

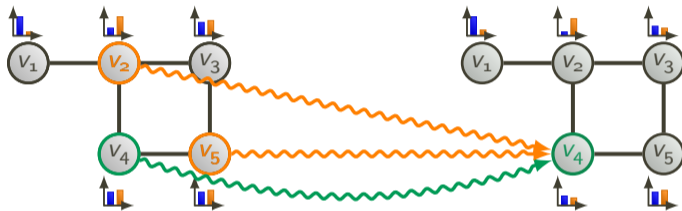
## WL meet VC

---

**Christopher Morris, Floris Geerts, Jan Tönshoff, Martin Grohe**

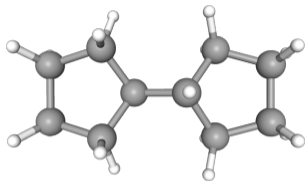
RWTH Aachen University, University of Antwerpen

# Expressivity of Graph Neural Networks

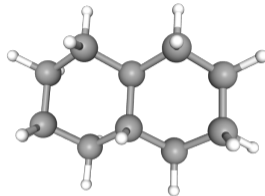


$$f^{(t)}(v) = f_{\text{merge}}^{W_1} \left( f^{(t-1)}(v), f_{\text{aggr}}^{W_2} \left( \{ \{ f^{(t-1)}(w) \mid w \in N(v) \} \} \right) \right)$$

# Expressivity of Graph Neural Networks



(a) Bicyclopentyl



(b) Decalin

## Key Insight

Any possible **GNN** architecture **misses crucial patterns** in the data!

C. Morris, M. Ritzert, M. Fey, W. L. Hamilton, J. Eric Lenssen, G. Rattan, and M. Grohe. "Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks". In: *AAAI*. 2019

K. Xu, W. Hu, J. Leskovec, and S. Jegelka. "How Powerful are Graph Neural Networks?" In: *ICLR*. 2019

W. Azizian and M. Lelarge. "Characterizing the Expressive Power of Invariant and Equivariant Graph Neural Networks". In: *ICLR*.

# Expressivity of Graph Neural Networks: Relationship between 1-WL and GNNs



## Theorem (Informal)

There exists a **GNN architecture** and corresponding **weights** such that it has the **same power** as the **1-Weisfeiler–Leman algorithm**.

C. Morris, M. Ritzert, M. Fey, W. L. Hamilton, J. Eric Lenssen, G. Rattan, and M. Grohe. “Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks”. In: *AAAI*. 2019

K. Xu, W. Hu, J. Leskovec, and S. Jegelka. “How Powerful are Graph Neural Networks?” In: *ICLR*. 2019

W. Azizian and M. Lelarge. “Characterizing the Expressive Power of Invariant and Equivariant Graph Neural Networks”. In: *ICLR*. 2021

# Weisfeiler and Leman go Machine Learning: The Story so far

**Christopher Morris**

*Department of Computer Science  
RWTH Aachen University  
Aachen, Germany*

**Yaron Lipman**

*Meta AI Research  
Department of Computer Science and Applied Mathematics  
Weizmann Institute of Science  
Rehovot, Israel*

**Haggai Maron**

*NVIDIA Research  
Tel Aviv, Israel*

**Bastian Rieck**

*AIDOS Lab, Institute of AI for Health  
Helmholtz Zentrum München and Technical University of Munich  
Munich, Germany*

**Nils M. Kriege**

*Faculty of Computer Science,  
Research Network Data Science  
University of Vienna  
Vienna, Austria*

**Martin Grohe**

*Department of Computer Science  
RWTH Aachen University  
Aachen, Germany*

**Matthias Fey**

*Kumo.AI  
Mountain View, CA*

**Karsten Borgwardt\***

*Machine Learning & Computer  
Department of Biosystems  
ETH Zürich  
Switzerland*

MORRIS@CS.RWTH-AACHEN.DE

YARON.LIPMAN@WEIZMANN.AC.IL

HMARON@NVIDIA.COM

BASTIAN.RIECK@HELMHOLTZ-MUENCHEN.ME

NILS.KRIEGE@UNIVIE.AC.AT

GROHE@INFORMATIK.RWTH-AACHEN.DE

What does the **graph isomorphism problem** *has to do with machine learning?*

How are **generalization** and **expressivity** related?

*We show a tight connection between GNNs' expressivity and their generalization ability.*

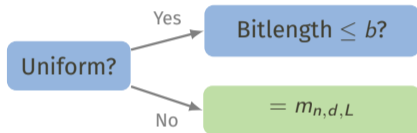


Uniform?

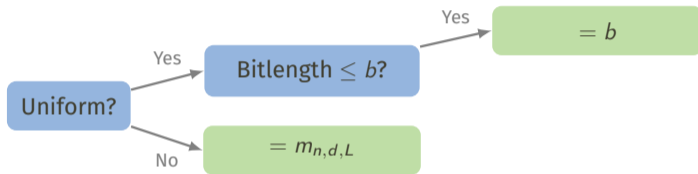
*We show a tight connection between GNNs' expressivity and their generalization ability.*



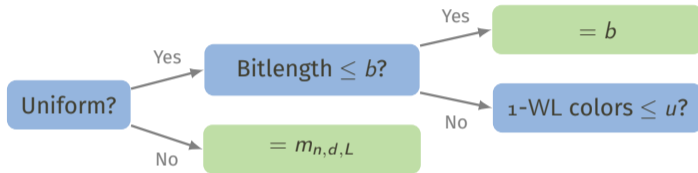
*We show a tight connection between GNNs' expressivity and their generalization ability.*



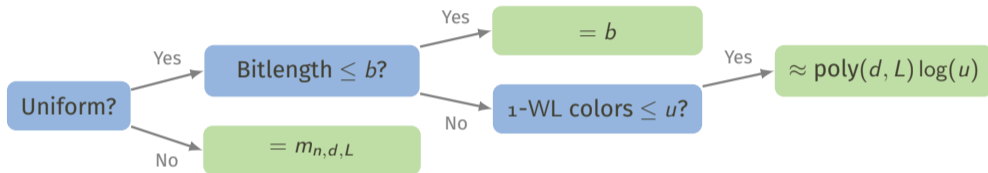
*We show a tight connection between GNNs' expressivity and their generalization ability.*



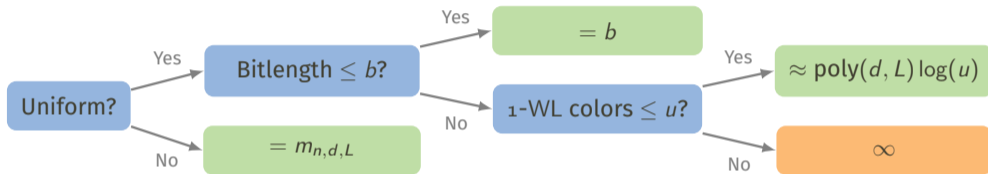
*We show a tight connection between GNNs' expressivity and their generalization ability.*



*We show a tight connection between GNNs' expressivity and their generalization ability.*



*We show a tight connection between GNNs' expressivity and their generalization ability.*



*We show a tight connection between GNNs' expressivity and their generalization ability.*

- [AL21] W. Azizian and M. Lelarge. “Characterizing the Expressive Power of Invariant and Equivariant Graph Neural Networks”. In: *ICLR*. 2021.
- [Mor+19] C. Morris, M. Ritzert, M. Fey, W. L. Hamilton, J. Eric Lenssen, G. Rattan, and M. Grohe. “Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks”. In: *AAAI*. 2019.
- [Xu+19] K. Xu, W. Hu, J. Leskovec, and S. Jegelka. “How Powerful are Graph Neural Networks?” In: *ICLR*. 2019.