Weisfeiler–Lehman goes Dynamic: An Analysis of the Expressive Power of Graph Neural Networks for Attributed and Dynamic Graphs

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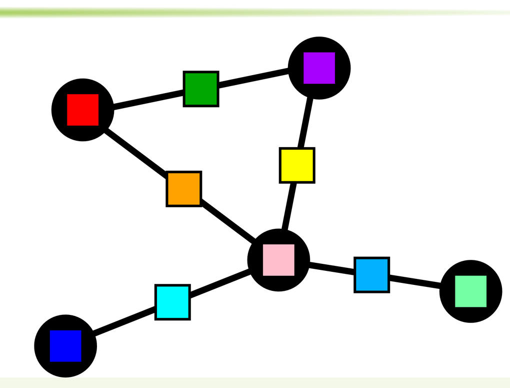
Motivation

- GNNs are as powerful as the Weisfeiler-Lehman test (1-WL) in their ability to distinguish graphs.
- It has been shown that the equivalence enforced by 1-WL equals unfolding equivalence.
- On the other hand, GNNs turned out to be universal approximators on graphs modulo the constraints enforced by 1-WL/unfolding equivalence.
- However, these results only apply to Static Attributed Undirected Homogeneous Graphs (SAUHG) with node attributes.
- This work provides 1-WL test and unfolding trees with corresponding equivalences for attributed and dynamic graphs
- Further, GNNs for attributed and dynamic graphs are analyzed regarding their expressive power

Attributed Graphs

Definition (SAUHG)

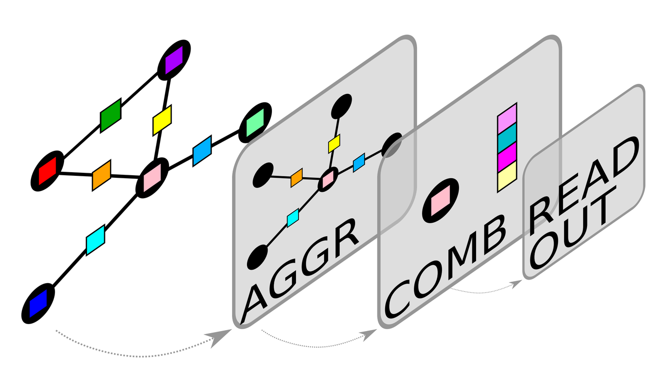
*A **SAUHG** is a static, node/edge attributed, undirected, homogeneous graph (SAUHG) graph.*



SGNN

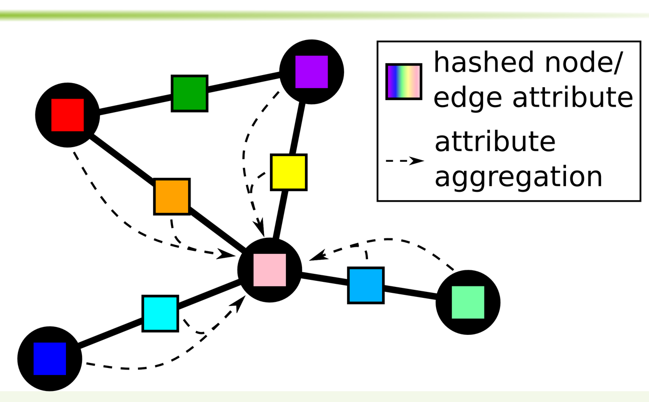
The propagation scheme of the SAUHG GNN is determined by:

- COMBINATION of the node representation of the previous iteration
- AGGREGATION of representations of neighbors and their edge attributes
- output is then determined via a suitable READOUT function.



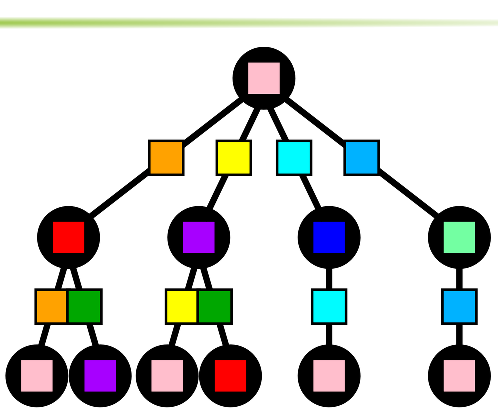
Attributed WL Test

The **attributed WL test** extends the standard 1-WL test by aggregating additionally over the edge attributes of the neighbour nodes.



Attributed Unfolding Tree

The **Attributed Unfolding Tree** of a node in a graph is iteratively determined by the concatenation of its neighbors incl. node and edge attributes up to a certain depth.

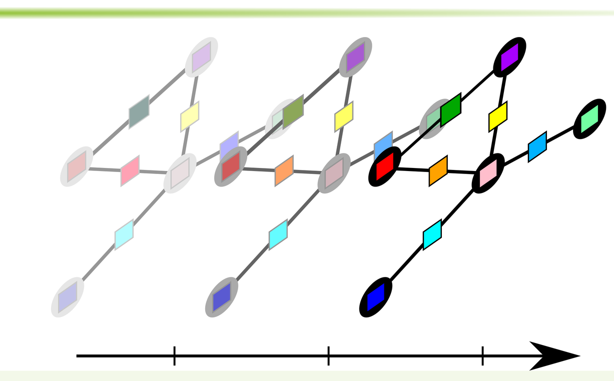


The attributed unfolding tree of the center node of depth 2.

Dynamic Graphs

Definition (Dynamic Graphs)

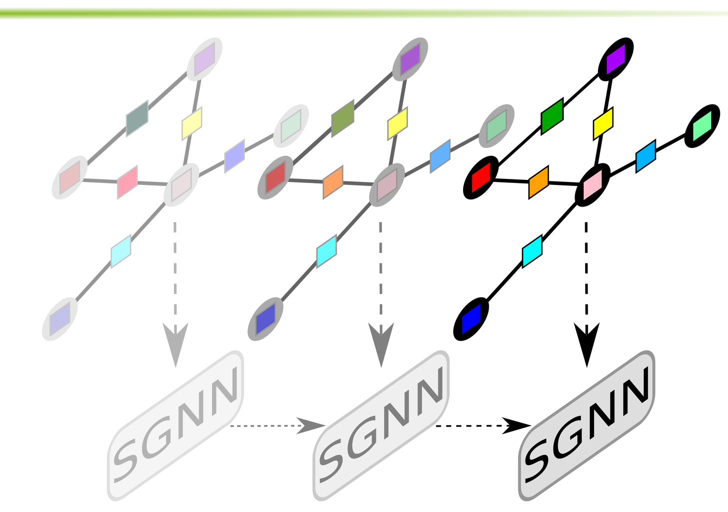
*A graph is **dynamic** if it is time dependent, here formalized as sequence of static graph snapshots.*



DGNN

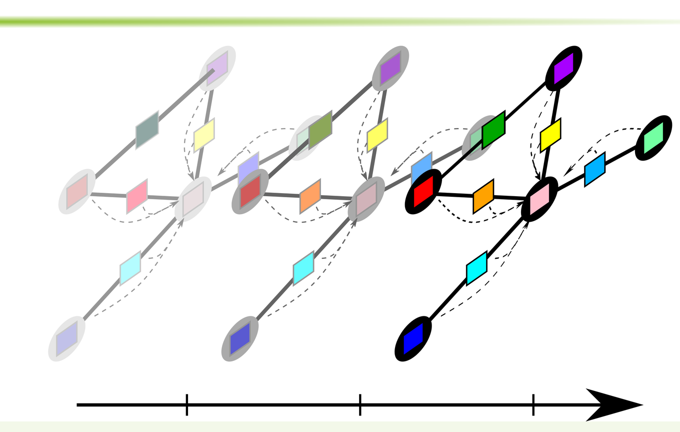
The propagation scheme of the Dynamic GNN is determined by:

- COMBINATION, AGGREGATION and READOUT as in SGNN
- stacked SGNN over time by temporal function



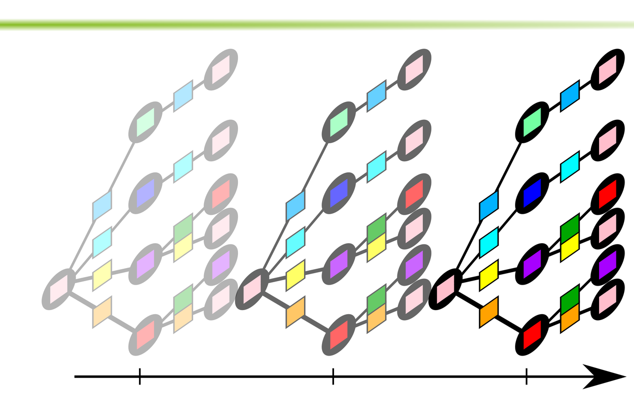
Dynamic WL Test

The **dynamic 1-WL test** is defined by applying 1-AWL on each timestamp. Therefore, here we have a colouring vector.



Dynamic Unfolding Tree

The **Dynamic Unfolding Tree** of a node in a dynamic graph is given by the set of attributed unfolding trees per timestamp.



The dynamic unfolding tree of depth 2 over 3 timestamps.

Universal Aproximation SGNN

For any attributed unfolding equivalence-preserving function, there exists an SGNN that can approximate it in probability and up to any precision.

Universal Aproximation DGNN

For any dynamic system, there exists a DGNN with N layers and SGNNs with hidden dimension 1, and RNN state dimension 1 **that can approximate it in probability and up to any precision.**

Dicussion and Future Work

- The theorems hold for any type of graph.
- Using a hidden and recurrent state dimension 1 is already sufficient.
- Future work includes the extension of the analysis to other GNN architectures and dynamic graph representations and the n-dimensional WL test

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