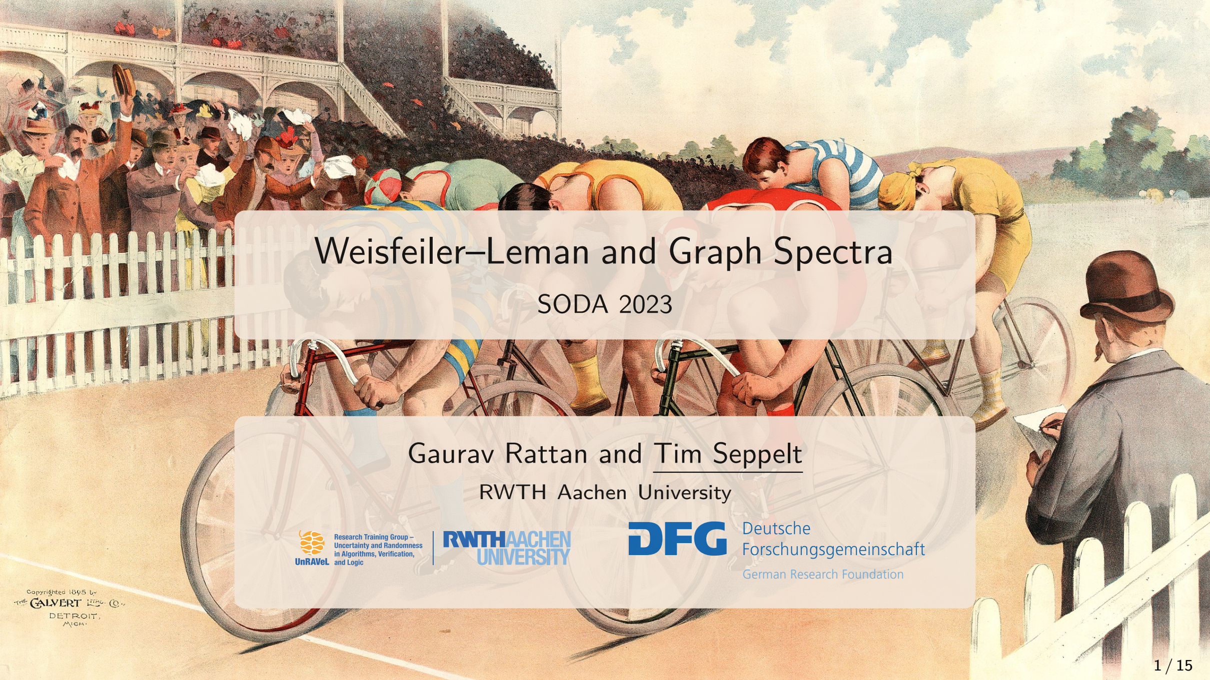

Weisfeiler–Leman and Graph Spectra

SODA 2023

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RWTH Aachen University

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

RWTH AACHEN UNIVERSITY

DFG Deutsche Forschungsgemeinschaft
German Research Foundation

What power does it need to distinguish graphs?

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Combinatorial Algorithms

Machine Learning Architectures

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Combinatorial Algorithms

Machine Learning Architectures

Spectral Properties

Weisfeiler–Leman Algorithm

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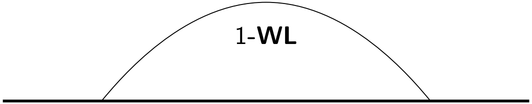

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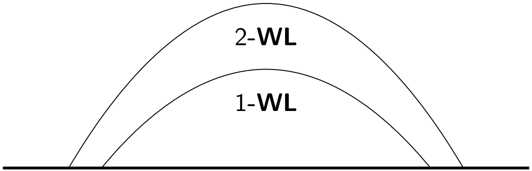

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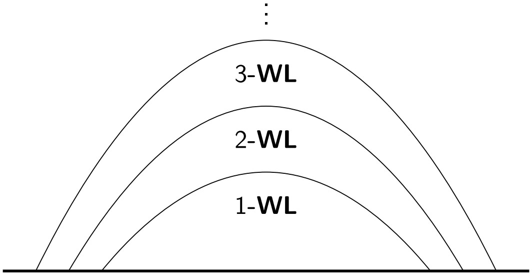

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Weisfeiler–Leman as a yardstick

k-WL

spectral properties

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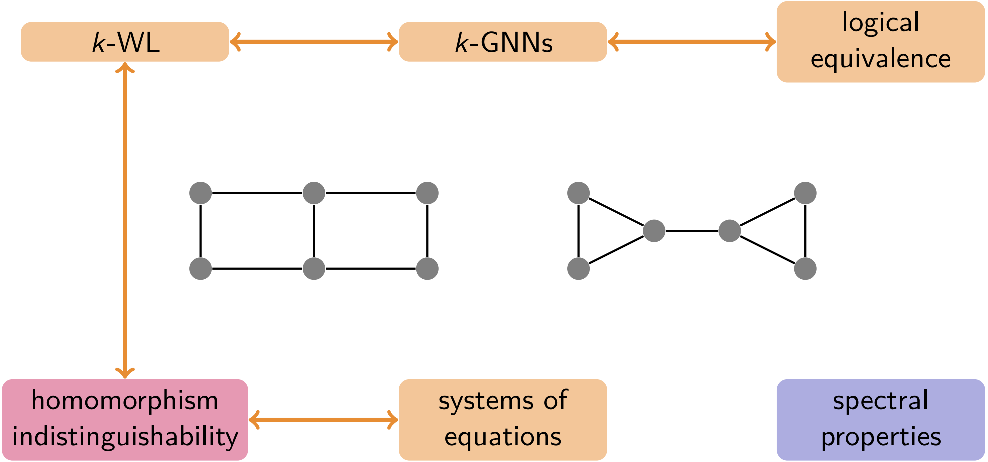

Spectral Graph Properties

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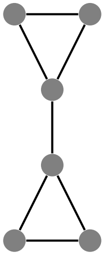
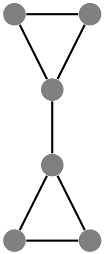


Graphs

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

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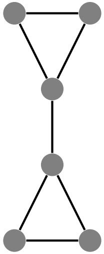
Laplacian Matrix

Graphs → Graph Matrices

Spectral Graph Properties



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Adjacency Matrix

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

Eigenvalues

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

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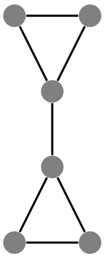
Eigenvectors

Graphs → Graph Matrices → Spectral Properties

Spectral Graph Properties



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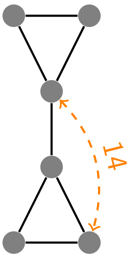


Commute Distances

Graphs → Graph Matrices → Spectral Properties → Derived Spectral Properties

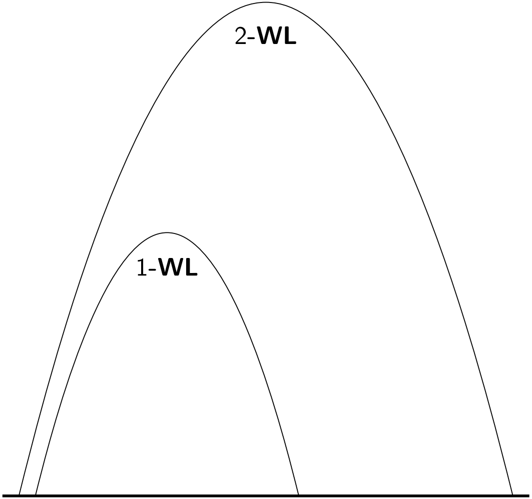
Outline

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

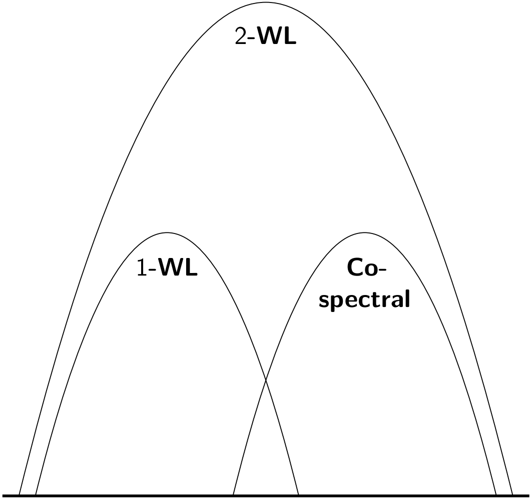
Spectra between 1-WL and 2-WL

Spectra beyond 2-WL

Stronger Spectral Invariants



Stronger Spectral Invariants



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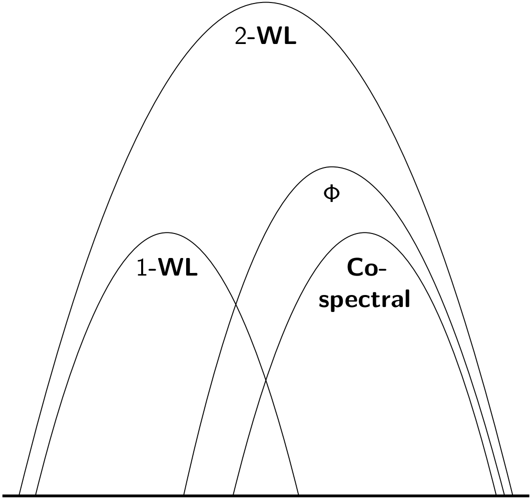

Definition (Fürer's spectral invariant)

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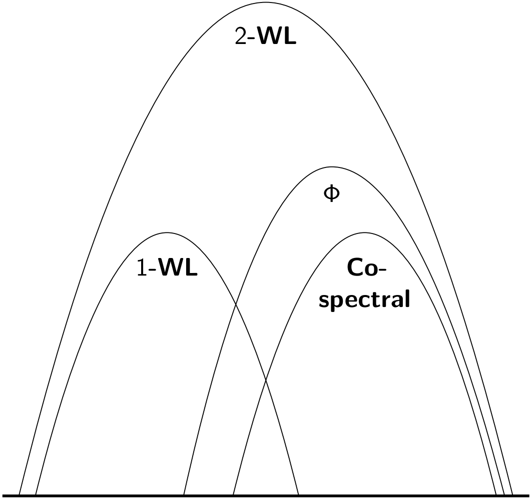

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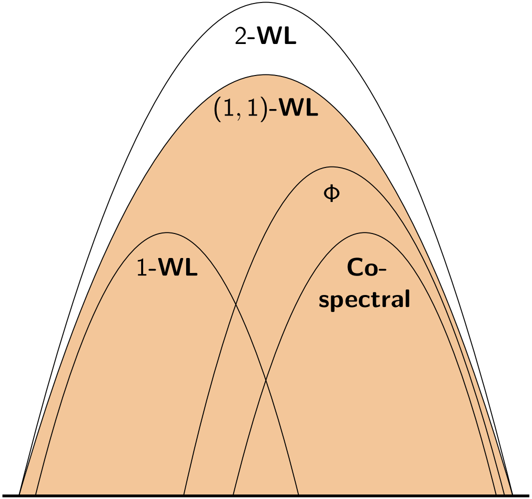
Question (Fürer (2010))

Is Φ as strong as 2-WL?

Stronger Spectral Invariants



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If G and H are (1, 1)-WL indistinguishable then $\Phi(G) = \Phi(H)$.

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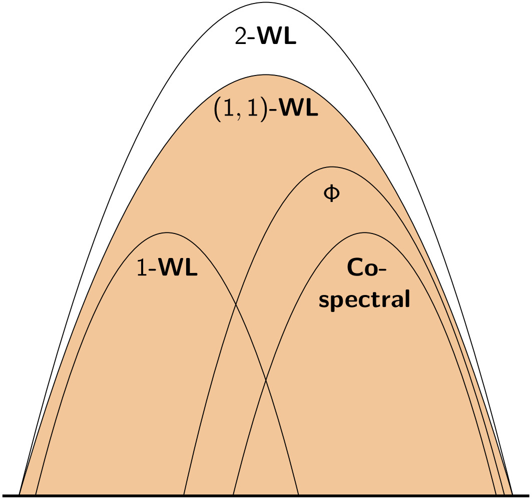

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Question (Fürer (2010))

Is Φ as strong as 2-WL? **No!**

Theorem

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

$(1,1)$-WL

Comparing vertex-individualised copies using 1-WL.

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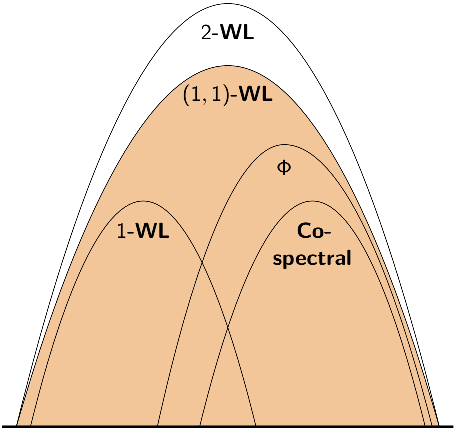
Two graphs G and H are $(1,1)$-WL indistinguishable if there is a bijection $\pi \colon V(G) \to V(H)$ such that the vertex-individualised copies G_v and $H_{\pi(v)}$ are 1-WL indistinguishable for all $v \in V(G)$.

$(1, 1)$-WL

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



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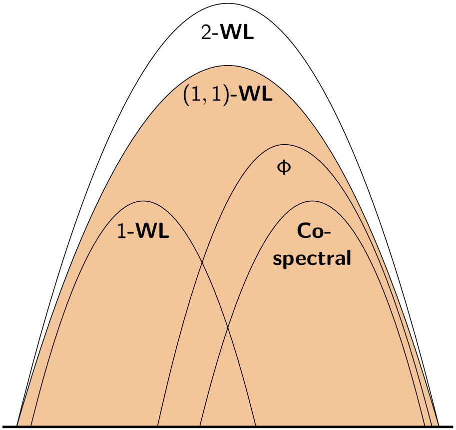

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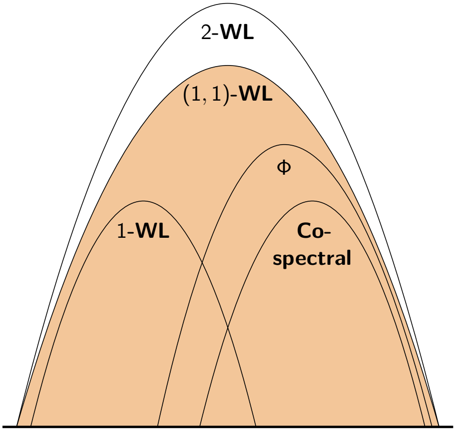

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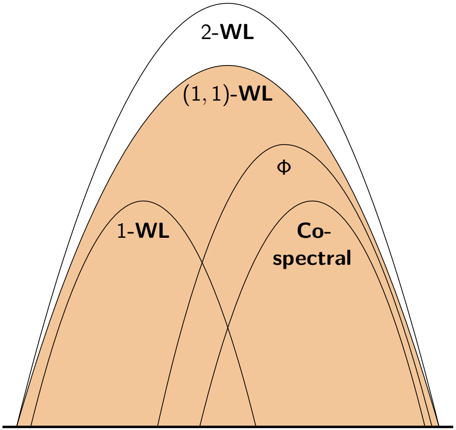

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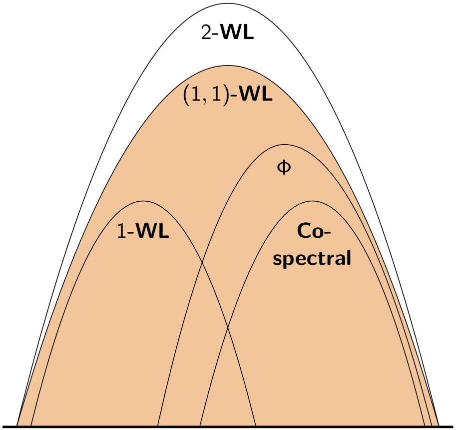

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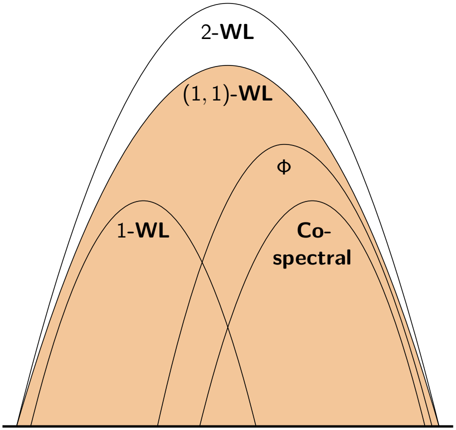
  - same multiset of commute distances, strengthens a result of Godsil (1981)
- augmenting 1-WL with spectral information does not allow to supersede $(1, 1)$-WL



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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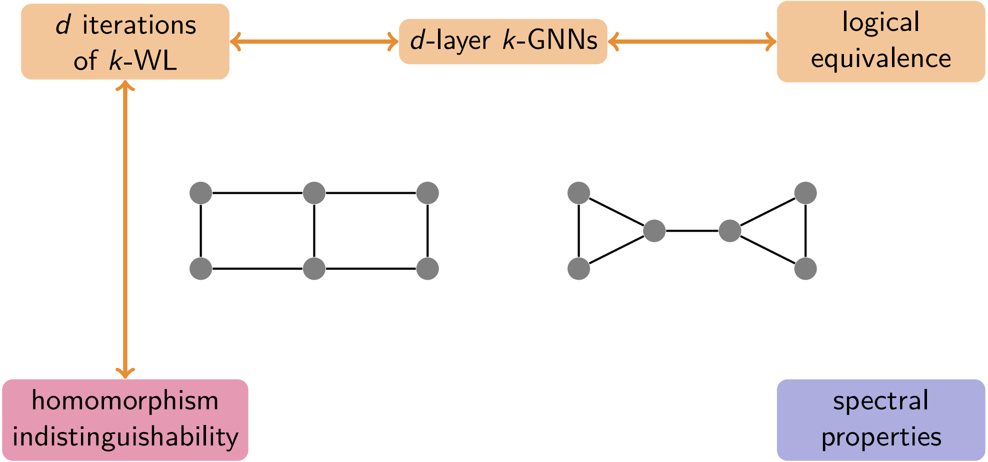

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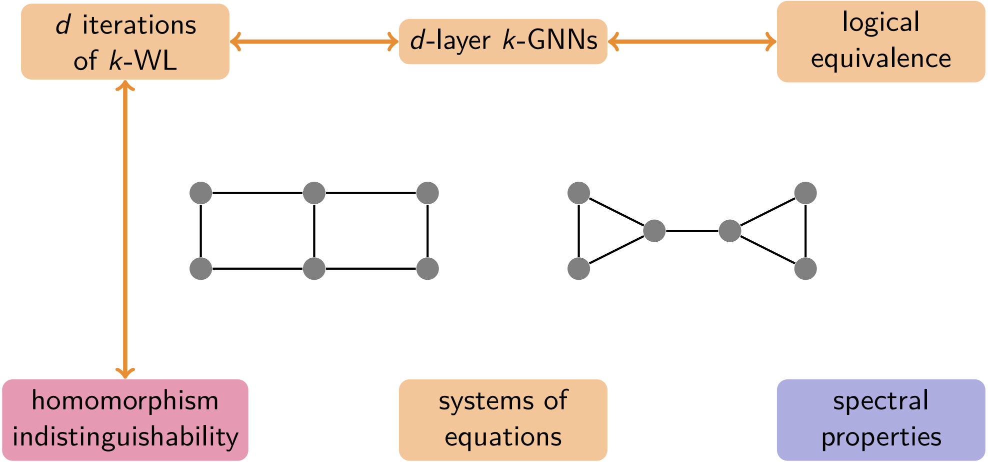


Spectra for k-WL after d iterations

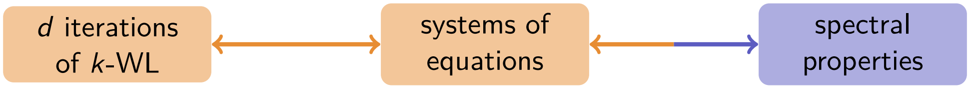
Spectra for k-WL after d iterations

d iterations of k-WL

systems of equations

spectral properties

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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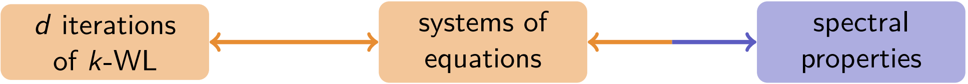
$$X\boldsymbol{A}_G = \boldsymbol{A}_H X \quad \text{for all } \boldsymbol{A} \in \mathcal{A}_{k,d}.$$



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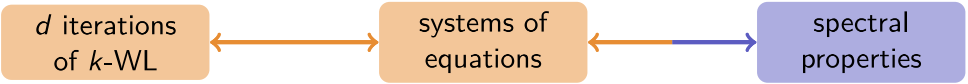

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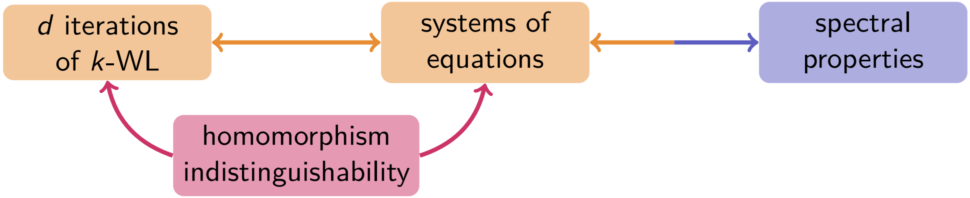
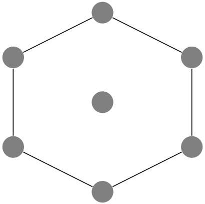


Homomorphism Indistinguishability



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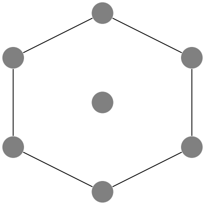

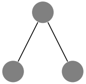

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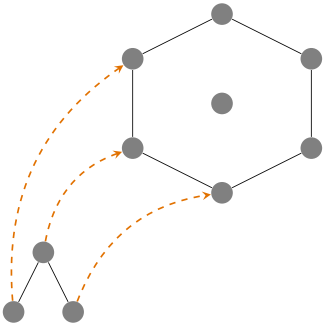

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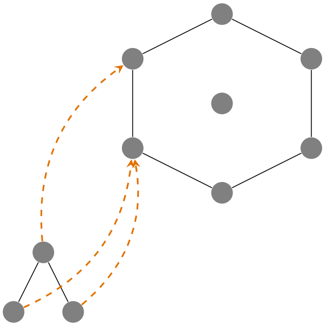

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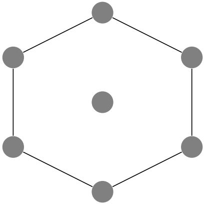

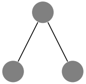

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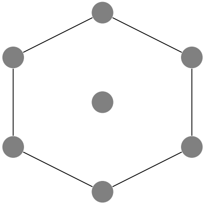
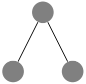
Homomorphism Indistinguishability





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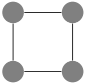

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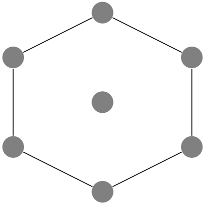
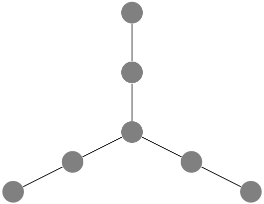
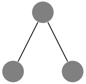
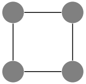
Homomorphism Indistinguishability

		
	24	24
	36	36

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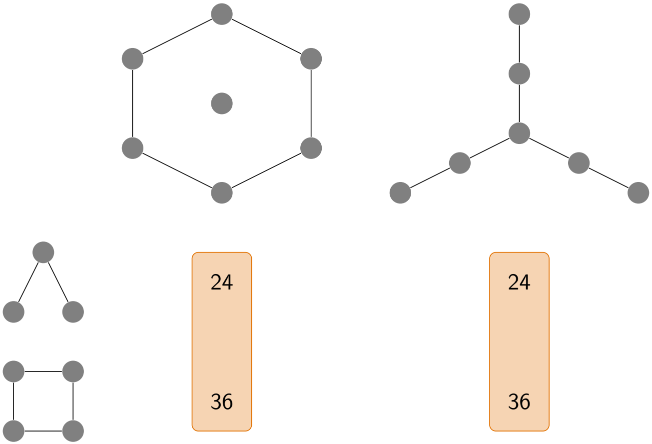
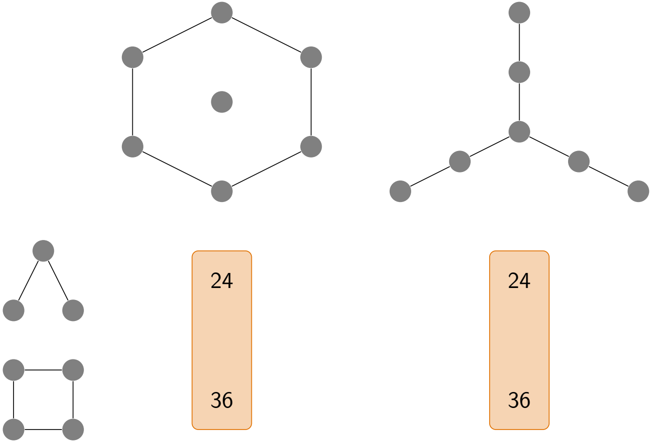
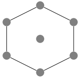
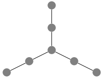


Homomorphism Indistinguishability



The graphs  and  are **homomorphism indistinguishable** over {, }.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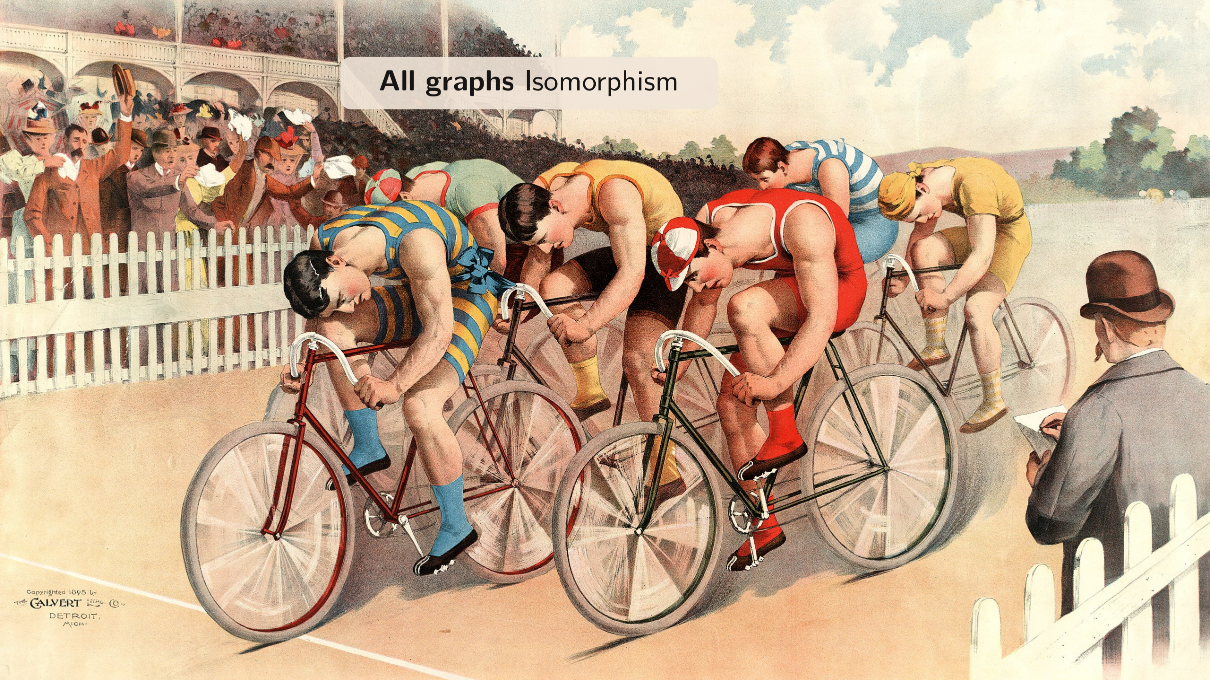
MICH.

All graphs Isomorphism

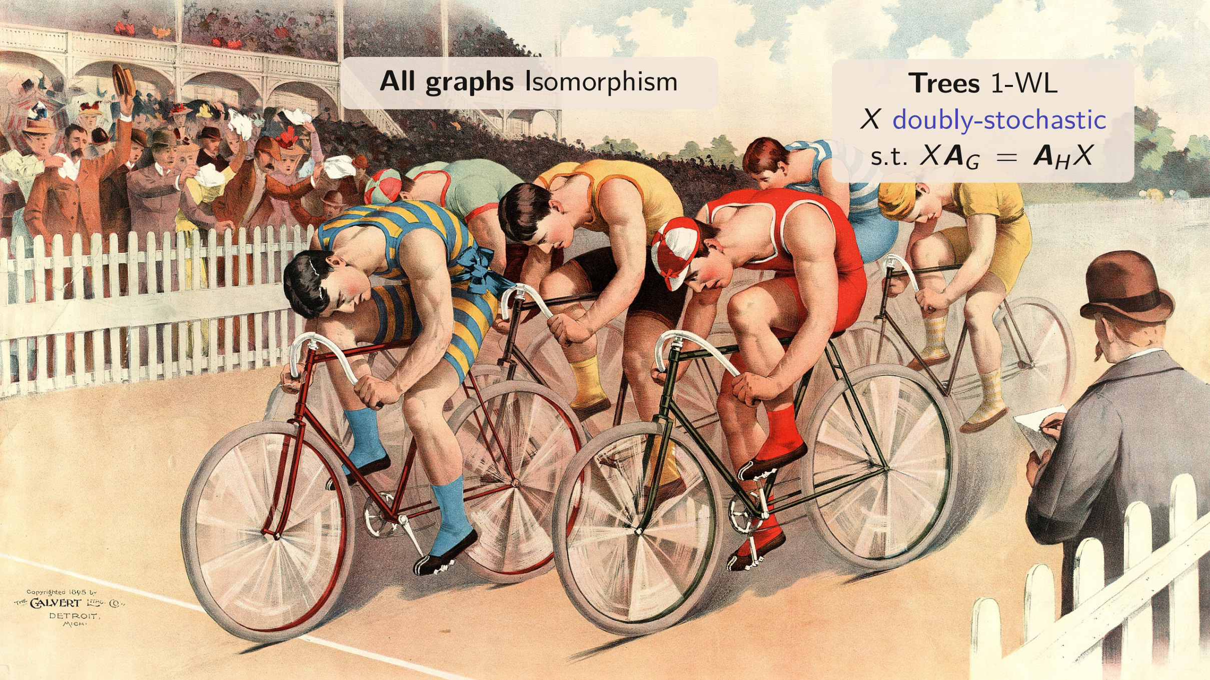


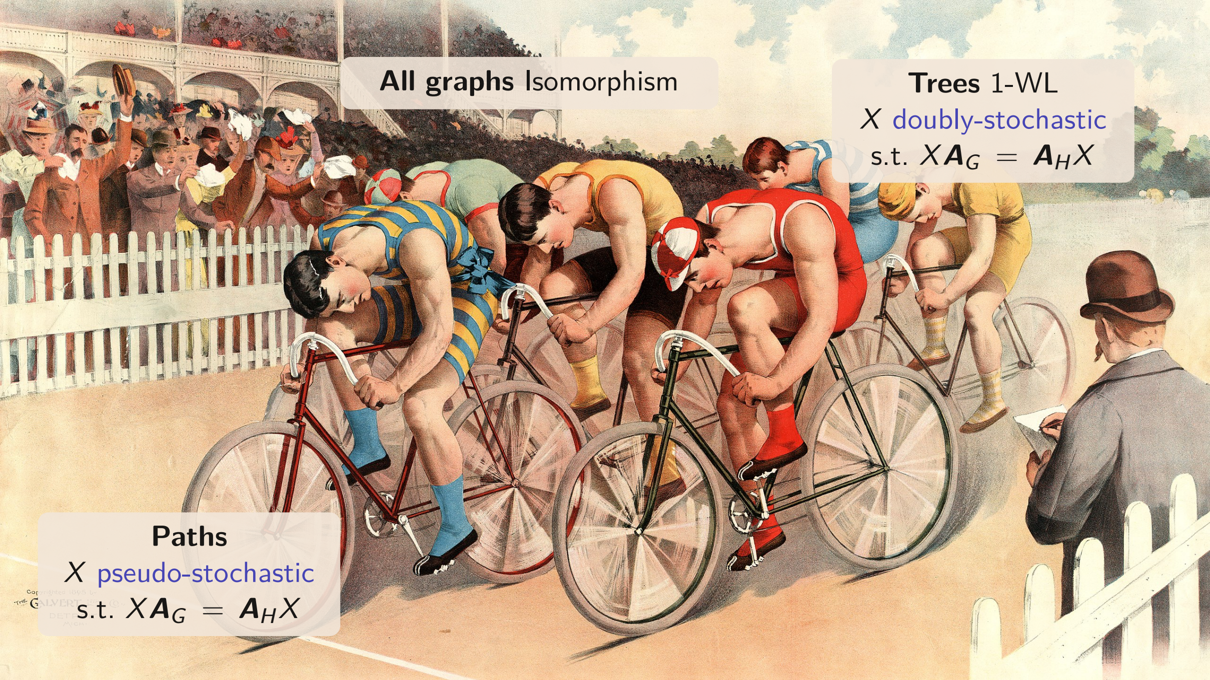
All graphs Isomorphism

Trees 1-WL

X doubly-stochastic

s.t. $X\boldsymbol{A}_G = \boldsymbol{A}_H X$





All graphs Isomorphism

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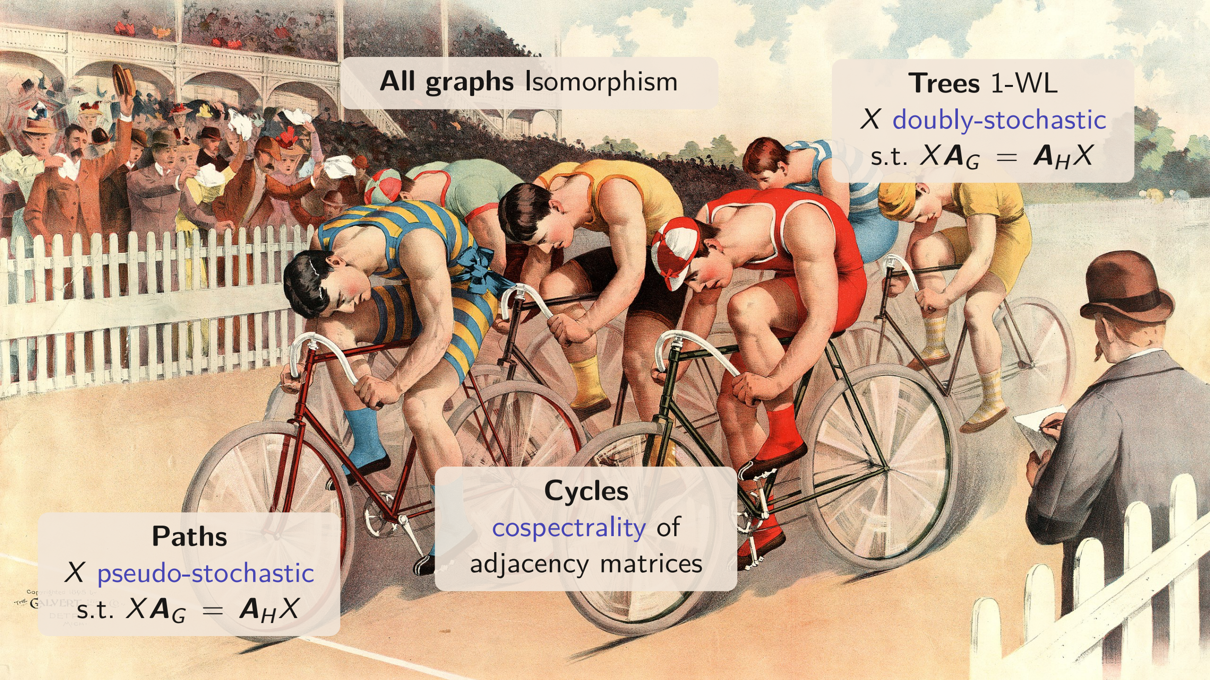
s.t. $X\boldsymbol{A}_G = \boldsymbol{A}_H X$

Paths
X pseudo-stochastic
s.t. $X\boldsymbol{A}_G = \boldsymbol{A}_H X$



All graphs Isomorphism

Trees 1-WL
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s.t. $X\boldsymbol{A}_G = \boldsymbol{A}_H X$

Cycles
cospectrality of
adjacency matrices

Paths
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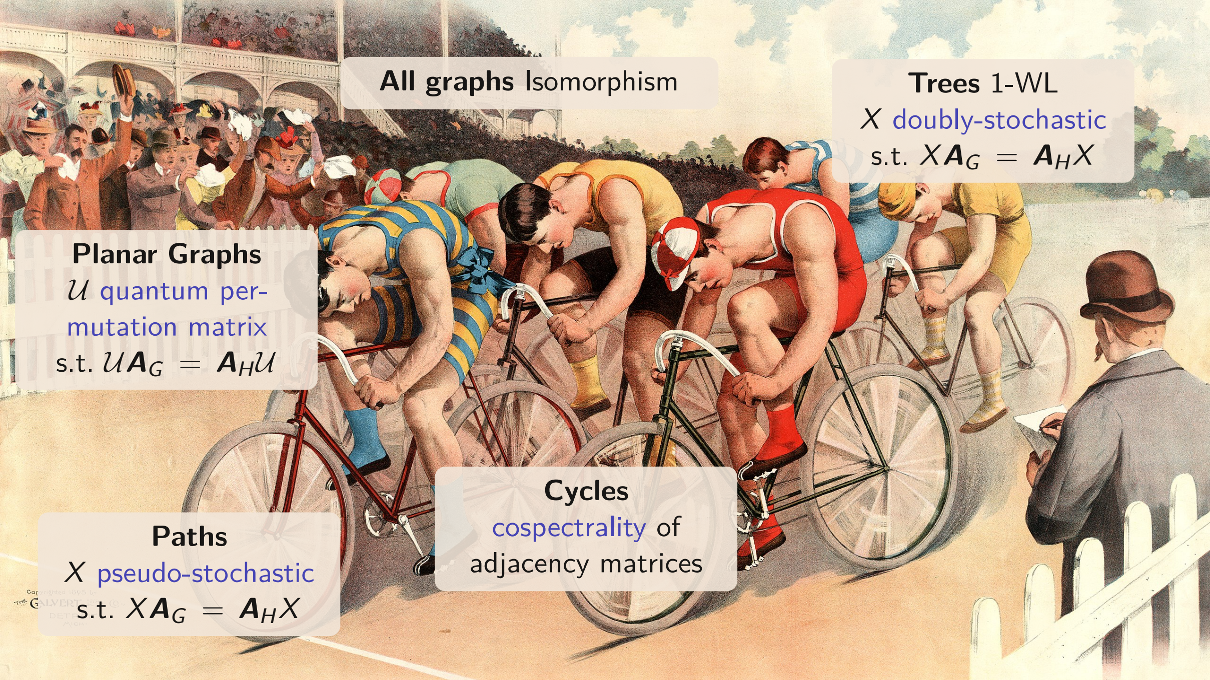

All graphs Isomorphism

Trees 1-WL
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Planar Graphs
$\mathcal{U}$ quantum permutation matrix
s.t. $\mathcal{U}\boldsymbol{A}_G = \boldsymbol{A}_H\mathcal{U}$

Cycles
cospectrality of adjacency matrices

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Unified Algebraic Framework

Grohe et al. (2022)

Mančinska and Roberson (2020)

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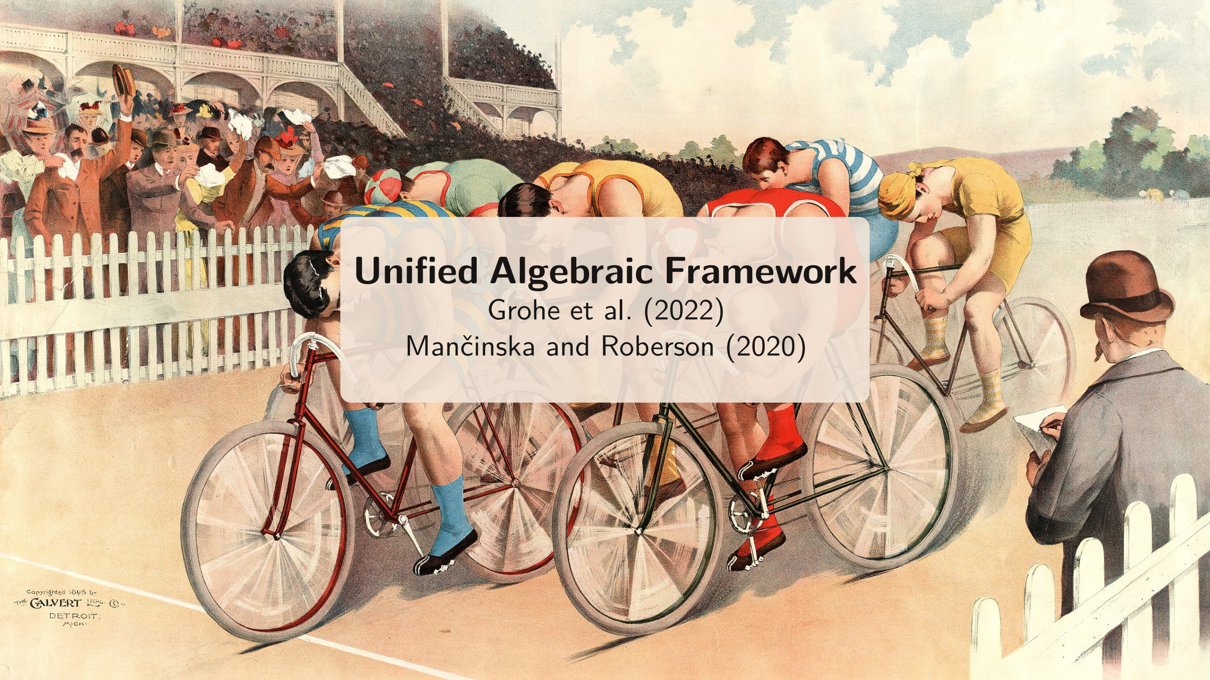
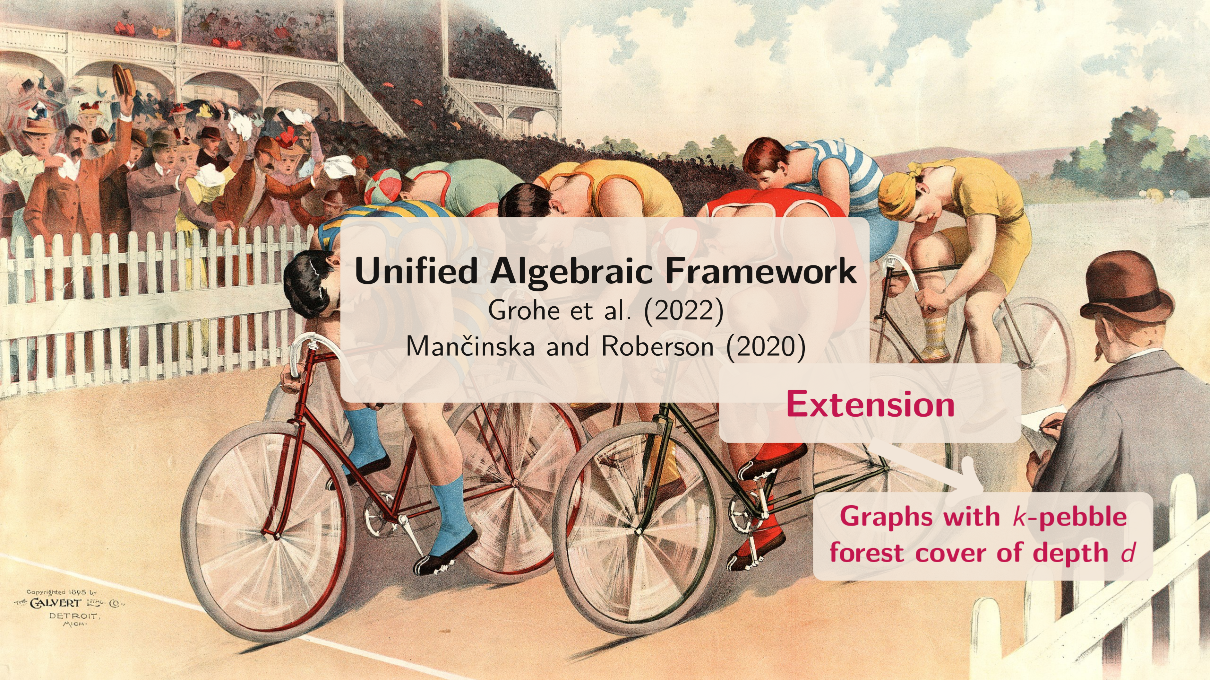




Unified Algebraic Framework

Grohe et al. (2022)

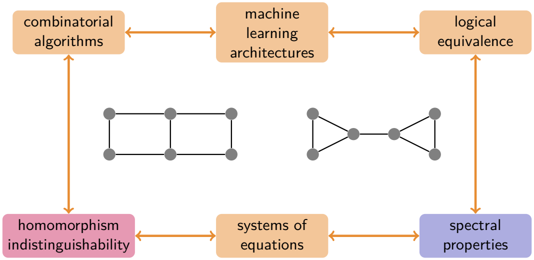
Mančinska and Roberson (2020)

Extension

Graphs with k-pebble forest cover of depth d

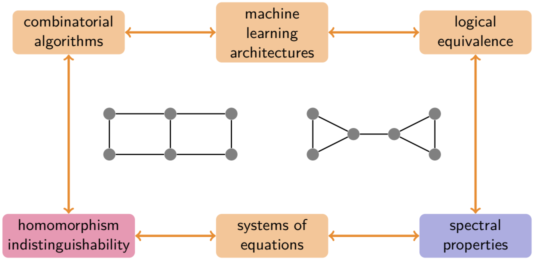
Conclusion

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



Conclusion

- we mapped out the relationship between combinatorial algorithms and spectral graph properties
  - classical spectral graph properties between 1-WL and 2-WL,



Conclusion

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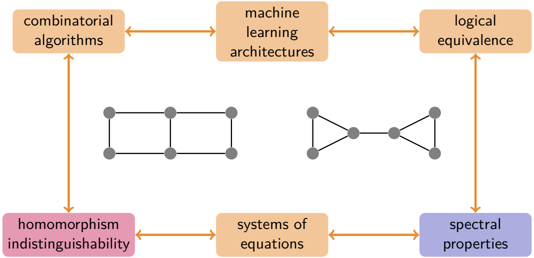

Conclusion

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  - classical spectral graph properties between 1-WL and 2-WL,
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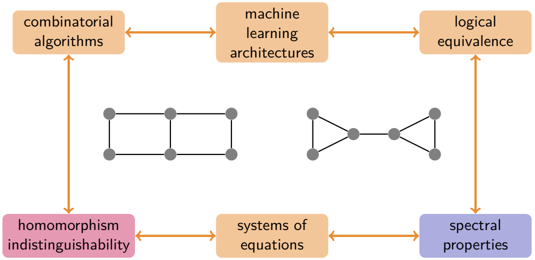
- we introduced $(1,1)$-WL, a linear space algorithm, separating 1-WL plus spectra from 2-WL.



Conclusion

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  - classical spectral graph properties between 1-WL and 2-WL,
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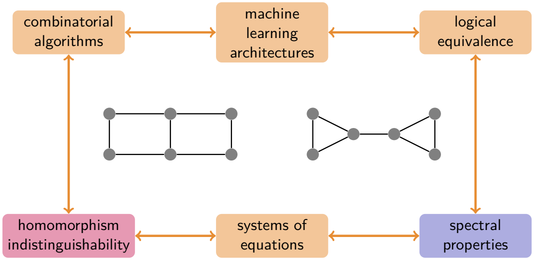
- we contributed algebraic tools for constructing systems of equations for homomorphism indistinguishability.



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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.

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