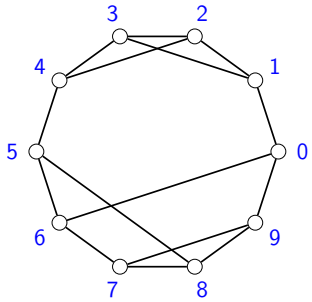
Graph Isomorphism and Beyond

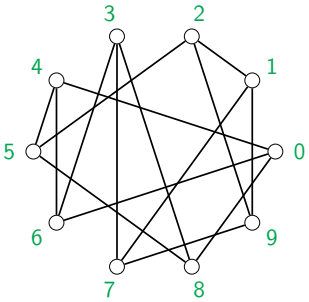
Daniel Neuen

TU Dresden

Workshop "Parameterized Complexity of Computational Reasoning"

Graph Isomorphism Problem





Graph Isomorphism Problem (GI)

Input: Two graphs G_1 and G_2
Problem: Is $G_1 \cong G_2$?

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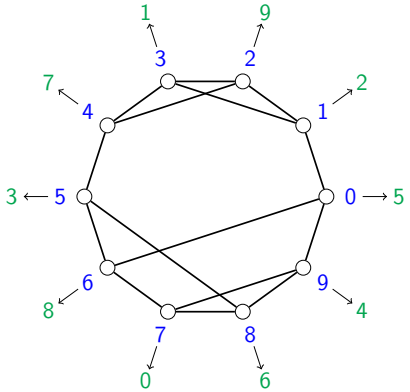

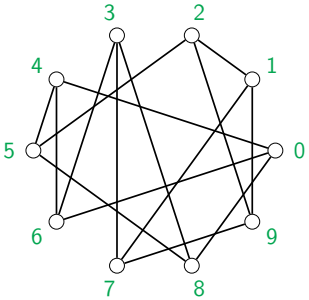

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Some Facts

- GI is in NP
- GI is in coAM
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Theorem (Babai 2016)

GI can be solved in time $n^{O((\log n)^2)}$.

Canonization

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A **canonization** is a mapping $\kappa\colon \mathcal{G} \to \mathcal{G}$ such that

- $\kappa(G) \cong G$ for all graphs G, and
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Theorem (Babai 2019)

There exists a canonization that can be computed in time $n^{O((\log n)^c)}$.

Restricted Graph Classes

Many graph classes admit polynomial-time isomorphism tests:

- planar graphs [Hopcroft, Wong '74]
- graphs of maximum degree d [Luks '82]
- graphs of bounded tree-width [Bodlaender '88]
- graphs excluding a fixed minor [Ponomarenko '91]
- graphs excluding a fixed topological subgraph [Grohe, Marx '12]
- graphs of bounded rank-width [Grohe, N. '19]

...

Parameterized Isomorphism Tests

Let k denote a graph parameter (such as maximum degree, genus, tree-width, Hadwiger number, rank-with, etc.)

XP Algorithms

$n^{f(k)}$

Parameterized Isomorphism Tests

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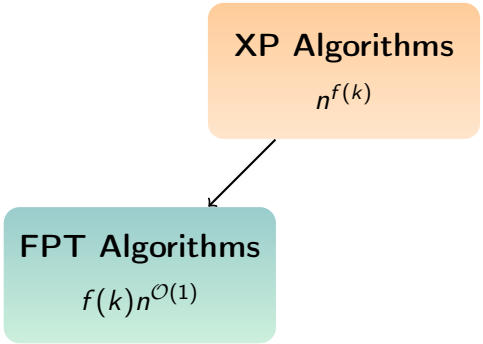

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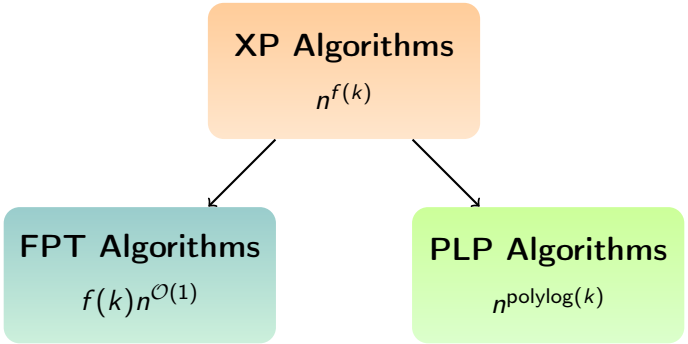

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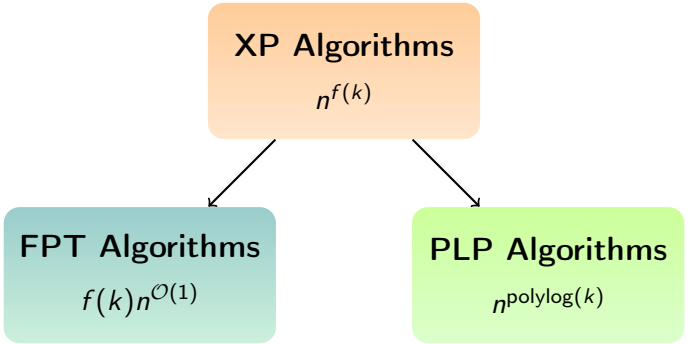
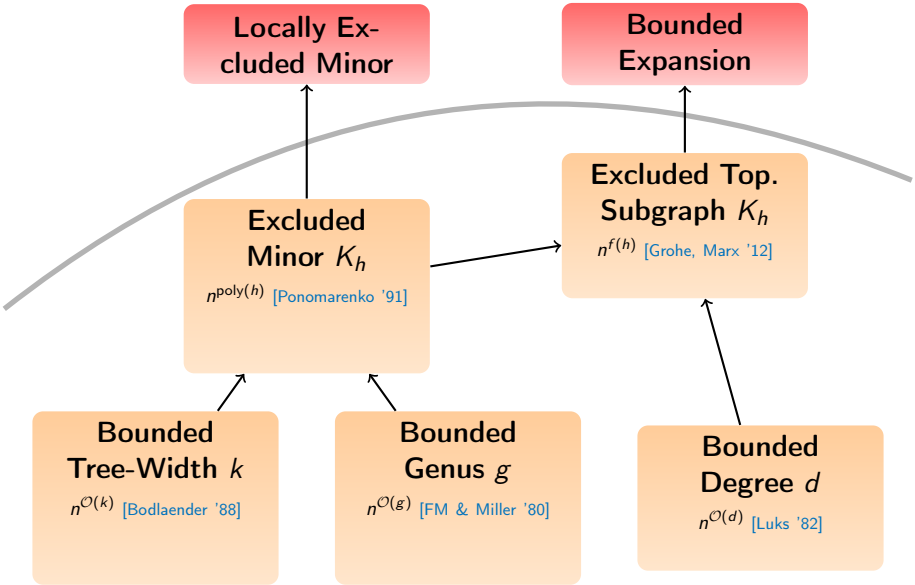


$n^{\text{polylog}(k)} = n^{(\log k)^{\mathcal{O}(1)}}$

$2^k n$ and $n^{\log k}$ are incomparable (consider $k = (\log n)^{1+\varepsilon}$)

Isomorphism Tests for Sparse Graphs



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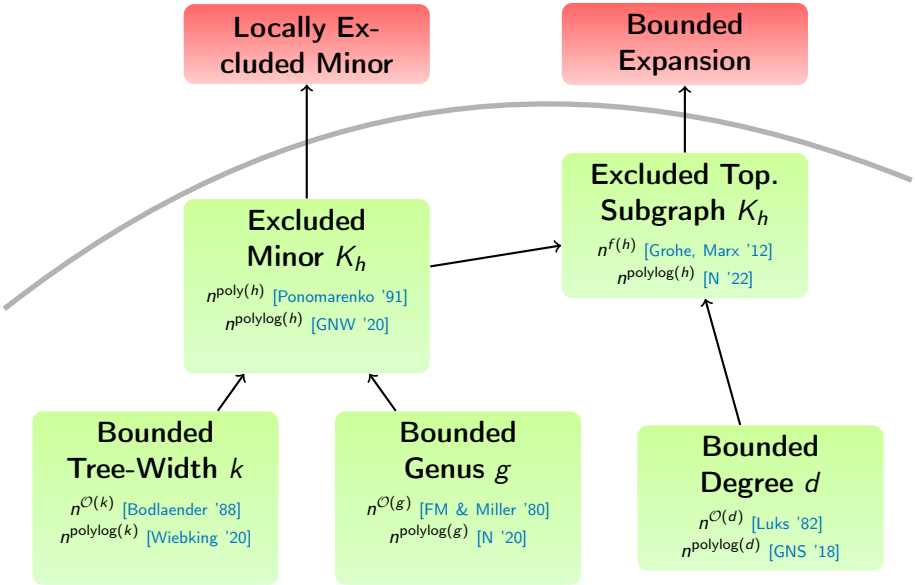

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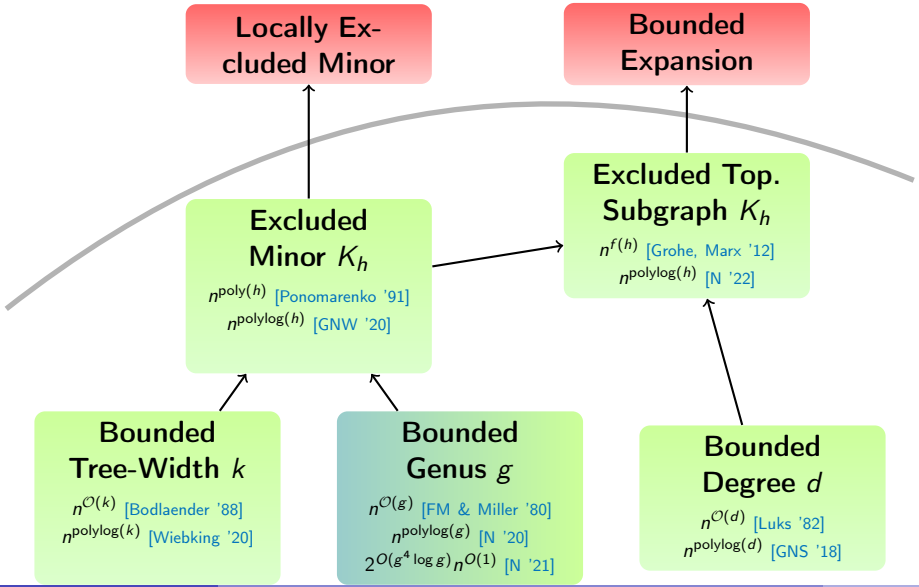

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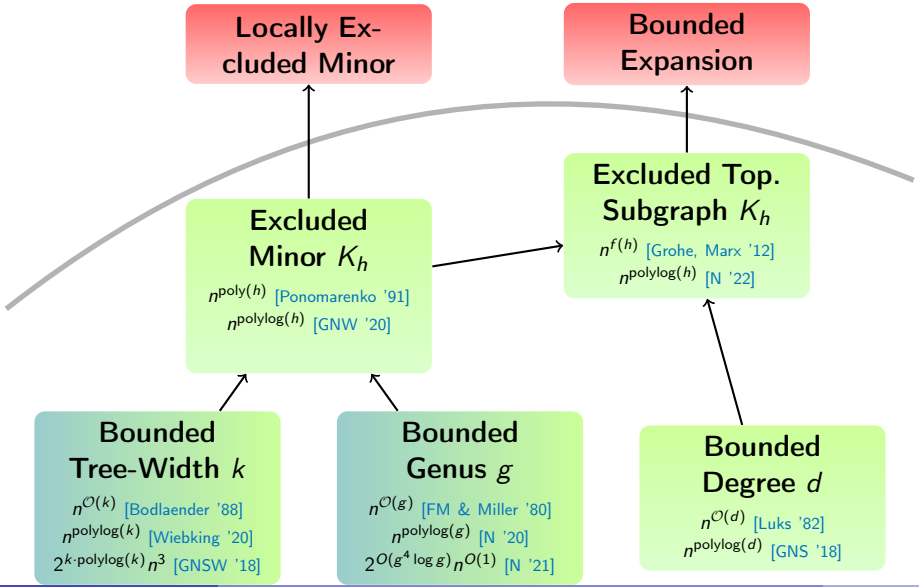

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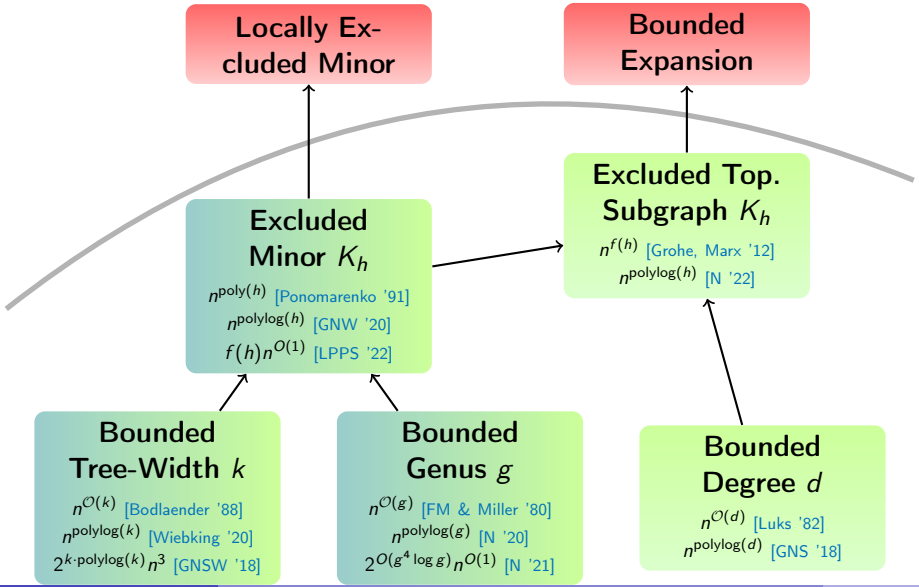

The Isomorphic Priors Model [Dorfman, Döring, Herold, Nanongkai, N., Spoerhase, Wu '26]

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- Suppose that in the past we have already solved instances $G_1, \ldots, G_k$ with optimal solutions $\mathrm{OPT}_1, \ldots, \mathrm{OPT}_k$
- Given an instance H, quickly (e.g., in polynomial time)
  - return an optimal solution for H, or
  - correctly conclude that $H \ncong G_i$ for all $i = 1, \ldots, k$ (and use heavy-computation fall-back)

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Fix a computational problem Π on graphs.

Preprocessing Phase

Input: A database of graph $\mathcal{S} = \{G_1, \ldots, G_k\}$ of **prior graphs**, and optimal solutions $\mathsf{OPT}_1, \ldots, \mathsf{OPT}_k$.

Task: Build a data structure $\mathcal{D}$ to accelerate future queries

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Query Phase

Input: A graph H.

Task: Given access to $\mathcal{D}$

(a) find an optimal solution for H, or

(b) deduce that $H \ncong G_i$ for all $i = 1, \ldots, k$.

Naive Approaches

Solve Π Directly:

Preprocessing Phase: Do nothing $O(1)$

Query Phase: Solve Π on H $T_\Pi(n, m)$

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Preprocessing Phase: Do nothing $O(1)$

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Use GI/Canonization Algorithms:

Let $\kappa\colon \mathcal{G} \to \mathcal{G}$ be a canonization that can be computed in time $T_{\text{canon}}(n, m)$

Preprocessing Phase: For each $i \in \{1, \ldots, k\}$ insert $\kappa(G_i)$ (viewed as a string) into a trie with value OPT_i $O(k \cdot T_{\text{canon}}(n, m))$

Query Phase: look up $\kappa(H)$ in the trie $O(T_{\text{canon}}(n, m))$

How to Improve?

Idea: Build **solution-preserving signatures** $\sigma : \mathcal{G} \to \{0,1\}^*$

- if $G \cong H$, then $f(G) = f(H)$
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The Color Refinement Algorithm

Color Refinement Algorithm (CR)

Initialization Every vertex gets the same color assigned

Refinement Two vertices v, w get different colors assigned if there is some color class C such that $|N(v) \cap C| \neq |N(w) \cap C|$.

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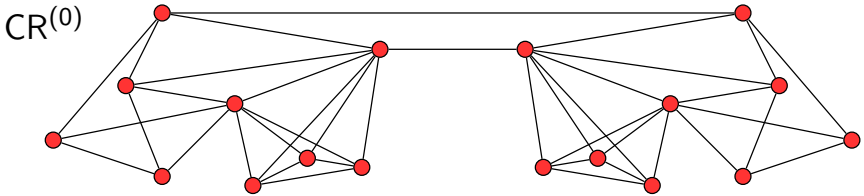

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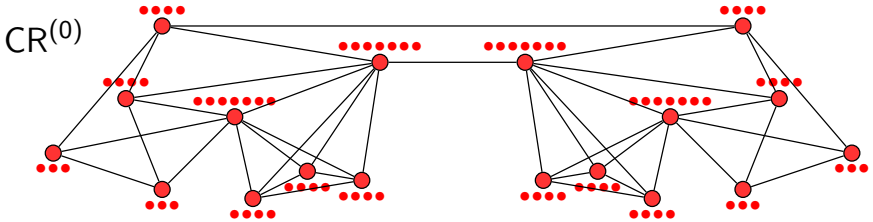

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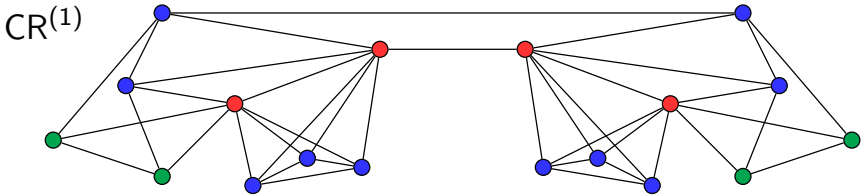

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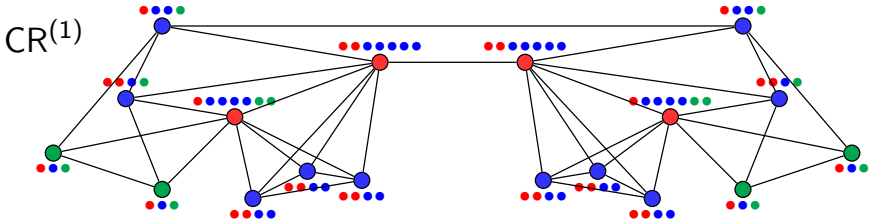

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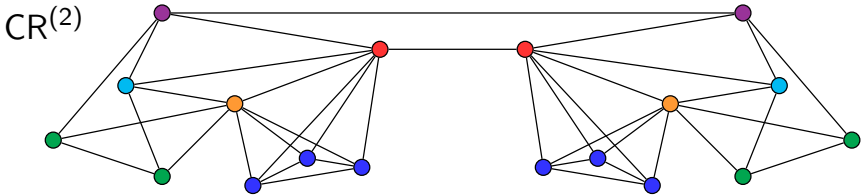

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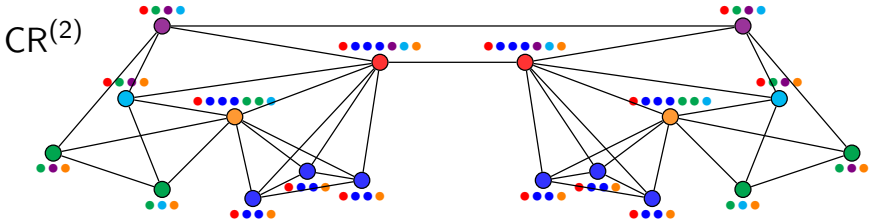

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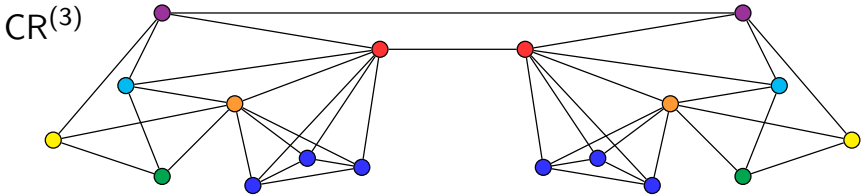
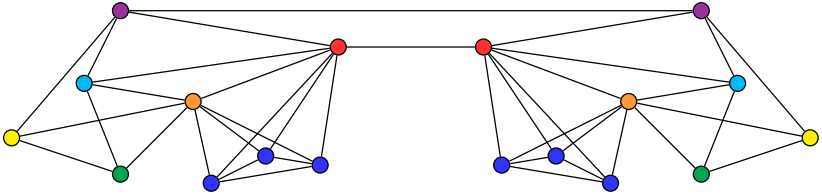
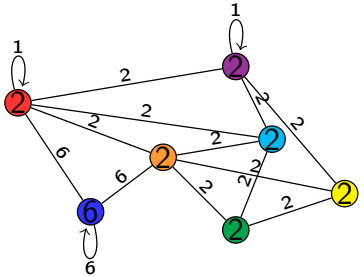


Signatures Based on CR



There is a mapping $\sigma_{\mathrm{CR}} \colon \mathcal{G} \to \{0,1\}^*$ such that

- $G \equiv_{\mathrm{CR}} H \iff \sigma_{\mathrm{CR}}(G) = \sigma_{\mathrm{CR}}(H)$
- $\sigma_{\mathrm{CR}}(G)$ can be computed in time $O((n+m)\log n)$



Constrained Shortest Path

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Input: A graph $G = (V, E)$, edge lengths $\ell \colon E \to \mathbb{R}_{\geq 0}$,
edge cost $c \colon E \to \mathbb{R}_{\geq 0}$, $s, t \in V$, budget $B \in \mathbb{R}_{\geq 0}$

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- CR-equivalent instances achieve the same OPT
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Theorem

Constrained Shortest Path can be solved in the Isomorphic Priors Model in $O(k(n+m)\log n)$ preprocessing time and $O((n+m)\log n)$ query time.

Negative Triangle

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Input: A graph $G = (V, E)$, edge weights $c\colon E \to \mathbb{Z}$
Question: Is there a negative triangle?

No algorithm with running time $O(n^{3-\varepsilon})$ is known.

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Theorem

Negative Triangle can be solved in the Isomorphic Priors Model in $\widetilde{O}(k \cdot n^{\omega})$ preprocessing time and $\widetilde{O}(n^{\omega})$ randomized query time.

Hard Problems

The following problems cannot be solved in polynomial time in the Isomorphic Priors Model, unless GI can be solved in polynomial time.

- Independent Set
- Clique
- 3-Coloring
- Hamiltonian Cycle
- Feedback Vertex Set
- Max Cut

...

Isomorphic Priors - Discussion

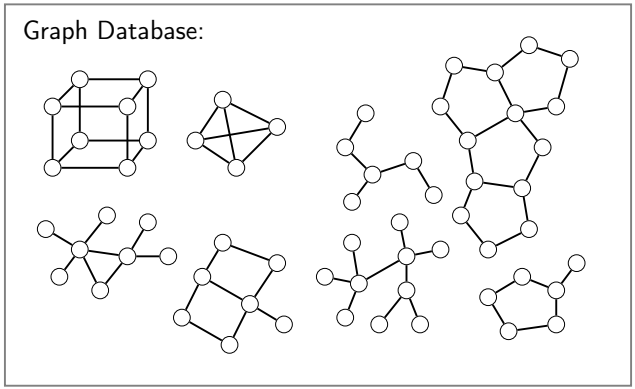
Isomorphic vs Similar Graphs

- Output approximately optimal solution if a prior is close to the query graph

Parameterized Complexity

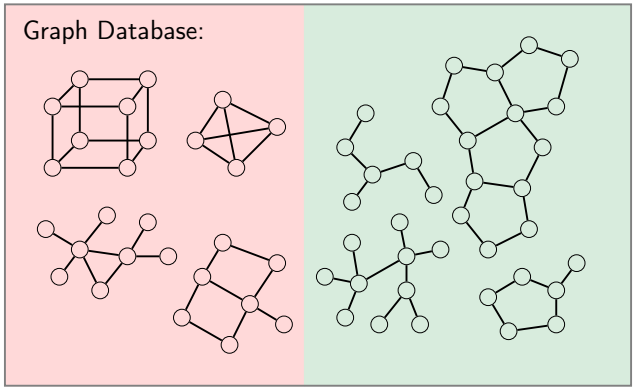
- Is Independent Set solvable in FPT time in the Isomorphic Priors Model?

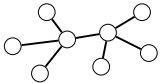
Graph Similarity



Is this graph in the database up to a small error?

Graph Similarity





How to classify this graph?

Edit Distance

Measure the number of operations to make graphs isomorphic.

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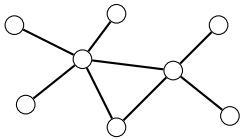
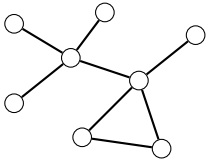
Graph Edit Distance

Minimal number $\delta_{\text{edit}}(G, H)$ of edge deletions and additions to make G, H isomorphic.





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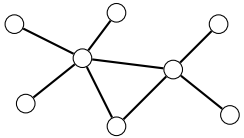

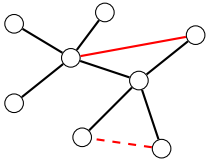

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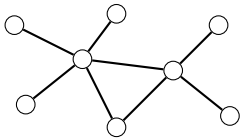

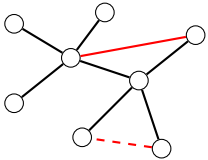

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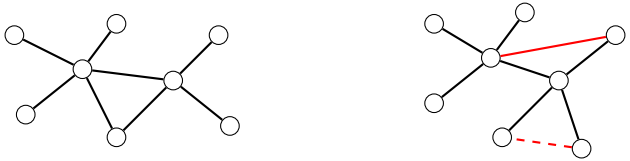

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Alternative View: Minimize $\|A_G^\pi - A_H\|$ over all permutations π.

How to Measure Graph Similarity

Many Ways to Measure Similarity

- graph edit distance
- minimize $\|A_G^\pi - A_H\|$ for other matrix norms
- distance based on spectrum
- distance based on counting small patterns
- Weisfeiler-Leman kernels

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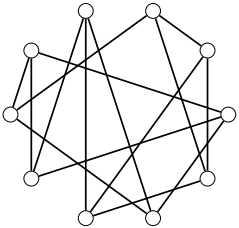
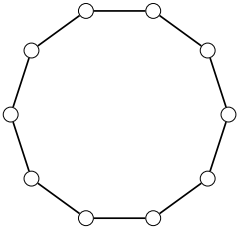
Appropriate Measure Depends on Application

Computational Complexity Can Vary a Lot

Hardness of Graph Edit Distance

- computing Graph Edit Distance is NP-hard





Hardness of Graph Edit Distance

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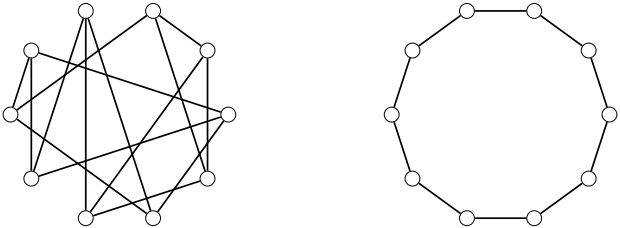

- computing Graph Edit Distance on trees is NP-hard [Grohe, Rattan, Woeginger '18]

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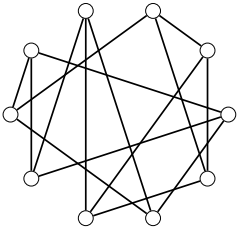

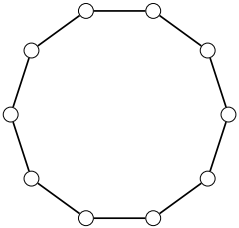

- computing Graph Edit Distance on trees is NP-hard [Grohe, Rattan, Woeginger '18]
- hard to approximate [Arvind, Köbler, Kuhnert, Vasudev '12]

Additive Approximation

Theorem (Arora, Frieze, and Kaplan '02)

There is an algorithm that, given graphs G, H and $\varepsilon > 0$, finds a bijection $\pi\colon V(G) \to V(H)$ such that

$$\|A_G^\pi - A_H\| \leq \delta_{edit}(G, H) + \varepsilon n^2$$

in time $n^{O(\varepsilon^{-2} \log n)}$.

Improvement for Bounded VC Dimension

Let $\mathcal{X}$ be a set system over V.

- $A \subseteq V$ is **shattered** if $\{A \cap X \mid X \in \mathcal{X}\} = 2^A$
- The **VC dimension** of $\mathcal{X}$ is maximum size of a shattered set

The VC dimension of a graph G is the VC dimension of $\{N_G(v) \mid v \in V(G)\}$.

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Theorem (Dahan, Grohe, N., Novotny '26)

There is an algorithm that, given graphs G, H of VC dimension d and $\varepsilon > 0$, finds a bijection $\pi \colon V(G) \to V(H)$ such that

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in time $n^{O(\varepsilon^{-2} d)}$.

Robust GI

ε-GI

Input:	Two graphs G and H
Promise:	$G \cong H$ or $\delta_{\text{edit}}(G, H) > \varepsilon n^2$
Question:	Is $G \cong H$?

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ε-GI on graphs of VC dimension at most d can be solved in time $n^{O(\varepsilon^{-1} d \log \varepsilon^{-1})}$.

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- Consider the set system $\{N_G(v) \triangle N_G(w) \mid v, w \in V(G)\}$; it has VC dimension $O(d)$

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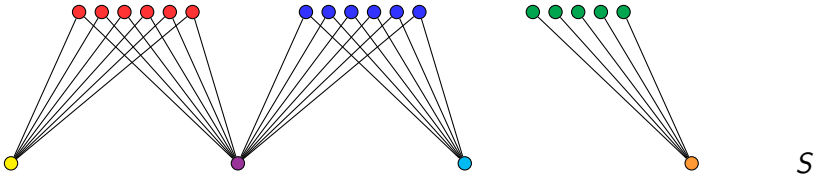

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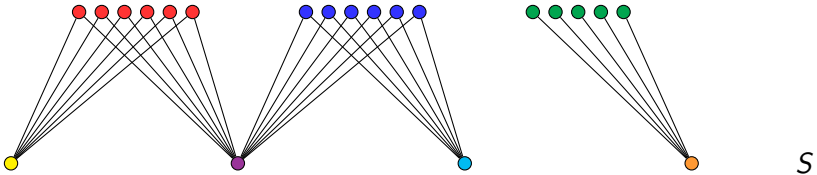

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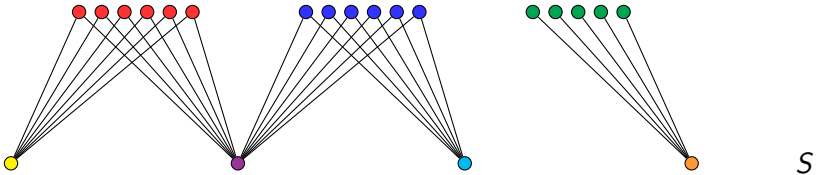

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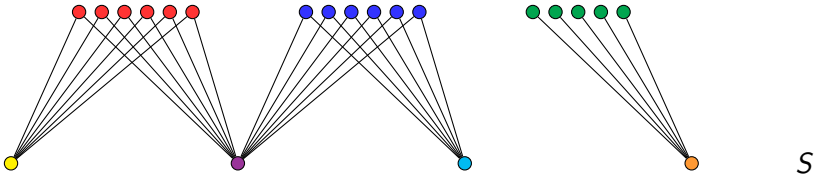

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- vertices of the same color have similar neighborhoods
- between any pair of color classes, either almost all or almost non of the edges are present
- either graphs are distinguished by CR or $\delta_{\text{edit}}(G, H) \leq \varepsilon n^2$

Further Open Problems

Theorem (Dahan, Grohe, N., Novotny '26)

ε-GI on graphs of VC dimension at most d can be solved in time $n^{O(\varepsilon^{-1} d \log \varepsilon^{-1})}$.

Questions:

- Is the dependence on d necessary?
- Can we obtain a running time of $f(\varepsilon, d)n^{O(1)}$?

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Question

What is the parameterized complexity of Graph Edit Distance on trees?

- What about Graph Cleaning (only edge deletions in G) on graphs of tree-width 2? The problem is FPT on trees [Marx, Schlotter '08].