Graph Decompositions via Counting Logics

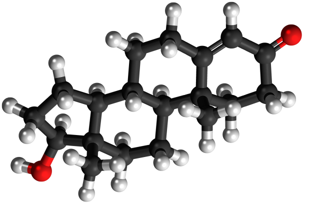
Sandra Kiefer

MAX PLANCK INSTITUTE
FOR SOFTWARE SYSTEMS

Structure Meets Power
Paris, France
July 4, 2022

Structure Identification

Find a description of **this molecule.**



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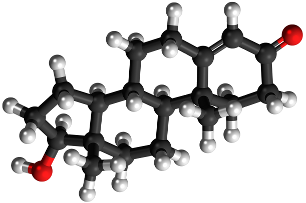

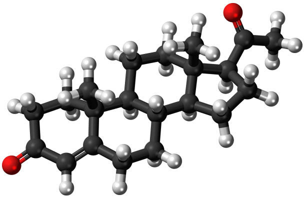

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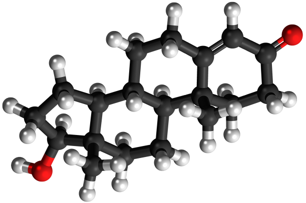

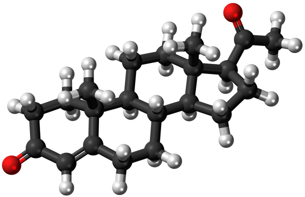

There is 1 red atom with
1 adjacent white atom.

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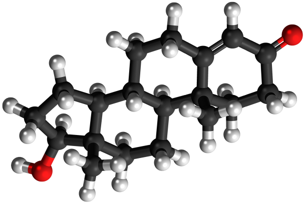

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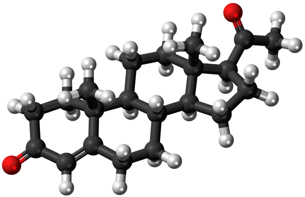

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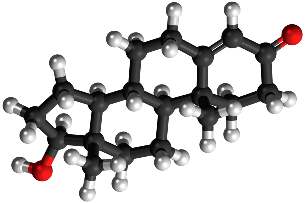

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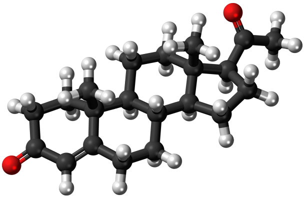

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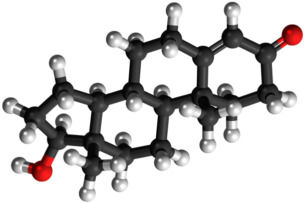

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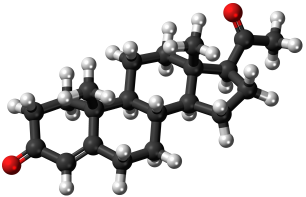

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$$\exists x \exists y \Big(\mathsf{Red}(x) \wedge \mathsf{White}(y) \wedge E(x,y) \Big)$$

Descriptive Complexity

There is 1 vertex with exactly 2 neighbours that both have exactly 3 neighbours.

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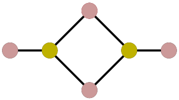

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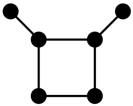

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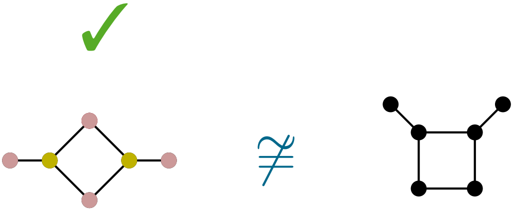

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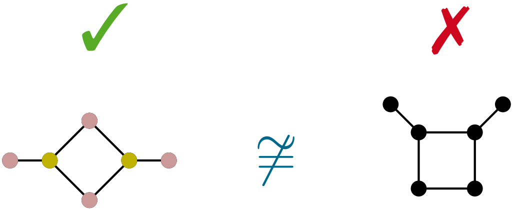

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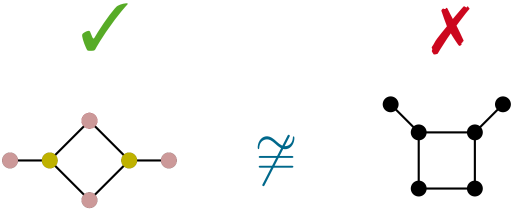

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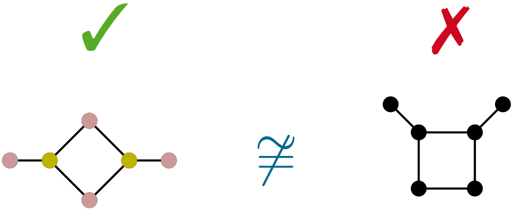

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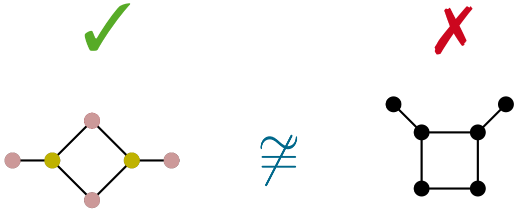

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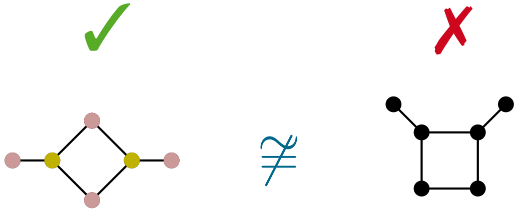

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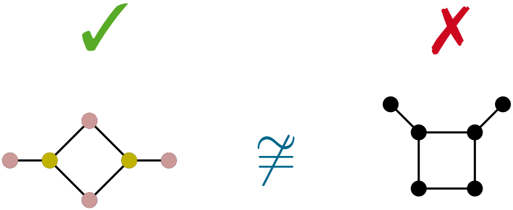

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2 variables, counting quantifiers, FO $\rightsquigarrow$ C^2-formula

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How can we measure the complexity of a logical formula?

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The complexity of a defining formula is a measure for the inherent complexity of the graphs.

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But how do we get from descriptions to actual algorithms?

Algorithmic Logics

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For graphs G, H, the following are equivalent.

1. The logic C^{k+1} distinguishes G and H.
2. The algorithm k-WL distinguishes G and H.

[Cai, Fürer, Immerman ’92]

Colour Refinement

Oldest (?) reference: *The generation of a unique machine description for chemical structures*

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1-WL

- *Initialisation*: All vertices have their initial colours.
- *Refinement*: Recolour vertices depending on colours in their neighbourhoods.
- *Stop* when colouring is stable.

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1-WL

- *Initialisation*: All vertices have their initial colours.
- *Refinement*: Recolour vertices depending on colours in their neighbourhoods.
- *Stop* when colouring is stable.

The induced partition respects orbits, so if two graphs result in different colourings, then they are non-isomorphic.

1-WL has an $O((m + n) \log n)$-implementation.

[Cardon & Crochemore '82]

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Fact

On paths of length n, 1-WL terminates after at most $\frac{n}{2}$ iterations.

Regular graphs

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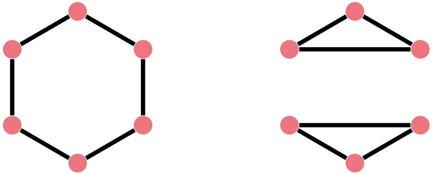

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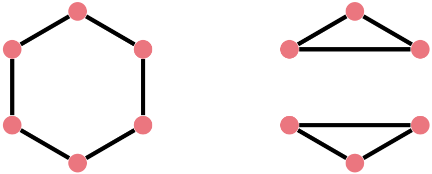

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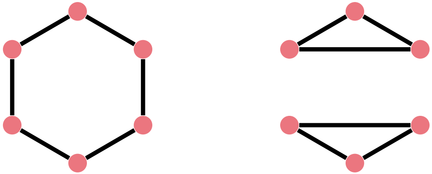

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On every regular graph, 1-WL terminates after one iteration.

1-WL does not distinguish d-regular graphs of equal order.

The WL-Algorithm

The more powerful k-WL iteratively computes a colouring of V^k.
It can be implemented to run in time $O(n^{k+1} \log n)$.

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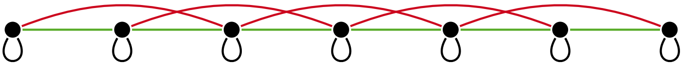

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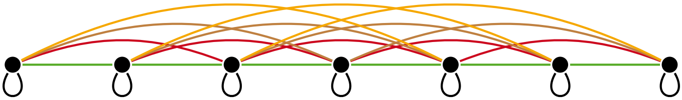

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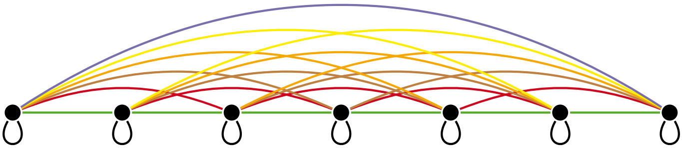

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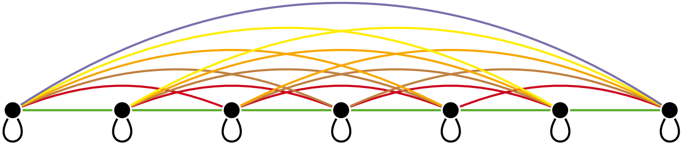

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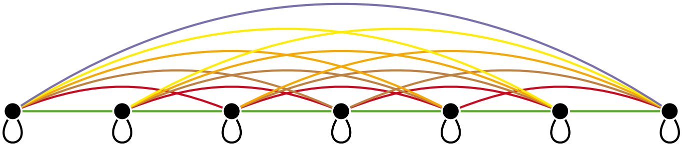

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2-WL does not distinguish strongly regular graphs with equal parameters.

Applications

Via the WL-algorithm, the logic C has connections to many areas:

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Via the WL-algorithm, the logic C has connections to many areas:

- Practical graph-isomorphism tests
- Linear programming

$$
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-1 & 1 & 3 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & -2 & 3 & \frac{1}{2} & \frac{1}{2} & 1 \\
1 & 3 & -1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 1 \\
\hline
0 & \frac{1}{3} & \frac{2}{3} & 0 & \frac{3}{2} & 0 & \frac{3}{2} & 2 & 0 & 1 & 0 & -1 & 0 & 1 \\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{3}{2} & 0 & \frac{3}{2} & 0 & 2 & 0 & 0 & 1 & 0 & -1 & 1 \\
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\hline
2 & 2 & 2 & \frac{3}{2} & \frac{3}{2} & \frac{3}{2} & \frac{3}{2} & 1 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \infty
\end{array}\right)
$$

$$
[\![\widetilde{A}]\!] = [[\widetilde{A}]] = \begin{pmatrix} 4 & 2 & 1 \\ 12 & 4 & \infty \end{pmatrix}
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Image source: [Grohe et al. ’14]

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\hline
0 & \frac13 & \frac23 & 0 & \frac32 & 0 & \frac32 & 2 & 0 & 1 & 0 & -1 & 0 & 1 \\
\frac13 & \frac13 & \frac13 & \frac32 & 0 & \frac32 & 0 & 2 & 0 & 0 & 1 & 0 & -1 & 1 \\
\frac13 & \frac13 & \frac13 & 0 & \frac32 & 0 & \frac32 & 0 & 2 & -1 & 0 & 1 & 0 & 1 \\
\frac23 & \frac13 & 0 & \frac32 & 0 & \frac32 & 0 & 0 & 2 & 0 & -1 & 0 & 1 & 1 \\
\hline
2 & 2 & 2 & \frac32 & \frac32 & \frac32 & \frac32 & 1 & 1 & \frac12 & \frac12 & \frac12 & \frac12 & \infty
\end{array}\right)$$

$$[\![\widetilde{A}]\!] = [[\widetilde{A}]] = \begin{pmatrix} 4 & 2 & 1 \\ 12 & 4 & \infty \end{pmatrix}$$

Image source: [Grohe et al. ’14]

Applications

Via the WL-algorithm, the logic C has connections to many areas:

- Practical graph-isomorphism tests
- Linear programming
- Graph kernels
- Graph neural networks
- Propositional proof complexity
- Homomorphism counting

$$\widetilde{A} = \left(\begin{array}{ccc|cccc|cc|cccc|c}
3 & -1 & 1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 3 & -2 & \frac{1}{2} & \frac{1}{2} & 1 \\
-1 & 1 & 3 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & -2 & 3 & \frac{1}{2} & \frac{1}{2} & 1 \\
1 & 3 & -1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 1 \\
\hline
0 & \frac{1}{3} & \frac{2}{3} & 0 & \frac{3}{2} & 0 & \frac{3}{2} & 2 & 0 & 1 & 0 & -1 & 0 & 1 \\
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Pebble Game for C^k

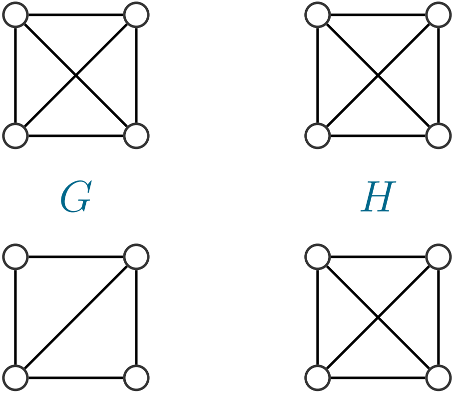
Spoiler and Duplicator dispose of k pairs of pebbles.

1

2

3

4



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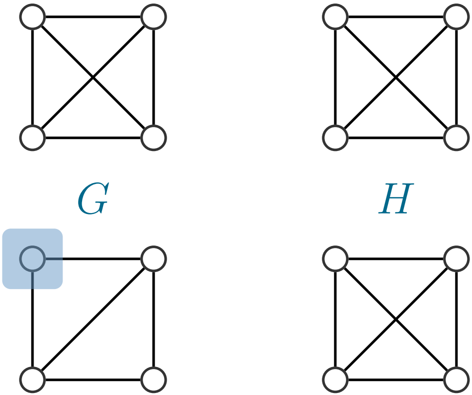
3

4



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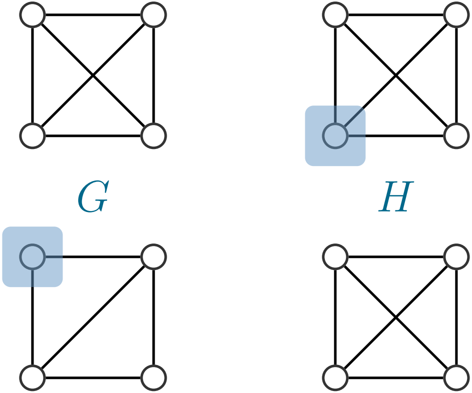
2 Duplicator takes the other pebble and selects a set S' of equal size in the other graph.

3

4



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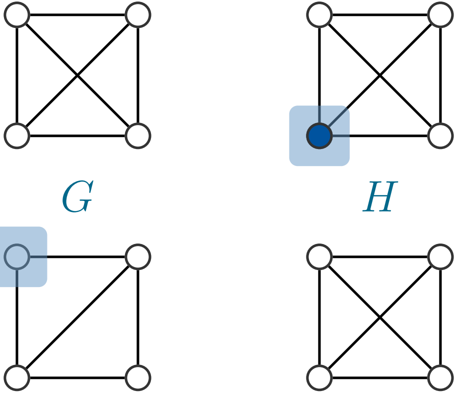

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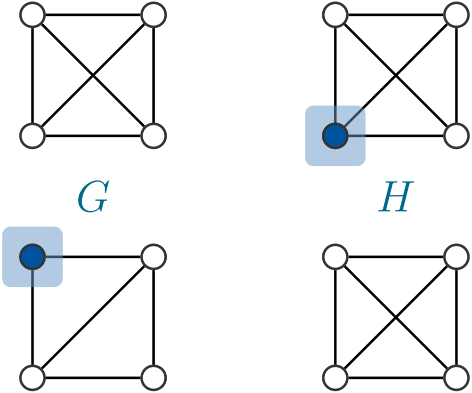

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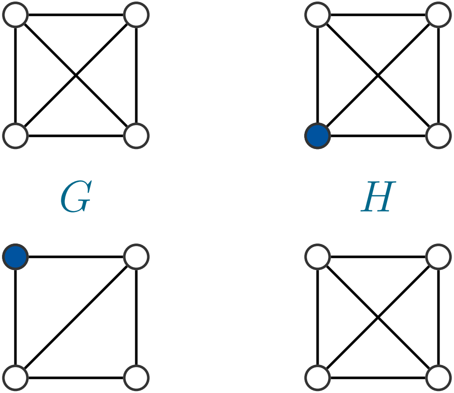

Are the pebbled subgraphs isomorphic? ✓

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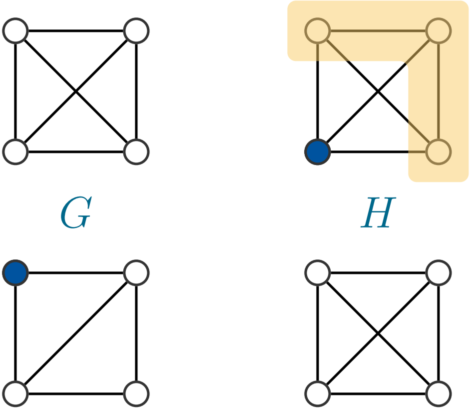

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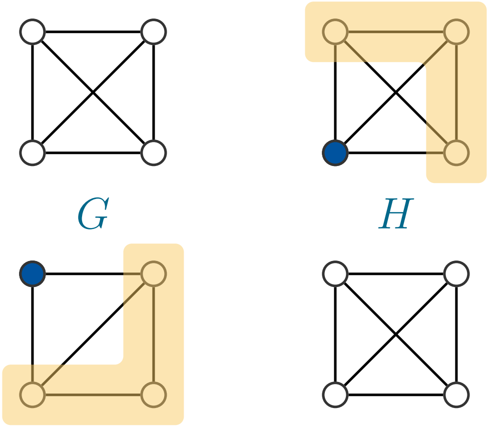

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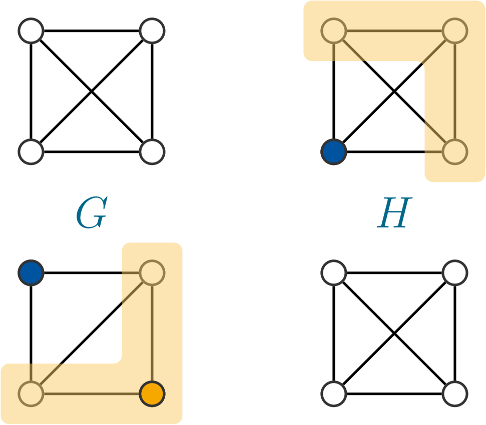

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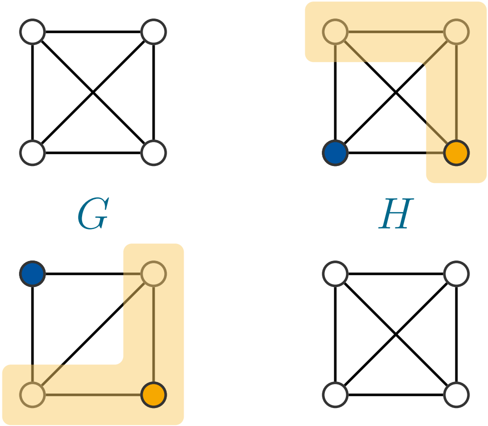

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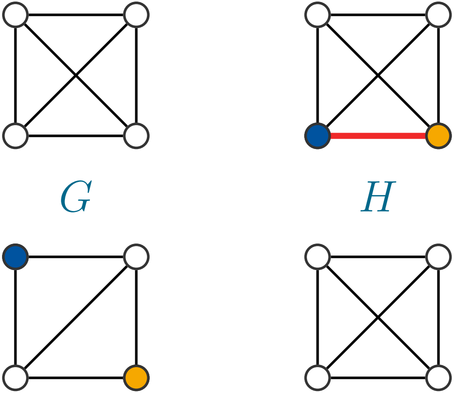

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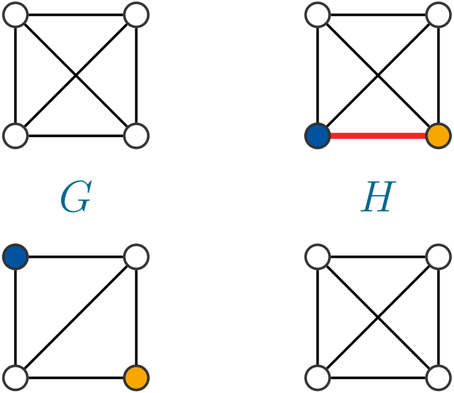

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Thus, Spoiler wins.

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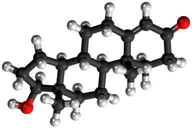
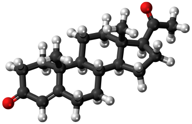
Nesting depth $\equiv$ Number of iterations $\equiv$ Rounds in game

Identification



$\ncong$



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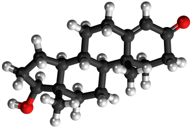
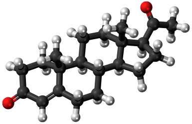
 $\ncong$ 

$$\exists x \exists y \Big(\mathsf{Red}(x) \land \mathsf{White}(y) \land E(x,y) \Big)$$

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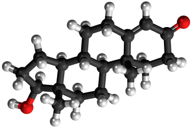
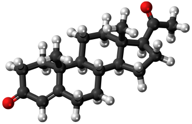
 $\not\cong$ 

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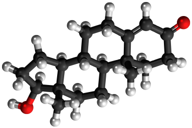

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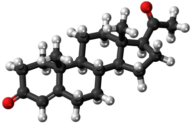

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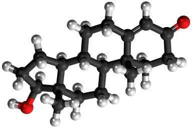
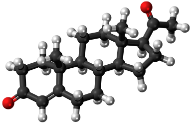
 $\ncong$ 

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Graphs that are not distinguished by C^k are *C^k-equivalent*.

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C^2 identifies almost all graphs. [Babai, Erdös, Selkow '80]

But it fails on very simple graphs! ($\mathsf{C}^2 \equiv 1$-WL)

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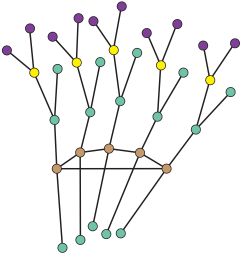

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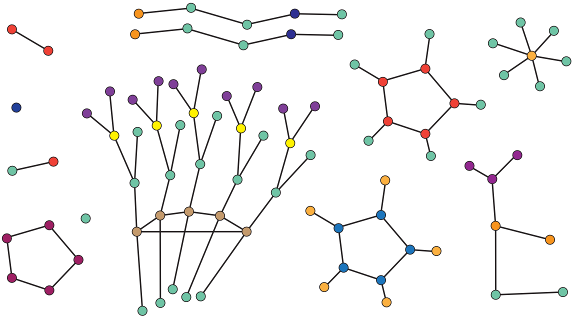
Bouquet forest: disjoint union of vertex-coloured trees and **non-isomorphic** bouquets



WL-Dimension

1-WL has an $O((m+n)\log n)$-implementation.

[Cardon & Crochemore '82]

k-WL can be implemented to run in time $O(n^{k+1}\log n)$.

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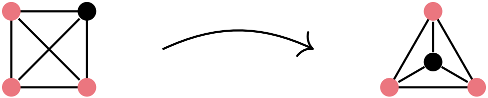
Graph class	WL-dimension		
	lower bound	upper bound	
Trees	1	1	
Interval graphs	2	2	[Evdokimov, Ponomarenko, Tinhofer '00]
Excluded minor H	$\Omega(\lvert V(H)\rvert)$	$f(H)$	[Grohe '10]
Planar graphs	2	$\cancel{14}$ **3**	**[K., Ponomarenko, Schweitzer '17]**
Treewidth k	$\cancel{\Omega(k)}$ $\frac{k}{2}-2$	$\cancel{k+2}$ k	**[K., Neuen '19]**
Genus g	$\Omega(g)$	$4g+3$	[Grohe, K. '19]
Clique width k	$\Omega(k)$	$3k+4$	[Grohe, Neuen '19]
Rank width k	$\Omega(k)$	$3k+4$	[Grohe, Neuen '19]

Planar Graphs

G is *planar* $:\Longleftrightarrow$ G can be embedded in the plane without any edge crossings.



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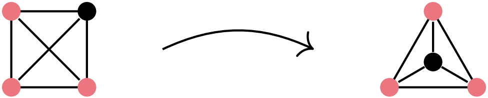

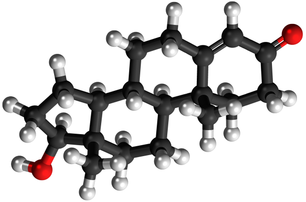

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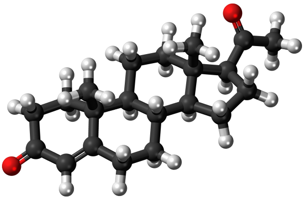
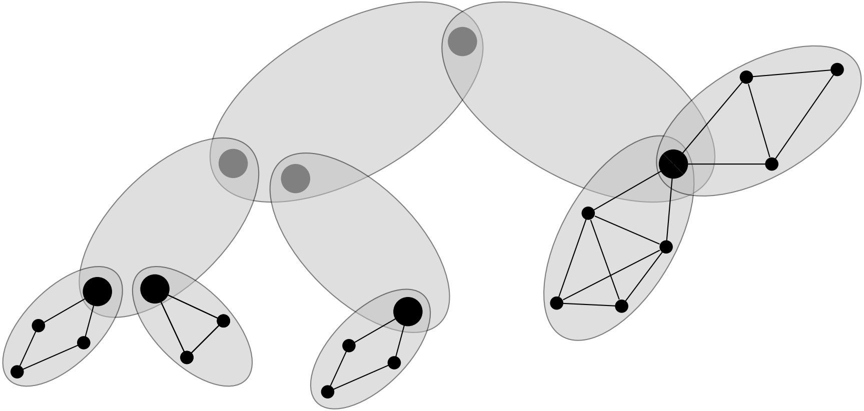


DECOMPOSITIONS



A decomposition of a connected graph into
2-connected components and cut vertices

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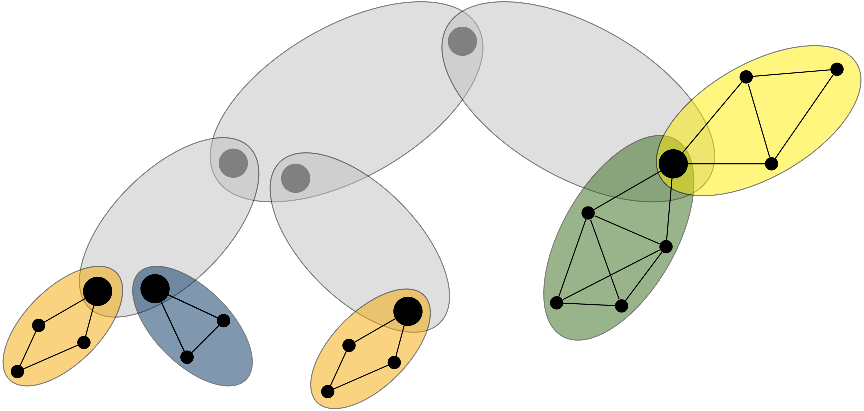

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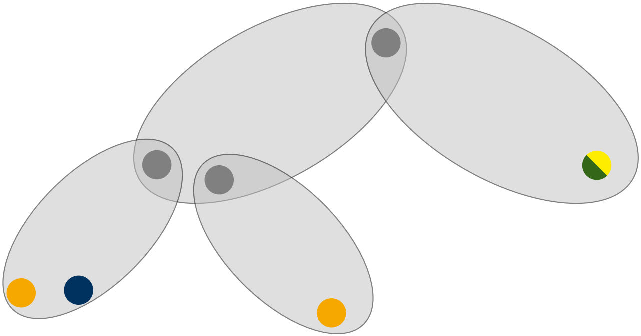

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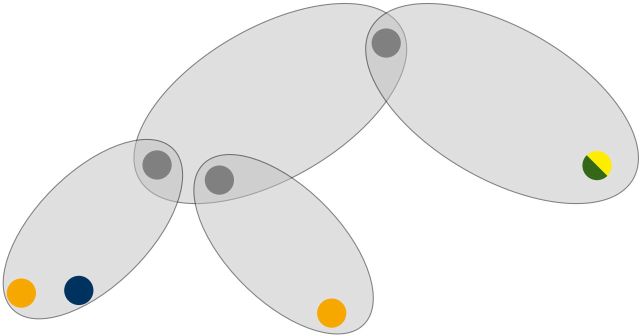

Reduction scheme:

1. planar $\leq$ vertex-coloured 2-connected planar
2. vertex-col. 2-conn. planar $\leq$ arc-col. 3-conn. planar
3. arc-coloured 3-connected planar case

Planar graphs

Theorem (K., Ponomarenko, Schweitzer 2017)

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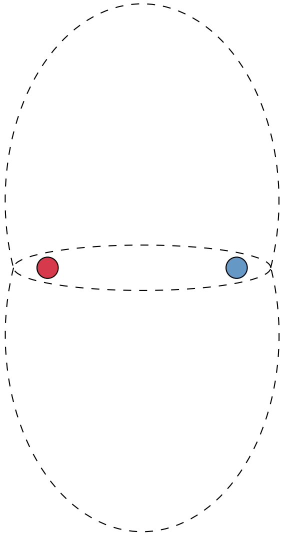
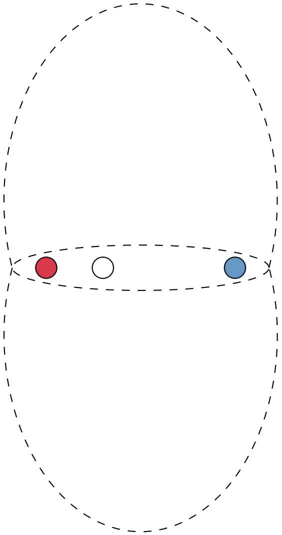
We show: 2-separators can be detected with 4-WL. (5 pebbles)

Detecting 2-Separators With 5 Pebbles





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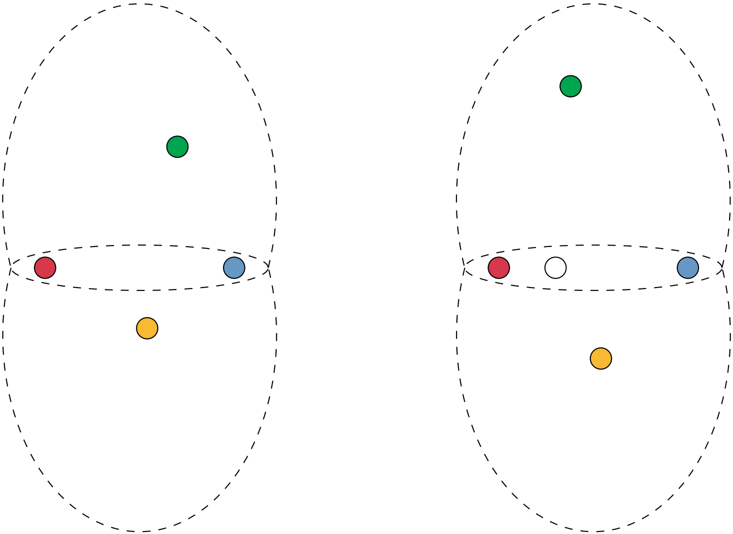

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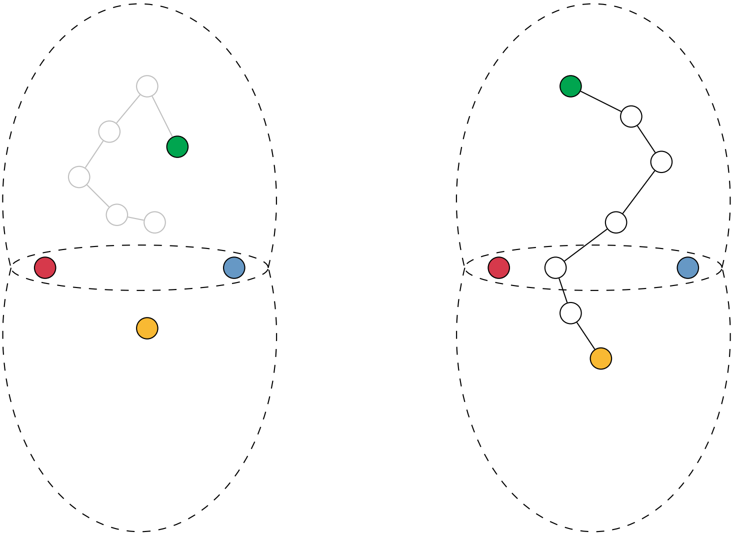

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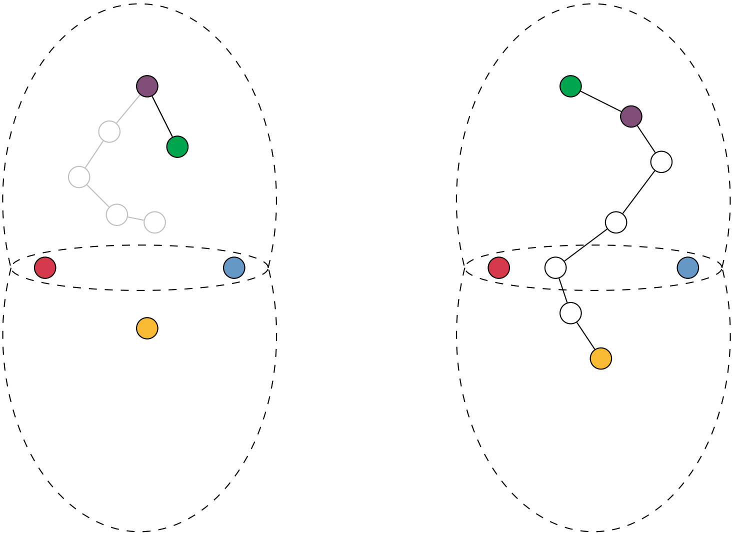

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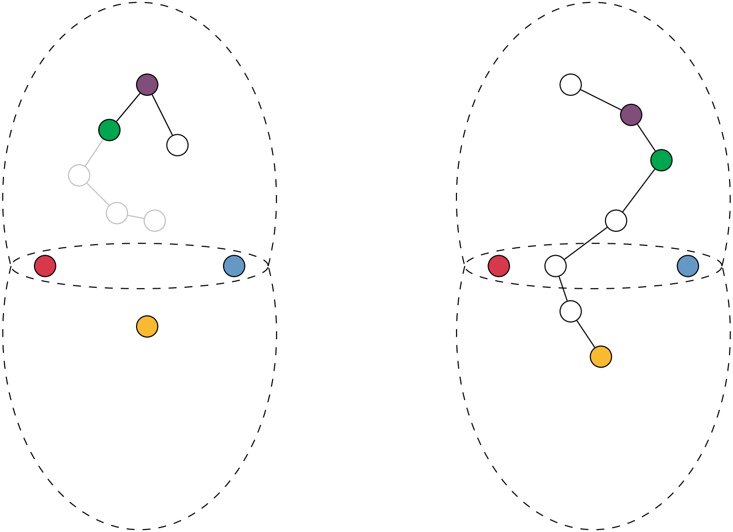

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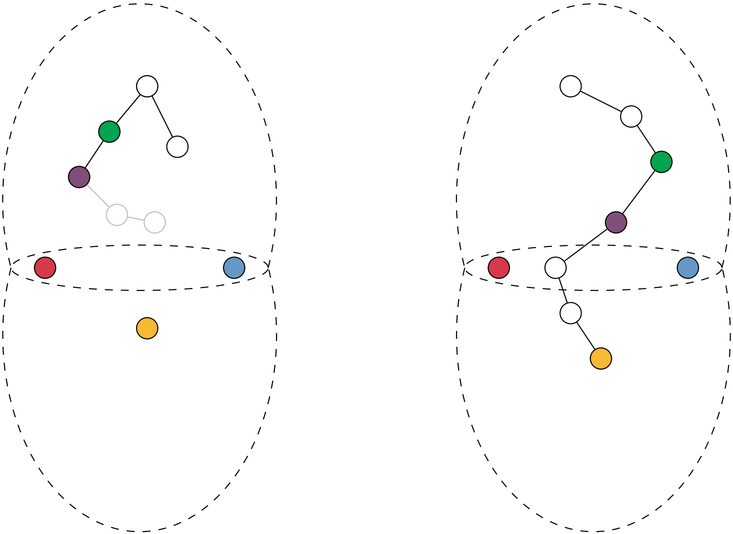

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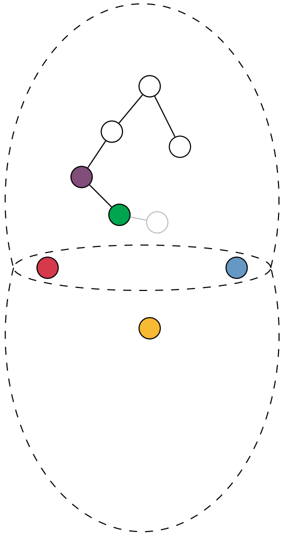

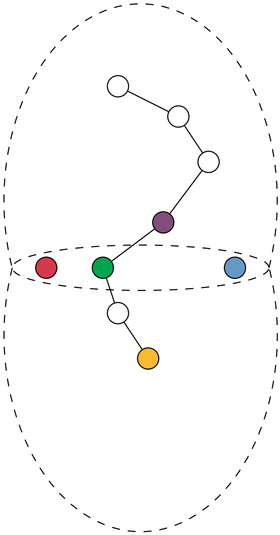

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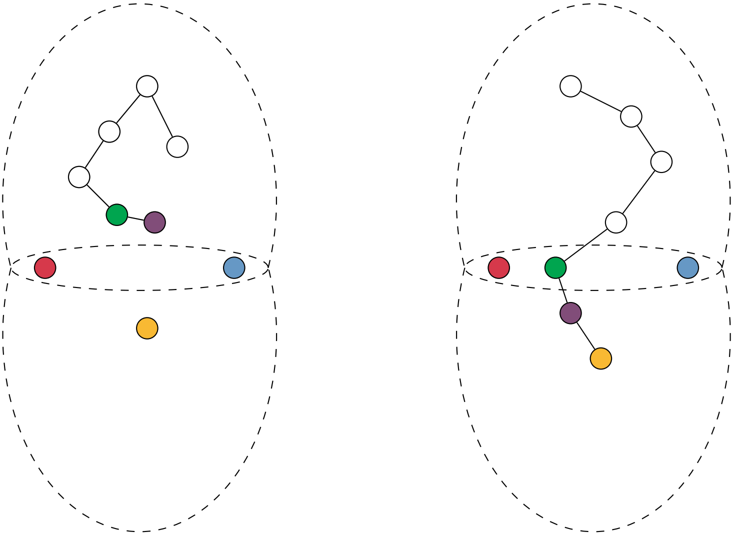

Spoiler wins.

Detecting Separators

Thus, 2-separators can be detected with **5 pebbles**. (4-WL)

Lemma (K., Ponomarenko, Schweitzer 2017)

*2-Separators can be detected with **4 pebbles**.* *(3-WL)*

Lemma (K., Neuen 2019)

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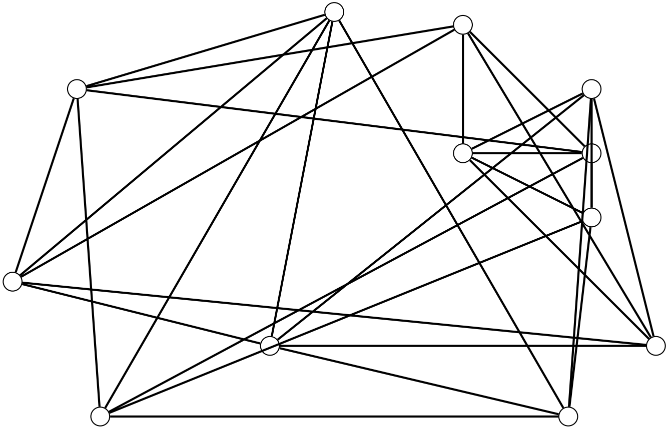
Reduction scheme:

1. planar $\leq$ vertex-coloured 2-connected planar **2-WL**
2. **vertex-col. 2-conn. planar $\leq$ arc-col. 3-conn. planar** **2-WL**
3. arc-coloured 3-connected planar case **3-WL**

3-CONNECTED PLANAR GRAPHS



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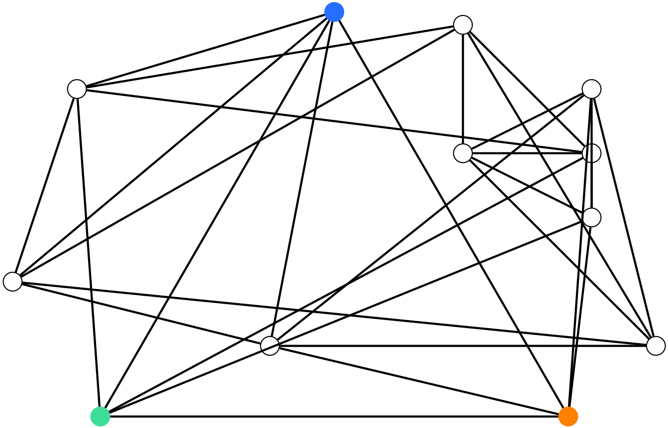

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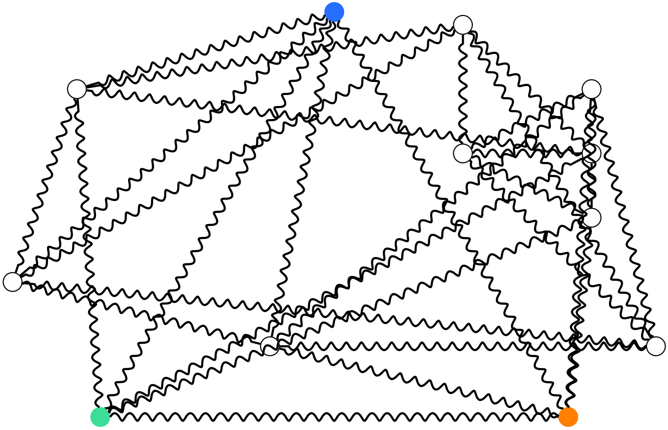

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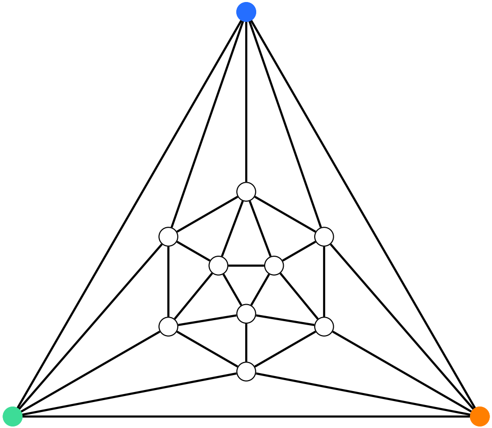

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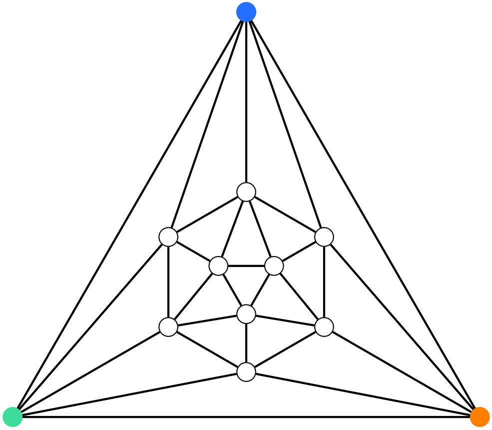

In **Tutte's Spring Embedding**, no two vertices are mapped to the same location.

We show: this implies that they get different colours w.r.t. 1-WL.

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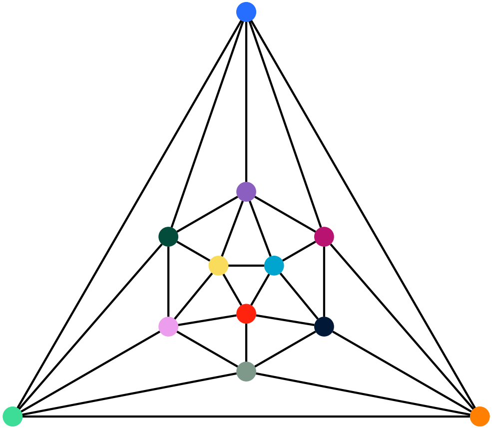

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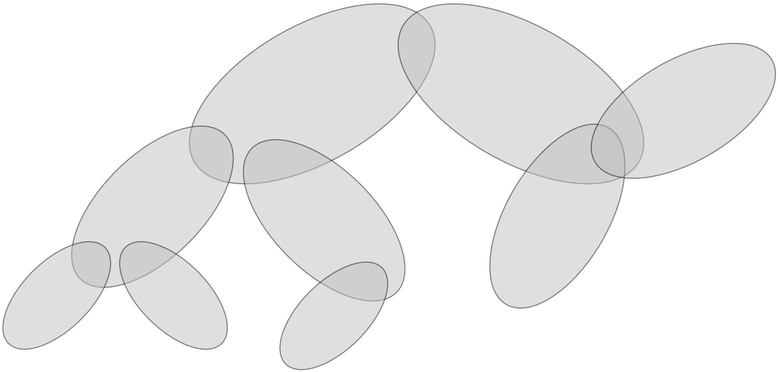
Bounded-Treewidth Graphs

Theorem (K., Neuen 2019)

Let G be a graph of treewidth at most $k \geq 2$. Then k-WL identifies G.



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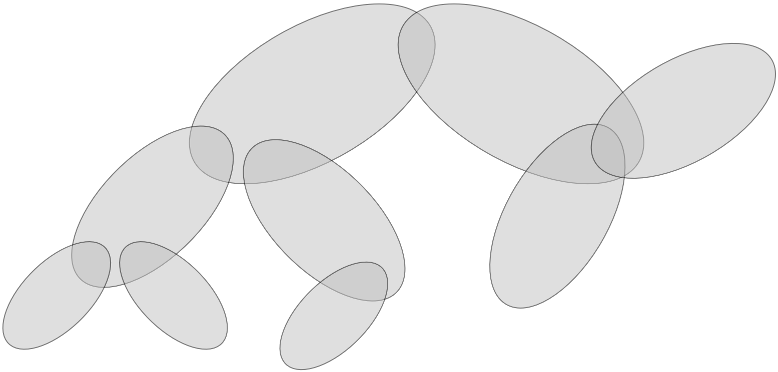
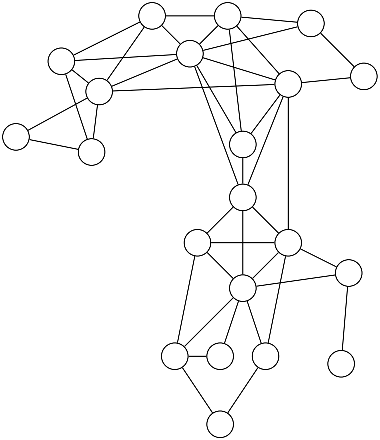


Spoiler enforces a descent of a tree decomposition of width at most k of G.

BOUNDED-TREEWIDTH GRAPHS



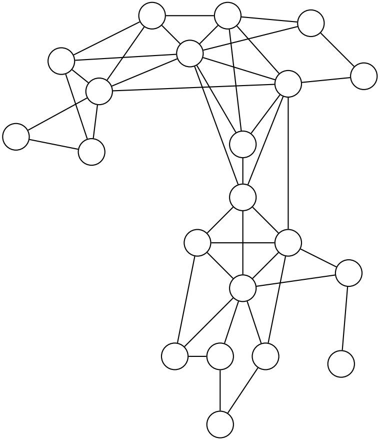
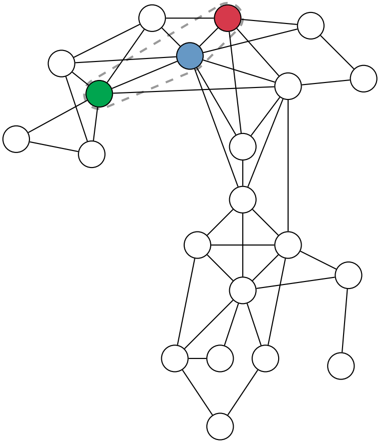
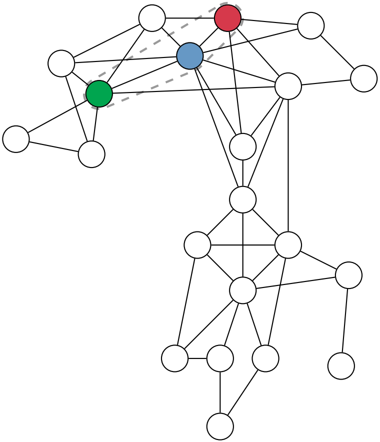


Image source: [Neuen]

Bounded-Treewidth Graphs





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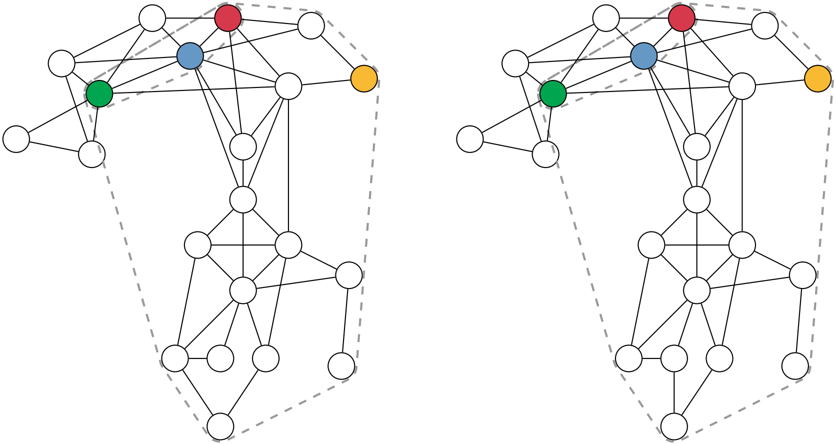

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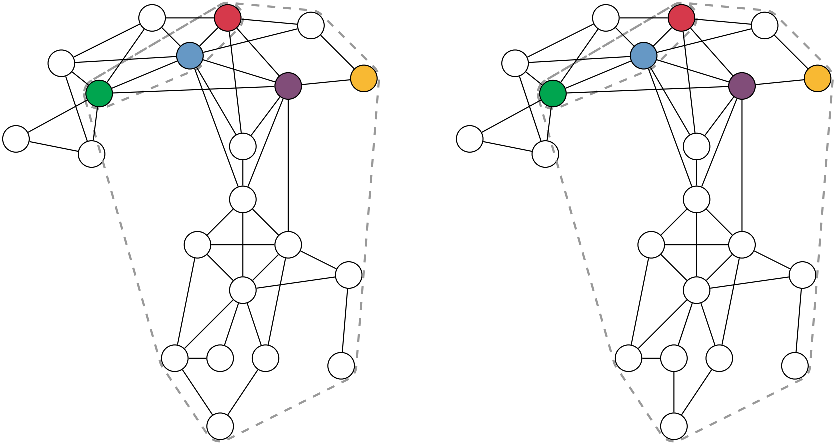

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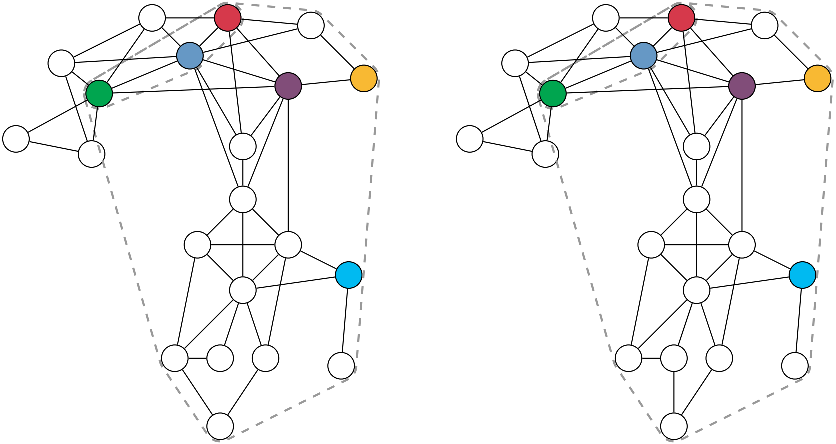

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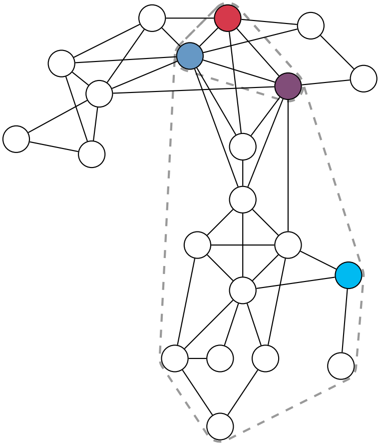

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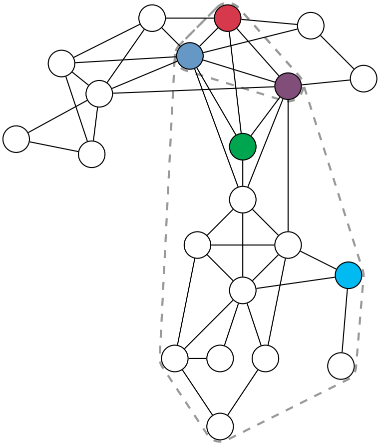

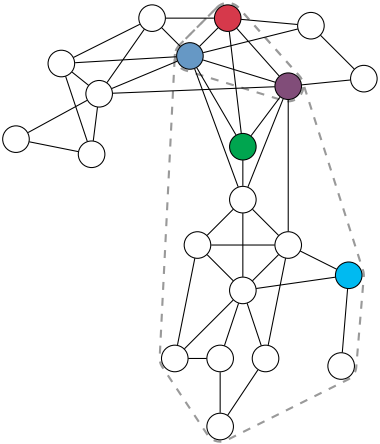

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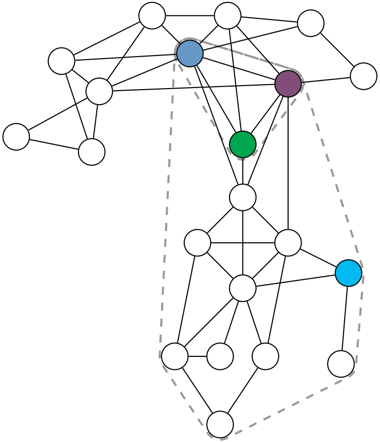

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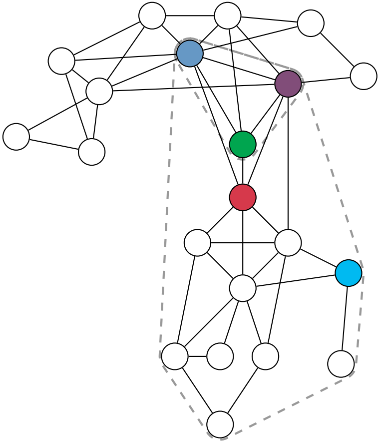
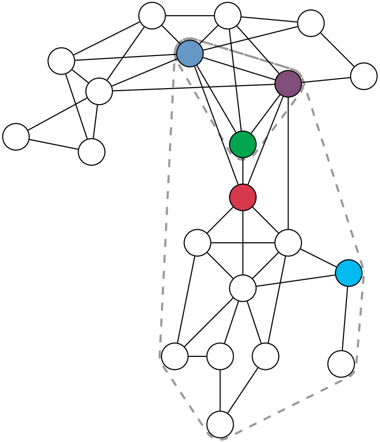

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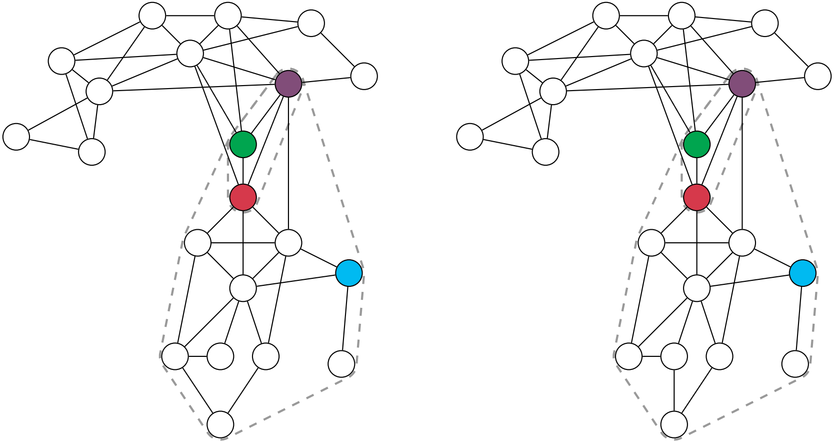

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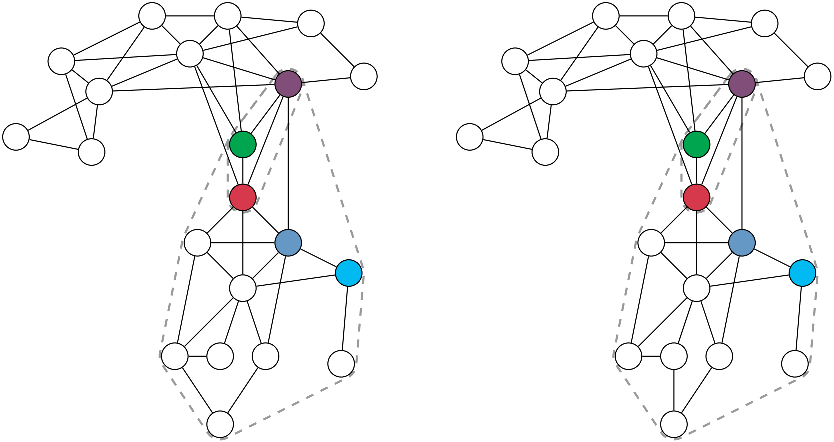

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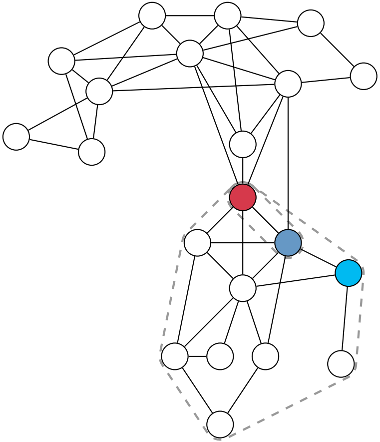

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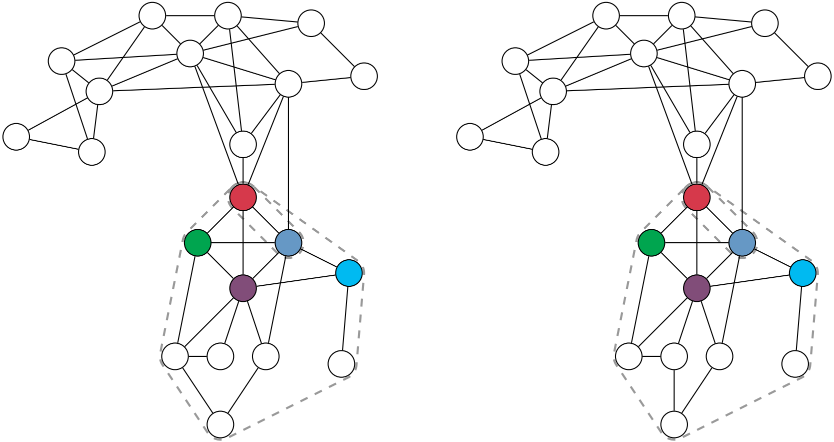

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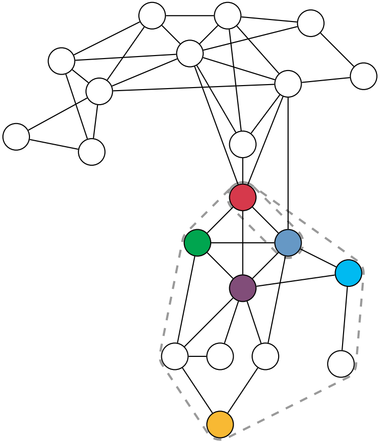

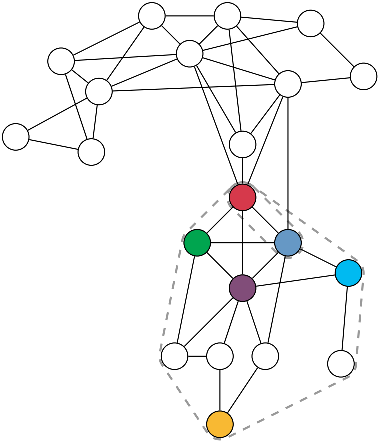

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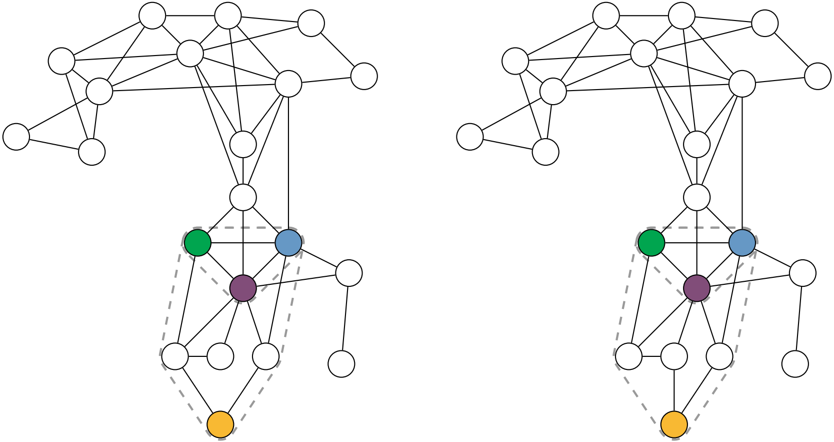

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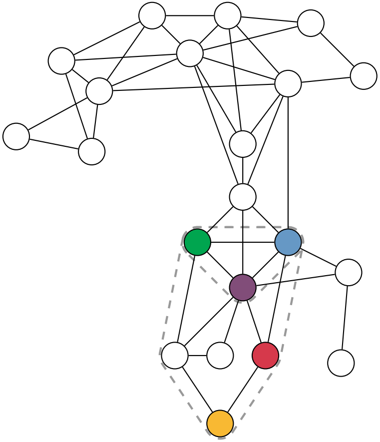

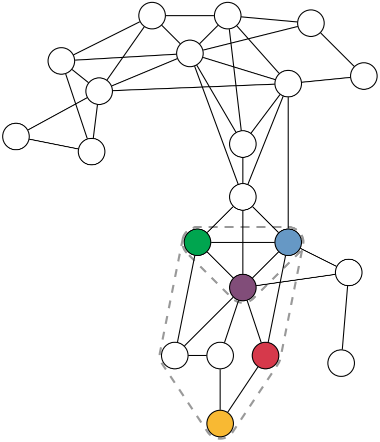

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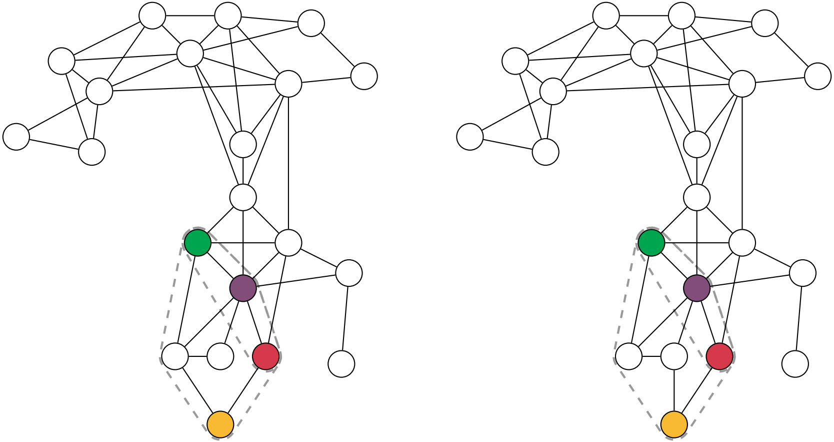

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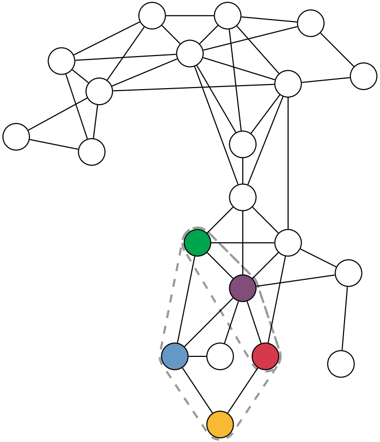

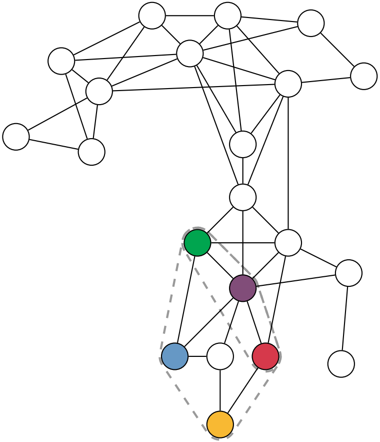

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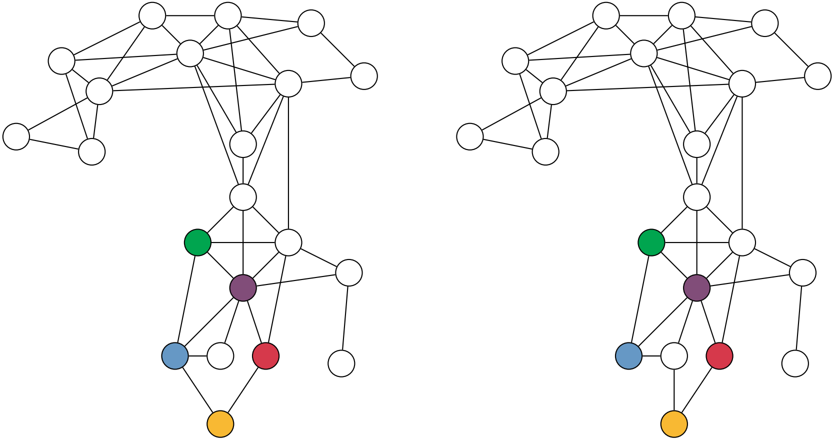

Spoiler wins.

Image source: [Neuen]

WL-DIMENSION

Definition

A graph G has *WL-dimension at most k* if k-WL identifies G.

Graph class	WL-dimension		
	lower bound	upper bound	
Trees	1	1	
Interval graphs	2	2	[Evdokimov, Ponomarenko, Tinhofer '00]
Excluded minor H	$\Omega(\lvert V(H)\rvert)$	$f(H)$	[Grohe '10]
Planar graphs	2	$\cancel{14}$ $\mathbf{3}$	**[K., Ponomarenko, Schweitzer '17]**
Treewidth k	$\cancel{\Omega(k)}$ $\frac{k}{2} - 2$	$\cancel{k+2}$ k	**[K., Neuen '19]**
Genus g	$\Omega(g)$	$4g+3$	[Grohe, K. '19]
Clique width k	$\Omega(k)$	$3k+4$	[Grohe, Neuen '19]
Rank width k	$\Omega(k)$	$3k+4$	[Grohe, Neuen '19]

Conclusion

Decompositions can be very helpful to bound the logical and algorithmic complexity of deciding isomorphism between graphs.

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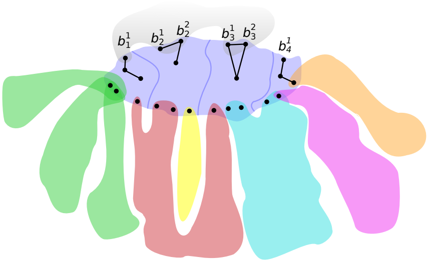

Theorem (Grohe, K. 2021)

There is a $k \in \mathbb{N}$ such that k-WL identifies all planar n-vertex graphs in $O(\log n)$ iterations.

Conclusion

The WL-dimension to distinguish two graphs is at most the dimension that distinguishes their decompositions into 3-connected components.

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WL-Dimension of Planar Graphs

1. Reduction to 2-connected graphs **2-WL**
2. Reduction to 3-connected graphs **3-WL**
3. 3-connected planar graphs **3-WL**

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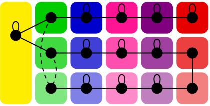
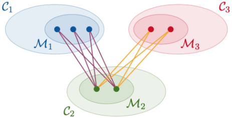
$\rightsquigarrow$ **ICALP-talk on Thursday** ☺

WL-Complexity



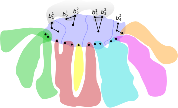
1-WL

Graphs with $n{-}1$ iterations



2-WL

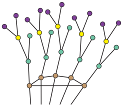
First nontrivial upper bound



Planar graphs

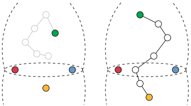
Logarithmic upper bound

WL-Power



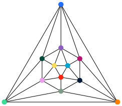
1-WL

Complete characterisation



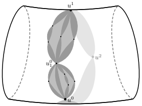
2-WL

Detects 2-separators



Planar graphs

WL-dim ≤ 3



Euler genus

WL-dim ≤ $4g{+}3$