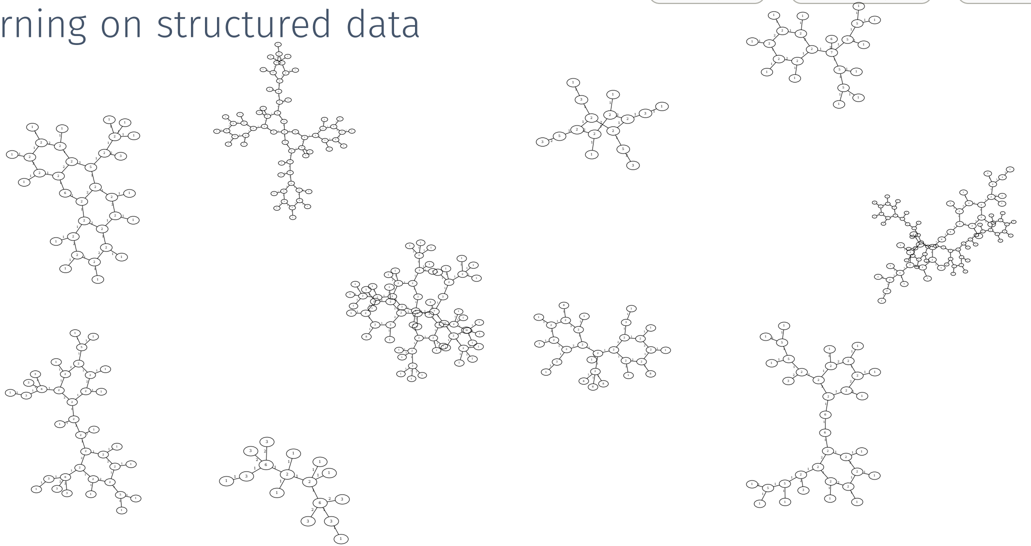
Expressive Graph Embeddings via Homomorphism Counts

Pascal Welke

CAIML Seminar on 25. November 2024

Hu et al (2020) Morris et al (2020) Dwivedi et al (2022)

Learning on structured data



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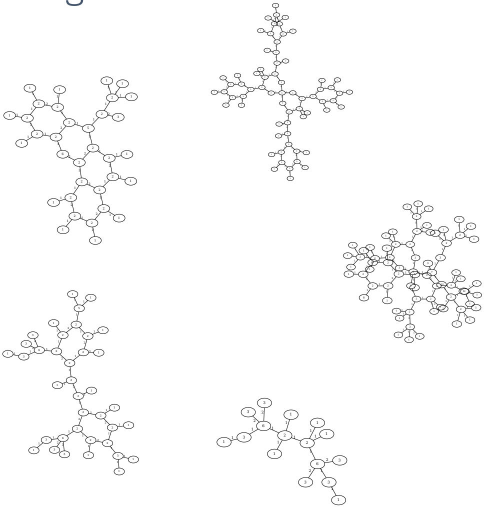

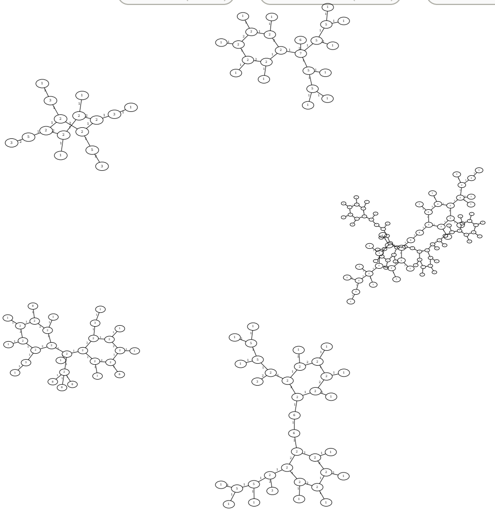

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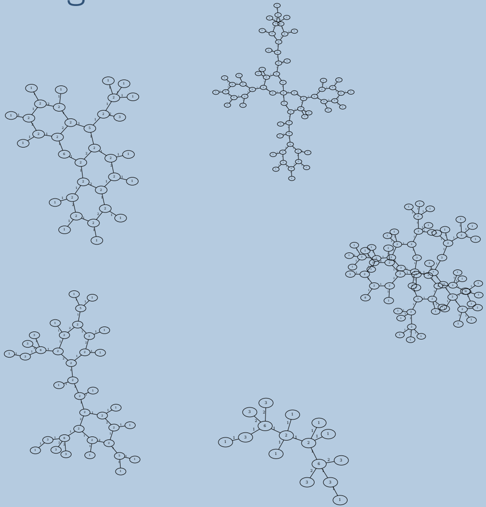

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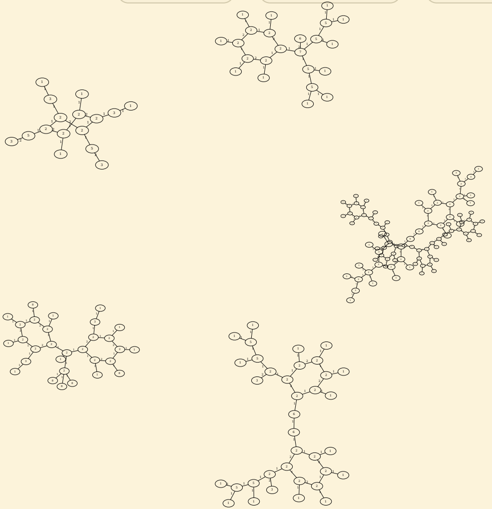

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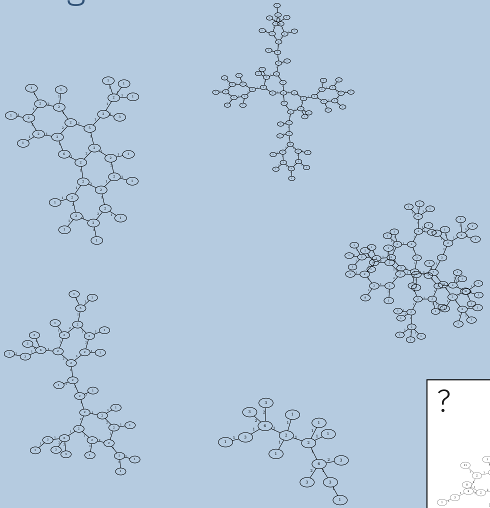
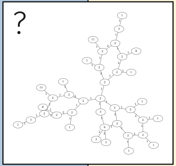
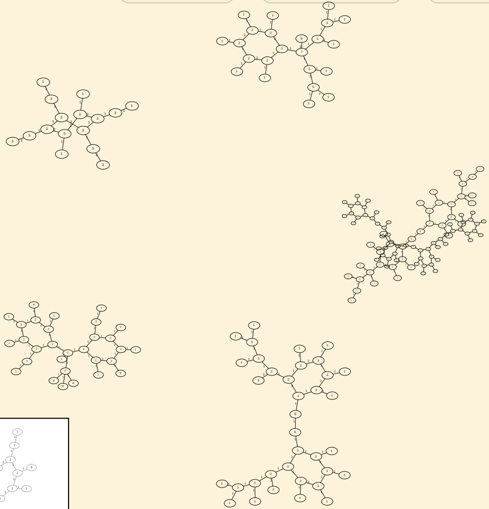
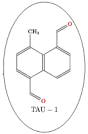






Learning on structured data

chemistry prof.



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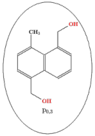
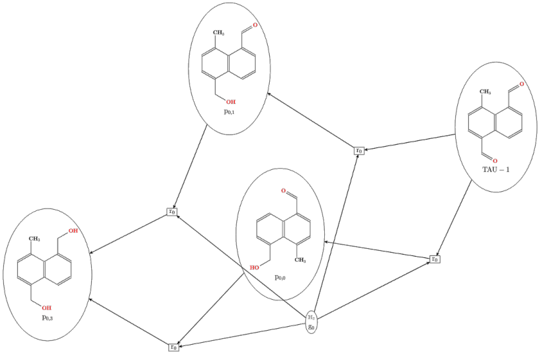


Learning on structured data

me



Problems in graph learning

Neural methods achieve remarkable results in graph learning

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- molecule synthesis and prediction
- modeling of human social behavior
- …

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Problems in graph learning

Neural methods achieve remarkable results in graph learning

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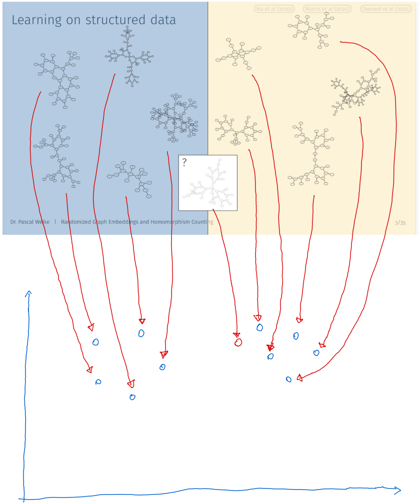
but come with

- significant resource demands
- too much complexity to be interpretable
- which hinders application in many scenarios

Graph Representation Learning

The goal

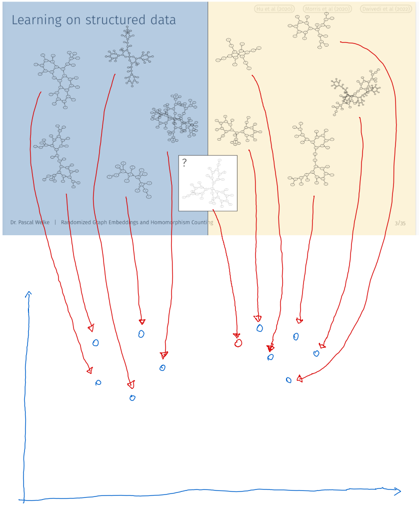
Vectorial graph representations
that



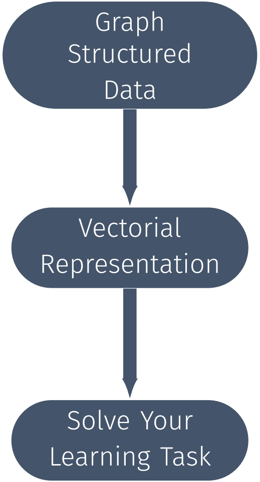
The goal

Vectorial graph representations that

- yield semantically and structurally meaningful distances
- are interpretable
- are adaptable to given data



Graph representation learning



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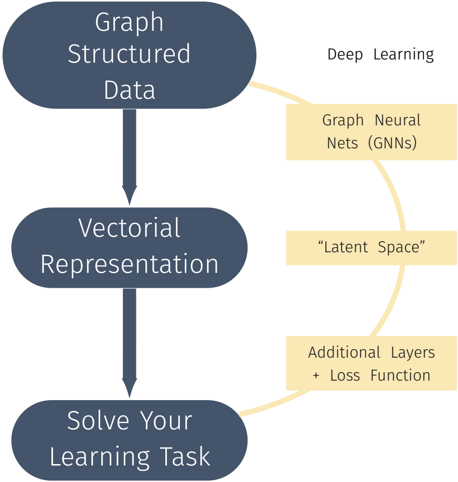

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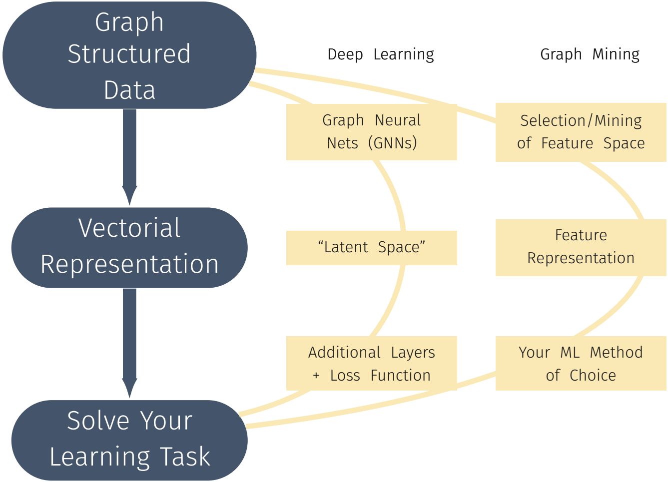

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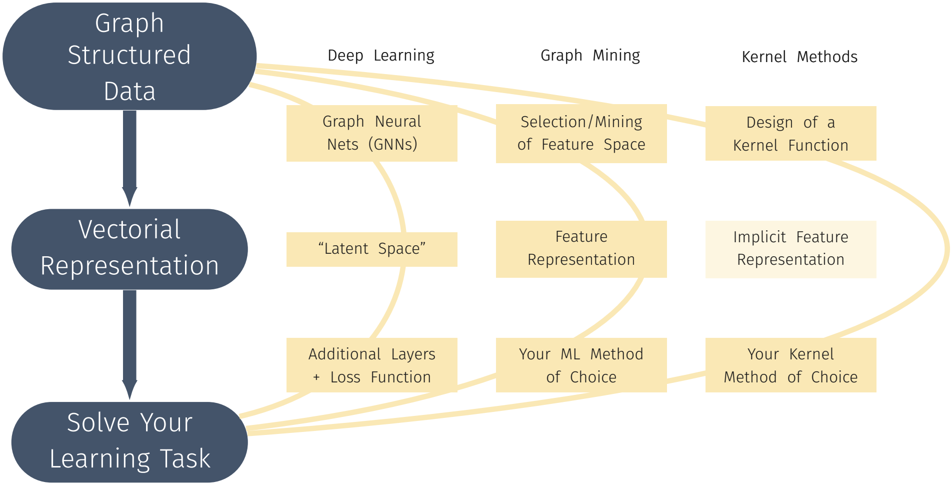
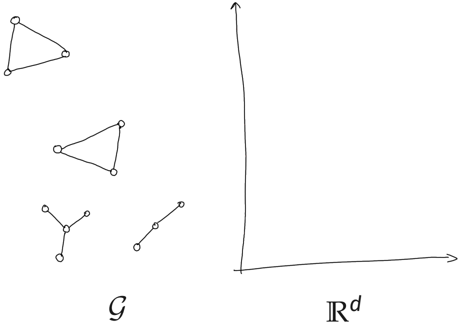


The problem with vectorial graph representations

We want our graph representation function ϕ to be



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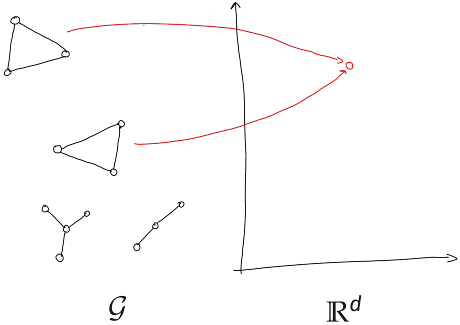
We want our graph representation function ϕ to be

- permutation-invariant

  for all isomorphic graphs

$$G \simeq H : \; \phi(G) = \phi(H)$$



The problem with vectorial graph representations

We want our graph representation function ϕ to be

- permutation-invariant

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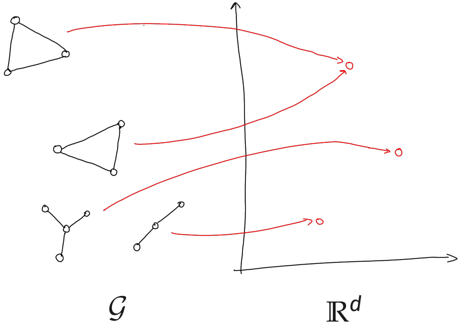
$$G \simeq H: \ \phi(G) = \phi(H)$$

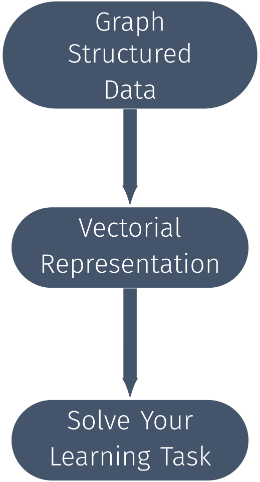
- complete

  for all non-isomorphic graphs

$$G \not\simeq H: \ \phi(G) \neq \phi(H)$$



Why do we care?



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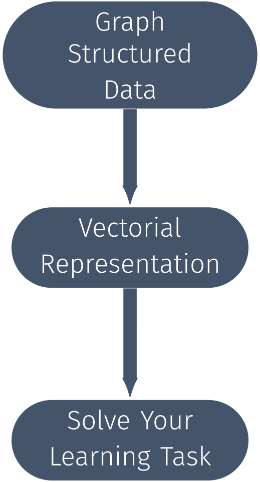
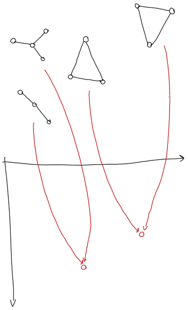




Why do we care?

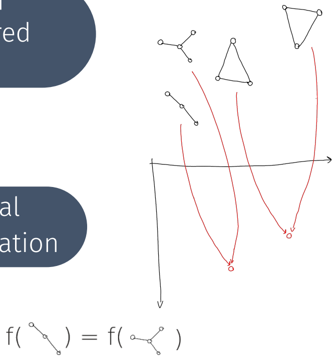
Graph Structured Data

↓

Vectorial Representation

↓

Solve Your Learning Task



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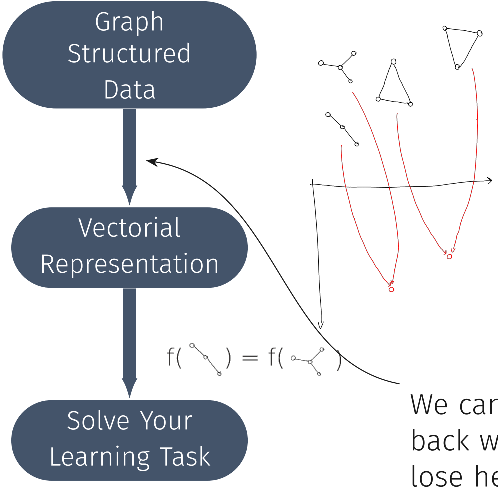

We cannot get back what we lose here

Why do we care?

Graph Structured Data

Vectorial Representation

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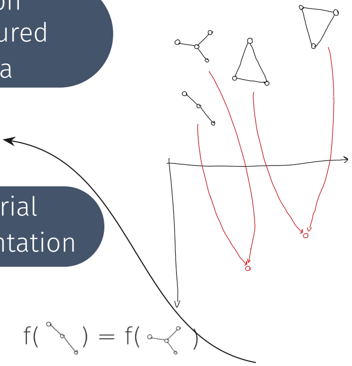

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- Unfortunately computing any permutation invariant and complete embedding (or kernel) is as hard as deciding graph isomorphism

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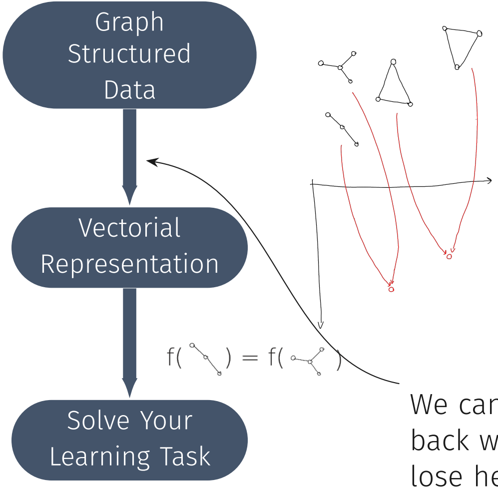

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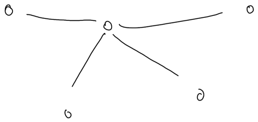
- Unfortunately computing any permutation invariant and complete embedding (or kernel) is as hard as deciding graph isomorphism
- **Typical solution**: drop completeness for efficiency
  - most practical graph kernels, GNNs, Weisfeiler Leman test, …

Message Passing and the Weisfeiler Leman Algorithm

Message Passing

- Let's assume that we have some feature representation $r_0 : V(G) \to \mathbb{R}^d$ for the vertices in our graph



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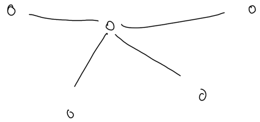

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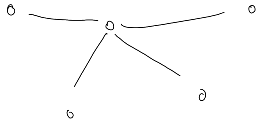

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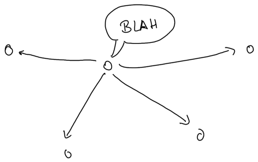
- In turn, neighbors might be influenced by that and hence spread (a variant of) that information (aka. "retweet")



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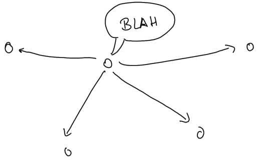
- Message passing models this kind of behavior as a simultaneous round based process



The message passing framework

$$r_{k+1}(v) = \mathrm{upd}_k\left(r_k(v),\ \mathrm{agg}_k\left(\{\{r_k(w) \mid w \in N(v)\}\}\right)\right)$$

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We will omit k in the notation of upd_k and agg_k when $\mathsf{upd}_0 = \mathsf{upd}_1 = \ldots$

Weisfeiler Leman (1)

$$r_{k+1}^{WL}(v) = \#_k \left(r_k^{WL}(v),\ \left\{ \left\{ r_k^{WL}(w) \mid w \in N(v) \right\} \right\} \right)$$

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- $\#_k : \mathcal{X}_k \times \mathbb{N}^{\mathcal{X}_k} \to \mathcal{X}_{k+1}$ is a perfect hash function

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Let's think of the hash values as colors of vertices

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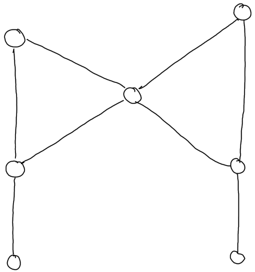

$k = 0$

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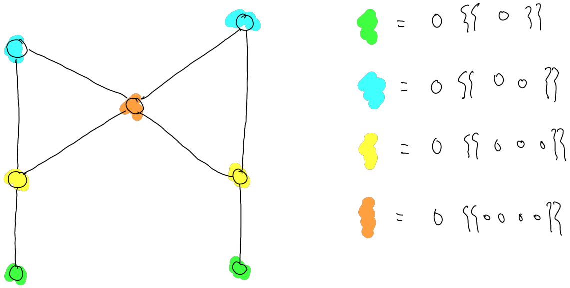

$k = 1$

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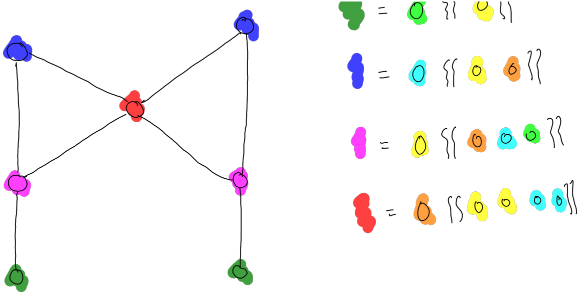

$k = 2$

Message passing graph neural networks (1)

$$r_{k+1}^{MPNN}(v) = \mathrm{MLP}_k^{\mathrm{UPD}}\left(r_k^{MPNN}(v),\ \mathrm{MLP}_k\left(\sum_{w \in N(v)} r_k^{MPNN}(w)\right)\right)$$

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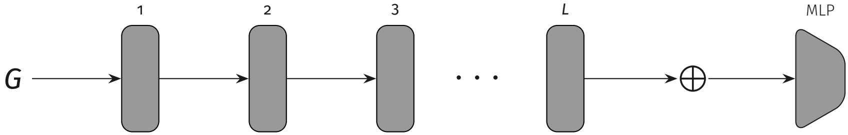

- MPNN layers are stacked on top of each other

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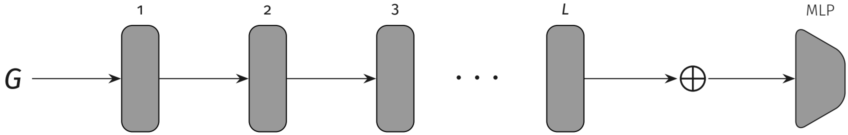
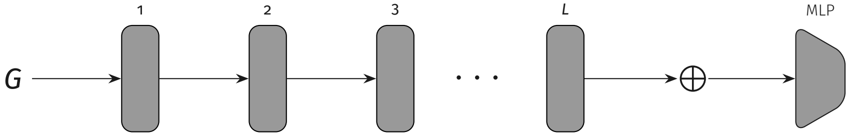


- MPNN layers are stacked on top of each other
- Graph level tasks are solved by summing together all node representations, then a final MLP

Message passing graph neural networks (2)

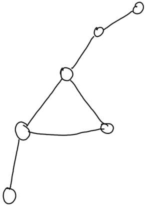


- MPNN layers are stacked on top of each other
- Graph level tasks are solved by summing together all node representations, then a final MLP
- Training can be done with gradient descent

Message Passing and the Weisfeiler Leman Algorithm | Issues

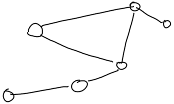
Isomorphic Graphs have Identical WL Label Histograms

G



$r_0^{WL,G}: \{\{\circ\ \circ\ \circ\ \circ\ \circ\ \circ\}\}$

H



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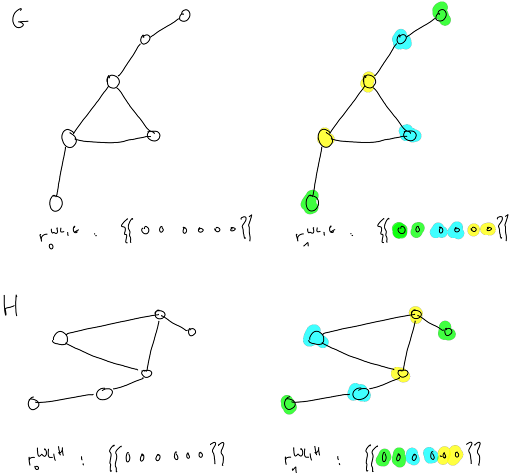

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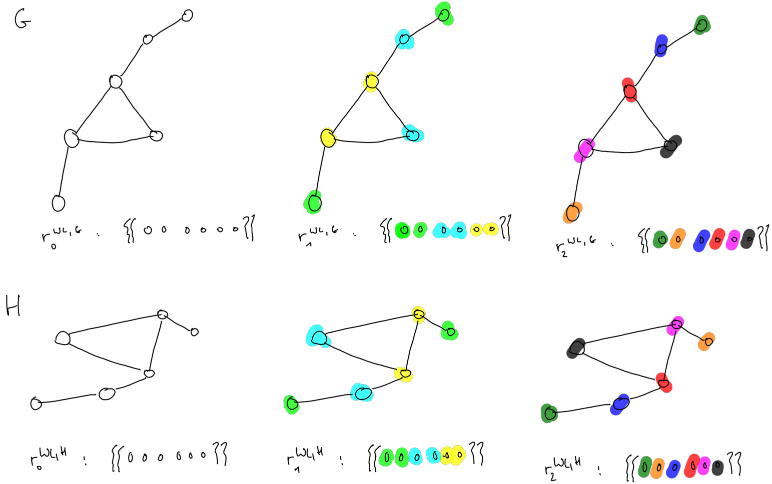

Nonisomorphic Graphs Can Have Identical Label Histograms

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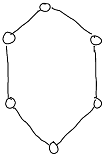
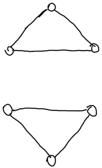


$r_2^{WL,G}$: $\{\{\circ\ \circ\ \circ\ \circ\ \circ\ \circ\}\}$

H



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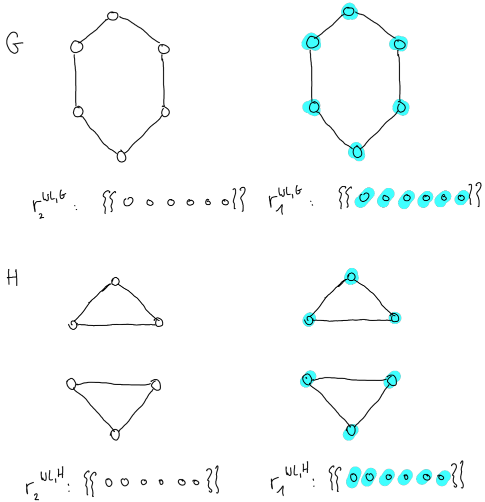

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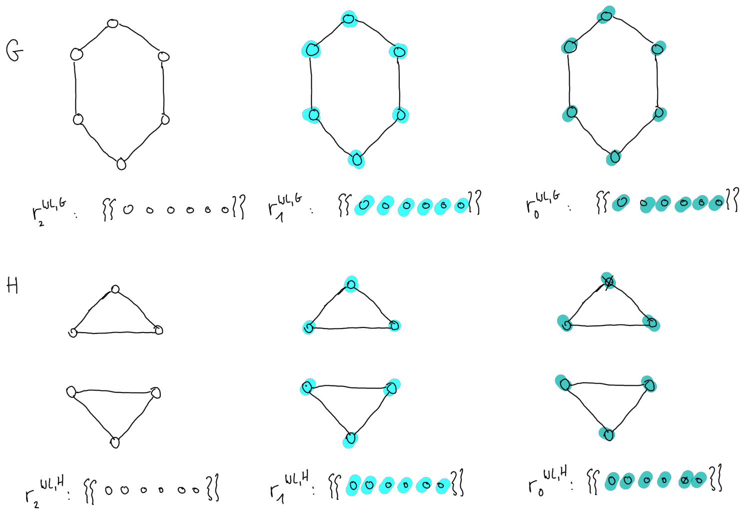

The connection between WL and MPNNs

$$r_k^{\mathrm{WL}}(G) = r_k^{\mathrm{WL}}(H) \Longrightarrow r_k^{\mathrm{MPNN}}(G) = r_k^{\mathrm{MPNN}}(H)$$

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- Whenever WL cannot distinguish two graphs, *any* MPNN cannot compute different representations
- MPNNs are incomplete
- Their incompleteness can be bounded by the incompleteness of the WL algorithm

Homomorphism Counts as Graph Representations

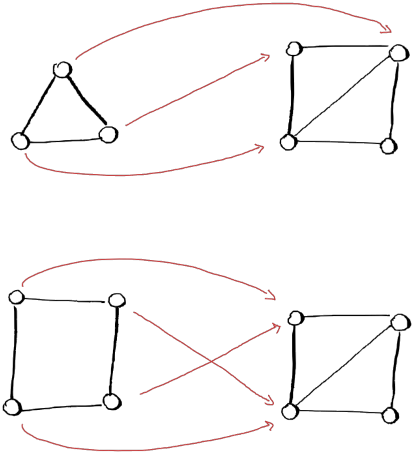
Homomorphism

A *homomorphism* from H to G is a function

$$h : V(H) \to V(G)$$

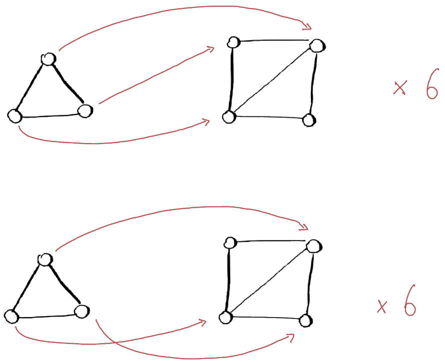
such that

$$(v, w) \in E(H) \implies (h(v), h(w)) \in V(G)$$



Counting Homomorphisms

Given ***H*** and ***G***, we can ask *how many* homomorphisms exist from ***H*** to ***G***?



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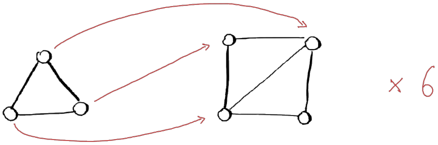
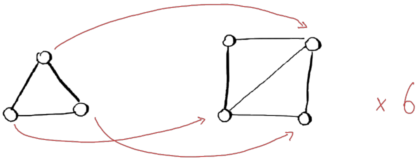
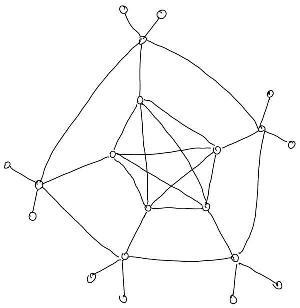




There are twelve homomorphisms from $\boldsymbol{H}$ to $\boldsymbol{G}$!

An intractable complete graph embedding

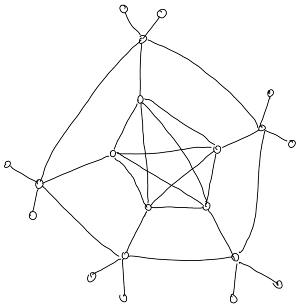
G



An intractable complete graph embedding

$\varphi_n(G)$

G



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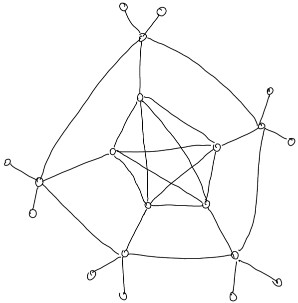

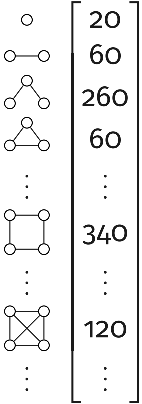

Theorem [Lovász 1967].
Two graphs G and H are isomorphic iff $\varphi_n(G) = \varphi_n(H)$

We can count homomorphisms (for some graphs) in practice!

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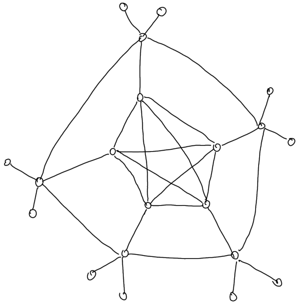
- Homomorphism counting is fixed parameter tractable
- The parameter is called tree-width
- If the pattern H has tree-width k, the homomorphisms from H to any G can be counted in $O(|V(G)|^k)$

An intractable complete graph embedding

G



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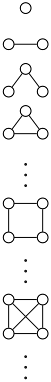
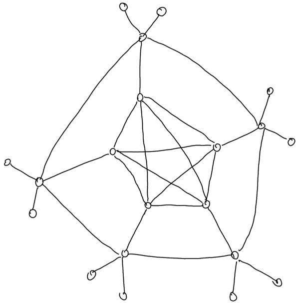


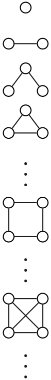
$$\begin{bmatrix} 20 \\ 60 \\ 260 \\ 60 \\ \vdots \\ 340 \\ \vdots \\ 120 \\ \vdots \end{bmatrix}$$

An intractable complete graph embedding

G



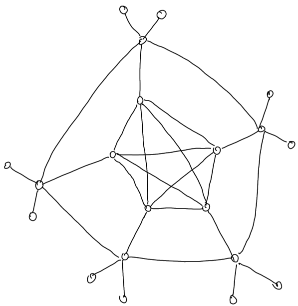
$\varphi_n(G)$

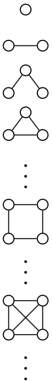


$$\begin{bmatrix} 20 \\ 60 \\ 260 \\ 60 \\ \vdots \\ 340 \\ \vdots \\ 120 \\ \vdots \end{bmatrix} \begin{array}{c} \\ \leftarrow \\ \\ \leftarrow \\ \\ \leftarrow \\ \\ \leftarrow \\ \\ \end{array}$$

~~An in~~tractable complete graph embedding

G





$$\varphi_n(G) = \begin{bmatrix} 20 \\ 60 \\ 260 \\ 60 \\ \vdots \\ 340 \\ \vdots \\ 120 \\ \vdots \end{bmatrix} \quad \begin{matrix} \\ \leftarrow \\ \\ \leftarrow \\ \\ \leftarrow \\ \\ \leftarrow \\ \\ \end{matrix} \quad \varphi_{\mathcal{F}}(G) = \begin{bmatrix} 0 \\ 60 \\ 0 \\ 60 \\ 0 \\ 340 \\ 0 \\ 120 \\ 0 \end{bmatrix}$$

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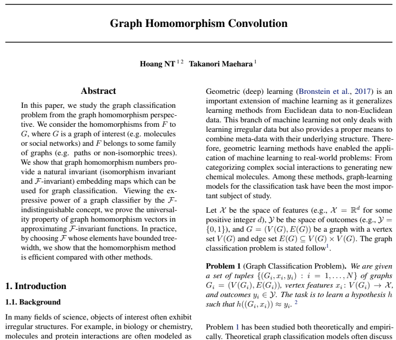
We will now see two variants how to select patterns

Graph Homomorphism Convolution (GHC)

NT and Maehara (2020)

- Introduce homomorphism counts as feature vectors of graphs



Graph Homomorphism Convolution

Hoang NT [1 2] Takanori Maehara [1]

Abstract

In this paper, we study the graph classification problem from the graph homomorphism perspective. We consider the homomorphisms from F to G, where G is a graph of interest (e.g. molecules or social networks) and F belongs to some family of graphs (e.g. paths or non-isomorphic trees). We show that graph homomorphism numbers provide a natural invariant (isomorphism invariant and $\mathcal{F}$-invariant) embedding maps which can be used for graph classification. Viewing the expressive power of a graph classifier by the $\mathcal{F}$-indistinguishable concept, we prove the universality property of graph homomorphism vectors in approximating $\mathcal{F}$-invariant functions. In practice, by choosing $\mathcal{F}$ whose elements have bounded tree-width, we show that the homomorphism method is efficient compared with other methods.

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In many fields of science, objects of interest often exhibit irregular structures. For example, in biology or chemistry, molecules and protein interactions are often modeled as

Geometric (deep) learning (Bronstein et al., 2017) is an important extension of machine learning as it generalizes learning methods from Euclidean data to non-Euclidean data. This branch of machine learning not only deals with learning irregular data but also provides a proper means to combine meta-data with their underlying structure. Therefore, geometric learning methods have enabled the application of machine learning to real-world problems: From categorizing complex social interactions to generating new chemical molecules. Among these methods, graph-learning models for the classification task have been the most important subject of study.

Let $\mathcal{X}$ be the space of features (e.g., $\mathcal{X} = \mathbb{R}^d$ for some positive integer d), $\mathcal{Y}$ be the space of outcomes (e.g., $\mathcal{Y} = \{0, 1\}$), and $G = (V(G), E(G))$ be a graph with a vertex set $V(G)$ and edge set $E(G) \subseteq V(G) \times V(G)$. The graph classification problem is stated follow[1].

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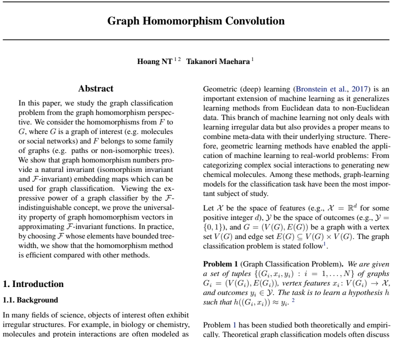

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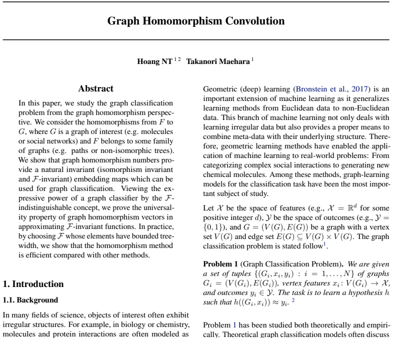

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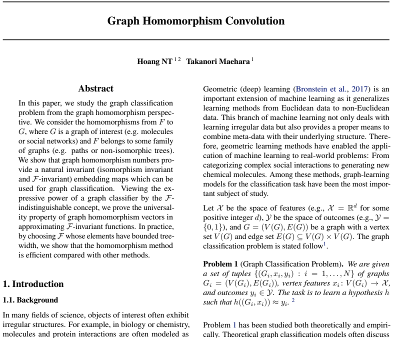

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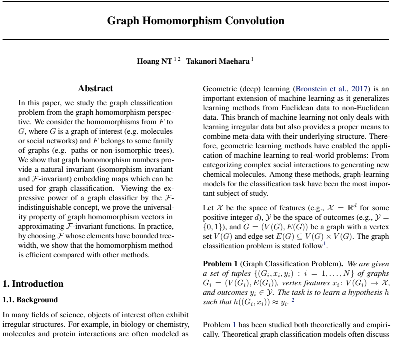
- Use an SVM with these features



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GHC: Experimental results

Table 2. Classification accuracy over 10 experiments
(a) Synthetic datasets

METHODS	CSL	BIPARTITE	PAULUS25
Practical models			
GIN	10.00 ± 0.00	55.75 ± 7.91	7.14 ± 0.00
GNTK	10.00 ± 0.00	58.03 ± 6.84	7.14 ± 0.00
Theory models			
Ring-GNN	$10 \sim 80 \pm 15.7$	55.72 ± 6.95	7.15 ± 0.00
GHC-Tree	10.00 ± 0.00	52.68 ± 7.15	7.14 ± 0.00
GHC-Cycle	$\mathbf{100.0} \pm \mathbf{0.00}$	$\mathbf{100.0} \pm \mathbf{0.00}$	7.14 ± 0.00

(b) Benchmark datasets

METHODS	MUTAG	IMDB-BIN	IMDB-MUL
Practical models			
GNTK	89.46 ± 7.03	75.61 ± 3.98	51.91 ± 3.56
GIN	89.40 ± 5.60	70.70 ± 1.10	43.20 ± 2.00
PATCHY-SAN	89.92 ± 4.50	71.00 ± 2.20	45.20 ± 2.80
WL kernel	90.40 ± 5.70	73.80 ± 3.90	50.90 ± 3.80
Theory models			
Ring-GNN	78.07 ± 5.61	73.00 ± 5.40	48.20 ± 2.70
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GHC: Experimental results

Table 2. Classification accuracy over 10 experiments
(a) Synthetic datasets

METHODS	CSL	BIPARTITE	PAULUS25
Practical models			
GIN	10.00 ± 0.00	55.75 ± 7.91	7.14 ± 0.00
GNTK	10.00 ± 0.00	58.03 ± 6.84	7.14 ± 0.00
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Ring-GNN	$10 \sim 80 \pm 15.7$	55.72 ± 6.95	7.15 ± 0.00
GHC-Tree	10.00 ± 0.00	52.68 ± 7.15	7.14 ± 0.00
GHC-Cycle	$\mathbf{100.0 \pm 0.00}$	$\mathbf{100.0 \pm 0.00}$	7.14 ± 0.00

(b) Benchmark datasets

METHODS	MUTAG	IMDB-BIN	IMDB-MUL
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GNTK	89.46 ± 7.03	75.61 ± 3.98	51.91 ± 3.56
GIN	89.40 ± 5.60	70.70 ± 1.10	43.20 ± 2.00
PATCHY-SAN	89.92 ± 4.50	71.00 ± 2.20	45.20 ± 2.80
WL kernel	90.40 ± 5.70	73.80 ± 3.90	50.90 ± 3.80
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- Good results on some synthetic datasets
- Competitive results on (smaller) benchmark datasets

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- GHC in practice requires a fixed, user defined choice of the pattern set $\mathcal{F}$

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- GHC in practice requires a fixed, user defined choice of the pattern set $\mathcal{F}$
- This allows to bound the expressivity of GHC by an extension of the WL algorithm: k-WL (Neuen (2024))

Expectation-Complete Graph Representations with Homomorphisms




ICML 2023

Pascal Welke*, Maximilian Thiessen*, Fabian Jogl, and Thomas Gärtner

TU Wien
Vienna | Austria
Research Unit Machine Learning

At a glance

- Expressiveness bounded by k-WL

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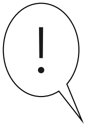

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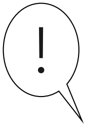

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$\Rightarrow$ allows to adapt to challenging learning tasks without domain knowledge

$\Rightarrow$ works well in practice

What if we keep completeness . . .

. . . in expectation?

Expectation complete graph embeddings

Let $\phi_X : \mathcal{G} \to V$ depend on a random variable X drawn from a distr. $\mathcal{D}$ over a set $\mathcal{X}$

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We call ϕ_X complete in expectation if the expectation

$$\mathop{\mathbb{E}}_{X \sim \mathcal{D}}[\phi_X(\cdot)] = \sum_{t \in \mathcal{X}} \Pr(X = t)\phi_t(\cdot)$$

is a complete graph embedding

What is the benefit?

Sampling $X_1, X_2, X_3, \ldots$ will eventually make the joint embedding

$$(\phi_{X_1}(G), \phi_{X_2}(G), \phi_{X_3}(G), \ldots)$$

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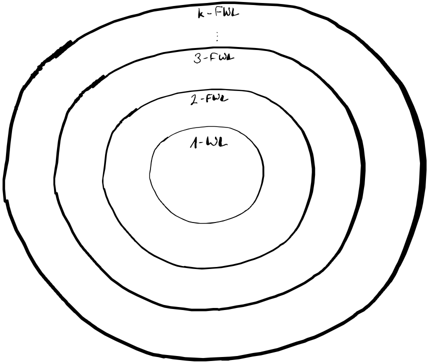

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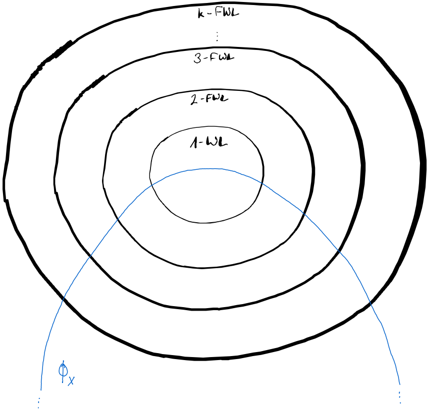

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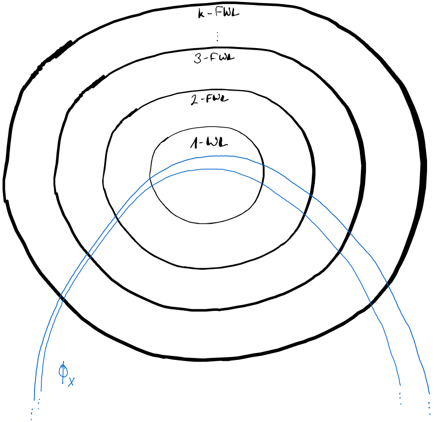

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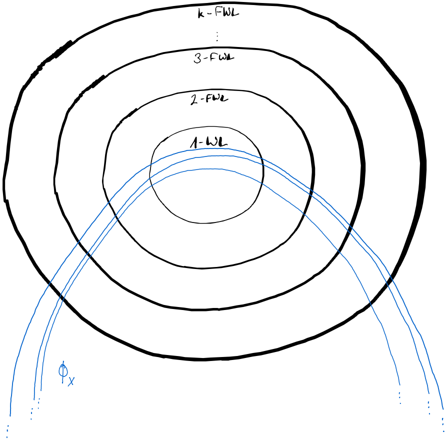

What if we keep completeness …

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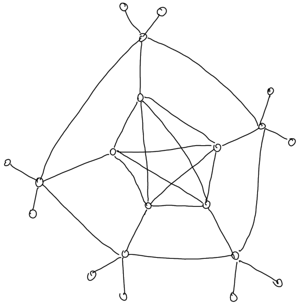
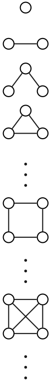
… efficiently

An intractable complete graph embedding

G



$\varphi_n(G)$



$$\begin{bmatrix}20\\60\\260\\60\\\vdots\\340\\\vdots\\120\\\vdots\end{bmatrix}$$

An intractable complete graph embedding

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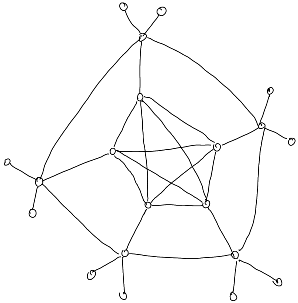

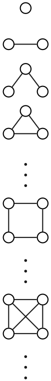

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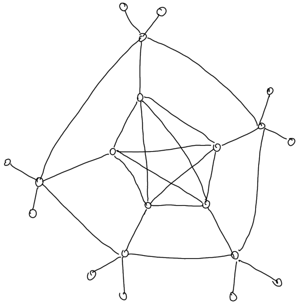

$$\varphi_n(G) = \begin{bmatrix} 20 \\ 60 \\ 260 \\ 60 \\ \vdots \\ 340 \\ \vdots \\ 120 \\ \vdots \end{bmatrix} \qquad \begin{matrix} \\ \leftarrow \\ \\ \leftarrow \\ \\ \leftarrow \\ \\ \leftarrow \\ \\ \end{matrix} \qquad \varphi_{\mathcal{F}}(G) = \begin{bmatrix} 0 \\ 60 \\ 0 \\ 60 \\ 0 \\ 340 \\ 0 \\ 120 \\ 0 \end{bmatrix}$$

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We can make any (message passing) GNN expectation-complete

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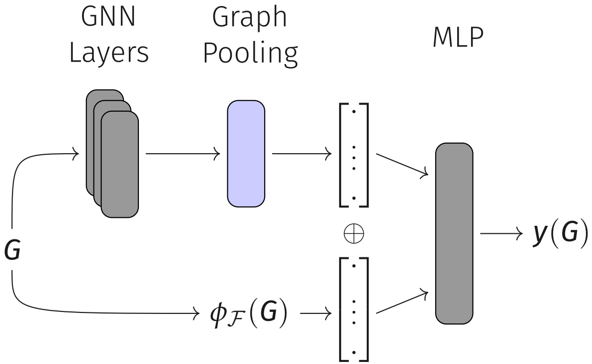
ICML 2023
LoG 2023



Empirical results

Table 1. Performance of different GNNs on 9 OGB benchmarks and `ZINC`. Baseline of a GNN with homorphism counts is the same GNN without homomorphism counts. Results for GNNs with homorphism counts are averaged over 9 different random samples of pattern graphs.

	Top 1 / 2 / 3	Beats baseline
GIN	0% / 0% / 0%	-
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GCN	0% / 0% / 0%	-
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Table 2. Accuracy on synthetic data

Method	CSL	PAULUS25
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Ours	37.67 ± 9.11	100.0 ± 0.00

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Homomorphism Counts as Node Representations

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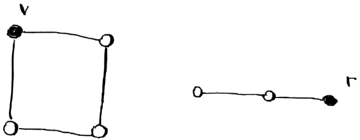

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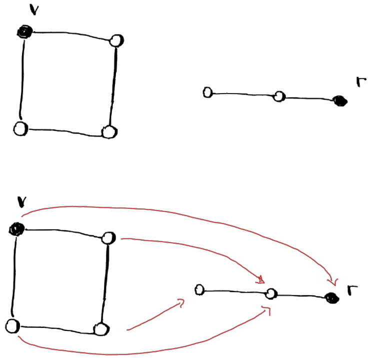

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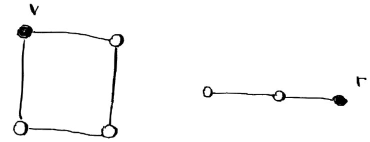

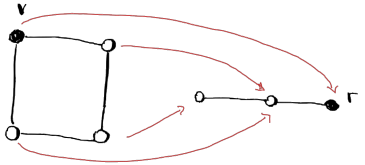

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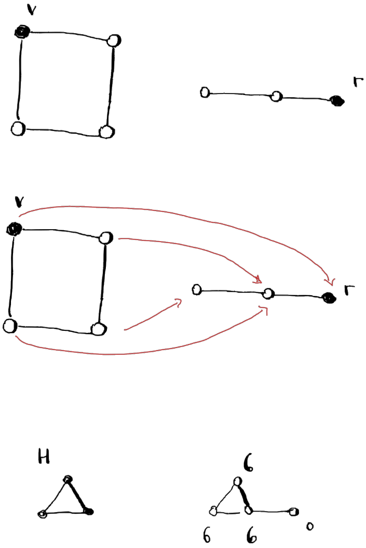

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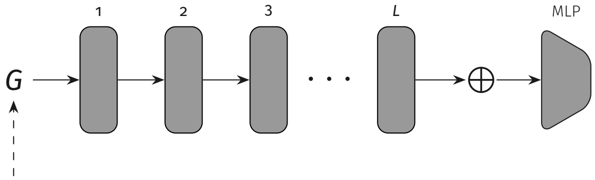
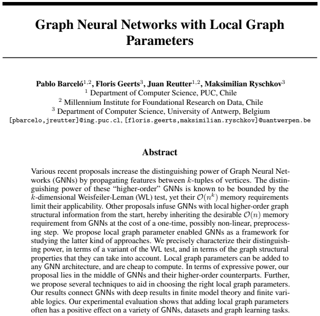


add hom-counts here

- This architecture is more expressive than WL



Graph Neural Networks with Local Graph Parameters

Pablo Barceló[1,2], Floris Geerts[3], Juan Reutter[1,2], Maksimilian Ryschkov[3]
[1] Department of Computer Science, PUC, Chile
[2] Millennium Institute for Foundational Research on Data, Chile
[3] Department of Computer Science, University of Antwerp, Belgium
[pbarcelo,jreutter]@ing.puc.cl, [floris.geerts,maksimilian.ryschkov]@uantwerpen.be

Abstract

Various recent proposals increase the distinguishing power of Graph Neural Networks (GNNs) by propagating features between k-tuples of vertices. The distinguishing power of these "higher-order" GNNs is known to be bounded by the k-dimensional Weisfeiler-Leman (WL) test, yet their $\mathcal{O}(n^k)$ memory requirements limit their applicability. Other proposals infuse GNNs with local higher-order graph structural information from the start, hereby inheriting the desirable $\mathcal{O}(n)$ memory requirement from GNNs at the cost of a one-time, possibly non-linear, preprocessing step. We propose local graph parameter enabled GNNs as a framework for studying the latter kind of approaches. We precisely characterize their distinguishing power, in terms of a variant of the WL test, and in terms of the graph structural properties that they can take into account. Local graph parameters can be added to any GNN architecture, and are cheap to compute. In terms of expressive power, our proposal lies in the middle of GNNs and their higher-order counterparts. Further, we propose several techniques to aid in choosing the right local graph parameters. Our results connect GNNs with deep results in finite model theory and finite variable logics. Our experimental evaluation shows that adding local graph parameters often has a positive effect on a variety of GNNs, datasets and graph learning tasks.

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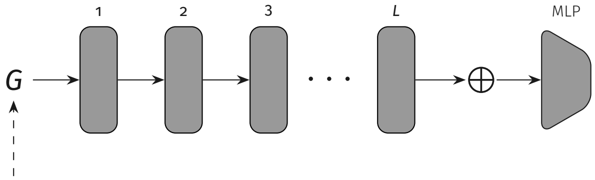
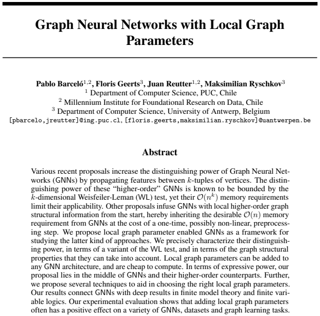


add hom-counts here

- This architecture is more expressive than WL
- It is incomparable to 2-WL



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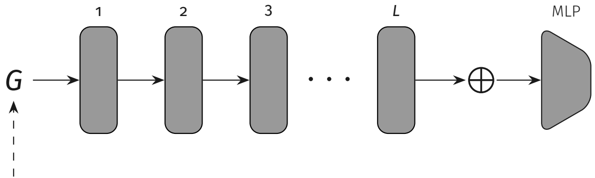
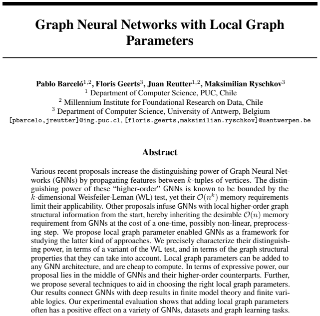


add hom-counts here

- This architecture is more expressive than WL
- It is incomparable to 2-WL
- Can be bounded by $\mathcal{F}$-WL (!)



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Abstract

Various recent proposals increase the distinguishing power of Graph Neural Networks (GNNs) by propagating features between k-tuples of vertices. The distinguishing power of these "higher-order" GNNs is known to be bounded by the k-dimensional Weisfeiler-Leman (WL) test, yet their $\mathcal{O}(n^k)$ memory requirements limit their applicability. Other proposals infuse GNNs with local higher-order graph structural information from the start, hereby inheriting the desirable $\mathcal{O}(n)$ memory requirement from GNNs at the cost of a one-time, possibly non-linear, preprocessing step. We propose local graph parameter enabled GNNs as a framework for studying the latter kind of approaches. We precisely characterize their distinguishing power, in terms of a variant of the WL test, and in terms of the graph structural properties that they can take into account. Local graph parameters can be added to any GNN architecture, and are cheap to compute. In terms of expressive power, our proposal lies in the middle of GNNs and their higher-order counterparts. Further, we propose several techniques to aid in choosing the right local graph parameters. Our results connect GNNs with deep results in finite model theory and finite variable logics. Our experimental evaluation shows that adding local graph parameters often has a positive effect on a variety of GNNs, datasets and graph learning tasks.

Experimental Results

(a) Results for the ZINC dataset show that homomorphism (hom) counts of cycles improve every model. We compare the mean absolute error (MAE) of each model without any homomorphism count (baseline), against the model augmented with the hom count, and with subgraph isomorphism (iso) counts of C_3–C_{10}.

MODEL	MAE (BASE)	MAE (HOM)	MAE (ISO)
GAT	0.47±0.02	**0.22±0.01**	0.24±0.01
GCN	0.35±0.01	**0.20±0.01**	0.22±0.01
GraphSage	0.44±0.01	**0.24±0.01**	0.24±0.01
MoNet	0.25±0.01	0.19±0.01	**0.16±0.01**
GatedGCN	0.34±0.05	**0.1353±0.01**	0.1357±0.01

(b) The effect of different cycles for the GAT model over the ZINC dataset, using mean absolute error.

SET ($\mathcal{F}$)	MAE
NONE	0.47±0.02
$\{C_3\}$	0.45±0.01
$\{C_4\}$	0.34±0.02
$\{C_6\}$	0.31±0.01
$\{C_5, C_6\}$	0.28±0.01
$\{C_3, \ldots, C_6\}$	0.23±0.01
$\{C_3, \ldots, C_{10}\}$	**0.22±0.01**

Table 2: Results for the PATTERN dataset show that homomorphism counts improve all models except GatedGCN. We compare weighted accuracy of each model without any homomorphism count (baseline) against the model augmented with the counts of the set $\mathcal{F}$ that showed best performance (best $\mathcal{F}$).

MODEL + BEST $\mathcal{F}$	ACCURACY BASELINE	ACCURACY BEST
GAT $\{K_3, K_4, K_5\}$	78.83 ± 0.60	85.50 ± 0.23
GCN $\{K_3, K_4, K_5\}$	71.42 ± 1,38	82.49 ± 0.48
GraphSage $\{K_3, K_4, K_5\}$	70.78 ± 0,19	85,85 ± 0.15
MoNet $\{K_3, K_4, K_5\}$	85.90 ± 0,03	**86.63 ± 0.03**
GatedGCN $\{\emptyset\}$	86.15 ± 0.08	86.15 ± 0.08

Table 3: All models improve the Hits@50 metric over the COLLAB dataset. We compare each model without any homomorphism count (baseline) against the model augmented with the counts of the set of patterns that showed best performance (best $\mathcal{F}$).

MODEL + BEST $\mathcal{F}$	HITS@50 BASELINE	HITS@50 BEST
GAT $\{K_3\}$	50.32±0.55	52.87±0.87
GCN $\{K_3, K_4, K_5\}$	51.35±1.30	**54.60±1.01**
GraphSage $\{K_5\}$	50.33±0.68	51.39±1.23
MoNet $\{K_4\}$	49.81±1.56	51.76±1.38
GatedGCN $\{K_3\}$	51.00±2.54	51.57±0.68

Insights?

- By adding homcounts to the node labels before message passing, we get an architecture that is at least as expressive as message passing

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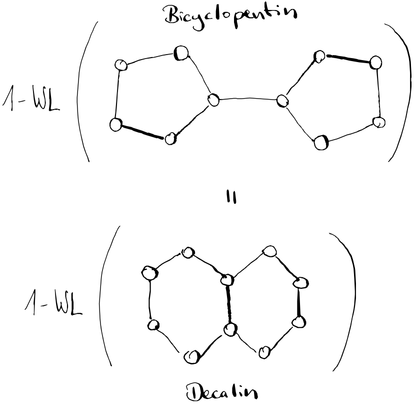
- By adding homcounts to the node labels before message passing, we get an architecture that is at least as expressive as message passing
- Cycle counting seems to be important ;)

GNNs can Count Homomorphisms – Implicitly

Practical problem

- 1-WL is sometimes not expressive enough



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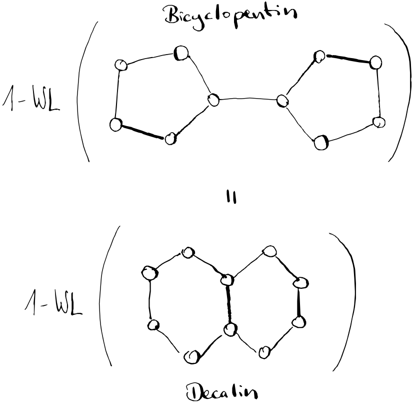

Practical problem

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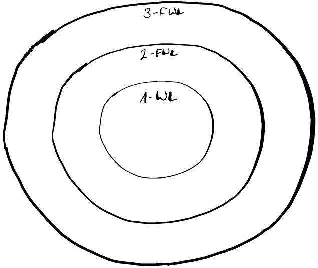
- 2-FWL is already impractical



Weisfeiler and Leman Go Loopy: A New Hierarchy for Graph Representational Learning




NeurIPS 2024 (oral)

Raffaele Paolino*, Sohir Maskey*, Pascal Welke, and Gitta Kutyniok

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

TU WIEN

At a glance

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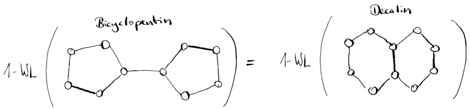

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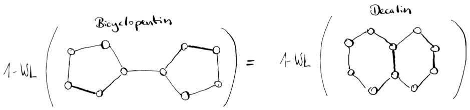

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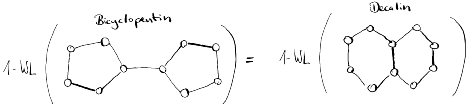

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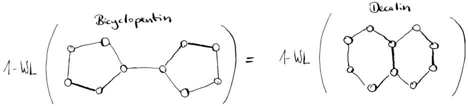

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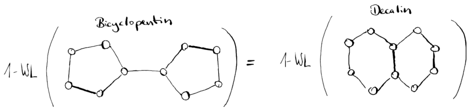

- we propose a generalized message passing architecture
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- fast in practice, s.o.t.a. results

Contributions

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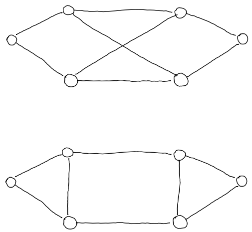

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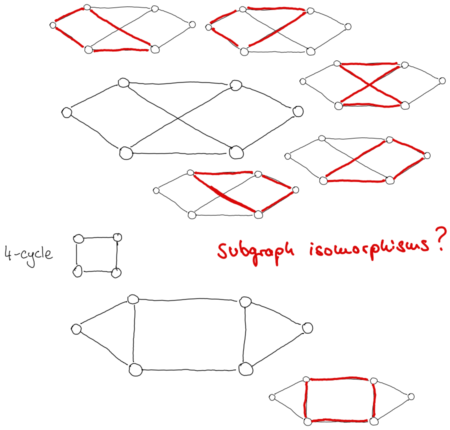

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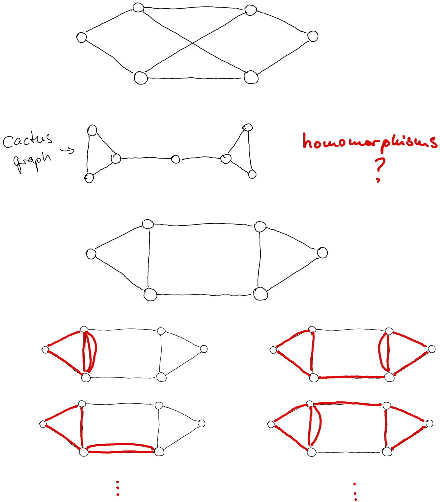
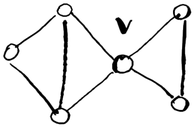


A glimpse at the implementation



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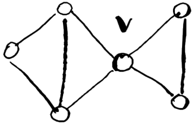

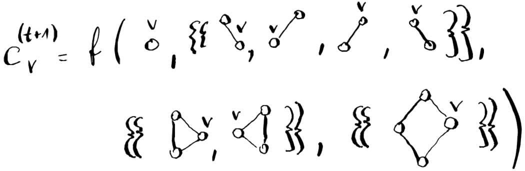

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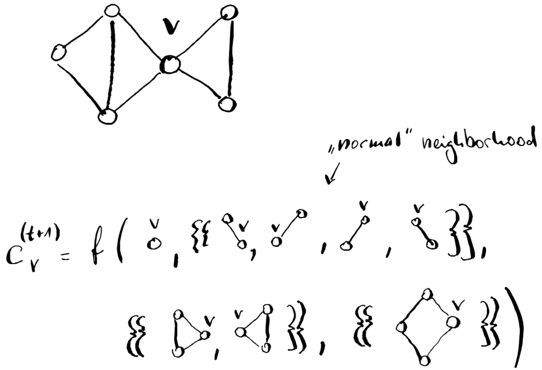

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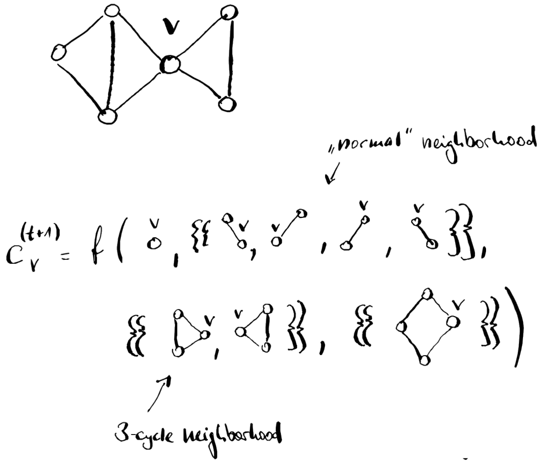

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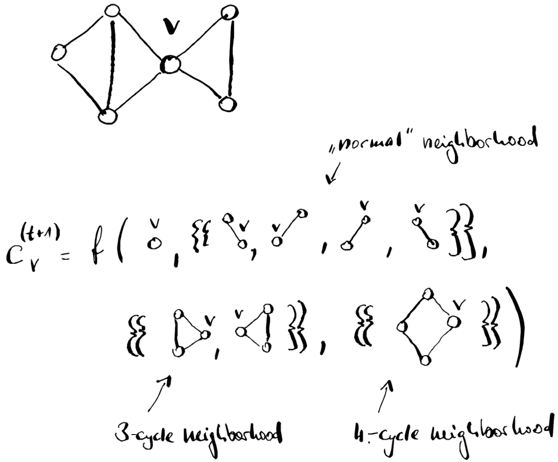

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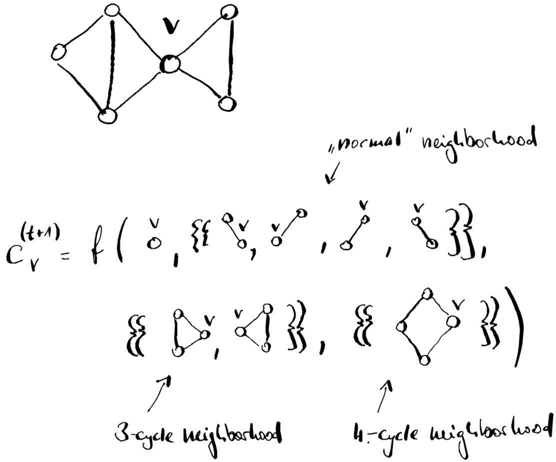

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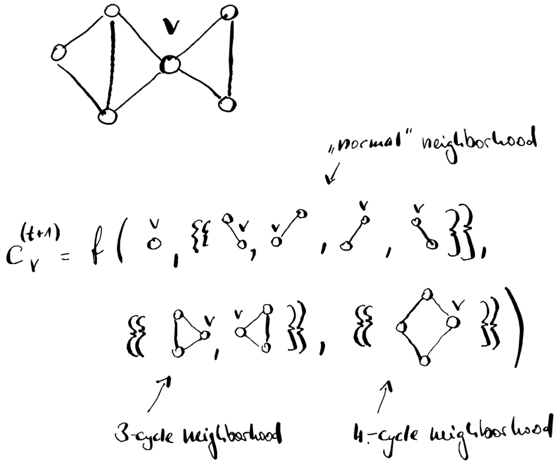

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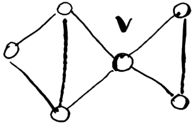

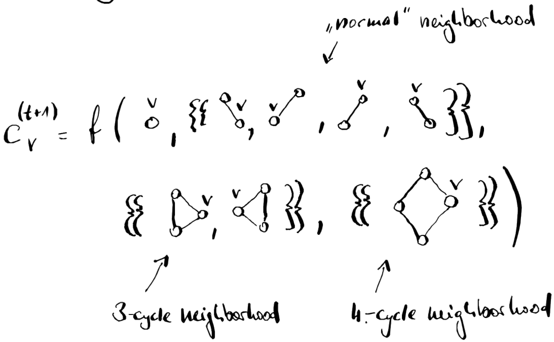

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A complete representation for cycles :

Empirical results

Table 4: Normalized test MAE (↓) on graph regression, QM9 dataset. Top three models as $\boxed{1^{\text{st}}}$, $\boxed{2^{\text{nd}}}$, $\underline{3^{\text{rd}}}$.

Model	μ	α	$\varepsilon_{\text{homo}}$
1-GNN	0.493	0.78	0.00321
1-2-3-GNN	0.476	0.27	0.00337
DTNN	$\boxed{0.244}$	0.95	0.00388
Deep LRP	0.364	0.298	$\underline{0.00254}$
PPGN	$\boxed{0.231}$	0.382	0.00276
NestedGNN	0.428	0.290	0.00265
I2-GNN	0.428	$\underline{0.230}$	0.00261
DRFWL GNN	$\underline{0.346}$	$\boxed{0.222}$	$\boxed{0.00226}$
5-ℓGIN	0.350 ± 0.011	$\boxed{0.217}$ ± 0.025	$\boxed{0.00205}$ ± 0.00005

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Table 3: Test MAE (↓) on graph regression, ZINC dataset. Top three models as 1[st], 2[nd], 3[rd].

Model	ZINC12K	ZINC250K
GIN	0.163 ± 0.004	0.088 ± 0.002
GCN	0.321 ± 0.009	-
GAT	0.384 ± 0.007	-
GSN	0.115 ± 0.012	-
CIN	0.079 ± 0.006	0.022 ± 0.002
NestedGNN	0.111 ± 0.003	0.029 ± 0.001
SUN	0.083 ± 0.003	-
GNNAK+	0.080 ± 0.001	-
I2-GNN	0.083 ± 0.001	0.023 ± 0.001
DRFWL GNN	0.077 ± 0.002	0.025 ± 0.003
SignNet	0.084 ± 0.004	0.024 ± 0.003
HIMP	0.151 ± 0.006	0.036 ± 0.002
PathNN	0.090 ± 0.004	-
5-ℓGIN	0.072 ± 0.002	0.022 ± 0.001

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How are they connected?

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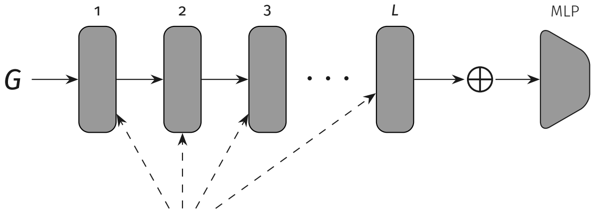
How are they connected?

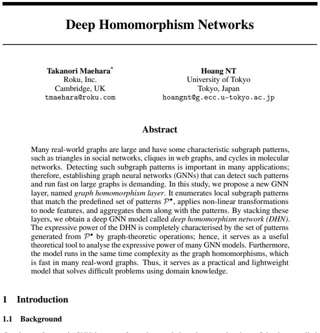
Can we collect most of our results in one architecture?

Deep Homomorphism Networks



change the layers

- Message passing can be generalized to homomorphism counting



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Abstract

Many real-world graphs are large and have some characteristic subgraph patterns, such as triangles in social networks, cliques in web graphs, and cycles in molecular networks. Detecting such subgraph patterns is important in many applications; therefore, establishing graph neural networks (GNNs) that can detect such patterns and run fast on large graphs is demanding. In this study, we propose a new GNN layer, named *graph homomorphism layer*. It enumerates local subgraph patterns that match the predefined set of patterns $\mathcal{P}^\bullet$, applies non-linear transformations to node features, and aggregates them along with the patterns. By stacking these layers, we obtain a deep GNN model called *deep homomorphism network (DHN)*. The expressive power of the DHN is completely characterised by the set of patterns generated from $\mathcal{P}^\bullet$ by graph-theoretic operations; hence, it serves as a useful theoretical tool to analyse the expressive power of many GNN models. Furthermore, the model runs in the same time complexity as the graph homomorphisms, which is fast in many real-word graphs. Thus, it serves as a practical and lightweight model that solves difficult problems using domain knowledge.

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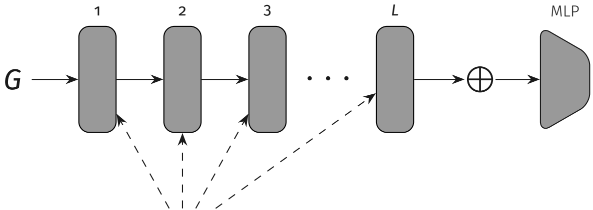
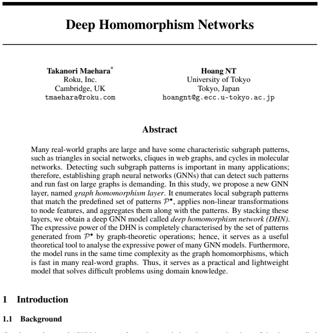


change the layers

- Message passing can be generalized to homomorphism counting
- We have to use a node-weighted variant of homomorphisms, though



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$$\mathrm{GHL}_{\mathcal{P}^\circ}\left((G^\circ, x); \rho, \{\mu_{P^\circ} : P^\circ \in \mathcal{P}^\circ\}\right) :=$$

$$\rho\left(\hom((P^\circ, \mu_{P^\circ}), (G^\circ, x)) : P^\circ \in \mathcal{P}^\circ\right)$$

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  - Homomorphism bases (aka spasms) of patterns allow to compute and learn(!) very powerful graph invariants Jin et al (2024) Dell et al (2018) Curticapean et al (2017)

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