A vintage-style illustration of a bicycle race. In the foreground, several cyclists in various colored jerseys (blue and yellow, green and red, red and white, blue and white striped, yellow) are hunched over their handlebars, racing on a dirt track. To the left, a large crowd of spectators in early 20th-century attire (hats, coats) watches from behind a white picket fence. In the background, a grand, multi-tiered grandstand with arches is visible. On the right, a jockey in a grey suit and brown bowler hat stands with his back to the viewer, looking at a clipboard. The sky is blue with light clouds.

Weisfeiler–Leman and Graph Spectra

SODA 2023

Gaurav Rattan and Tim Seppelt

RWTH Aachen University



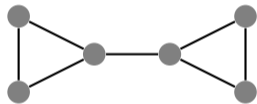
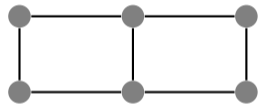
Research Training Group –
Uncertainty and Randomness
in Algorithms, Verification,
and Logic

RWTHAACHEN
UNIVERSITY

DFG

Deutsche
Forschungsgemeinschaft
German Research Foundation

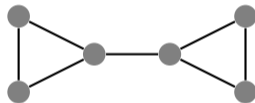
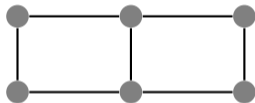
What power does it need to distinguish graphs?



What power does it need to distinguish graphs?

Combinatorial
Algorithms

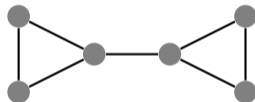
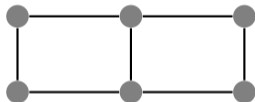
Machine Learning
Architectures



What power does it need to distinguish graphs?

Combinatorial
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Spectral
Properties

Weisfeiler–Leman Algorithm

- ▶ **1-WL** iteratively colours vertices by the colours of their neighbouring vertices.

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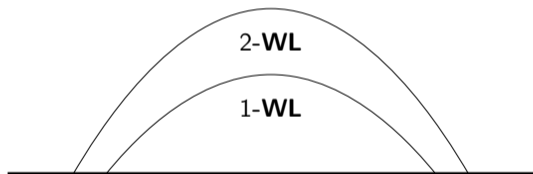
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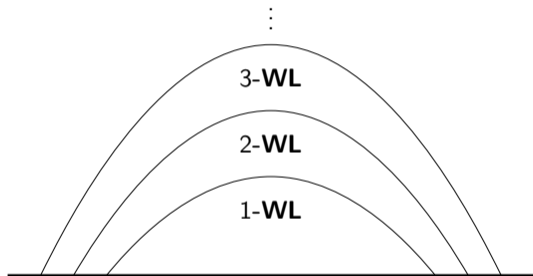
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Weisfeiler–Leman Algorithm

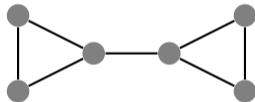
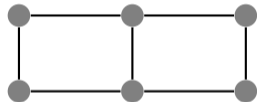
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Weisfeiler–Leman as a yardstick

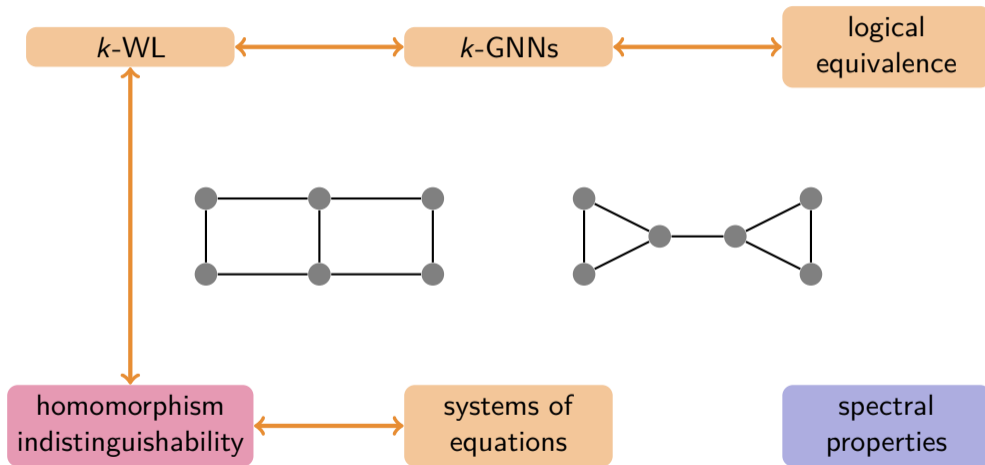
k -WL



spectral
properties

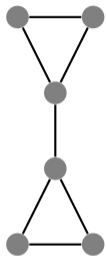
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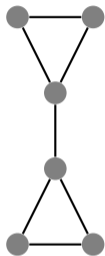
Spectral Graph Properties

Spectral Graph Properties



Graphs

Spectral Graph Properties



$$\begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency Matrix

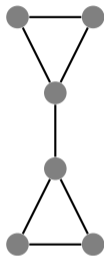
$$\begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{pmatrix}$$

Laplacian Matrix

Graphs

Graph Matrices

Spectral Graph Properties



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Adjacency Matrix

$$\pm\sqrt{3}, 1 \pm \sqrt{2}, \dots$$

Eigenvalues

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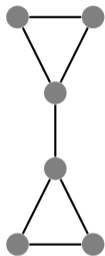
Eigenvectors

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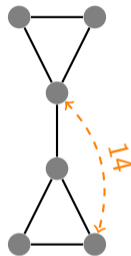
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Eigenvectors



Commute Distances

Graphs

Graph Matrices

Spectral
Properties

Derived Spectral
Properties

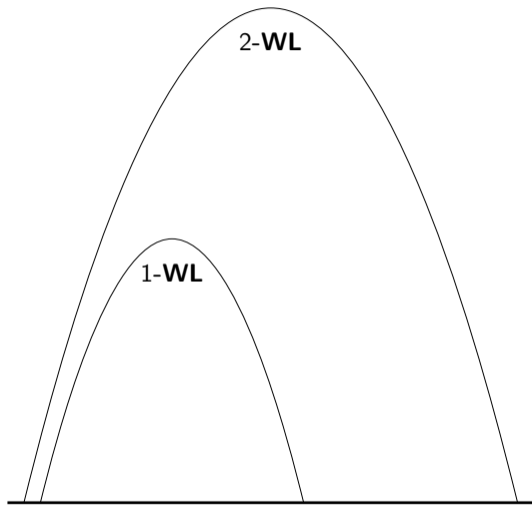
Outline

Central Questions: How does the power of **combinatorial invariants** (k -WL) and **spectral invariants** to distinguish graphs compare?

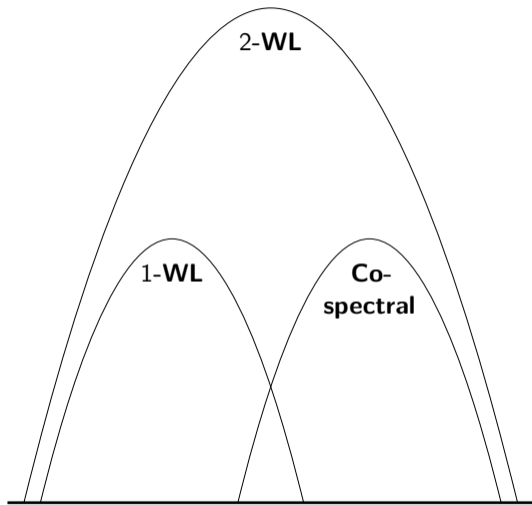
Spectra between 1-WL and 2-WL

Spectra beyond 2-WL

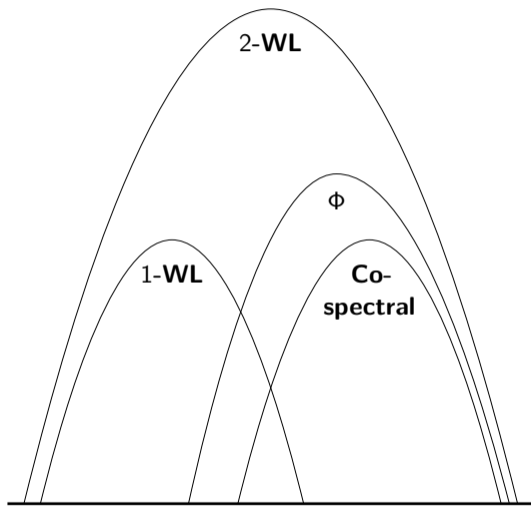
Stronger Spectral Invariants



Stronger Spectral Invariants



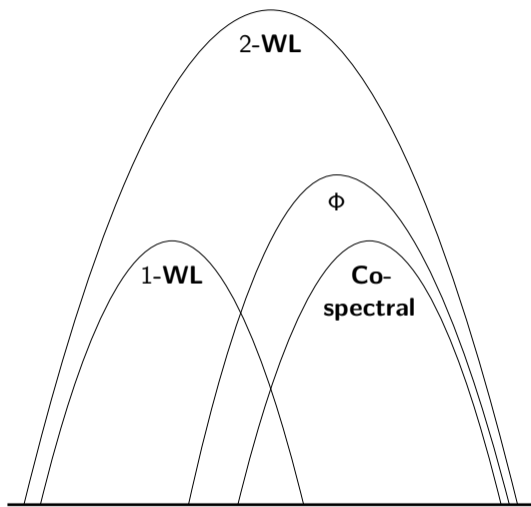
Stronger Spectral Invariants



Definition (Fürer's spectral invariant)

$\Phi(G) := (\text{Spec } A(G), \{\{P_v \mid v \in V(G)\}\})$
where $P_v := (p_{vv}, \{\{p_{vw} \mid w \in V(G)\}\})$
aggregates entries of projections onto
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Stronger Spectral Invariants



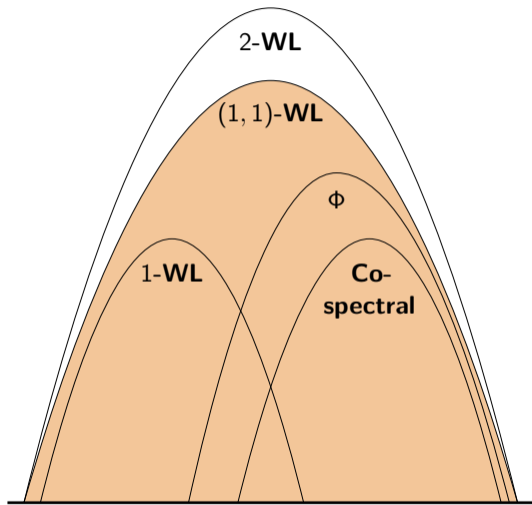
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Is Φ as strong as 2-WL?

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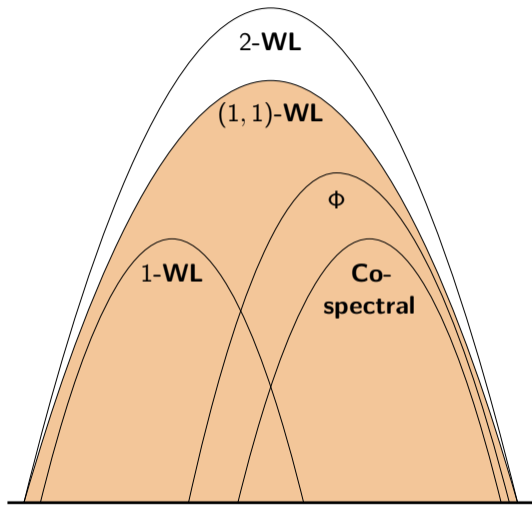
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Theorem

*If G and H are (1,1)-WL indistinguishable
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Question (Fürer (2010))

Is Φ as strong as 2-WL? **No!**

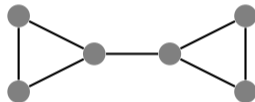
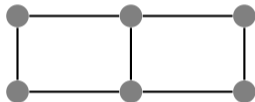
Theorem

If G and H are (1,1)-WL indistinguishable
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Hence, Φ is strictly weaker than 2-WL.

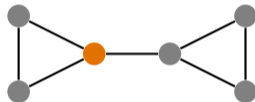
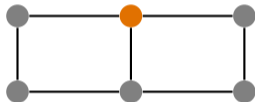
(1, 1)-WL

Comparing vertex-individualised copies using 1-WL.



(1, 1)-WL

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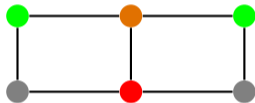
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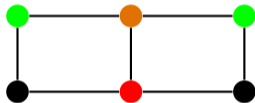
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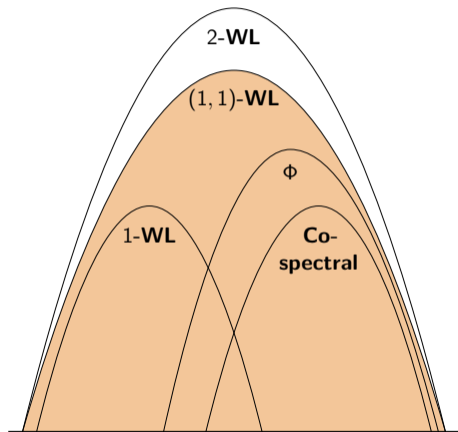
Comparing vertex-individualised copies using 1-WL.



Two graphs G and H are **(1, 1)-WL indistinguishable** if there is a bijection $\pi: V(G) \rightarrow V(H)$ such that the vertex-individualised copies G_v and $H_{\pi(v)}$ are 1-WL indistinguishable for all $v \in V(G)$.

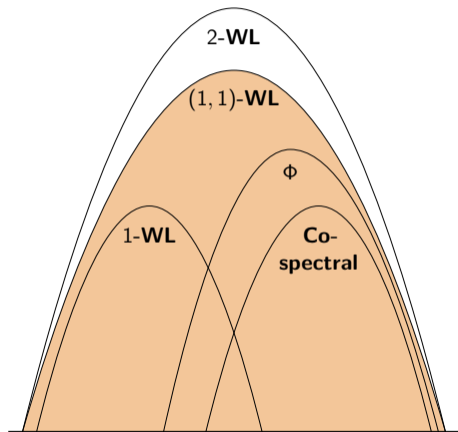
(1, 1)-WL

- ▶ strictly between **1-WL** and **2-WL** w.r.t. distinguishing power



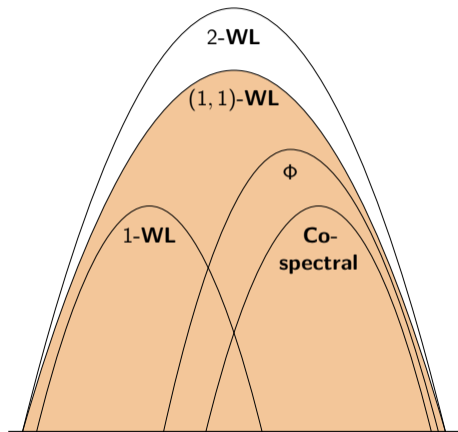
(1, 1)-WL

- ▶ strictly between **1-WL** and **2-WL** w.r.t. distinguishing power
- ▶ linear space complexity outperforming **2-WL**'s quadratic space complexity



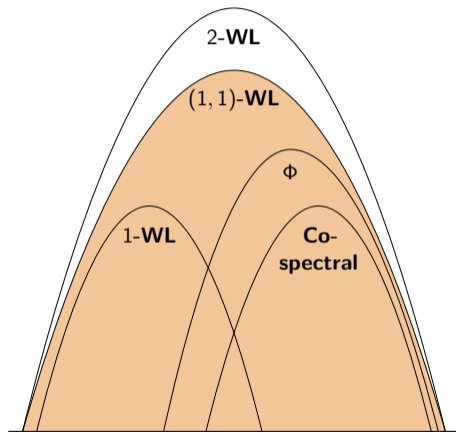
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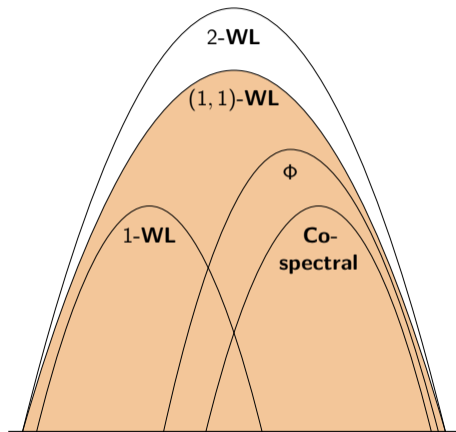
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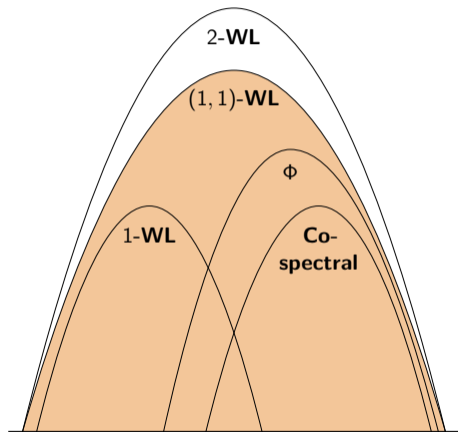
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 - ▶ have cospectral adjacency, Laplacian, etc. matrices, agree in Fürer's spectral invariant answers question of Fürer (2010) negatively
 - ▶ same multiset of commute distances, strengthens a result of Godsil (1981)
- ▶ augmenting 1-WL with spectral information does not allow to supersede (1, 1)-WL



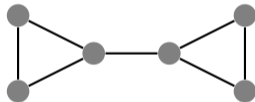
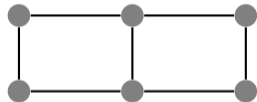
What power does it need to distinguish graphs?

Weisfeiler–Leman as a yardstick

d iterations
of k -WL



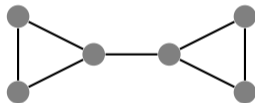
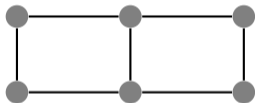
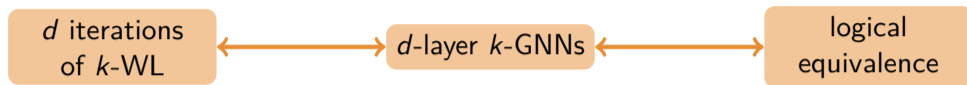
d -layer k -GNNs



spectral
properties

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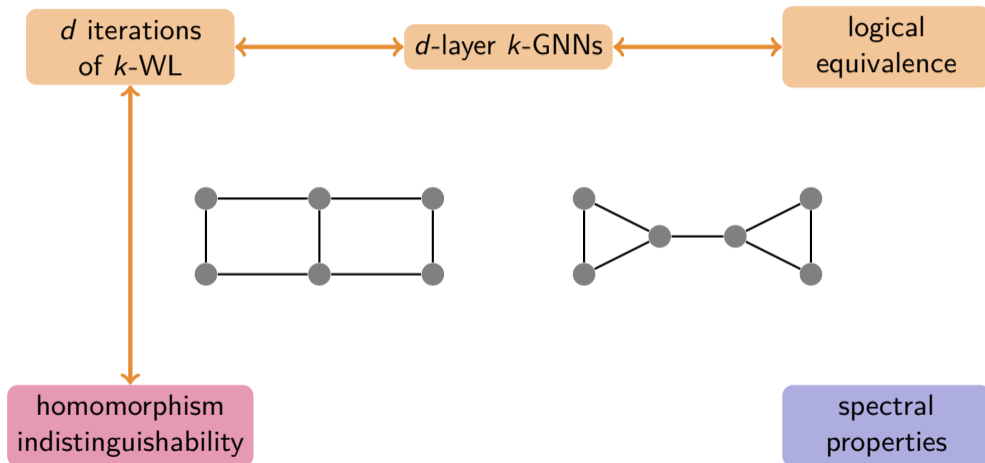
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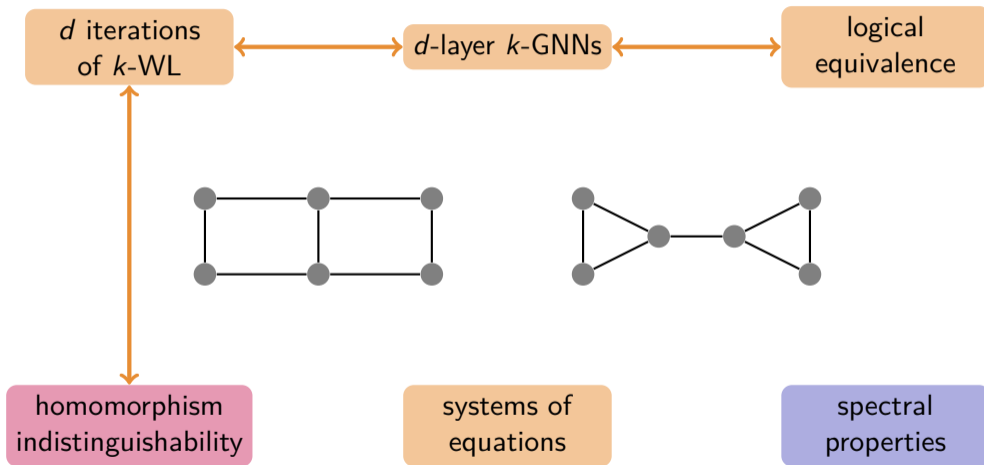
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Spectra for k -WL after d iterations

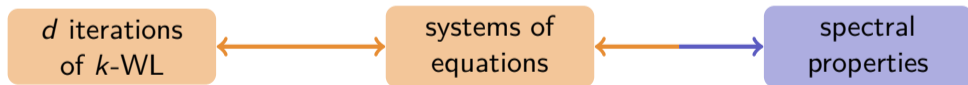
Spectra for k -WL after d iterations

d iterations
of k -WL

systems of
equations

spectral
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Spectra for k -WL after d iterations



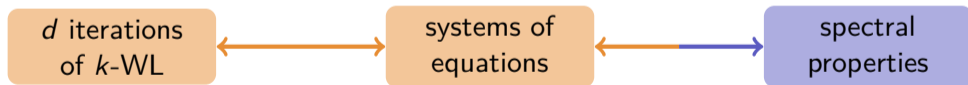
Spectra for k -WL after d iterations

Theorem

For graphs G and H and $k \geq 1$, $d \geq 0$, the following are equivalent:

1. G and H are *not distinguished by k -WL after d iterations*,
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$$X\mathbf{A}_G = \mathbf{A}_H X \quad \text{for all } \mathbf{A} \in \mathcal{A}_{k,d}.$$



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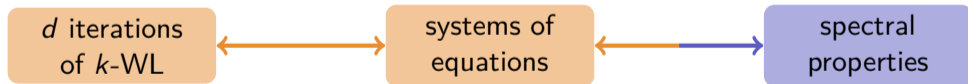
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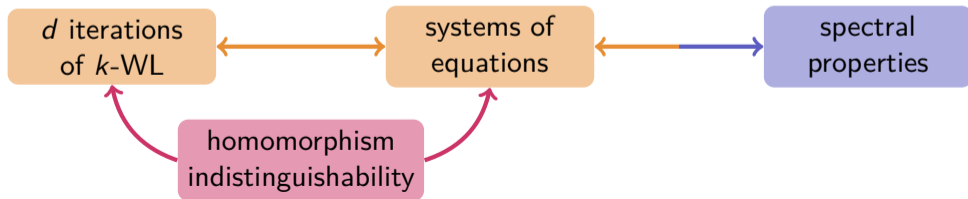
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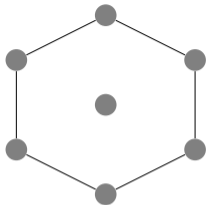
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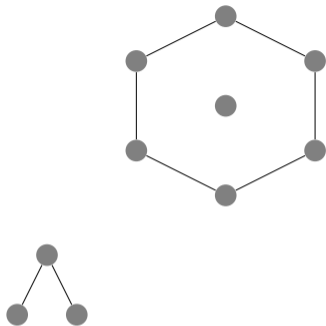
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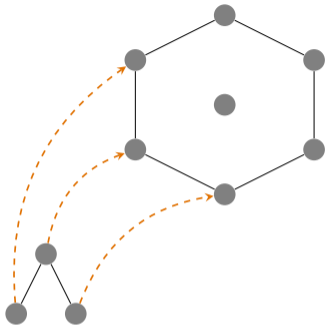
Homomorphism Indistinguishability



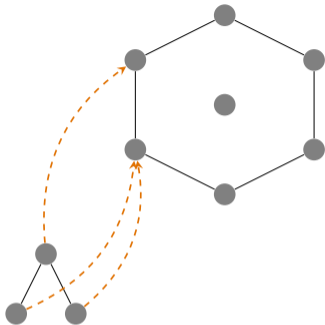
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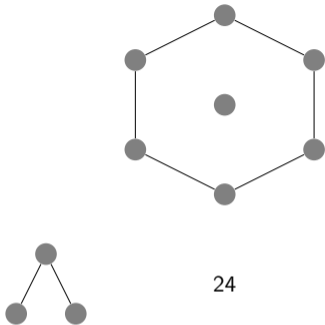
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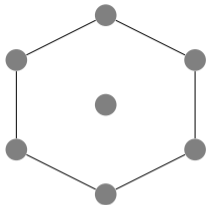
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Homomorphism Indistinguishability



Homomorphism Indistinguishability

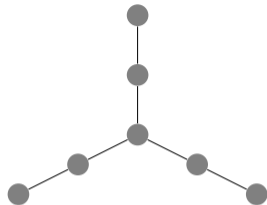
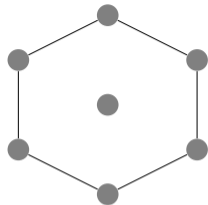


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Homomorphism Indistinguishability



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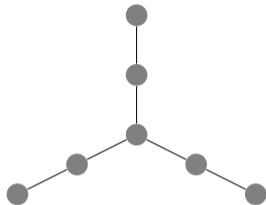
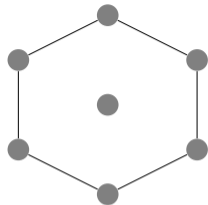
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Homomorphism Indistinguishability



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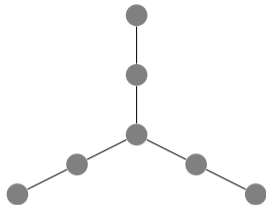
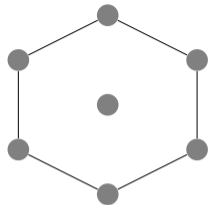


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Homomorphism Indistinguishability



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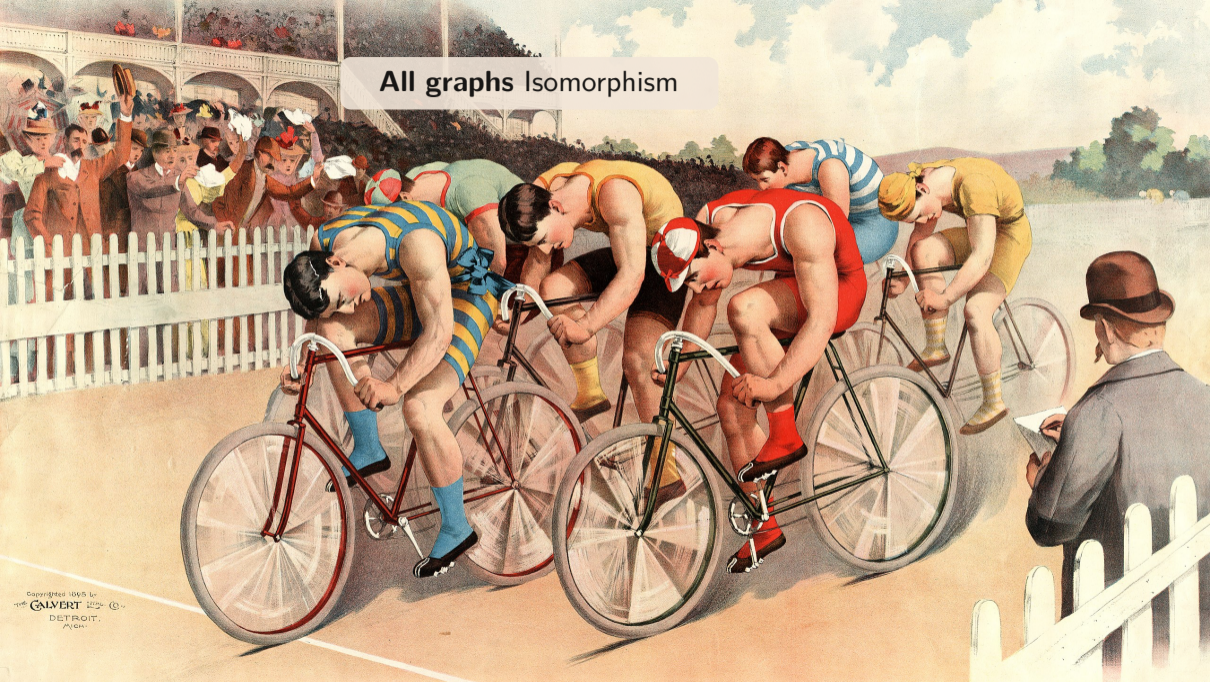
36

The graphs  and  are **homomorphism indistinguishable** over $\left\{ \begin{array}{c} \text{---} \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \end{array} , \begin{array}{c} \bullet \quad \bullet \\ \text{---} \\ \bullet \quad \bullet \end{array} \right\}$.



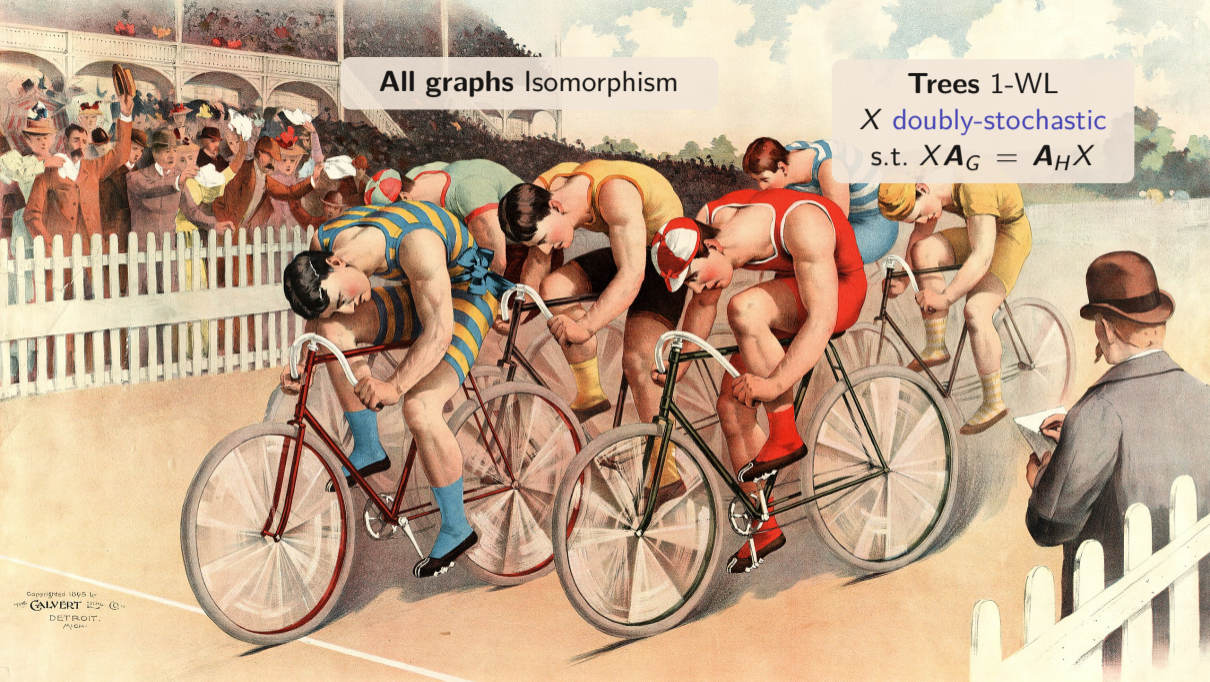
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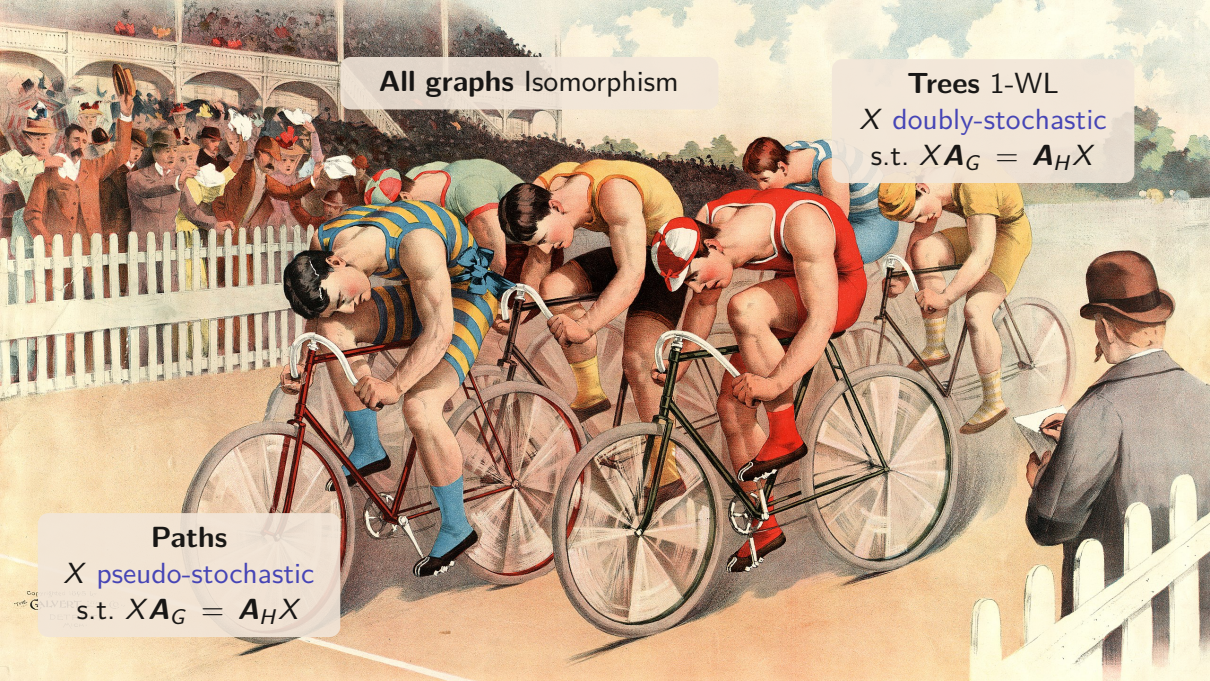
All graphs Isomorphism



All graphs Isomorphism

Trees 1-WL
 X doubly-stochastic
s.t. $XA_G = A_HX$

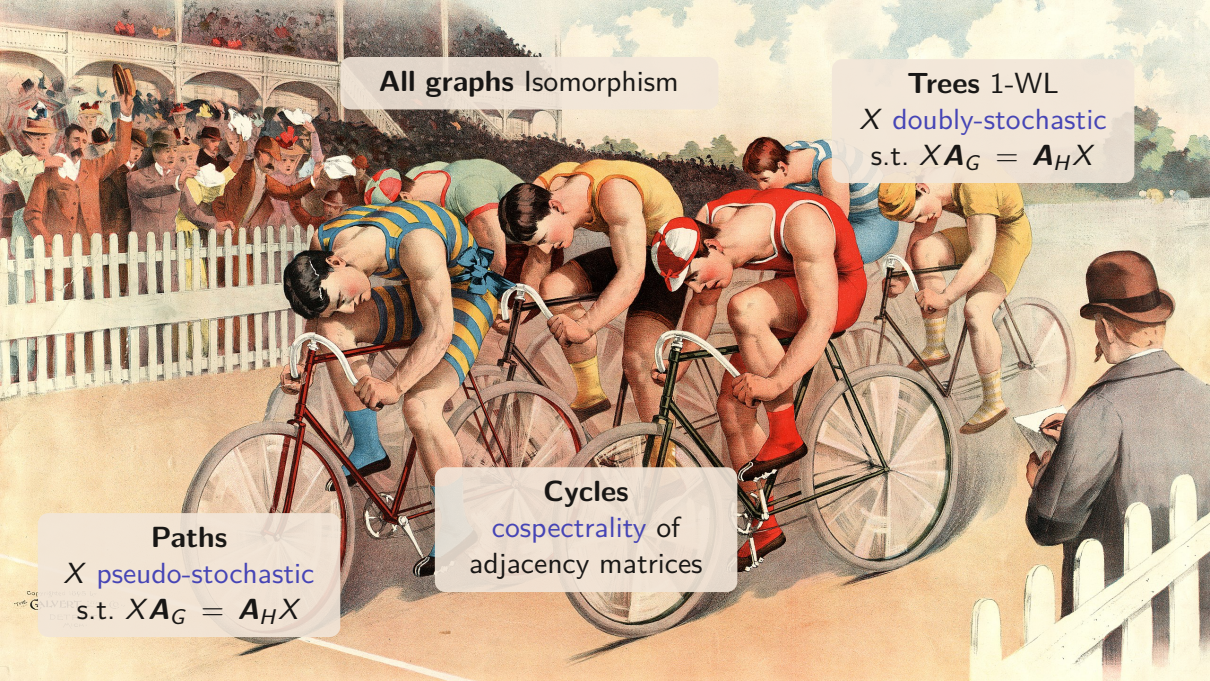


A vintage illustration of a bicycle race. Several cyclists in colorful, form-fitting suits are racing on a dirt track. In the background, a large crowd of spectators in early 20th-century attire watches from a grandstand. A jockey in a grey suit and brown hat is visible on the right, holding a clipboard. The scene is set outdoors under a blue sky with light clouds.

All graphs Isomorphism

Trees 1-WL
 X doubly-stochastic
s.t. $XA_G = A_HX$

Paths
 X pseudo-stochastic
s.t. $XA_G = A_HX$

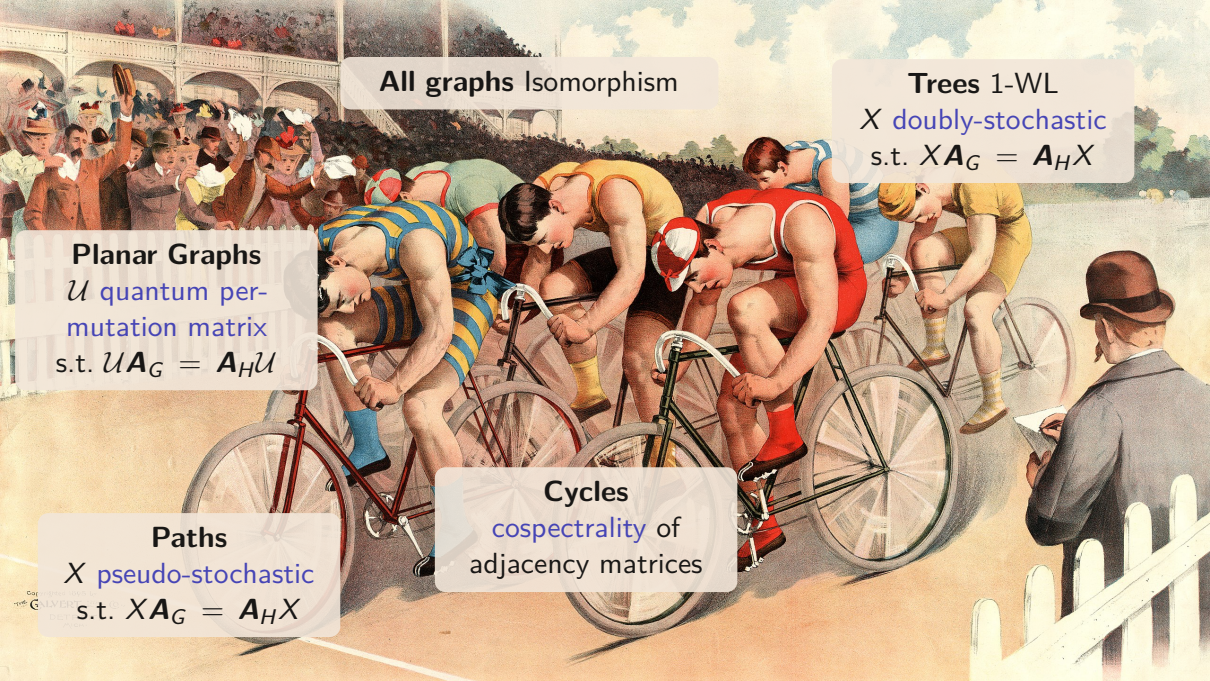
A vintage illustration of a bicycle race. Several cyclists in colorful, form-fitting suits are racing on a dirt track. In the background, a large crowd of spectators in early 20th-century attire watches from behind a white picket fence. A jockey in a grey suit and brown hat is visible on the right side of the track, looking towards the race. The scene is set outdoors under a blue sky with light clouds.

All graphs Isomorphism

Trees 1-WL
 X doubly-stochastic
s.t. $XA_G = A_HX$

Paths
 X pseudo-stochastic
s.t. $XA_G = A_HX$

Cycles
cospectrality of
adjacency matrices

A vintage illustration of a bicycle race. Several cyclists in colorful, form-fitting suits are racing on a dirt track. A crowd of spectators in early 20th-century attire is visible in the background, some waving. In the foreground, a jockey in a grey suit and brown hat is writing on a clipboard. The scene is set outdoors under a blue sky with light clouds.

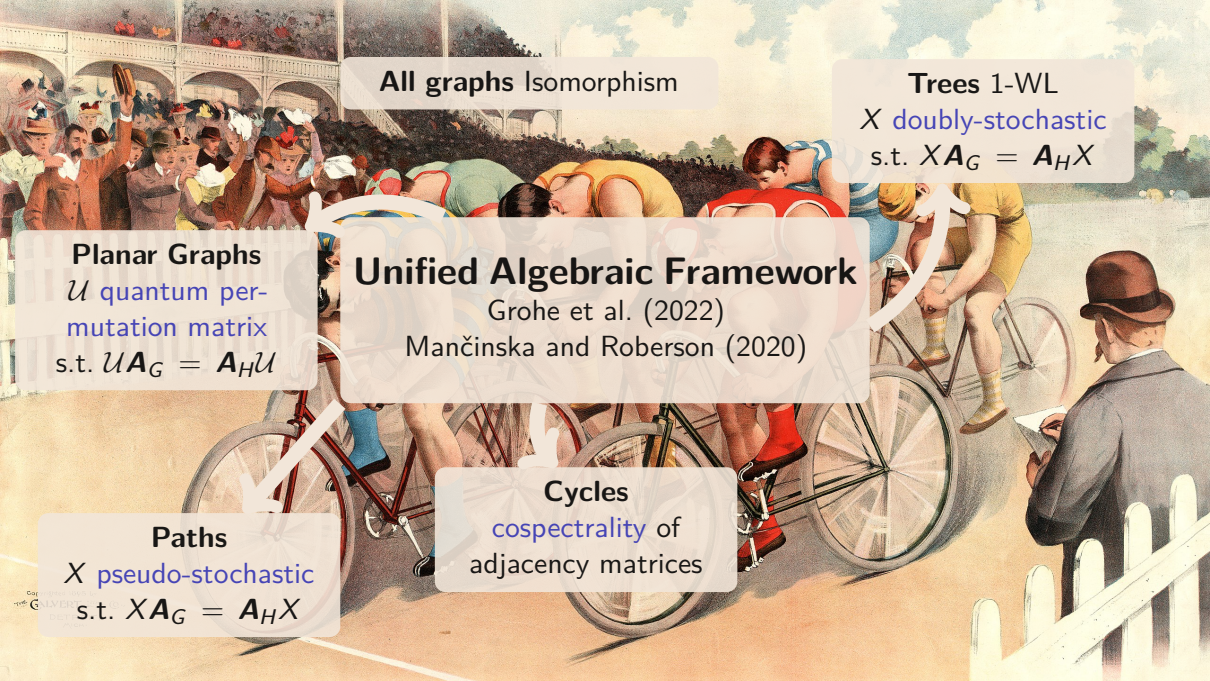
All graphs Isomorphism

Trees 1-WL
 X doubly-stochastic
s.t. $XA_G = A_HX$

Planar Graphs
 U quantum per-
mutation matrix
s.t. $UA_G = A_HU$

Cycles
cospectrality of
adjacency matrices

Paths
 X pseudo-stochastic
s.t. $XA_G = A_HX$

A vintage painting of a bicycle race. In the foreground, several cyclists in colorful jerseys (yellow, red, blue, green) are hunched over their handlebars, racing on a dirt track. A jockey in a grey suit and brown hat stands on the right, holding a clipboard and looking towards the race. In the background, a large crowd of spectators in period clothing watches from a raised platform. The scene is set outdoors under a blue sky with light clouds.

All graphs Isomorphism

Trees 1-WL
 X doubly-stochastic
s.t. $XA_G = A_HX$

Planar Graphs
 \mathcal{U} quantum permutation matrix
s.t. $\mathcal{U}A_G = A_H\mathcal{U}$

Unified Algebraic Framework

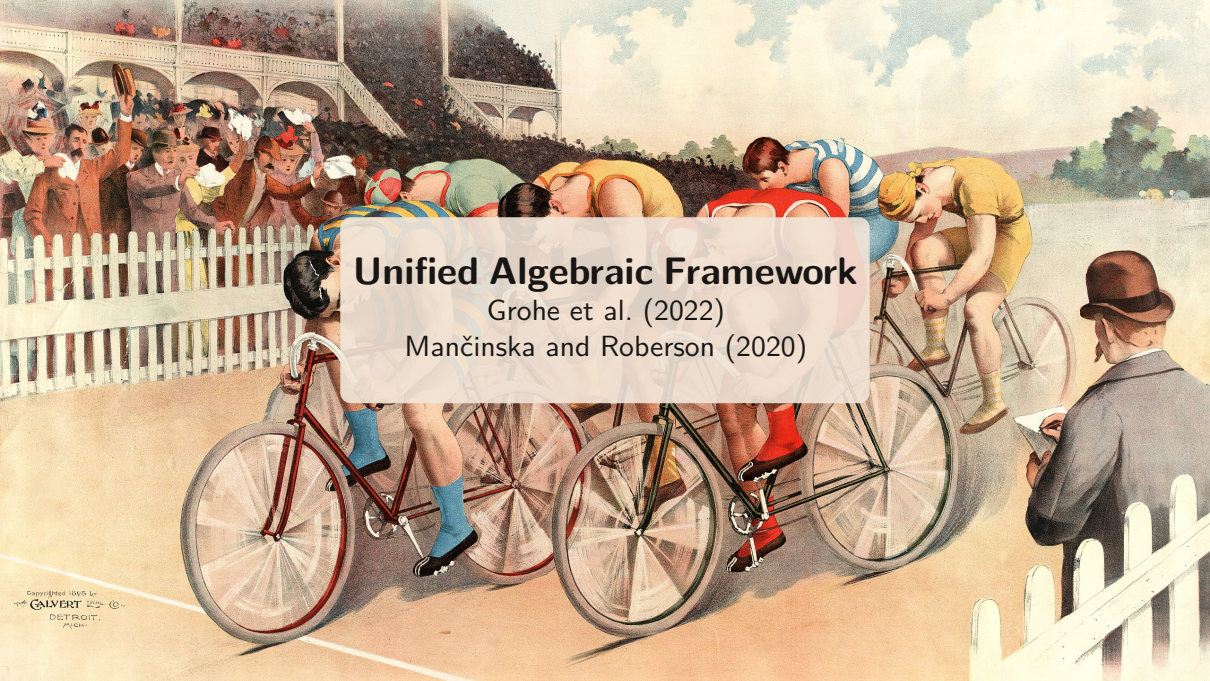
Grohe et al. (2022)

Mančinska and Roberson (2020)

Cycles

cospectrality of
adjacency matrices

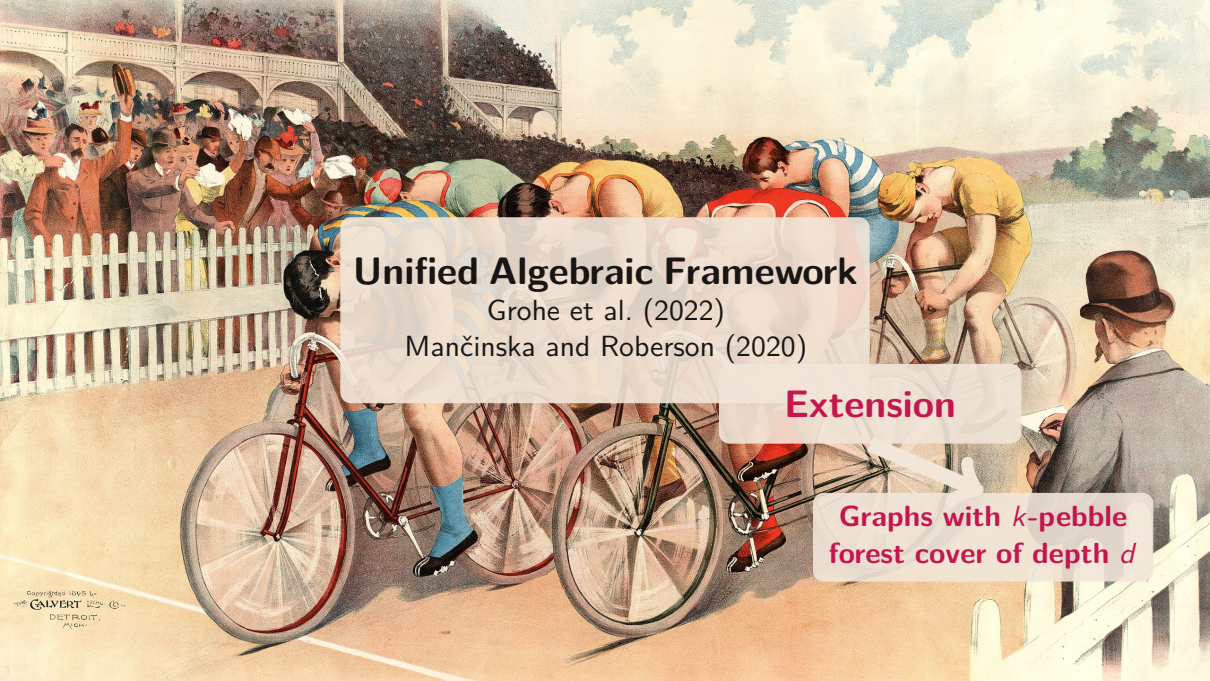
Paths
 X pseudo-stochastic
s.t. $XA_G = A_HX$

A vintage-style illustration of a bicycle race. Several cyclists in various colored jerseys (blue and white stripes, yellow, red, green) are leaning forward on their bikes, racing on a dirt track. A large crowd of spectators in early 20th-century attire is gathered behind a white picket fence on the left, watching the race. In the foreground on the right, a man in a grey suit and a brown bowler hat is seen from the back, looking at a clipboard. The background shows a large, ornate grandstand with multiple tiers and arches, filled with more spectators. The sky is bright with some clouds. A semi-transparent white box with black text is overlaid in the center of the image.

Unified Algebraic Framework

Grohe et al. (2022)

Mančinska and Roberson (2020)

A vintage-style illustration of a bicycle race. In the foreground, several cyclists are hunched over their handlebars, racing on a dirt track. They are wearing colorful, form-fitting cycling gear. To the left, a large crowd of spectators, including men in suits and hats and women in elaborate dresses and hats, watches from behind a white picket fence. In the background, a grand, multi-tiered grandstand with arches is visible. On the right side, a jockey in a brown suit and hat sits on a bicycle, looking towards the race. The overall scene is set in a bright, sunny outdoor environment.

Unified Algebraic Framework

Grohe et al. (2022)

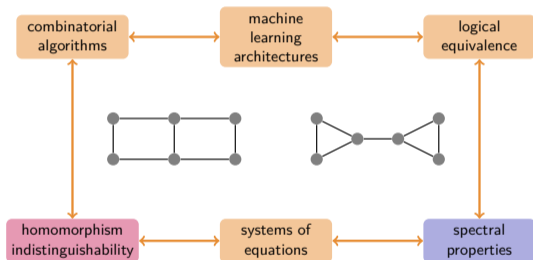
Mančinska and Roberson (2020)

Extension

**Graphs with k -pebble
forest cover of depth d**

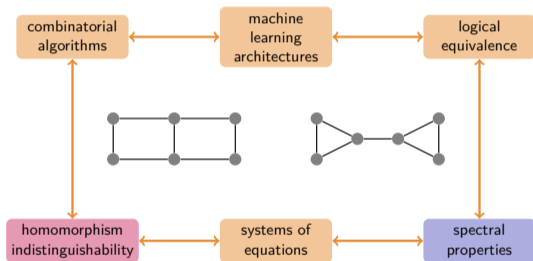
Conclusion

- ▶ we mapped out the relationship between **combinatorial algorithms** and **spectral graph properties**



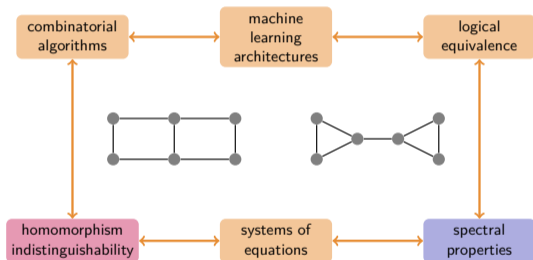
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 - ▶ classical **spectral graph properties** between **1-WL** and **2-WL**,



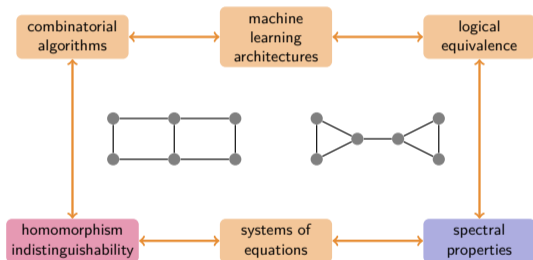
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 - ▶ classical **spectral graph properties** between **1-WL** and **2-WL**,
 - ▶ novel **spectral characterisations** for **k -WL** after d iterations.



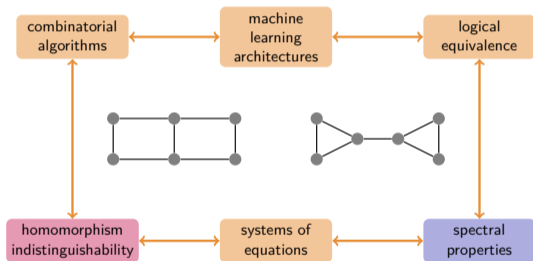
Conclusion

- ▶ we mapped out the relationship between **combinatorial algorithms** and **spectral graph properties**
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- ▶ we introduced **(1, 1)-WL**, a linear space algorithm, separating **1-WL** plus **spectra** from **2-WL**.



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- ▶ we introduced **(1, 1)-WL**, a linear space algorithm, separating **1-WL** plus **spectra** from **2-WL**.
- ▶ we contributed algebraic tools for constructing systems of equations for **homomorphism indistinguishability**.



Bibliography I

- Fürer, M. (2010). On the power of combinatorial and spectral invariants. *Linear Algebra and its Applications*, 432(9):2373–2380.
- Godsil, C. D. (1981). Equiarboreal graphs. *Combinatorica*, 1(2):163–167.
- Grohe, M., Rattan, G., and Seppelt, T. (2022). Homomorphism Tensors and Linear Equations. In Bojańczyk, M., Merelli, E., and Woodruff, D. P., editors, *49th International Colloquium on Automata, Languages, and Programming, ICALP 2022, July 4-8, 2022, Paris, France*, volume 229 of *LIPICs*. Schloss Dagstuhl - Leibniz-Zentrum für Informatik.
- Lovász, L. (1967). Operations with structures. *Acta Mathematica Academiae Scientiarum Hungarica*, 18(3):321–328.
- Mančinska, L. and Roberson, D. E. (2020). Quantum isomorphism is equivalent to equality of homomorphism counts from planar graphs. In *2020 IEEE 61st Annual Symposium on Foundations of Computer Science (FOCS)*, pages 661–672.
- Picture: “Bicycle race scene. A peloton of six cyclists crosses the finish line in front of a crowded grandstand, observed by a referee.” (1895) by Calvert Lithographic Co., Detroit, Michigan, Public Domain, via Wikimedia Commons.
- https://commons.wikimedia.org/wiki/File:Bicycle_race_scene,_1895.jpg