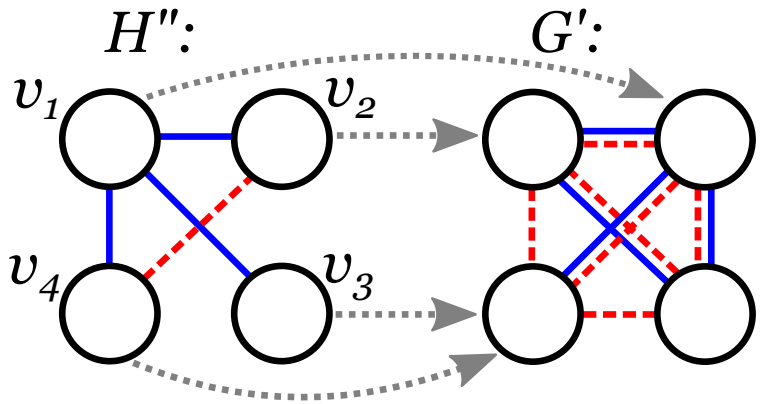
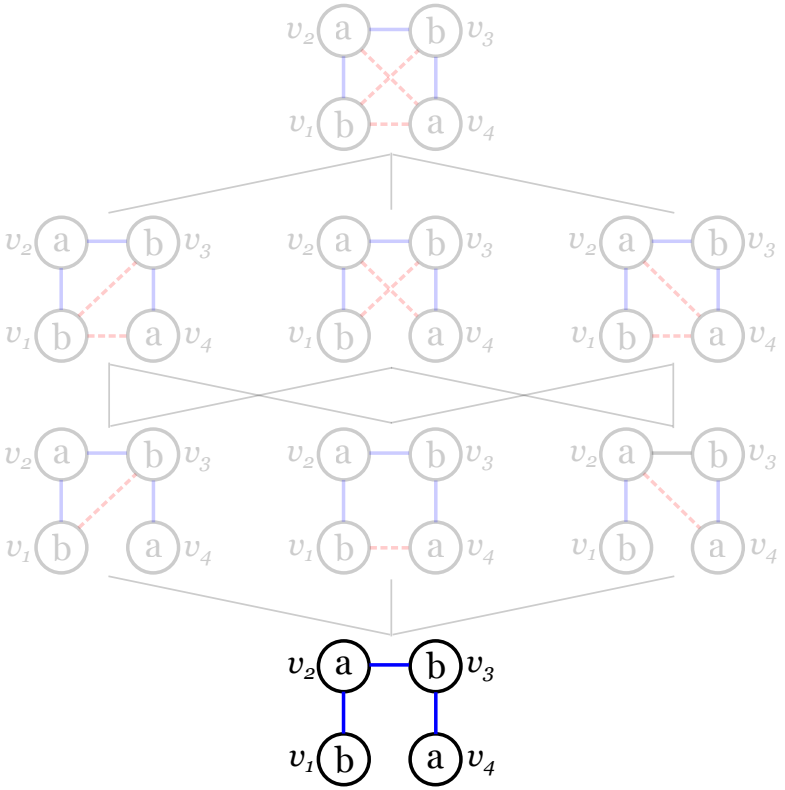


v_2 and v_4 of H'' must be mapped to distinct vertices in G'

Main Idea



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subgraph-isomorphism

partial injective homorphisms with two red edges

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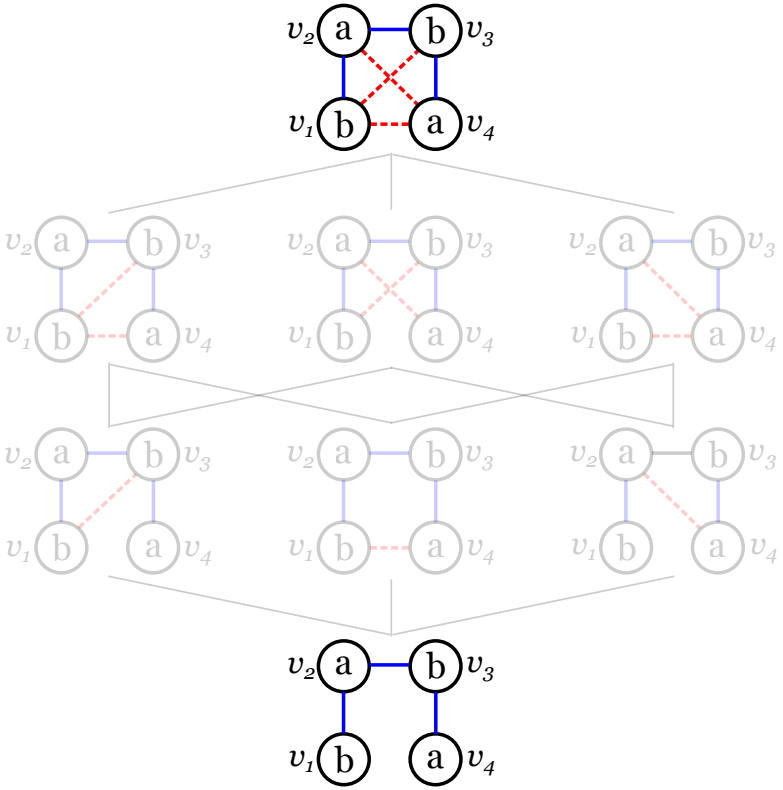

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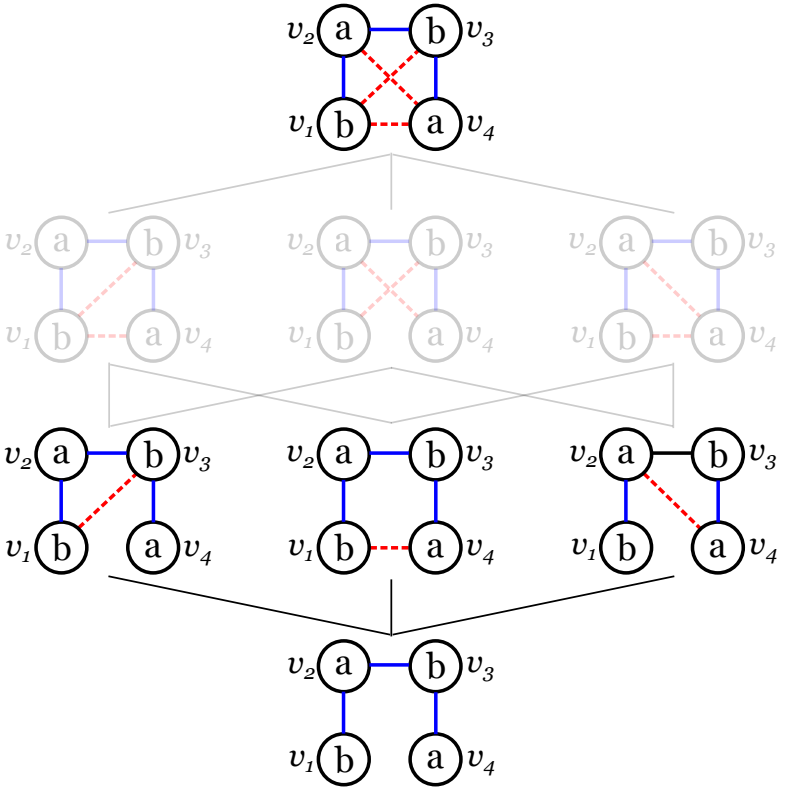

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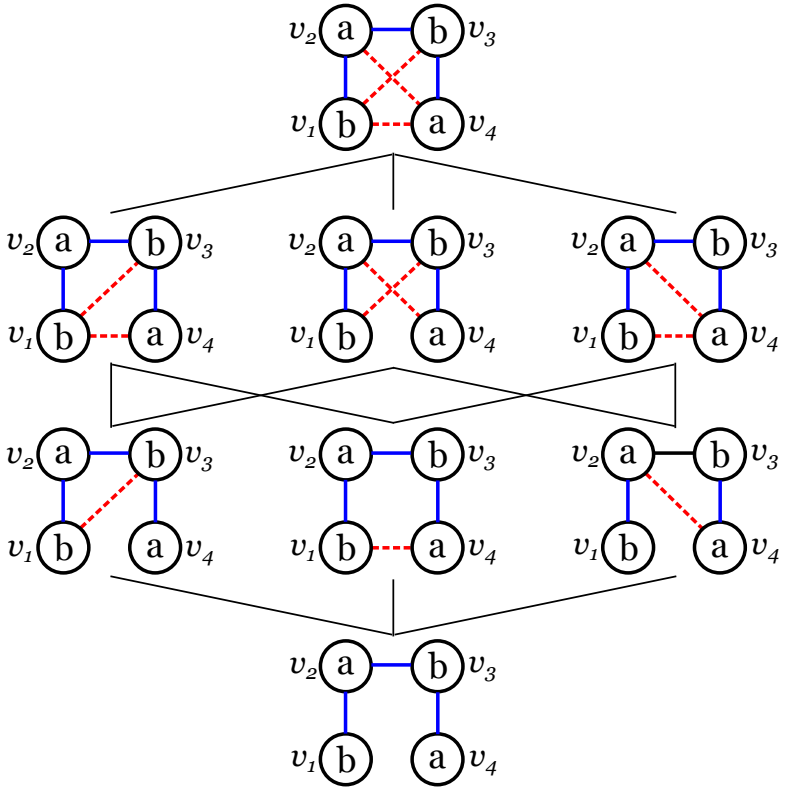

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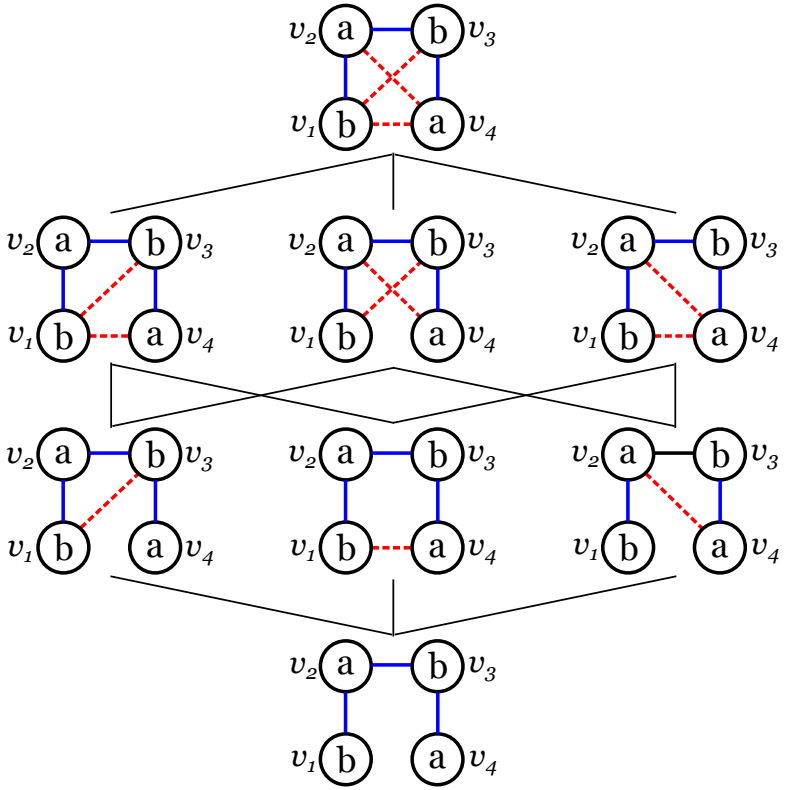

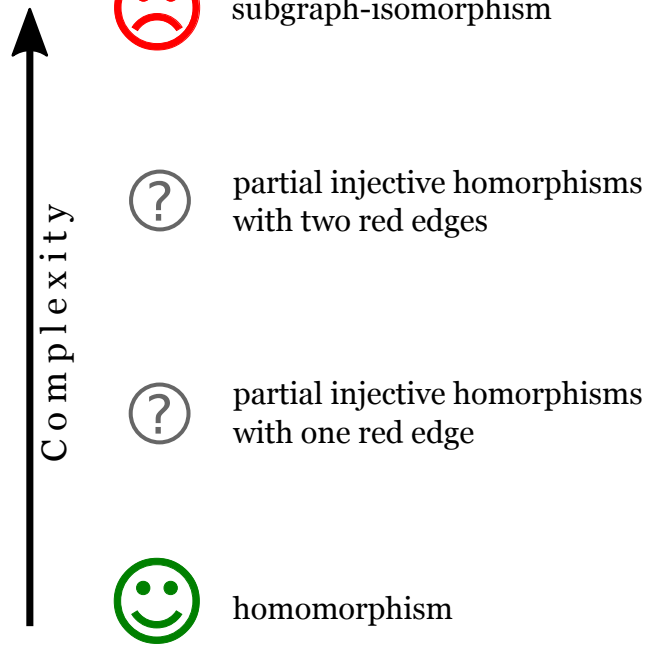

☺ **Partially injective homomorphism can be decided in polynomial time if the pattern graph (blue + red edges) has bounded tree-width.**

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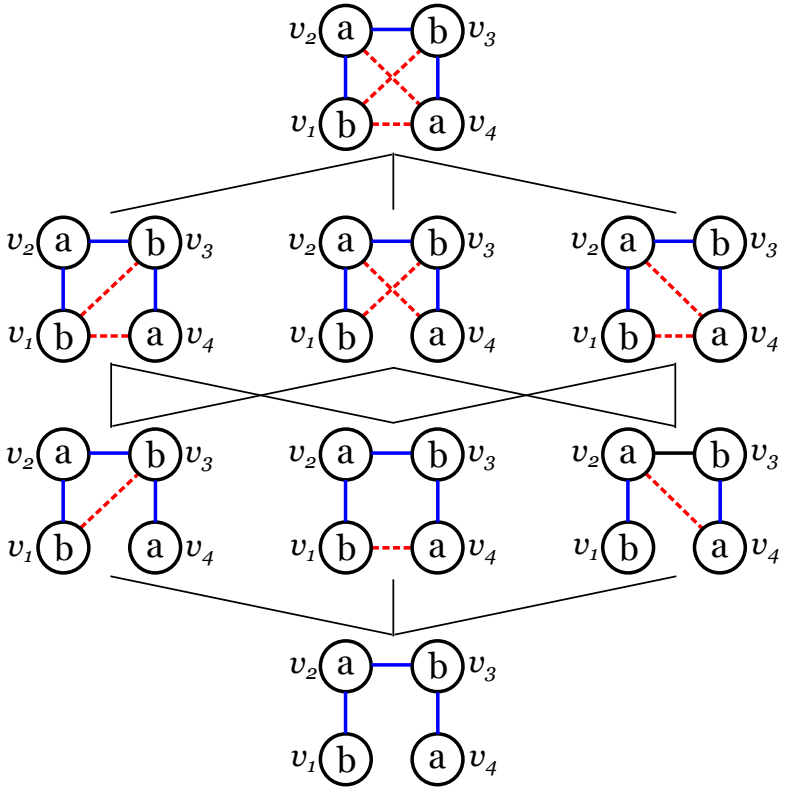

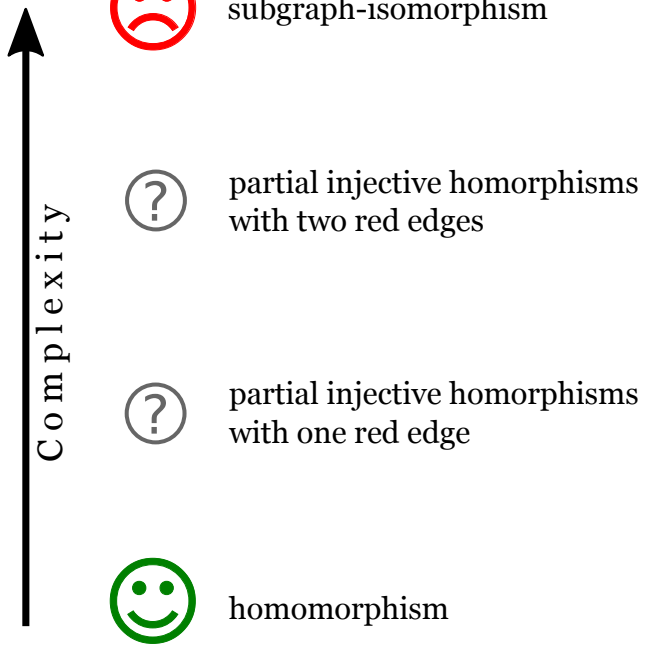

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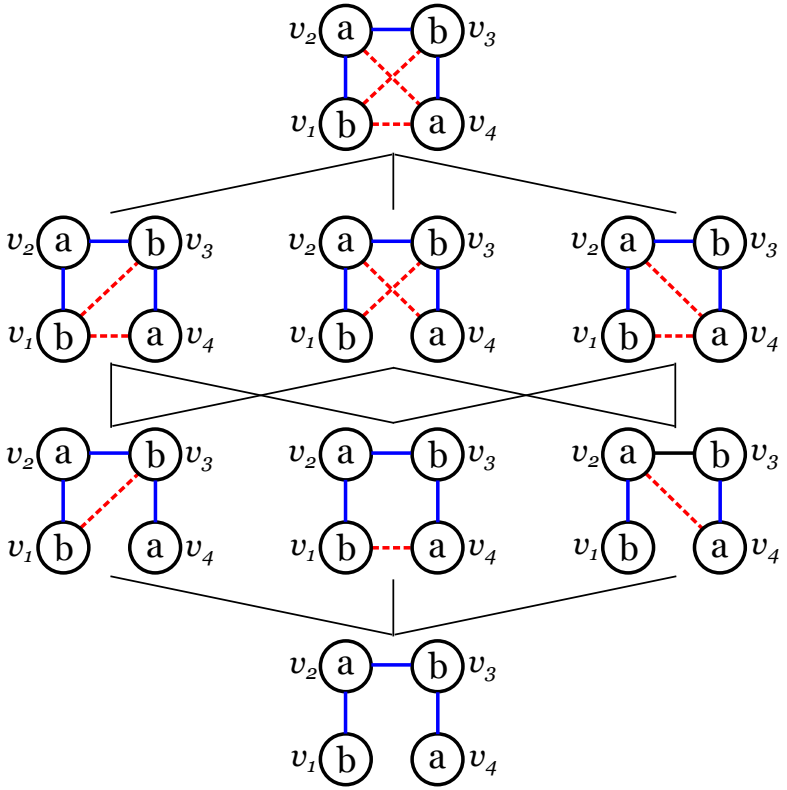

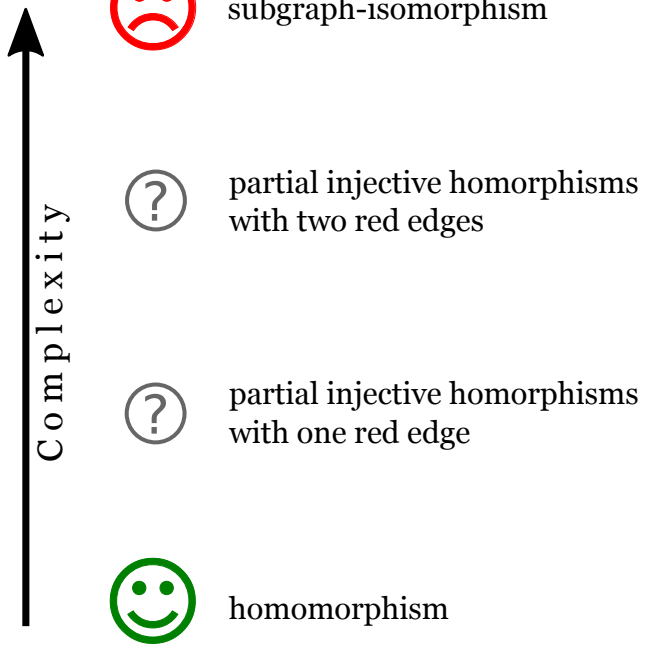

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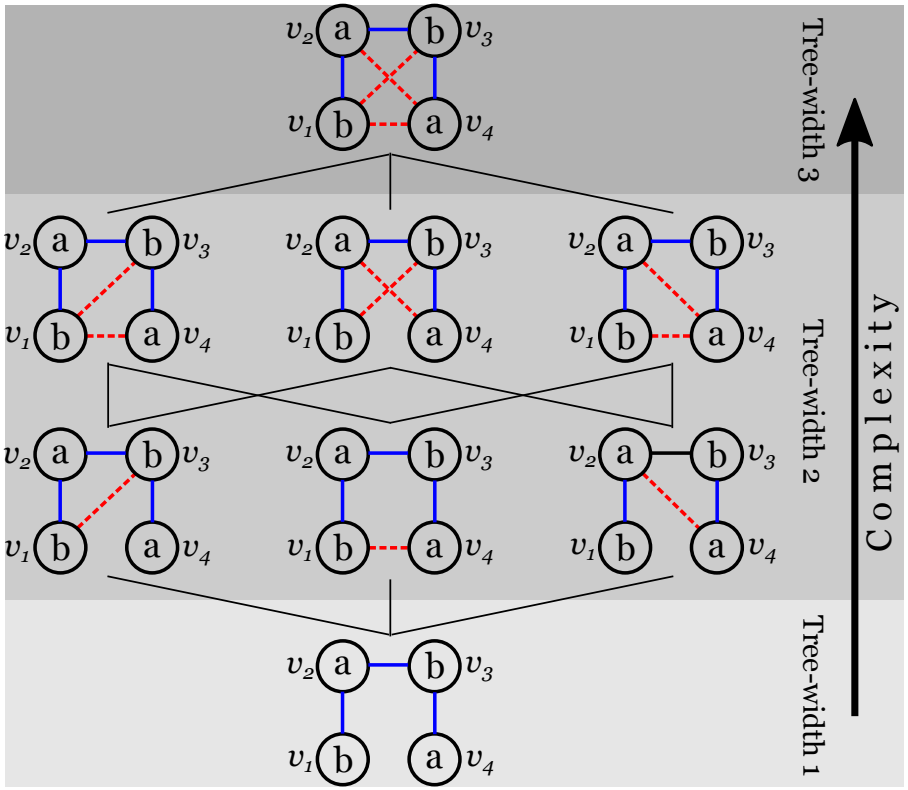

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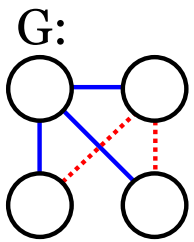
Pattern generation is based on refinement operator.

Refinement Operator

Refinement step (utilizes definition of *k-trees*):

Idea for tree-width $k = 2$:



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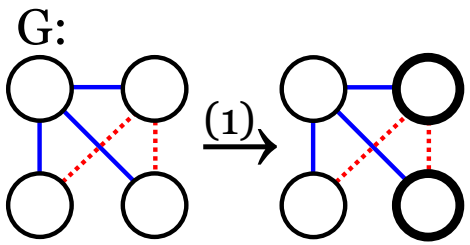

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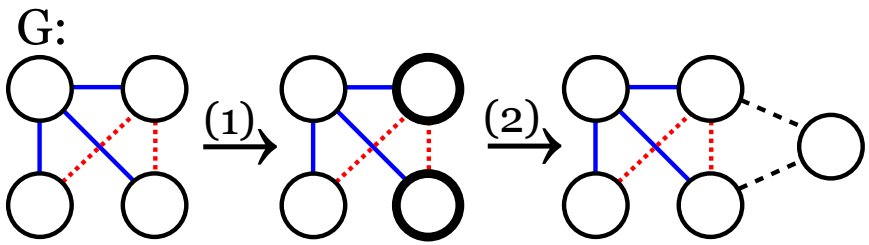

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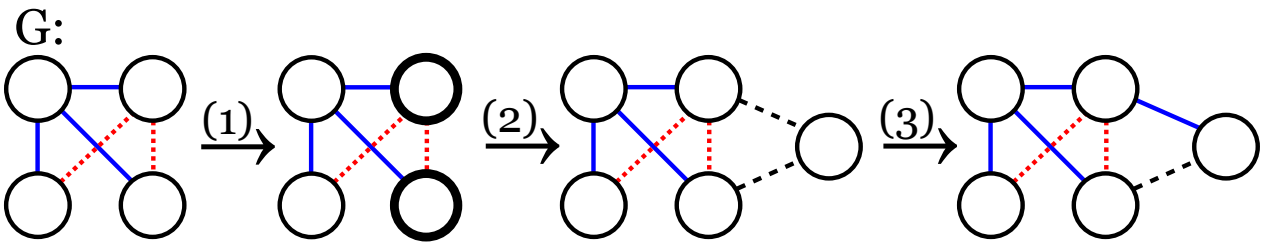

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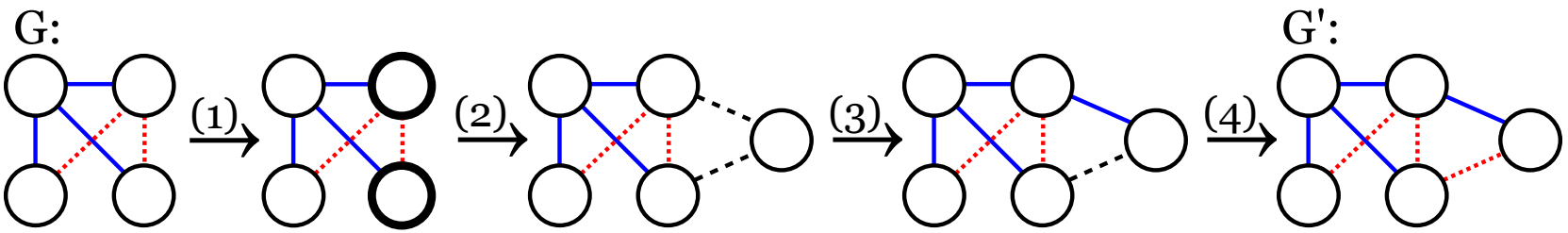

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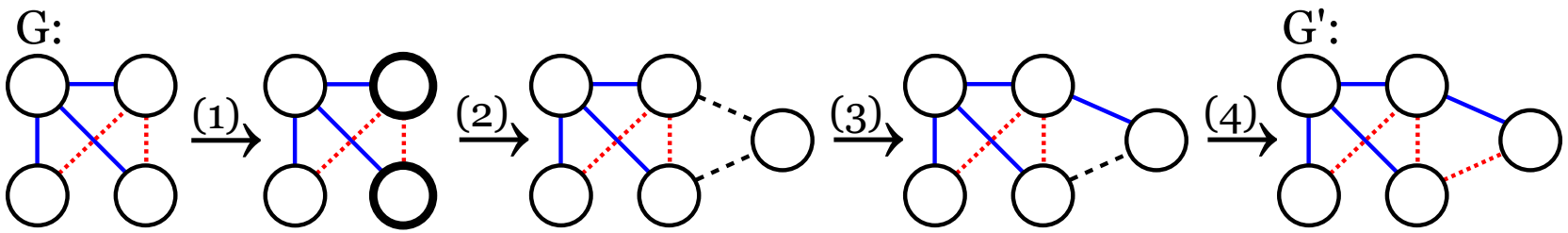

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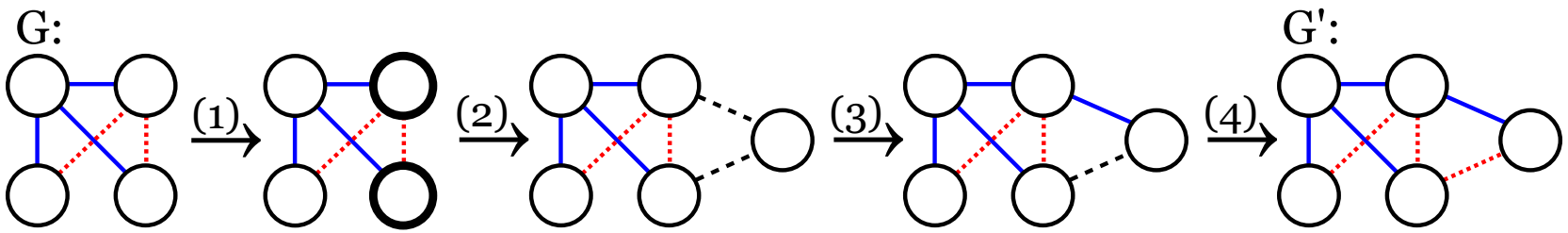

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Properties:

- graphs are *maximally* constrained (i.e. adding another red edge increases the tree-width)

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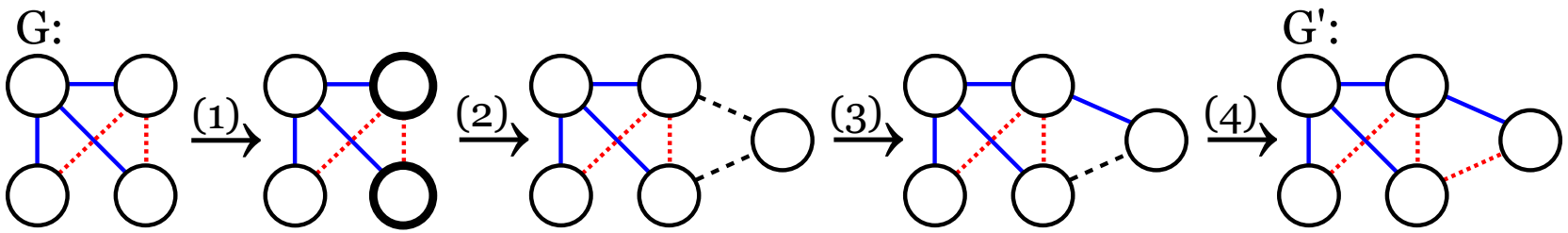

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SVMs were used to separate points representing molecular graphs in feature space spanned by patterns

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s.g.i. graphs	91.99 ± 6.65	73.07 ± 9.34	89.33 ± 1.13	88.55 ± 1.77
s.g.i. trees	91.63 ± 5.89	73.08 ± 9.39	89.14 ± 1.19	88.37 ± 1.72
p.i.h. trees ($k = 4$)	90.49 ± 6.98	72.38 ± 8.02	88.30 ± 1.29	87.54 ± 2.03
p.i.h. trees ($k = 3$)	90.21 ± 8.36	73.24 ± 8.55	88.77 ± 1.32	87.77 ± 2.02
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A: For already tree-width $k = 3$, the results are very close to those of ordinary frequent trees (subgraph isomorphism).

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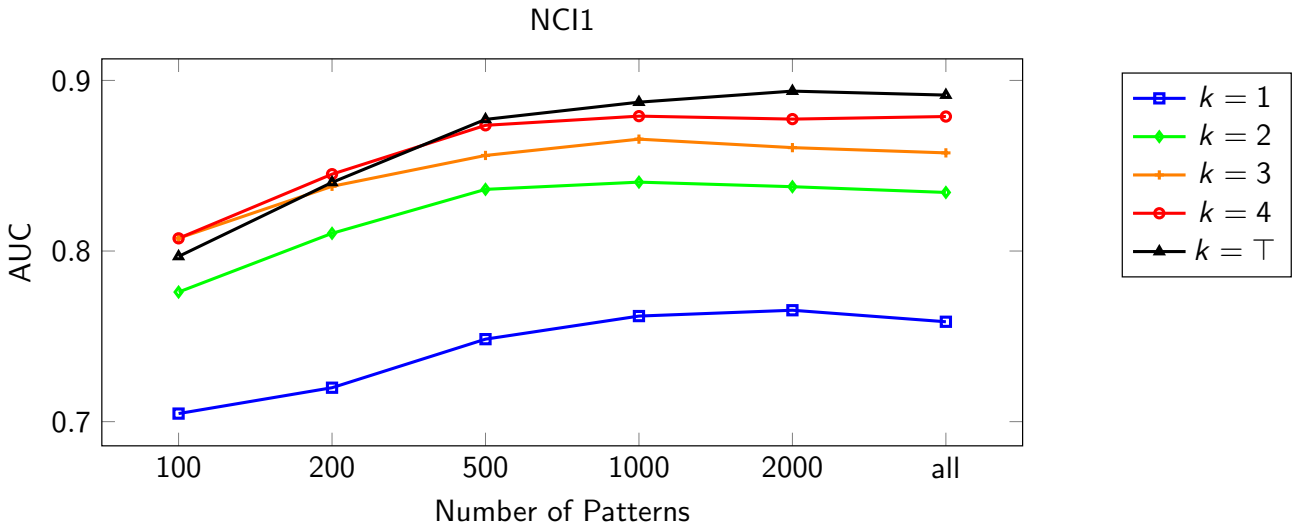

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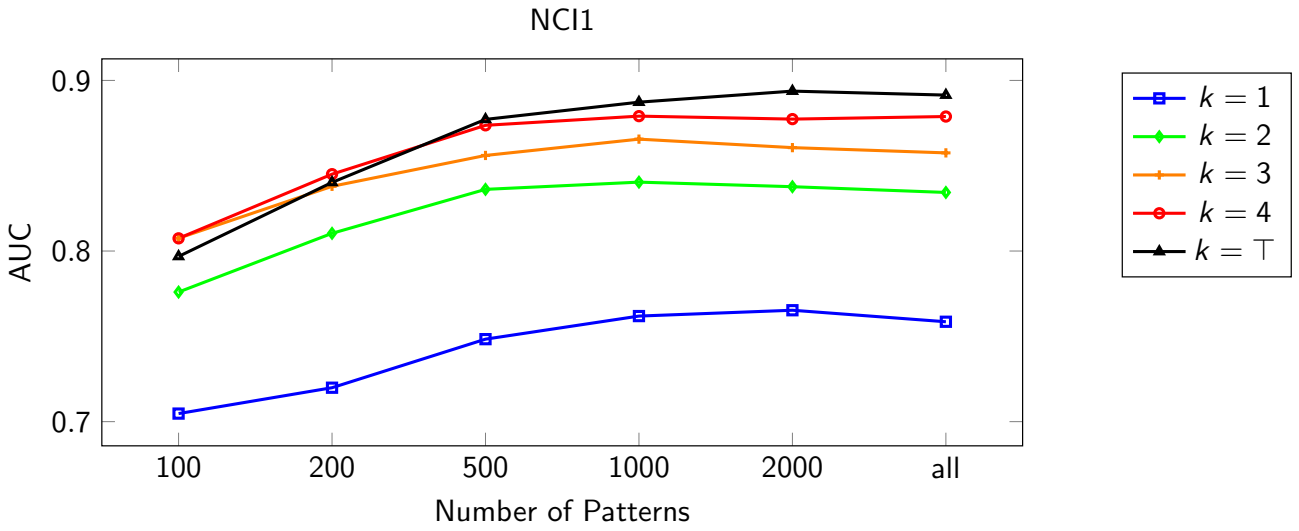

A: The predictive performance scales with the degree of injectivity of the underlying pattern matching operator.

Experiments III: Runtimes

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	MUTAG	PTC	NCI1	NCI109	Erdős-Rényi random graphs (unlabeled)			
					$q = 1.0$	$q = 1.5$	$q = 2.0$	$q = 3.0$
GASTON (EL)	0.1	0.2	2.6	2.7	2.8	54.6	*mem err*	*mem err*
GASTON (RE)	0.3	1.0	8.5	8.6	5.0	39.5	1163.0	31061.4
FSG	0.7	4.1	30.2	29.9	194.2	10584.9	10888.4	10852.5
PIH Miner ($k = 3$)	0.8	3.4	27.3	24.1	0.3	1.3	2.8	8.4

Runtimes (in sec.) of our algorithm in comparison to GASTON and FSG on molecular and artificial datasets.

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Runtimes (in sec.) of our algorithm in comparison to GASTON and FSG on molecular and artificial datasets.

A: While our algorithm is slower on real-world datasets, it is much faster on (unlabeled) graphs of a higher structural complexity (i.e., higher value q).

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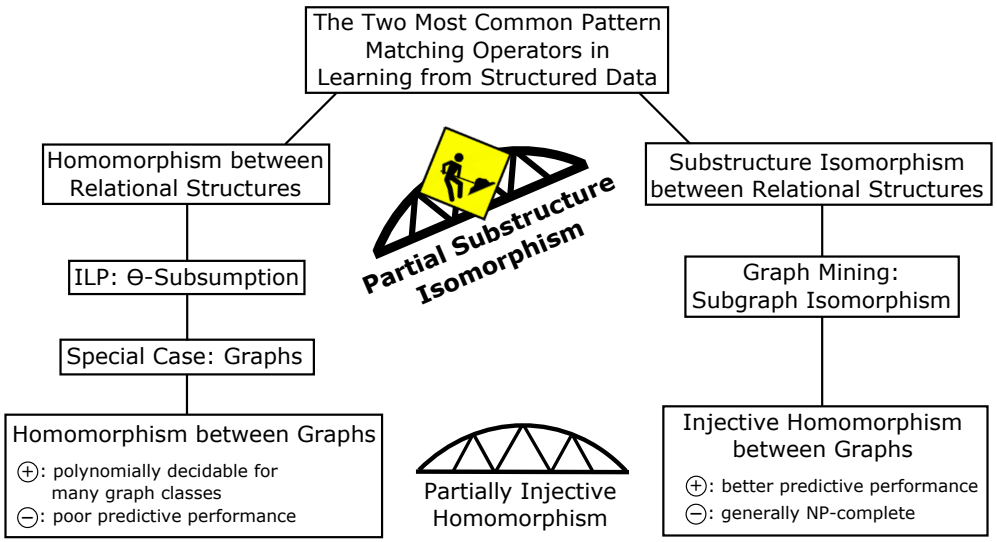
Upcoming work:

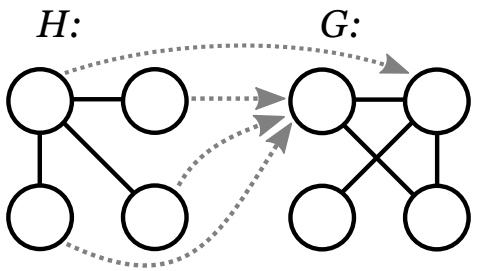


Appendix

Homomorphism & Subgraph Isomorphism

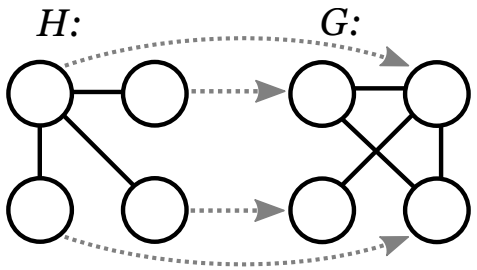
A **homomorphism** from a graph H (the *pattern*) into a graph G (the *text*) is a mapping $\varphi : V(H) \to V(G)$ that preserves the edges (i.e., $uv \in E(H)$ implies $\varphi(u)\varphi(v) \in E(G)$ for all $u, v \in V(H)$).

Example:



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

Example:



Tree-width

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

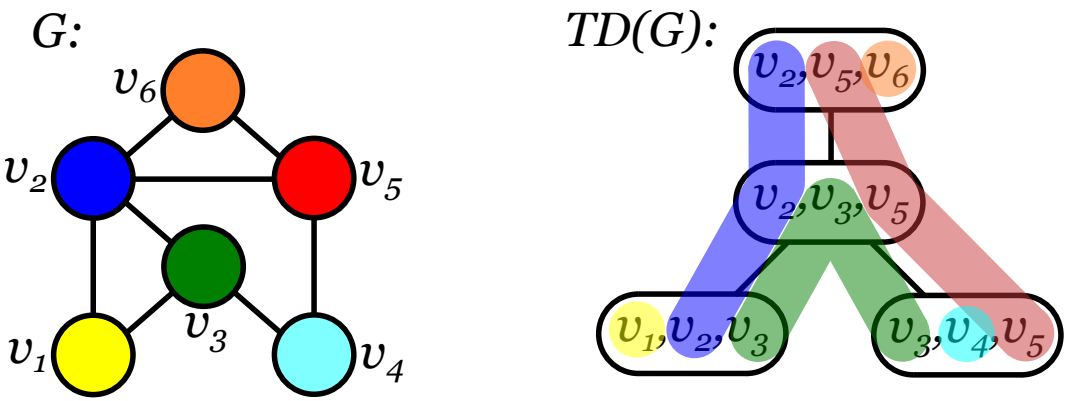
- $T = (I, F)$ is an unordered tree,
- $X = \{bag(i) : i \in I\}$ is a family of subsets of V, s.t.

  (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

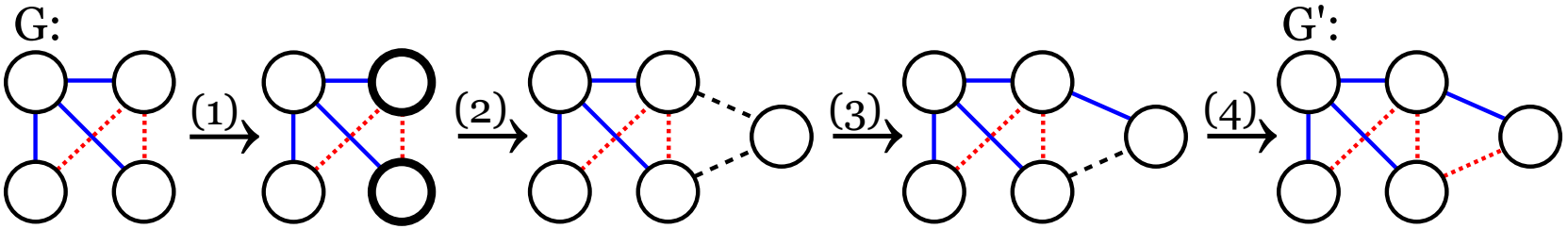
(ii) given a k-tree T_k with n vertices, a k-tree with $n+1$ vertices is obtained from T_k by adding a new vertex v to T_k and connecting v to all vertices of a k-clique of T_k.

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

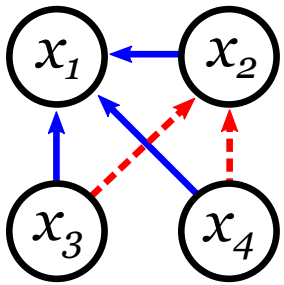
Partially Injective Homomorphisms can be generalized to first-order logic:

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 θ such that $A\theta \subseteq B$ and for all $xy \in \mathcal{C}$, $x\theta \neq y\theta$.

Example:

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

A':



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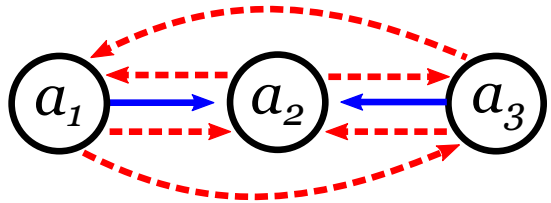

There is a partial substructure isomorphism from A to B w.r.t. constraints $\mathcal{C}$ iff A' subsumes B'.