The Weisfeiler-Leman dimension of graphs and isomorphism testing

Symmetry vs Regularity, 50 years of WL
(6th July 2018)

Pascal Schweitzer

based on joint work with
Sandra Kiefer, Ilia Ponomarenko, Erkal Selman

TECHNISCHE UNIVERSITÄT
KAISERSLAUTERN

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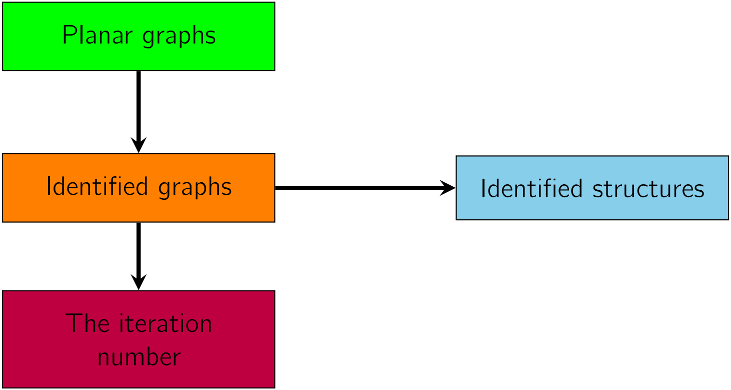
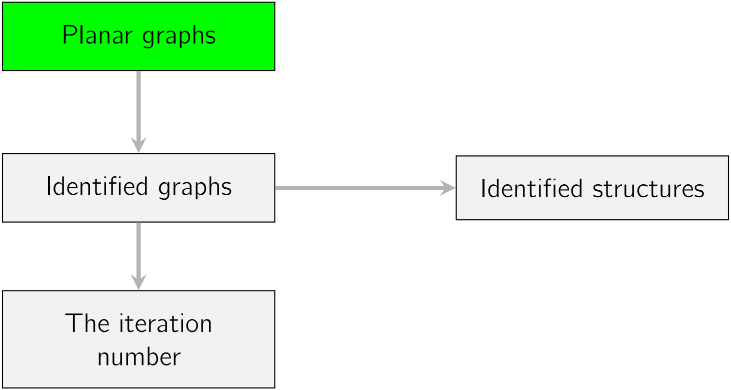
- the k-dimensional Weisfeiler-Leman algorithm distinguishes G from every other graph, [Babai]
- the graph is definable in fixed point logic with counting using at most $k+1$ variables C^{k+1} [Cai,Fürer,Immerman](1992)
- spoiler wins the bijective $k+1$ pebble game [Cai,Fürer,Immerman](1992)
- the k-th level (± 1) of the Sherali-Adams hierarchy solves some suitable constraint system for isomorphism of G [Malkin][Atserias,Maneva][Grohe,Otto](2012)
- the graph is uniquely determined by homomorphism counts to it of graphs of treewidth at most k [Dell,Grohe,Rattan] (2018)
- k players can win the quantum isomorphism game with a non-signaling strategy [Lupini,Roberson] (2018+)


Planar graphs
Identified graphs
Identified structures
The iteration number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Bounds on the WL-dimension

Theorem (Cai, Fürer, Immerman (1992))

There is an infinite family of 3-regular graphs whose WL-dimension is linear in the number of vertices.

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Theorem (Grohe (2012))

The WL-dimension in every graph class with a forbidden minor is bounded.

Examples

- trees
- planar graphs
- graphs embeddable on a fixed surface.
- graphs of bounded tree width
- K_t-minor-free graphs

WL-dimension of Planar graphs

Theorem (Kiefer, Ponomarenko, S. (2017))

Planar graphs have WL-dimension at most 3.

(previously ≤ 14 [Verbitsky] (2006) [Redies] (2014))

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Two step proof:

1.) reduce to 3-connected graphs

2.) handle 3-connected graphs (use **Tutte's Spring Embedder**)

WL-dimension of non-3-connected graphs

For a graph G let $\dim_{\mathrm{WL}}(G)$ denote its Weisfeiler-Leman dimension.

Lemma

Let G be a graph.

- *If $\dim_{\mathrm{WL}}(G) \geq 2$ then $\dim_{\mathrm{WL}}(G)$ is the maximum $\dim_{\mathrm{WL}}(C)$ over all connected components C of G.*

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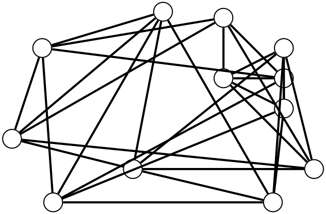
- *If $\dim_{\mathrm{WL}}(G) \geq 3$ then $\dim_{\mathrm{WL}}(G)$ is the maximum $\dim_{\mathrm{WL}}((C,\chi))$ over all vertex/edge-colored 3-connected components C of G.*

Automorphisms of 3-connected planar graphs

Tutte's Spring Embedder



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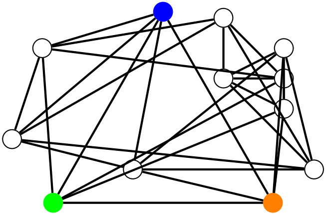

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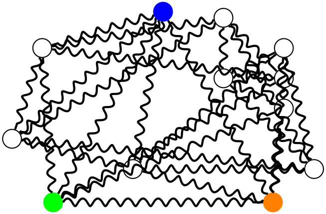

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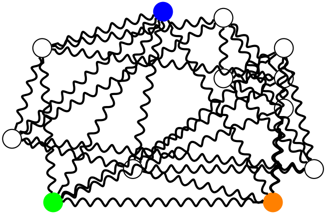

some physics

Automorphisms of 3-connected planar graphs

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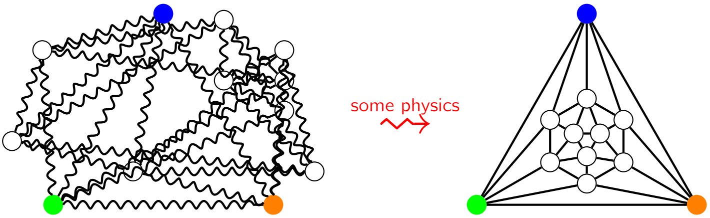

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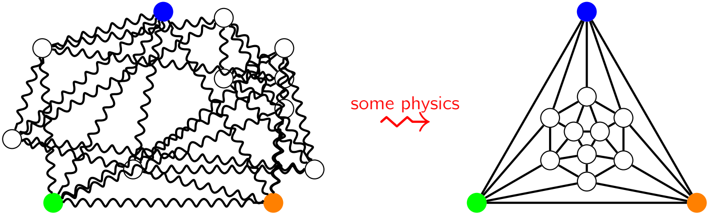

Lemma (Kiefer, Ponomarenko, S. (2017))

Let G be a planar graph. If vertices end up at different locations in the Spring Embedder then they have different colors under 1-dim WL.

Fixing number of planar graphs

Fixing number of a graph is the number of vertices that need to be fixed to destroy all automorphisms.

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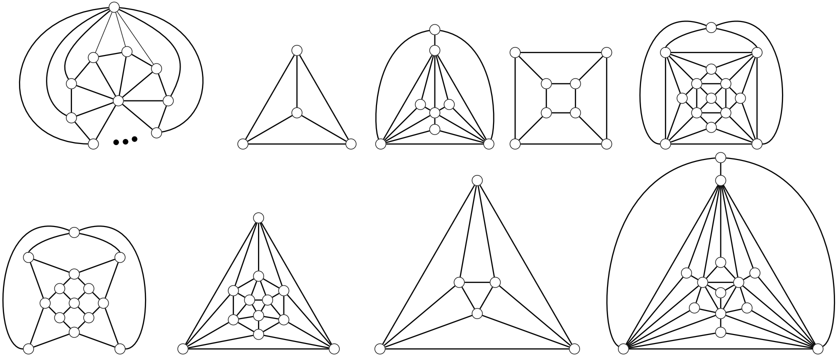
Theorem (Kiefer, Ponomarenko, S. (2017))

The 3-connected planar graphs with fixing number 3 are:



Loos' apartment:

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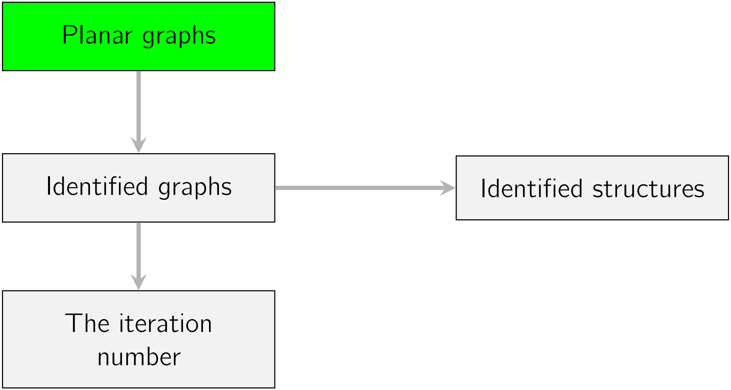
fixing number 2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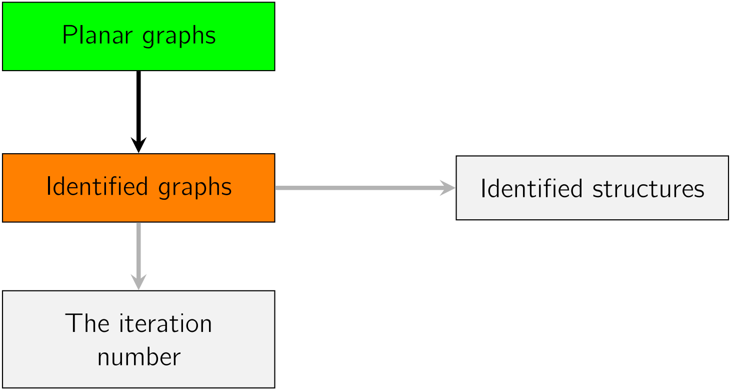
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Graphs identified by color refinement

A graph has WL-dimension 1, if it is distinguished from every non-isomorphic graph by color refinement (1-dim WL).

We say the graph is identified.

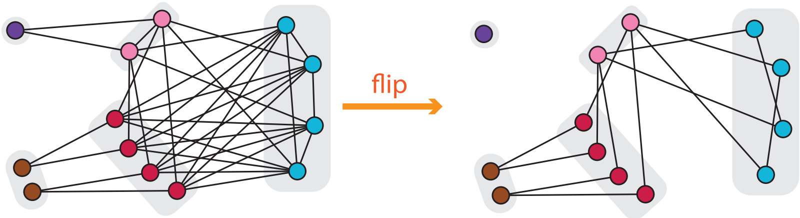
Question:
Which graphs are identified by color refinement?

- trees
- almost all graphs [Babai, Erdős, Selkow] (1980)

The flip of a graph

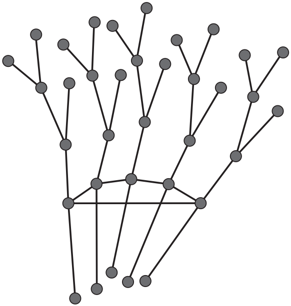
The flip of G is the vertex-colored graph obtained as follows:

- Consider the coarsest equitable partition of G.
- Complement edges within a class if this reduces number of edges.
- Complement edges between classes if this reduces number of edges.



Bouquet Forest

To obtain a bouquet, take 5 copies $(T_1, v_1), \ldots, (T_5, v_5)$ of a rooted tree (T, v) and connect them via a 5-cycle on $\{v_1, \ldots, v_5\}$.



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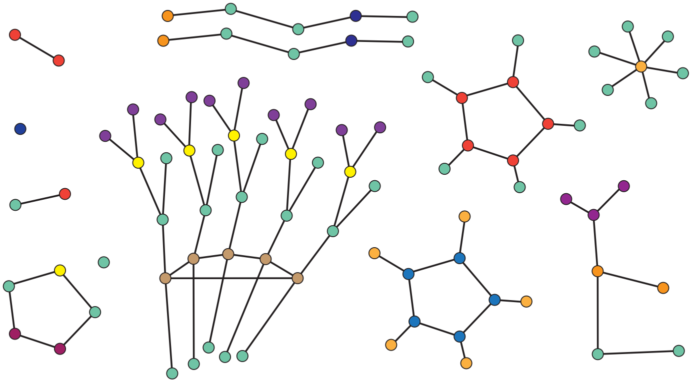
A bouquet forest is a disjoint union of vertex-colored trees and <u>non-isomorphic</u> vertex-colored bouquets.



Characterization via bouquet forests

Theorem (Kiefer, S., Selman (2015))

A graph is identified by color refinement if and only if its flip is a bouquet forest.

Similar results were independently obtained by [Arvind, Köbler, Rattan, Verbitsky].

Corollaries

Corollary

Given a graph on n vertices and m edges, one can decide in time $O((m+n)\log n)$ whether it is identified by color refinement.

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Given a graph on n *vertices and* m *edges, one can decide in time* $O((m+n)\log n)$ *whether it is identified by color refinement.*

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If a graph is identified by color refinement, then its coarsest equitable partition is the orbit partition.

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If a graph is identified by color refinement, then all vertex-colored versions of it are also identified.

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Side remark:
The last two statements do not hold for higher dimensional Weisfeiler-Leman algorithms.

Regular graphs that are identified

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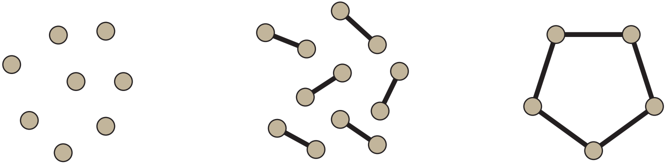
Lemma

A regular graph is identified if it has no edges, is a perfect matching a 5-cycle, or a complement of one of these graphs.



Biregular graphs that are identified

Recall: A graph is (d_1, d_2)-biregular if it has a bipartition (V_1, V_2) such that vertices in V_i have exactly d_i neighbors in the other class.

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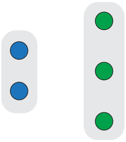
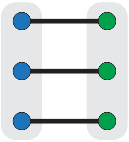
Recall: A graph is (d_1, d_2)-biregular if it has a bipartition (V_1, V_2) such that vertices in V_i have exactly d_i neighbors in the other class.

Lemma

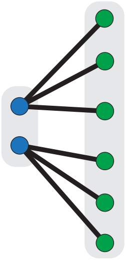
A bipartite (k, ℓ)-biregular graph is identified by color refinement if and only if $k \leq 1$, $\ell \leq 1$ or the bipartite complement has these properties.



$P \,\square\, Q$

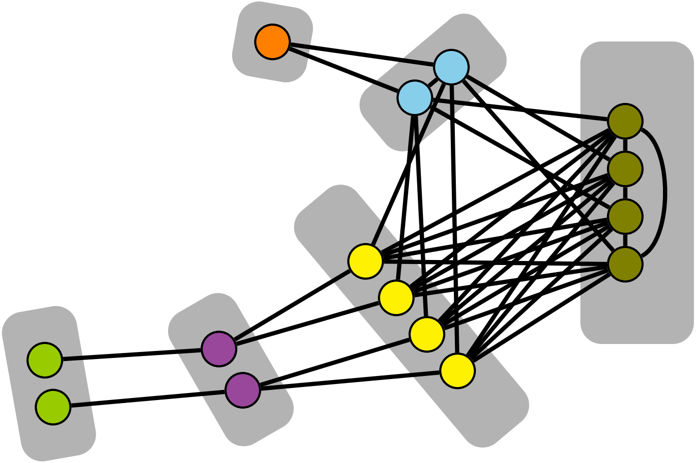


$P \equiv Q$



$P \ll Q$

The skeleton



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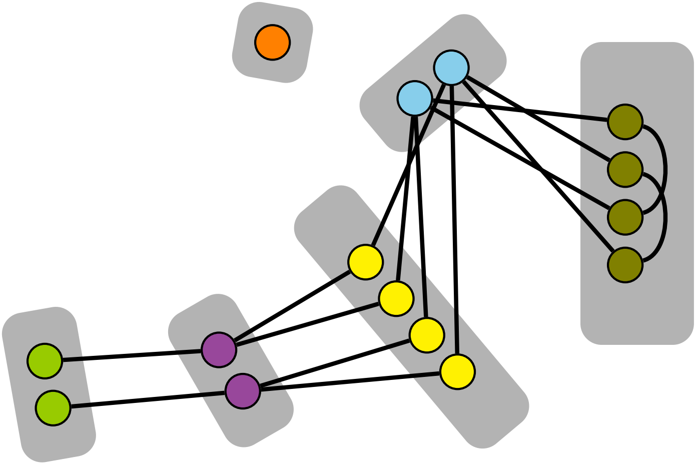

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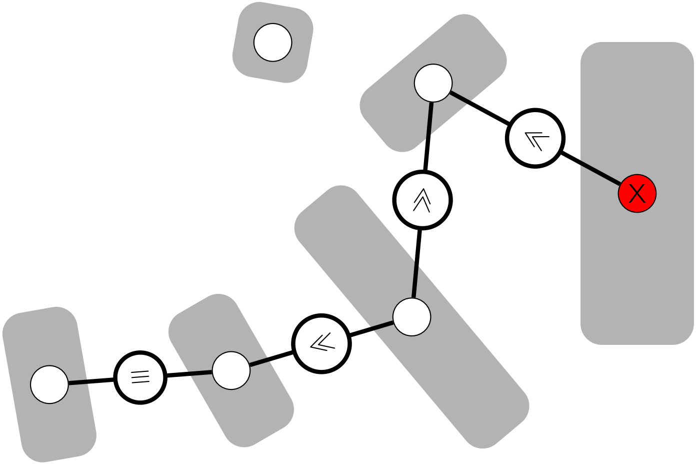
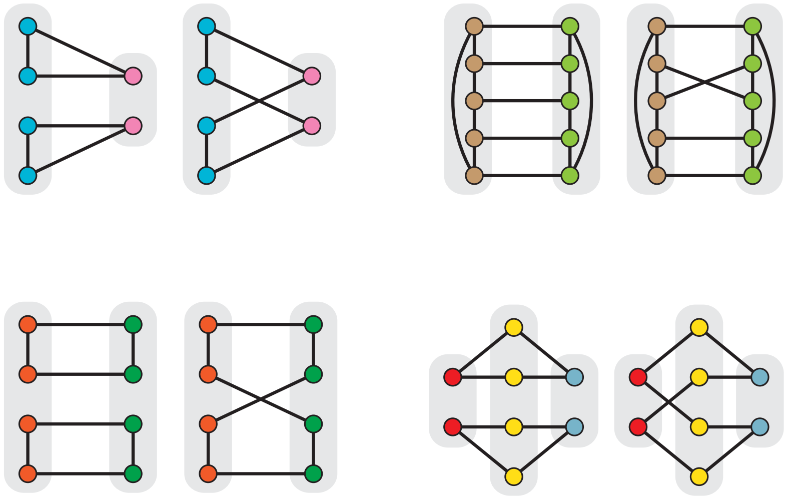


Conditions on the skeleton (Illustration)



Characterization via the skeleton

Call a color class P an exception if it induces a 5-cycle, a matching or the complement of a matching.

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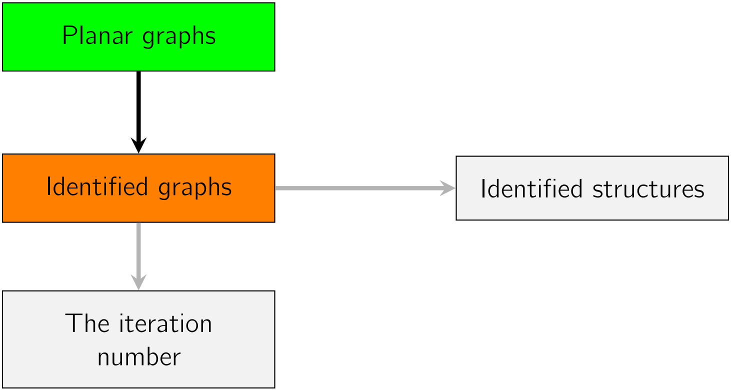
Theorem (Kiefer, S., Selman (2015))

A graph G with stable coloring χ is identified by color refinement if and only if the following hold:

1. *Each color class induces a graph identified by color refinement (i.e., empty graph, matching, a 5-cycle, or the complement of such),*
2. *for all pairs of distinct color classes P and Q we have $P \square Q$, $P \equiv Q$, $P \ll Q$ or $Q \ll P$,*
3. *the skeleton S_G is a forest,*
4. *there is no path $P_0, P_1, \dots, P_t$ in S_G with $P_0 \ll P_1$ and $P_{t-1} \gg P_t$*
5. *there is no path $P_0, P_1, \dots, P_t$ in S_G where $P_0 \ll P_1$ and P_t is an exception, and*
6. *in every connected component of S_G there is at most one exception.*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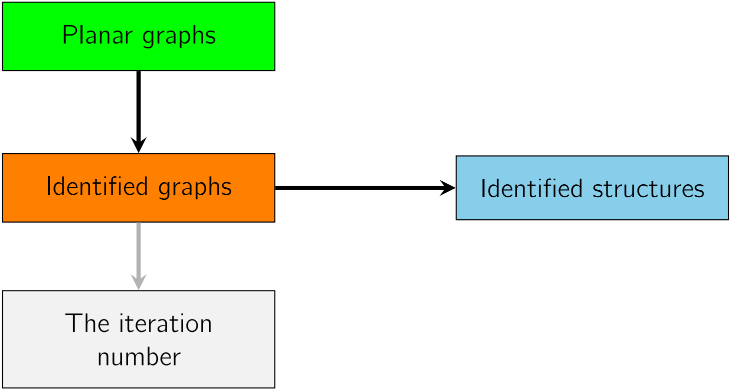
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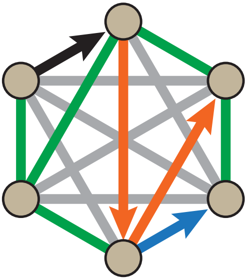
Generalization to relational structures

We can investigate which relational structures are identified by color refinement.
It suffices to consider edge colored partially oriented complete graphs (i.e., rainbows).

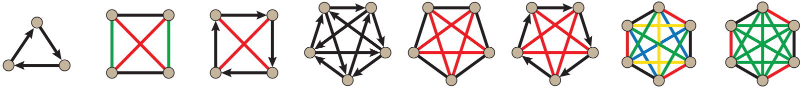


Regular structures identified

Theorem (Kiefer, S., Selman)

Let G be an color-regular rainbow. Then color refinement identifies G if and only if G is

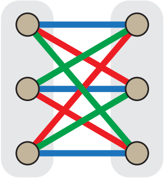
1. *an undirected complete graph with only one edge color,*
2. *undirected and has two edge colors, one of which induces a perfect matching, or*
3. *one of the following objects:*



Cases 2 and 3 are called exceptions.

A bipartite exception

- There is a new kind of biregular **exception** on 6 vertices:



The exception $P \equiv_3^3 Q$ involving two color classes

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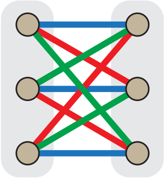


The exception $P \equiv_3^3 Q$ involving two color classes

Classification of identified sturctures

Theorem (Kiefer, S., Selman)

Let G be a rainbow. Then G is identified by color refinement if and only if the following hold:

1. *Each color class of the stable coloring induces a graph identified by color refinement*
2. *for all distinct pairs of color classes of the stable coloring P and Q we have $P \square Q$, $P \equiv Q$, $P \ll Q$, $Q \ll P$ or $P \equiv_3^3 Q$,*
3. *the skeleton S_G is a forest,*
4. *there is no path $P_0, P_1, \ldots, P_t$ in S_G with $P_0 \ll P_1$ and $P_{t-1} \gg P_t$,*
5. *there is no path $P_0, P_1, \ldots, P_t$ in S_G where $P_0 \ll P_1$ and P_t is an exception, and*
6. *in every connected component of S_G there is at most one exception.*

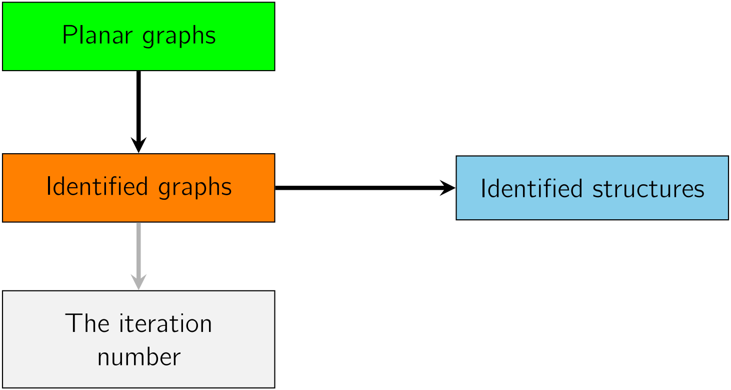
Consequences of the classification

Corollary

Given a rainbow on n vertices we can decide whether it is identified by color refinement in time $O(n^2 \log n)$.

Corollary

If a rainbow is identified by color refinement, then all its fissions are also identified.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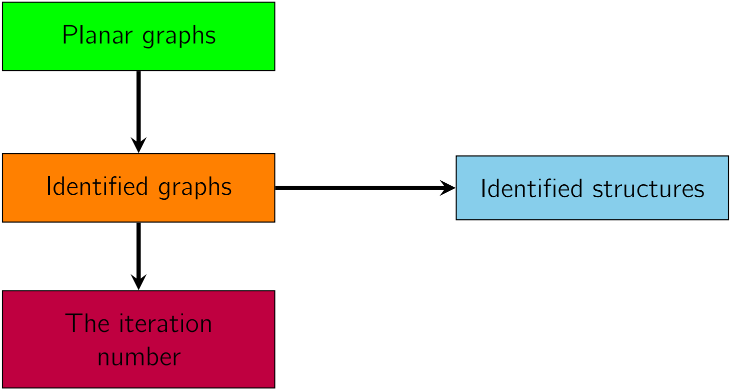
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Iteration number

How many rounds can the WL-process take to stabilize?

- An obvious upper bound is $n^k - 1$.
- For each k, a linear lower bound $\Omega(n)$ is known. [Fürer] (2001)
- For $k > 2$, better lower bounds are known only for relational structures. [Berkholz,Nordström] (2016)

- For $k = 2$ there is an upper bound of $n^2/\log n$. ← now

Upper bound for classical WL iterations

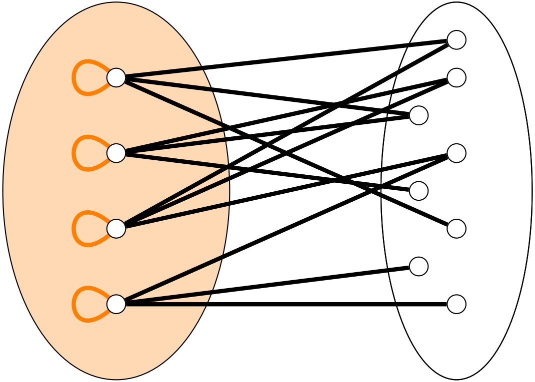
Theorem (Kiefer, S.)

The number of iterations of the 2-dimensional Weisfeiler-Leman algorithm on n-vertex graphs is at most $O(n^2/\log(n))$.

Two step proof:

1. big vertex color classes
2. small vertex color classes

Big color classes



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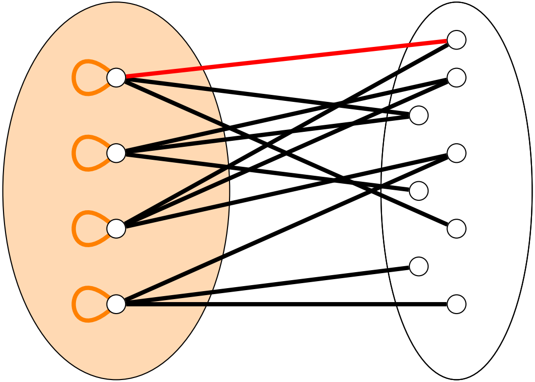

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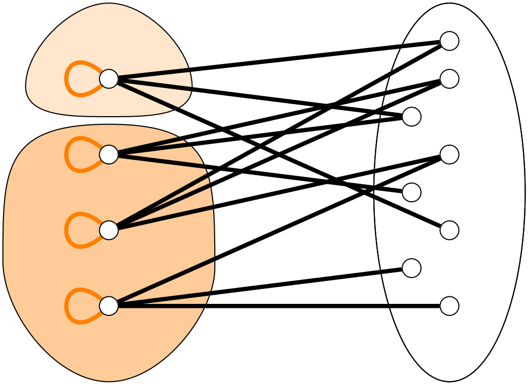

Small color classes

Lemma

For configurations with vertex color class size at most k the number of iterations of the 2-dimensional Weisfeiler-Leman algorithm on n-vertex graphs is at most $2^{O(k)} \cdot n$.

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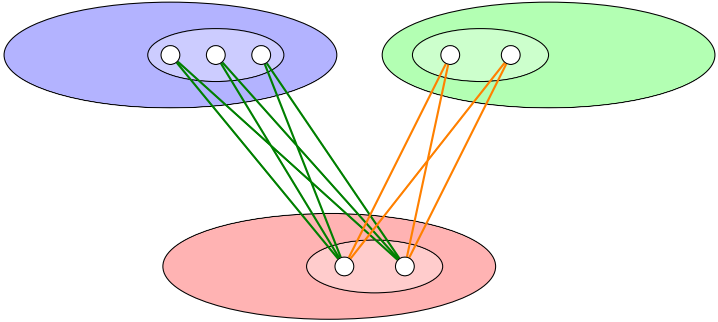

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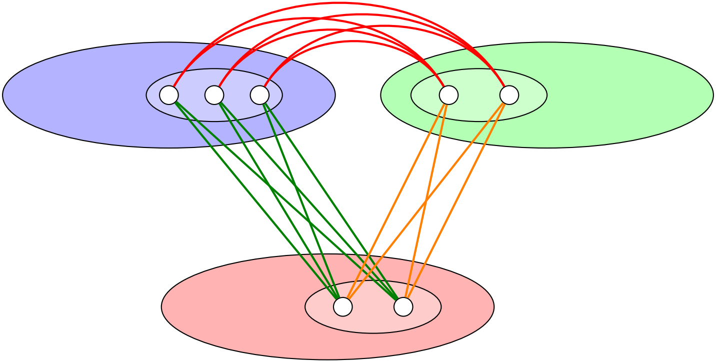

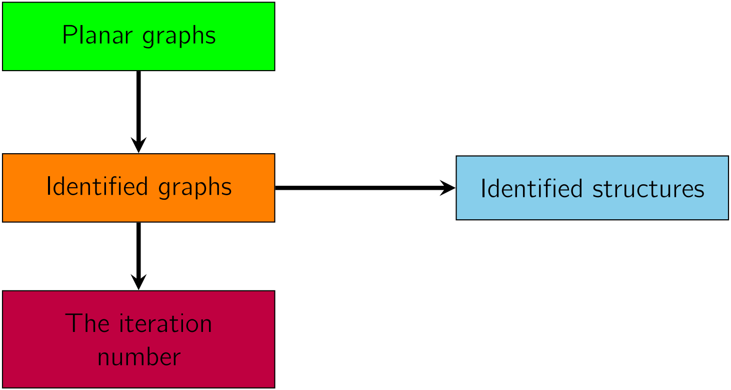

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Prize Money

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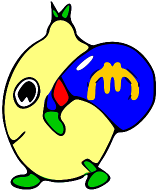
Prize for a proof that $GI \in \mathrm{P}$ or that $GI \notin \mathrm{P}$!



225 Euro

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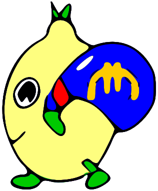

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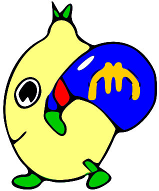
Prize Money

Prize for a proof that $GI \in \mathrm{P}$ or that $GI \notin \mathrm{P}$!



230 Euro