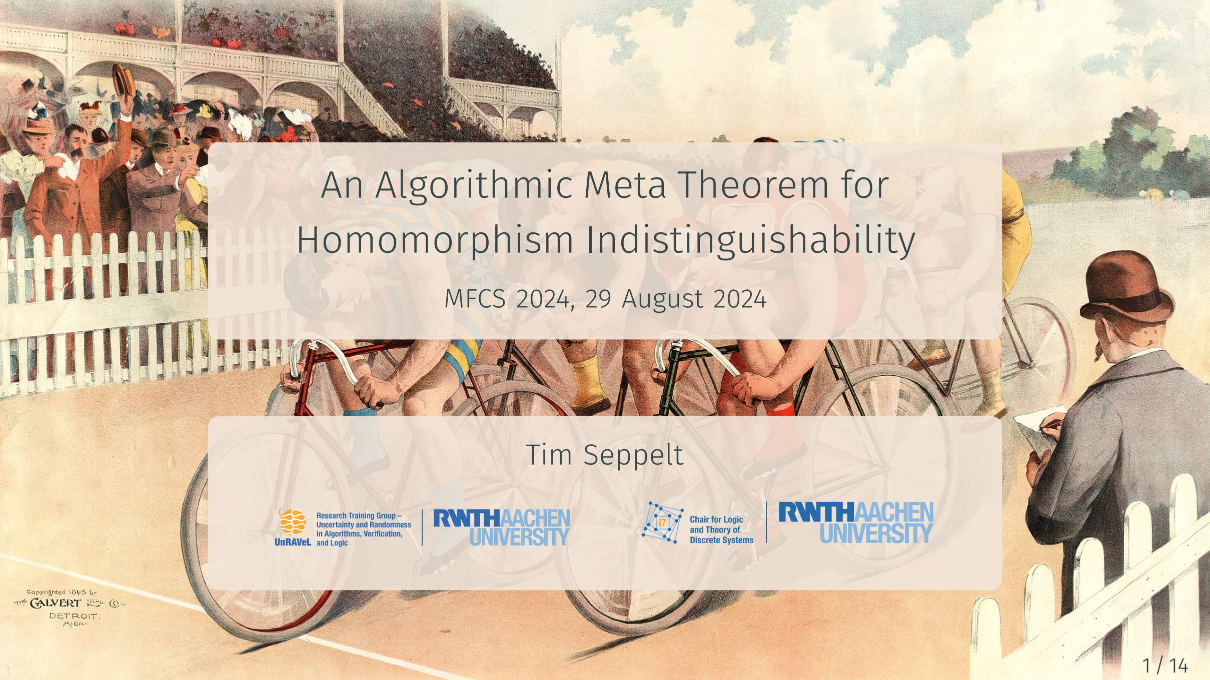


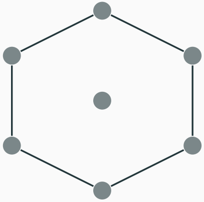
An Algorithmic Meta Theorem for Homomorphism Indistinguishability

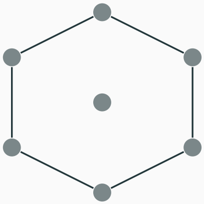
MFCS 2024, 29 August 2024

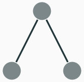
Tim Seppelt

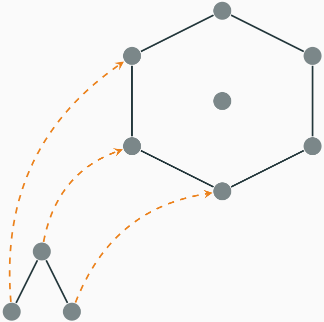
Research Training Group – Uncertainty and Randomness in Algorithms, Verification, and Logic (UnRAVeL) | RWTH Aachen University

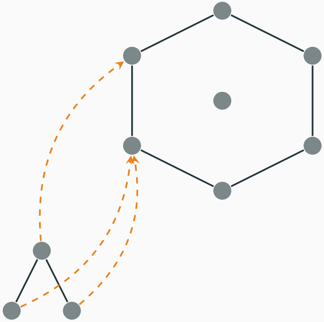
Chair for Logic and Theory of Discrete Systems (i7) | RWTH Aachen University

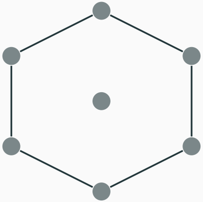


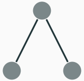




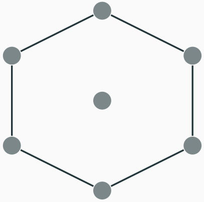


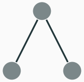




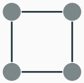


24

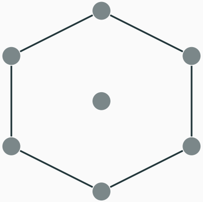
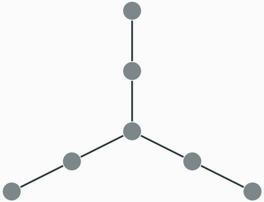
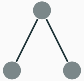
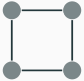


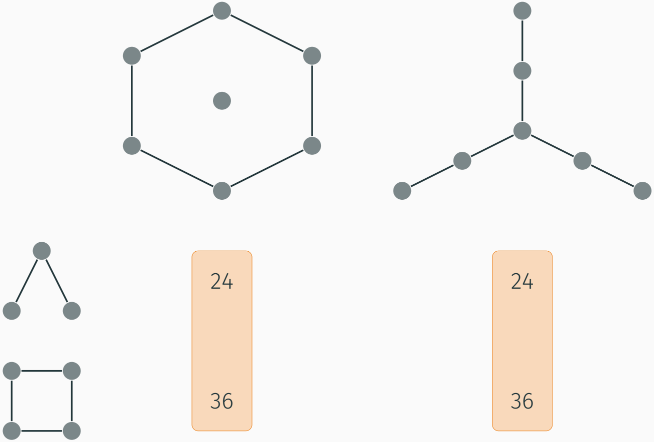


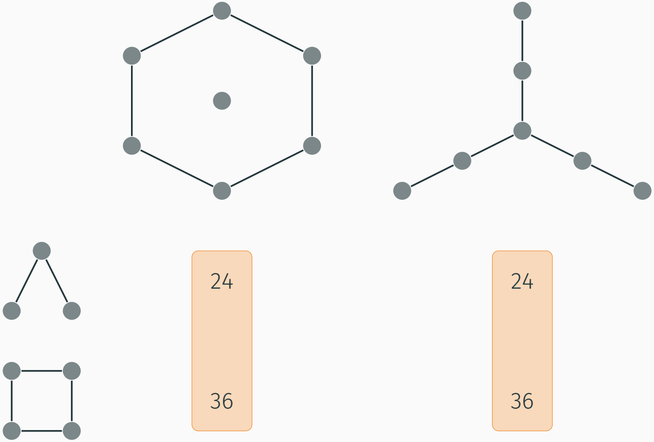
24

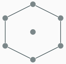
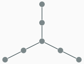


36

		
	24	24
	36	36


24
36
24
36



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

First Motivation: Characterisations and Connections

graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)

First Motivation: Characterisations and Connections

graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)
$\mathcal{C}$	cospectral adjacency matrices	Folklore

First Motivation: Characterisations and Connections

graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)
$\mathcal{C}$	cospectral adjacency matrices	Folklore
$\mathcal{P}$	quantum isomorphism	Mančinska and Roberson (2020)

First Motivation: Characterisations and Connections

graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)
$\mathcal{C}$	cospectral adjacency matrices	Folklore
$\mathcal{P}$	quantum isomorphism	Mančinska and Roberson (2020)
$\mathcal{TW}_k$	C^{k+1}-equivalence	Dvořák (2010); Dell, Grohe, and Rattan (2018)

First Motivation: Characterisations and Connections

graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)
$\mathcal{C}$	cospectral adjacency matrices	Folklore
$\mathcal{P}$	quantum isomorphism	Mančinska and Roberson (2020)
$\mathcal{TW}_k$	C^{k+1}-equivalence	Dvořák (2010); Dell, Grohe, and Rattan (2018)
	Weisfeiler–Leman algorithm	Cai, Fürer, and Immerman (1992)

First Motivation: Characterisations and Connections

graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)
$\mathcal{C}$	cospectral adjacency matrices	Folklore
$\mathcal{P}$	quantum isomorphism	Mančinska and Roberson (2020)
$\mathcal{TW}_k$	C^{k+1}-equivalence	Dvořák (2010); Dell, Grohe, and Rattan (2018)
	Weisfeiler–Leman algorithm	Cai, Fürer, and Immerman (1992)
	Sherali–Adams hiearchy	Atserias and Maneva (2012); Grohe and Otto (2015)

First Motivation: Characterisations and Connections

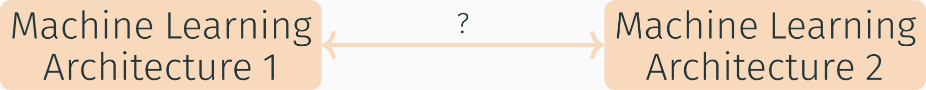
graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)
$\mathcal{C}$	cospectral adjacency matrices	Folklore
$\mathcal{P}$	quantum isomorphism	Mančinska and Roberson (2020)
$\mathcal{TW}_k$	C^{k+1}-equivalence	Dvořák (2010); Dell, Grohe, and Rattan (2018)
	Weisfeiler–Leman algorithm	Cai, Fürer, and Immerman (1992)
	Sherali–Adams hiearchy	Atserias and Maneva (2012); Grohe and Otto (2015)
	$\mathbb{P}_k$-coKleisli-isomorphism	Dawar, Jakl, and Reggio (2021)

First Motivation: Characterisations and Connections

graph class $\mathcal{F}$	relation $\equiv_{\mathcal{F}}$	
$\mathcal{G}$	isomorphism	Lovász (1967)
$\mathcal{C}$	cospectral adjacency matrices	Folklore
$\mathcal{P}$	quantum isomorphism	Mančinska and Roberson (2020)
$\mathcal{TW}_k$	C^{k+1}-equivalence	Dvořák (2010); Dell, Grohe, and Rattan (2018)
	Weisfeiler–Leman algorithm	Cai, Fürer, and Immerman (1992)
	Sherali–Adams hiearchy	Atserias and Maneva (2012); Grohe and Otto (2015)
	$\mathbb{P}_k$-coKleisli-isomorphism	Dawar, Jakl, and Reggio (2021)
	Graph Neural Networks	Xu et al. (2018); Morris et al. (2019)
...	...	

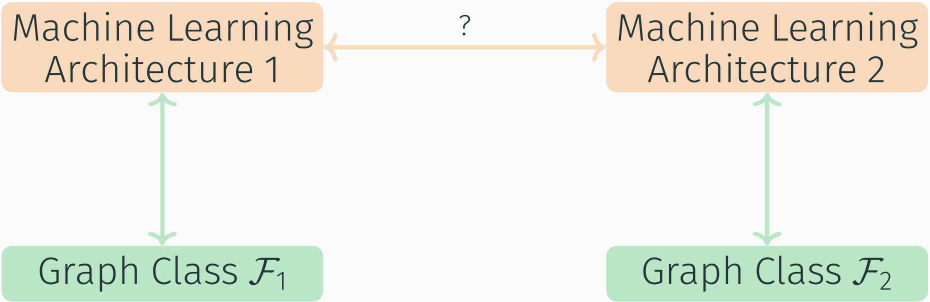
Second Motivation: Measuring Distinguishing Power

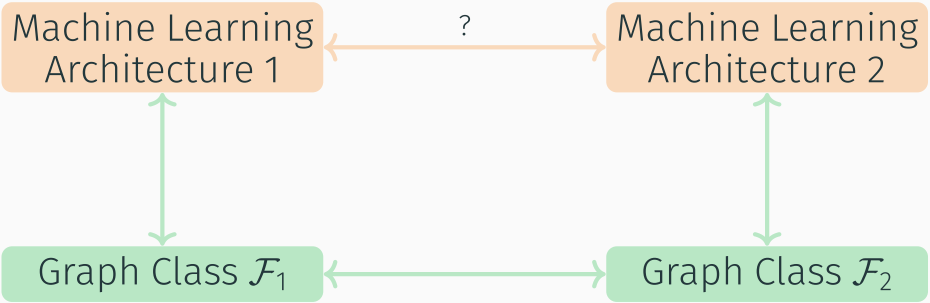
Roberson and S. (2023), Zhang et al. (2024)



Second Motivation: Measuring Distinguishing Power

Roberson and S. (2023), Zhang et al. (2024)





Machine Learning Architecture 1
?
Machine Learning Architecture 2
Graph Class $\mathcal{F}_1$
Graph Class $\mathcal{F}_2$

Complexity of Homomorphism Indistinguishability

HomInd($\mathcal{F}$)

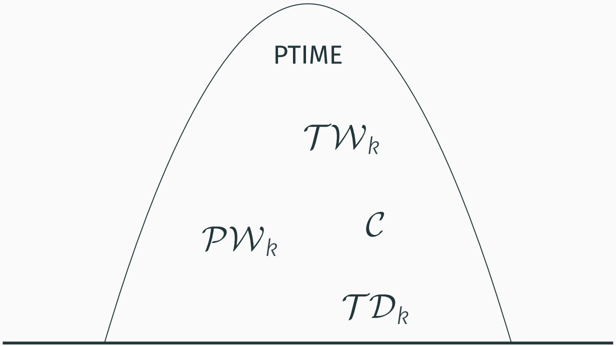
Input Graphs G and H.

Decide $G \equiv_{\mathcal{F}} H$.

HomInd($\mathcal{F}$)

Input Graphs G and H.

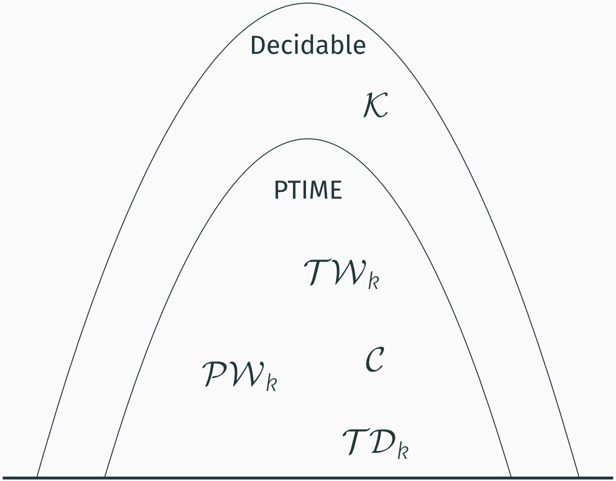
Decide $G \equiv_{\mathcal{F}} H$.



HomInd($\mathcal{F}$)

Input Graphs G and H.

Decide $G \equiv_{\mathcal{F}} H$.



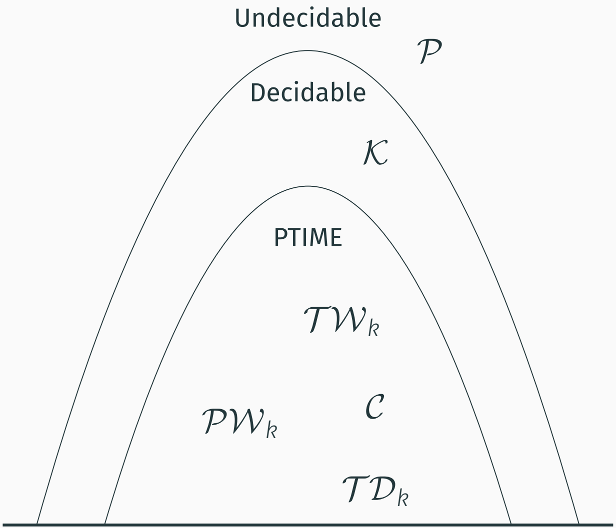
Complexity of Homomorphism Indistinguishability

Mančinska and Roberson (2020); Böker et al. (2019)

HomInd($\mathcal{F}$)

Input Graphs G and H.

Decide $G \equiv_{\mathcal{F}} H$.



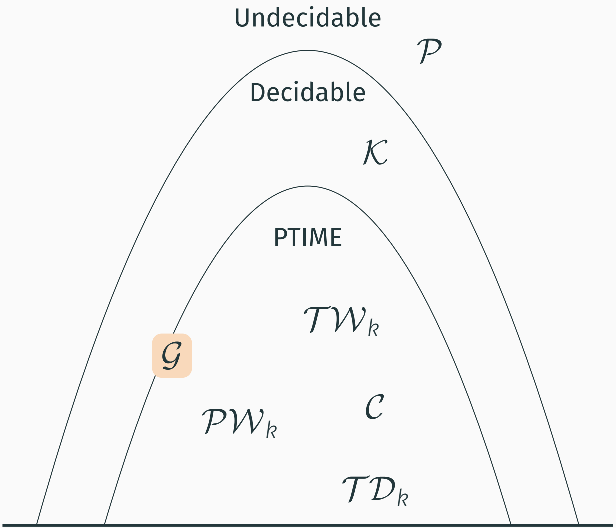
Complexity of Homomorphism Indistinguishability

Mančinska and Roberson (2020); Böker et al. (2019)

HomInd($\mathcal{F}$)

Input Graphs G and H.

Decide $G \equiv_{\mathcal{F}} H$.



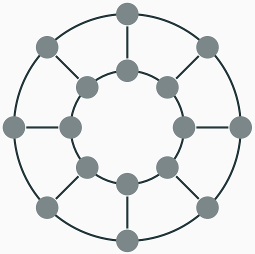
An Algorithmic Meta Theorem

Theorem

For every recognisable graph class $\mathcal{F}$ of bounded treewidth, $\textsc{HomInd}(\mathcal{F})$ *is in* coRP.

Theorem

For every recognisable graph class $\mathcal{F}$ of bounded treewidth, HomInd($\mathcal{F}$) *is in* coRP.

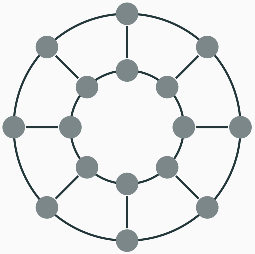


Minor-closed and bounded treewidth

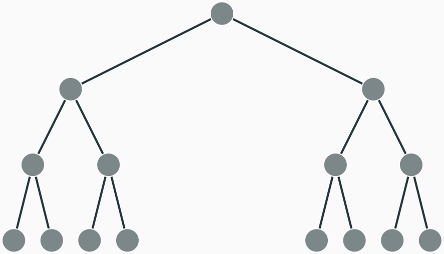
An Algorithmic Meta Theorem

Theorem

For every recognisable graph class $\mathcal{F}$ of bounded treewidth, HomInd($\mathcal{F}$) *is in* coRP.



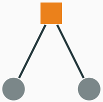
Minor-closed and bounded treewidth



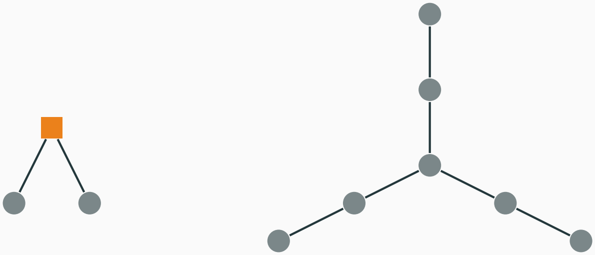
$CMSO_2$-definable and bounded treewidth

Courcelle (1990); Bojańczyk and Pilipczuk (2016)

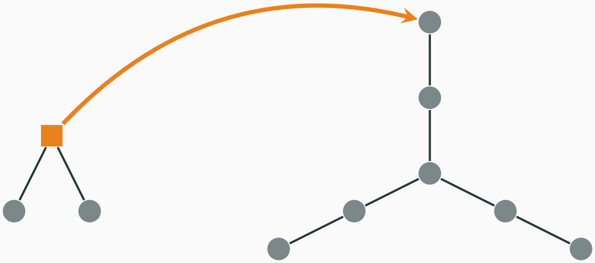
Labelled Graphs and Homomorphism Vectors



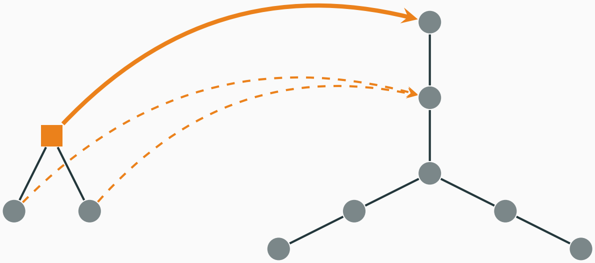
Labelled Graphs and Homomorphism Vectors



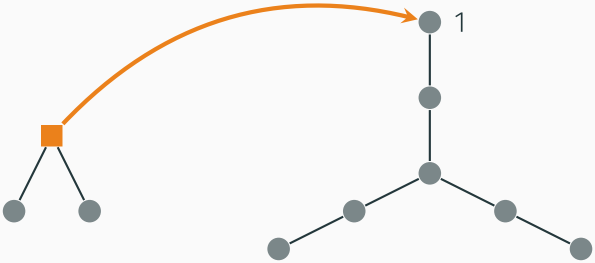
Labelled Graphs and Homomorphism Vectors

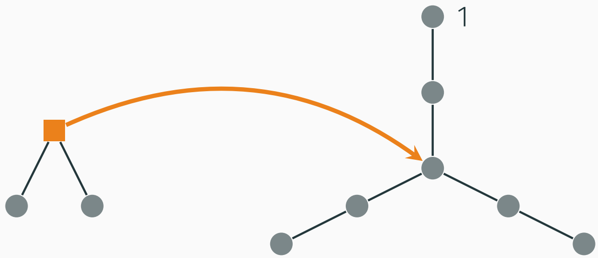


Labelled Graphs and Homomorphism Vectors

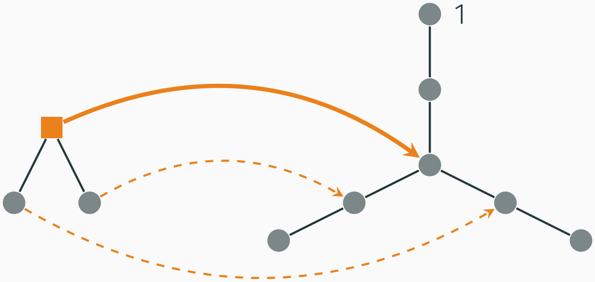


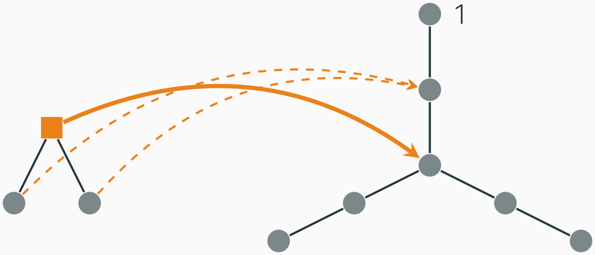
Labelled Graphs and Homomorphism Vectors



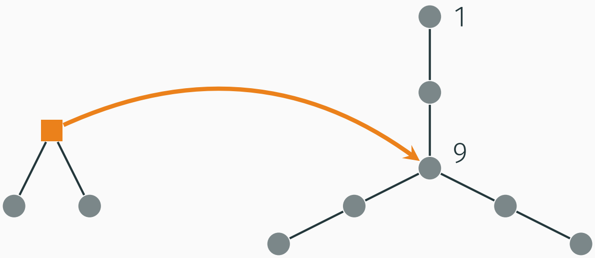

1

Labelled Graphs and Homomorphism Vectors



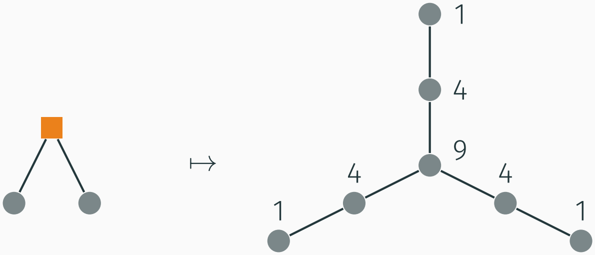

1

Labelled Graphs and Homomorphism Vectors

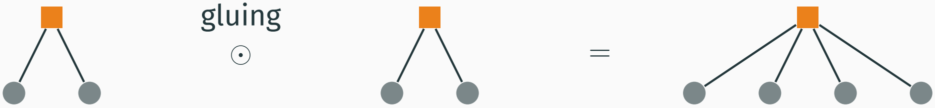


Labelled Graphs and Homomorphism Vectors

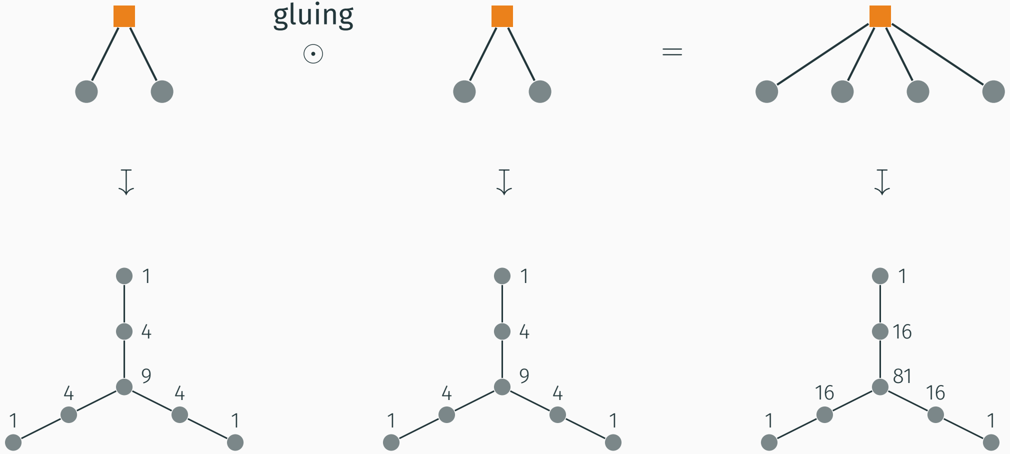
$$\mathcal{F} \longrightarrow \mathbb{R}^{V(G)}$$



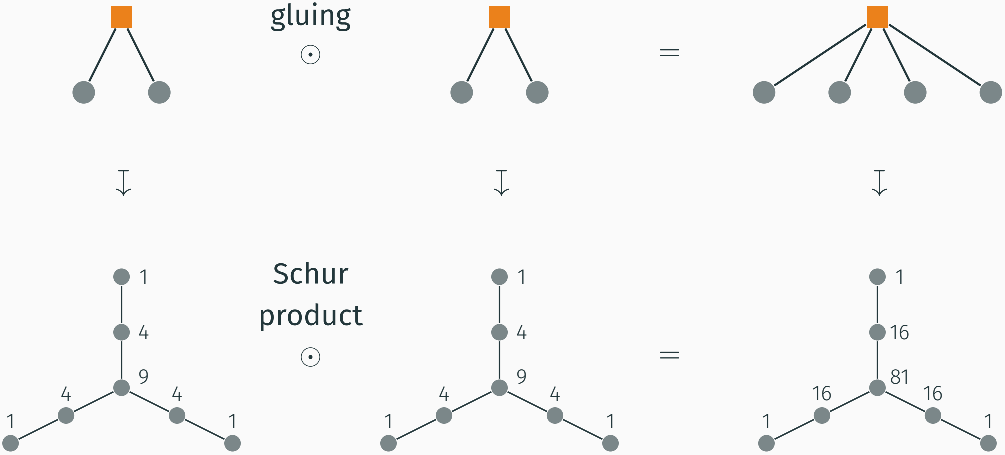
Combinatorial and Algebraic Operations: Gluing and Schur Product



Combinatorial and Algebraic Operations: Gluing and Schur Product



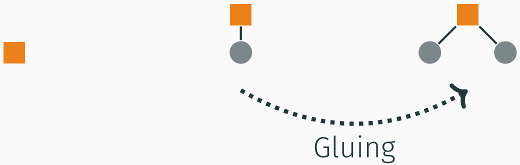
Combinatorial and Algebraic Operations: Gluing and Schur Product



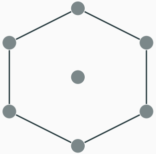
Homomorphism Indistinguishability over Trees

Homomorphism Indistinguishability over Trees

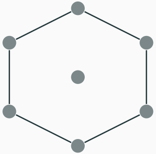
Attaching new edge


Gluing

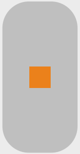

Attaching new edge

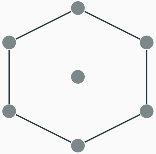


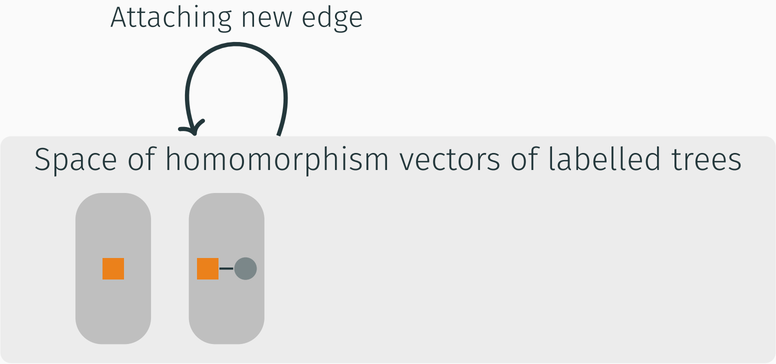
Space of homomorphism vectors of labelled trees



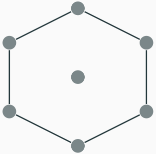
Space of homomorphism vectors of labelled trees





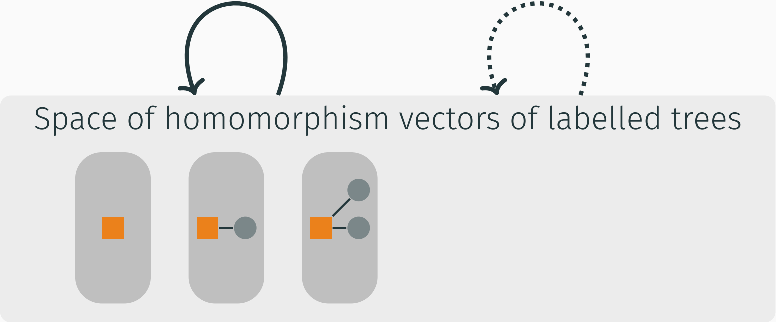


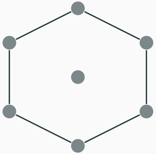
Attaching new edge
Space of homomorphism vectors of labelled trees

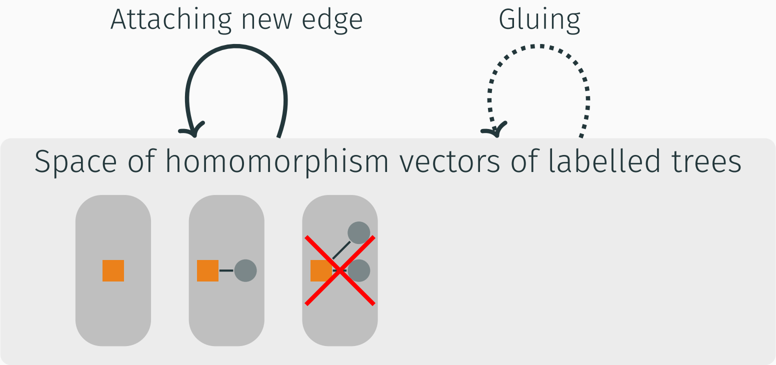


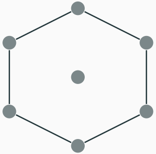
Attaching new edge

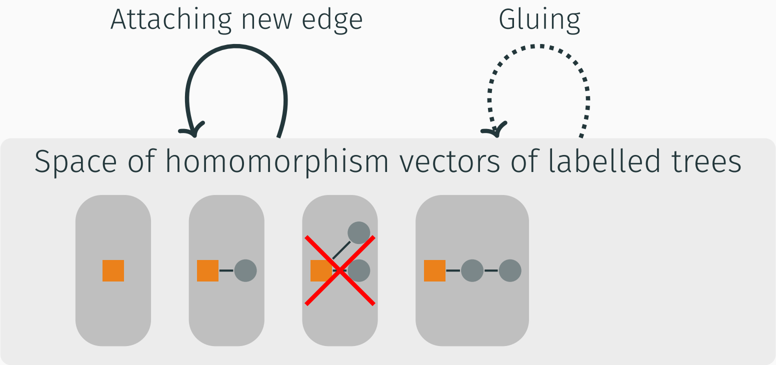
Gluing

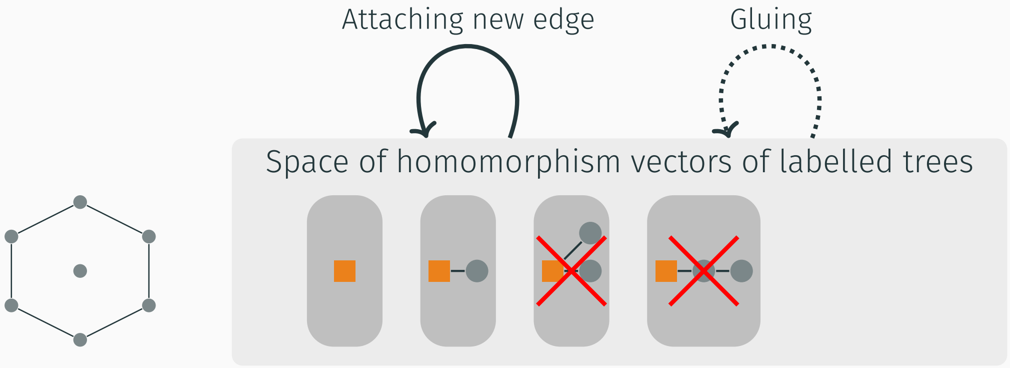


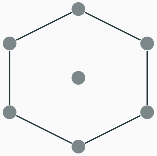


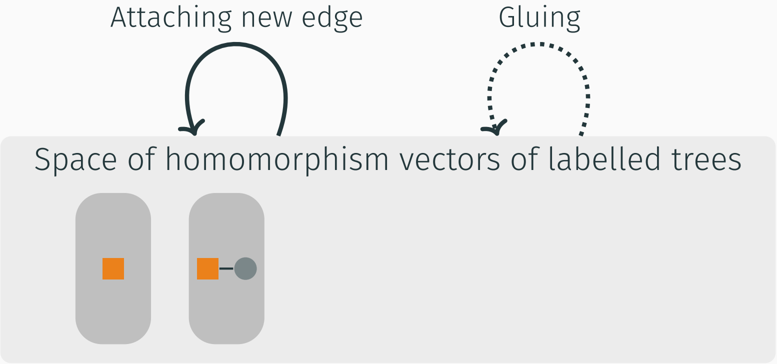

Attaching new edge
Gluing
Space of homomorphism vectors of labelled trees




Attaching new edge
Gluing
Space of homomorphism vectors of labelled trees


Attaching new edge
Gluing
Space of homomorphism vectors of labelled trees

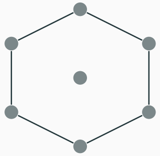


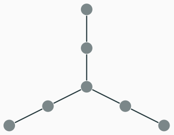


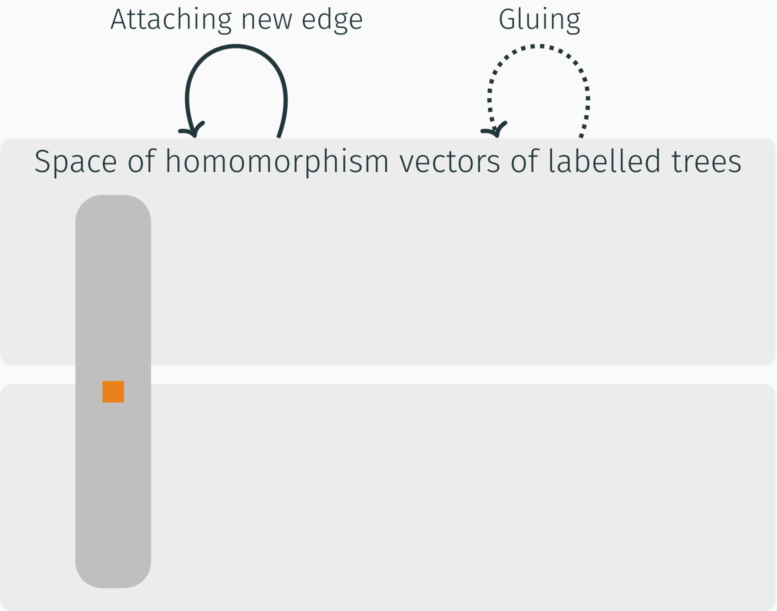
Attaching new edge
Gluing
Space of homomorphism vectors of labelled trees

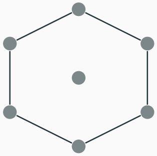
Attaching new edge   Gluing

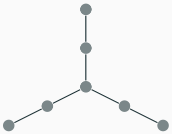
Space of homomorphism vectors of labelled trees

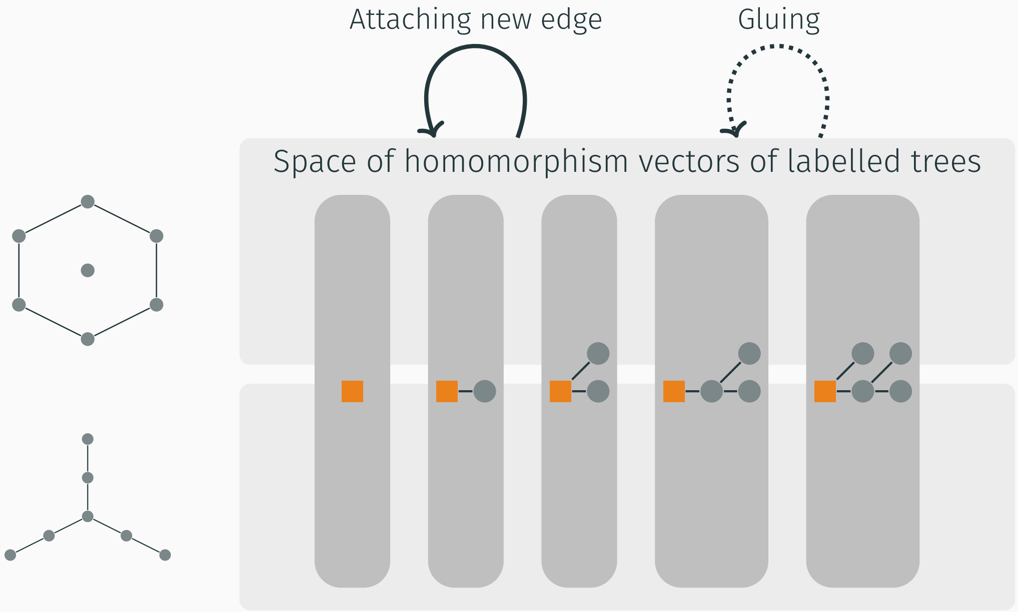




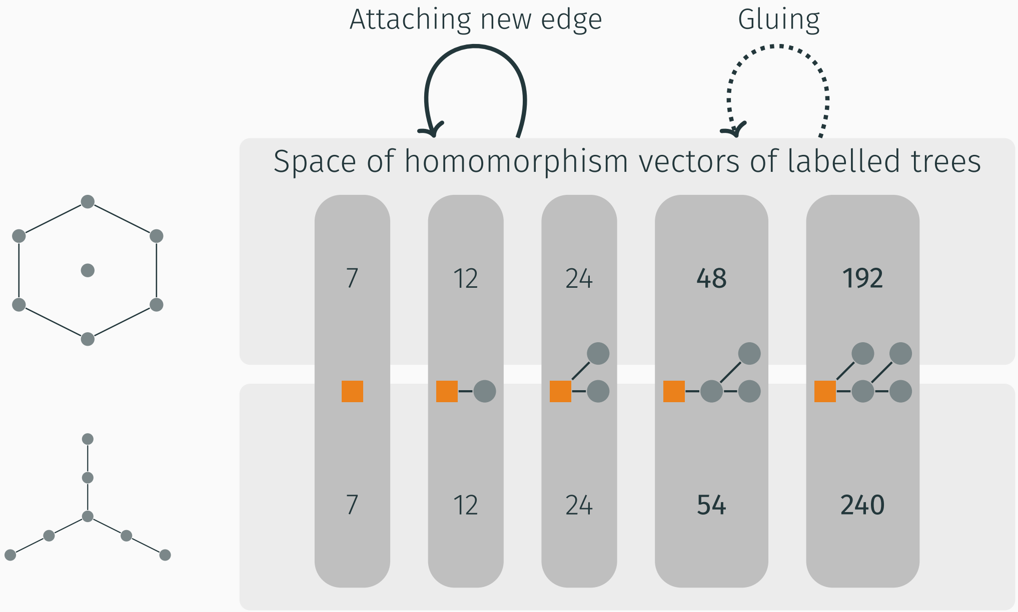

Attaching new edge
Gluing
Space of homomorphism vectors of labelled trees







Attaching new edge
Gluing
Space of homomorphism vectors of labelled trees



Attaching new edge
Gluing
Space of homomorphism vectors of labelled trees
7
12
24
48
192
7
12
24
54
240

Let $\mathcal{F}$ be a graph class. Let $F_1 \sim_{\mathcal{F}} F_2$ if and only if for all labelled graphs K

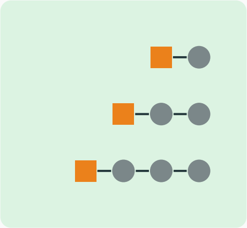
$$\mathrm{unlabel}(K \odot F_1) \in \mathcal{F} \iff \mathrm{unlabel}(K \odot F_2) \in \mathcal{F}.$$

Homomorphism Indistinguishability over Paths: Recognisability

Courcelle (1990)

Let $\mathcal{F}$ be a graph class. Let $F_1 \sim_{\mathcal{F}} F_2$ if and only if for all labelled graphs K

$$\mathrm{unlabel}(K \odot F_1) \in \mathcal{F} \iff \mathrm{unlabel}(K \odot F_2) \in \mathcal{F}.$$

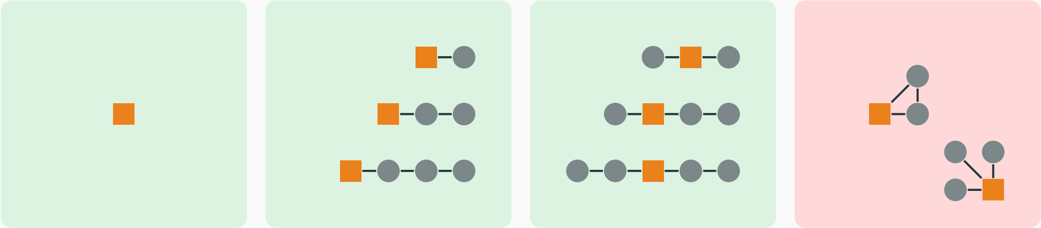


Homomorphism Indistinguishability over Paths: Recognisability

Courcelle (1990)

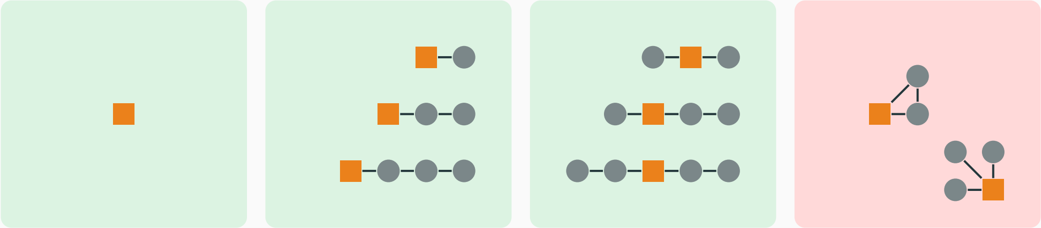
Let $\mathcal{F}$ be a graph class. Let $F_1 \sim_{\mathcal{F}} F_2$ if and only if for all labelled graphs K

$$\mathrm{unlabel}(K \odot F_1) \in \mathcal{F} \iff \mathrm{unlabel}(K \odot F_2) \in \mathcal{F}.$$



Let $\mathcal{F}$ be a graph class. Let $F_1 \sim_{\mathcal{F}} F_2$ if and only if for all labelled graphs K

$$\mathrm{unlabel}(K \odot F_1) \in \mathcal{F} \iff \mathrm{unlabel}(K \odot F_2) \in \mathcal{F}.$$

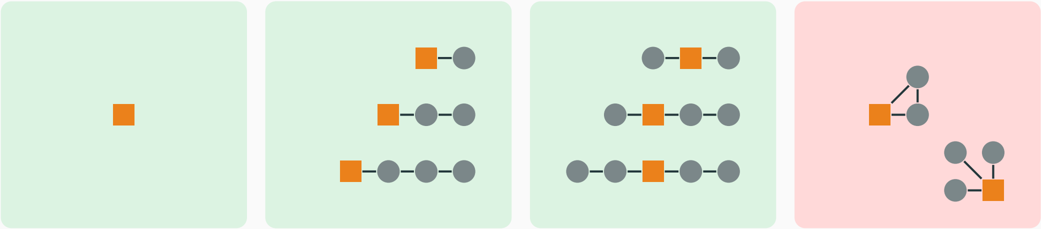


Definition

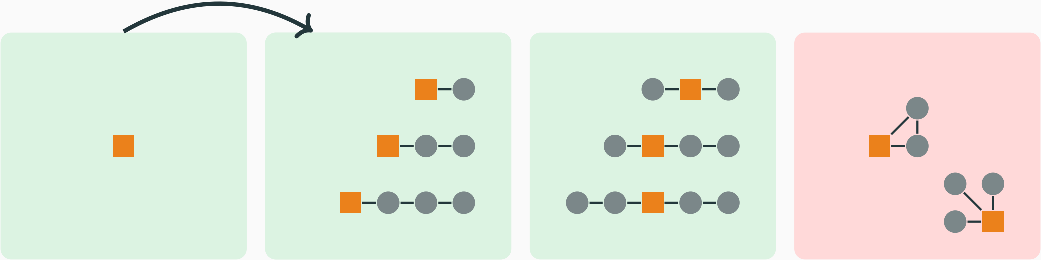
$\mathcal{F}$ is *recognisable* if $\sim_{\mathcal{F}}$ has finitely many equivalence classes.

Attaching a new edge

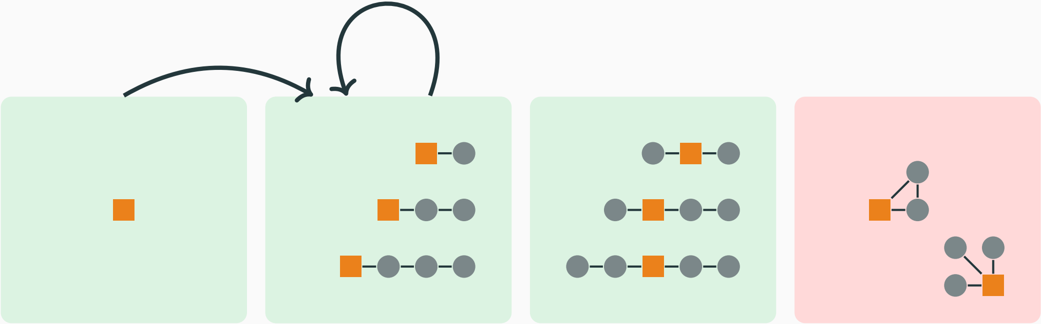
Attaching a new edge



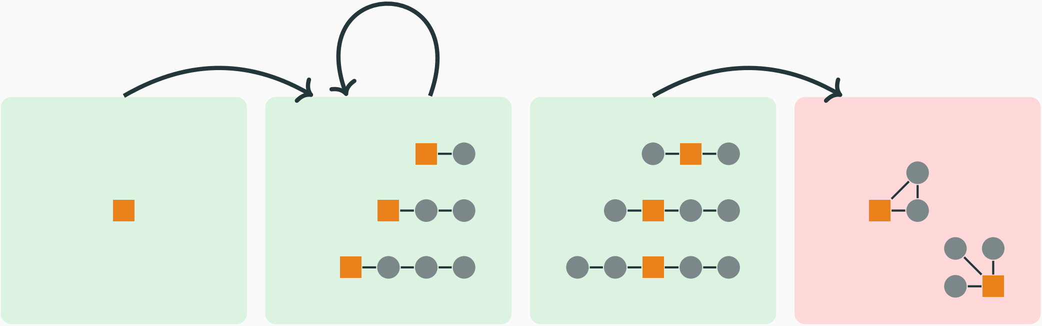
Attaching a new edge



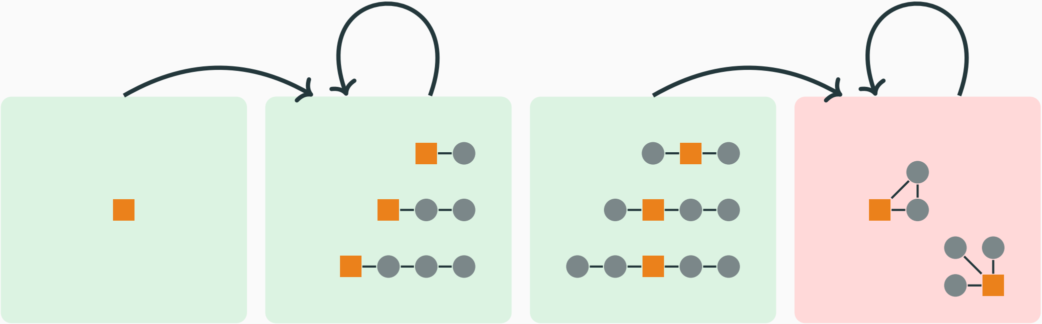
Attaching a new edge

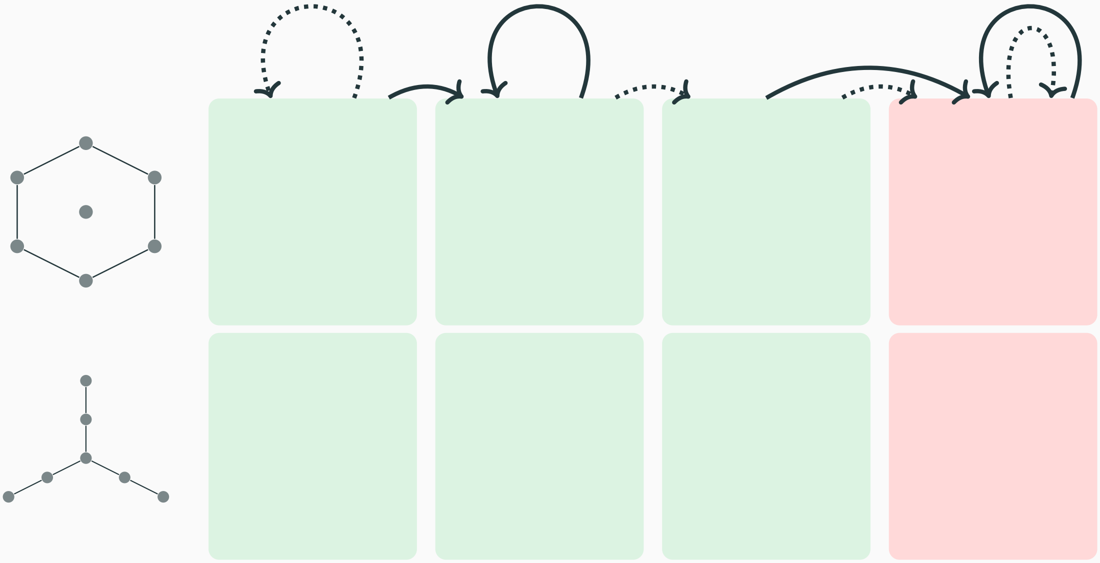


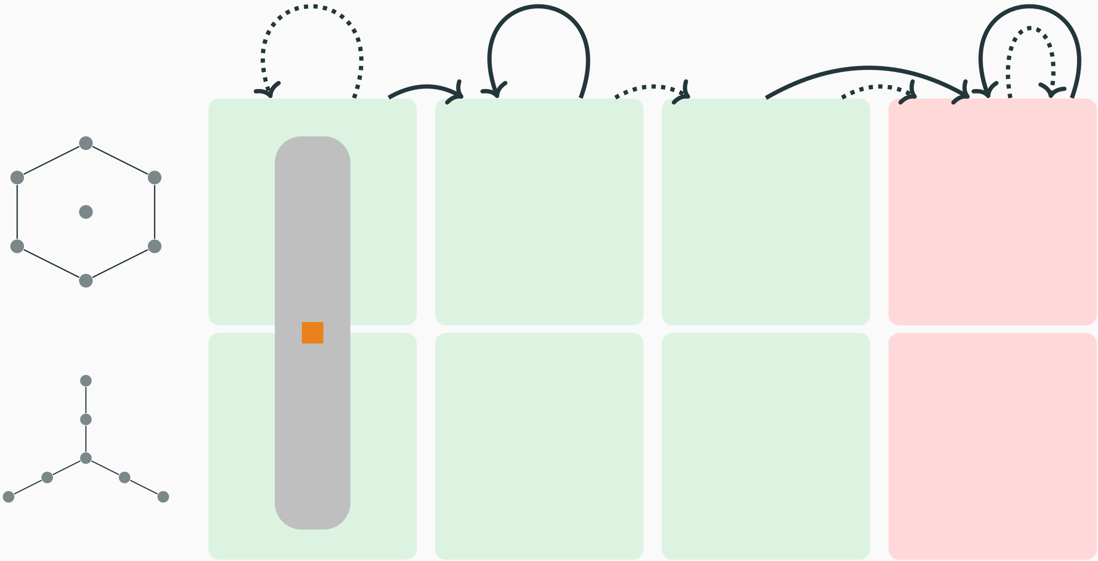
Attaching a new edge

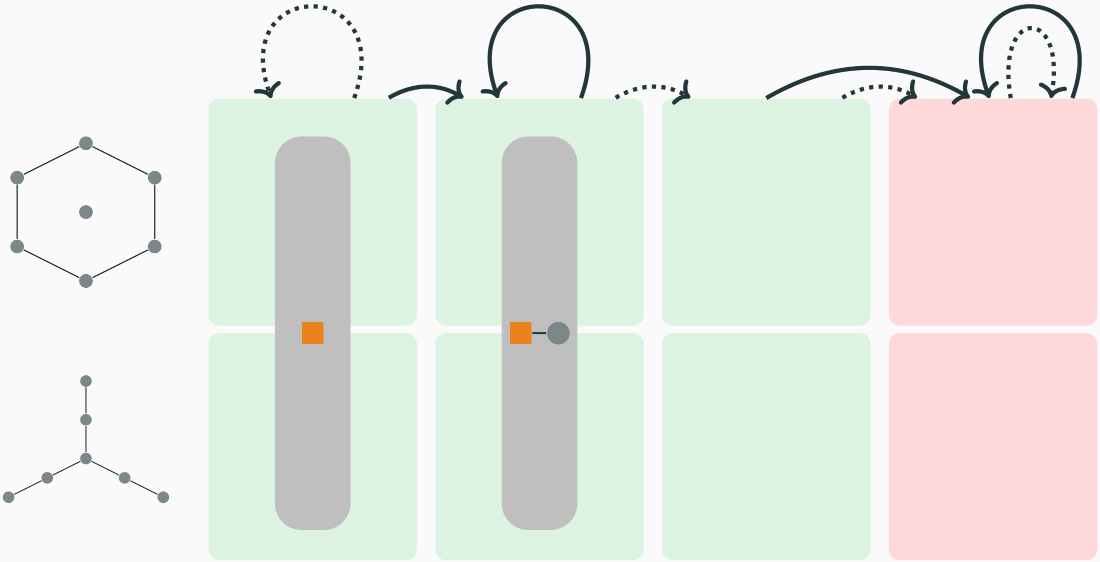


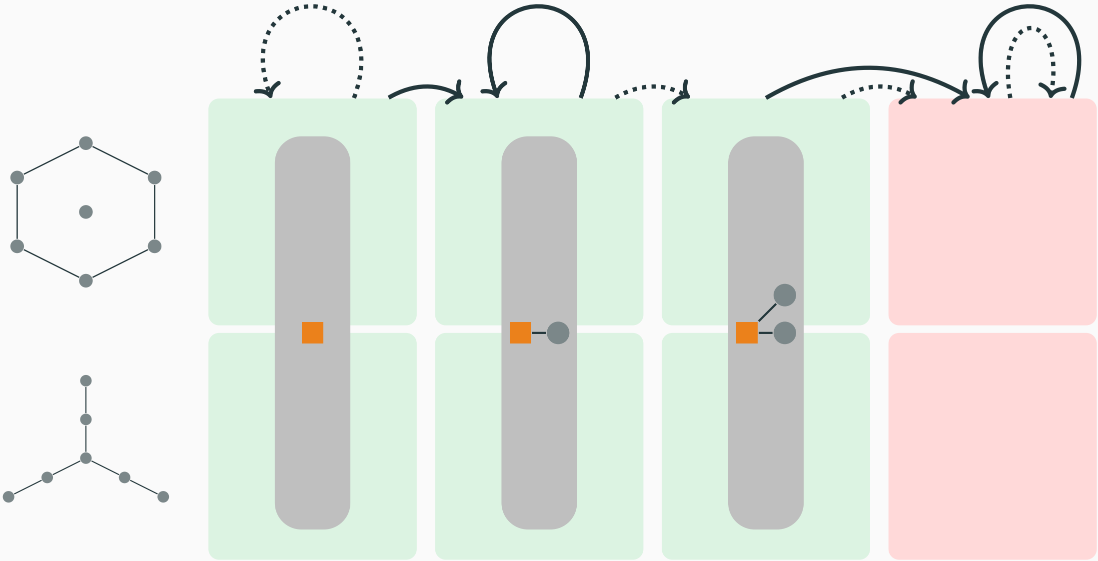
Attaching a new edge

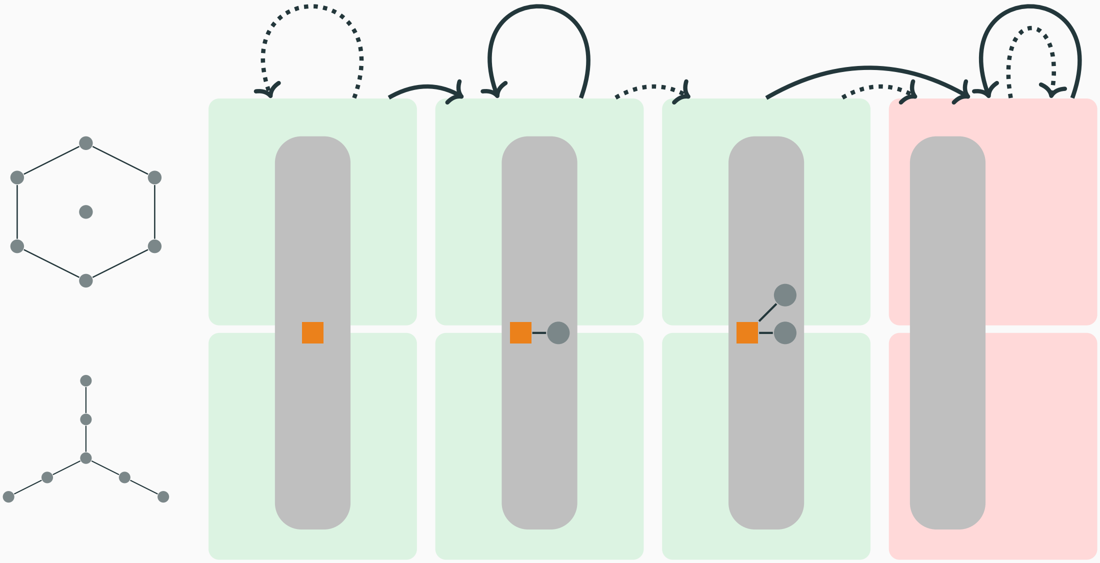


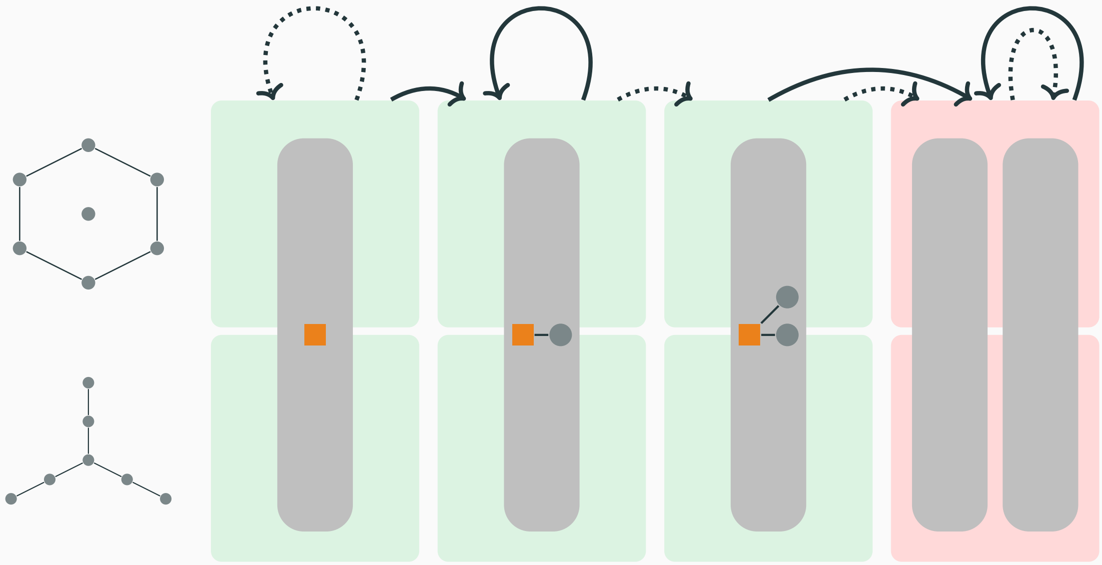


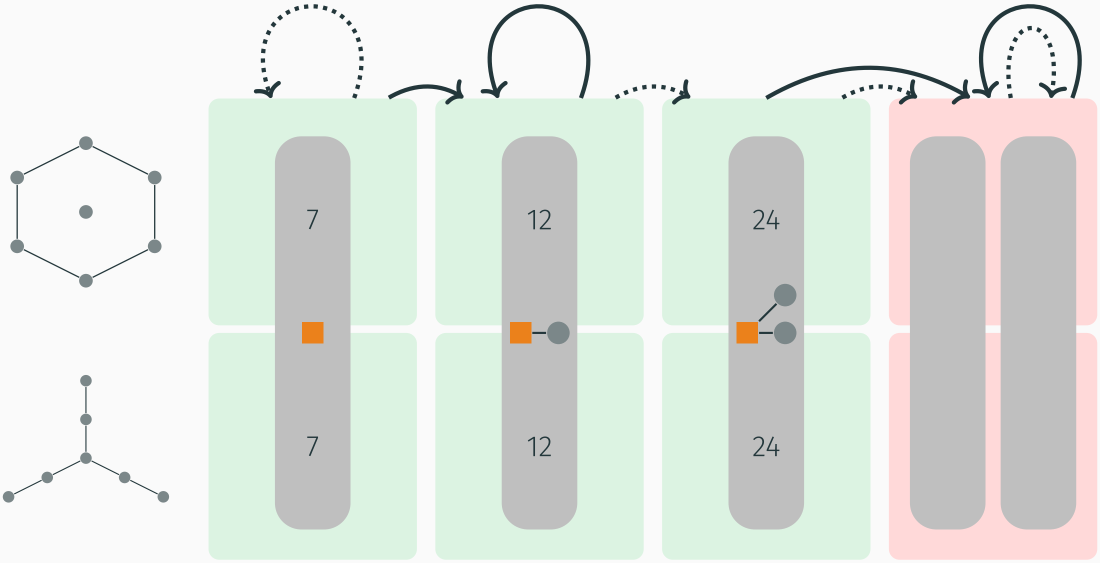










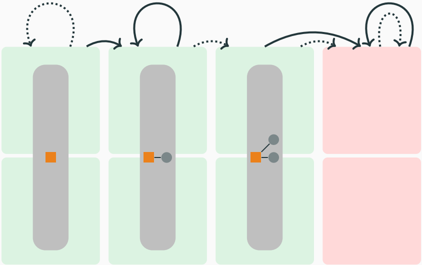

7
7
12
12
24
24

Conclusion

Theorem

For every recognisable graph class $\mathcal{F}$ of bounded treewidth, HomInd($\mathcal{F}$) *is in* coRP.

- New algorithms for known problems: Lasserre semidefinite program in coRP.



A conjecture

Conjecture

For a minor-closed graph class $\mathcal{F}$, either

$\mathcal{F}$ *contains all graphs* *and* $\textsc{HomInd}(\mathcal{F})$ *is Graph Isomorphism*,

A conjecture

Conjecture

For a minor-closed graph class $\mathcal{F}$, either

- $\mathcal{F}$ *contains all graphs* *and* $\textsc{HomInd}(\mathcal{F})$ *is Graph Isomorphism*,
- $\mathcal{F}$ *has bounded treewidth* *and* $\textsc{HomInd}(\mathcal{F})$ *is in polynomial time*, *or*

A conjecture

Conjecture

For a minor-closed graph class $\mathcal{F}$, either

- $\mathcal{F}$ *contains all graphs* *and* $\textsc{HomInd}(\mathcal{F})$ *is Graph Isomorphism,*
- $\mathcal{F}$ *has bounded treewidth* *and* $\textsc{HomInd}(\mathcal{F})$ *is in polynomial time, or*
- $\mathcal{F}$ *has unbounded treewidth* *and* $\textsc{HomInd}(\mathcal{F})$ *is undecidable.*

Atserias, Albert and Elitza Maneva (2012). "Sherali–Adams Relaxations and Indistinguishability in Counting Logics". In: *Proceedings of the 3rd Innovations in Theoretical Computer Science Conference*. ITCS '12. Cambridge, Massachusetts: Association for Computing Machinery, pp. 367–379. ISBN: 9781450311151. DOI: 10.1145/2090236.2090265. URL: https://doi.org/10.1145/2090236.2090265.

Bojańczyk, Mikołaj and Michał Pilipczuk (July 2016). "Definability equals recognizability for graphs of bounded treewidth". In: *Proceedings of the 31st Annual ACM/IEEE Symposium on Logic in Computer Science*. New York NY USA: ACM, pp. 407–416. ISBN: 978-1-4503-4391-6. DOI: 10.1145/2933575.2934508. URL: https://dl.acm.org/doi/10.1145/2933575.2934508.

- Böker, Jan, Yijia Chen, Martin Grohe, and Gaurav Rattan (2019). "The Complexity of Homomorphism Indistinguishability". en. In: Artwork Size: 13 pages Medium: application/pdf Publisher: Schloss Dagstuhl - Leibniz-Zentrum fuer Informatik GmbH, Wadern/Saarbruecken, Germany, 13 pages. DOI: 10.4230/LIPICS.MFCS.2019.54. URL: http://drops.dagstuhl.de/opus/volltexte/2019/10998/.
- Cai, Jin-Yi, Martin Fürer, and Neil Immerman (1992). "An optimal lower bound on the number of variables for graph identification". In: *Combinatorica* 12.4, pp. 389–410. ISSN: 1439-6912. DOI: 10.1007/BF01305232. URL: https://doi.org/10.1007/BF01305232.

Courcelle, Bruno (Mar. 1990). “The monadic second-order logic of graphs. I. Recognizable sets of finite graphs”. In: *Information and Computation* 85.1, pp. 12–75. ISSN: 0890-5401. DOI: `10.1016/0890-5401(90)90043-H`. URL: `https://www.sciencedirect.com/science/article/pii/089054019090043H`.

Dawar, Anuj, Tomáš Jakl, and Luca Reggio (2021). “Lovász-Type Theorems and Game Comonads”. In: *36th Annual ACM/IEEE Symposium on Logic in Computer Science, LICS 2021, Rome, Italy, June 29 - July 2, 2021*. IEEE, pp. 1–13. DOI: `10.1109/LICS52264.2021.9470609`.

Dell, Holger, Martin Grohe, and Gaurav Rattan (2018). “Lovász Meets Weisfeiler and Leman”. en. In: *45th International Colloquium on Automata, Languages, and Programming (ICALP 2018)*, 40:1–40:14. DOI: `10.4230/LIPICS.ICALP.2018.40`.

Bibliography iv

- Dvořák, Zdeněk (Aug. 2010). “On recognizing graphs by numbers of homomorphisms”. en. In: *Journal of Graph Theory* 64.4, pp. 330–342. ISSN: 03649024. DOI: `10.1002/jgt.20461`. URL: `http://doi.wiley.com/10.1002/jgt.20461`.
- Grohe, Martin and Martin Otto (2015). “Pebble Games and Linear Equations”. In: *The Journal of Symbolic Logic* 80.3, pp. 797–844. ISSN: 00224812, 19435886. DOI: `10.1017/jsl.2015.28`. URL: `http://www.jstor.org/stable/43864249`.
- Lovász, László (Sept. 1967). “Operations with structures”. In: *Acta Mathematica Academiae Scientiarum Hungarica* 18.3, pp. 321–328. ISSN: 1588-2632. DOI: `10.1007/BF02280291`. URL: `https://doi.org/10.1007/BF02280291`.

Mančinska, Laura and David E. Roberson (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)*, pp. 661–672. DOI: 10.1109/FOCS46700.2020.00067.

Morris, Christopher, Martin Ritzert, Matthias Fey, William L. Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe (July 2019). "Weisfeiler and Leman Go Neural: Higher-Order Graph Neural Networks". In: *Proceedings of the AAAI Conference on Artificial Intelligence* 33, pp. 4602–4609. ISSN: 2374-3468, 2159-5399. DOI: 10.1609/aaai.v33i01.33014602. URL: https://aaai.org/ojs/index.php/AAAI/article/view/4384.

- Roberson, David E. and Tim Seppelt (2023). “Lasserre Hierarchy for Graph Isomorphism and Homomorphism Indistinguishability”. In: *50th International Colloquium on Automata, Languages, and Programming, ICALP 2023, July 10-14, 2023, Paderborn, Germany*. Ed. by Kousha Etessami, Uriel Feige, and Gabriele Puppis. Vol. 261. LIPIcs. Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 101:1–101:18. DOI: 10.4230/LIPICS.ICALP.2023.101. URL: https://doi.org/10.4230/LIPIcs.ICALP.2023.101.
- Xu, Keyulu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka (Dec. 21, 2018). “How Powerful are Graph Neural Networks?” In: *International Conference on Learning Representations*. URL: https://openreview.net/forum?id=ryGs6iA5Km.

Zhang, Bohang, Jingchu Gai, Yiheng Du, Qiwei Ye, Di He, and Liwei Wang (2024). "Beyond Weisfeiler–Lehman: A Quantitative Framework for GNN Expressiveness". In: *The Twelfth International Conference on Learning Representations*. URL: https://openreview.net/forum?id=HSKaGOi7Ar.

Title 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