Lecture 6: Higher-Order Graph Neural Networks

Relational Learning
Overview
Overview

• Motivation
Overview

- Motivation
- The Weisfeiler-Lehman hierarchy
Overview

• Motivation
• The Weisfeiler-Lehman hierarchy
• Higher-order graph neural networks
Overview

• Motivation
• The Weisfeiler-Lehman hierarchy
• Higher-order graph neural networks
  • Higher-order message passing neural networks: k-GNNs
Overview

• Motivation

• The Weisfeiler-Lehman hierarchy

• Higher-order graph neural networks
  • Higher-order message passing neural networks: k-GNNs
  • Invariant/Equivariant graph networks
Overview

• Motivation

• The Weisfeiler-Lehman hierarchy

• Higher-order graph neural networks
  • Higher-order message passing neural networks: k-GNNs
  • Invariant/Equivariant graph networks
  • Provably powerful graph networks
Overview

• Motivation
• The Weisfeiler-Lehman hierarchy
• Higher-order graph neural networks
  • Higher-order message passing neural networks: k-GNNs
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• Expressive power in real-world data
Overview

• Motivation

• The Weisfeiler-Lehman hierarchy

• Higher-order graph neural networks
  • Higher-order message passing neural networks: k-GNNs
  • Invariant/Equivariant graph networks
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• Homophily and heterophily: Comparative perspectives
Overview

• Motivation
• The Weisfeiler-Lehman hierarchy
• Higher-order graph neural networks
  • Higher-order message passing neural networks: k-GNNs
  • Invariant/Equivariant graph networks
  • Provably powerful graph networks
• Expressive power in real-world data
• Homophily and heterophily: Comparative perspectives
• Summary
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One way of achieving more expressive models is through a richer message passing approach — and this is related to Weisfeiler-Lehman hierarchy.
The Weisfeiler-Lehman Hierarchy
A Tale of Two Graphs
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What if we extend the 1-WL algorithm to consider, e.g., pairs of nodes when colouring?
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This extended algorithm is called the 2-dimensional WL algorithm, and it can distinguish these two graphs!
$k$-dimensional Weisfeiler-Lehman
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- We consider a colouring function $\lambda : V_G^k \rightarrow C$ that colours each $k$-tuple of nodes of the graph with a colour from a set $C$ of colours. This colour will depend on the isomorphism type of the tuple, e.g., a $k$-cycle and a $k$-tree will have different colours.
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We denote a $k$-tuple as $t = (u_1, \ldots, u_k)$, and define a substitution as $t[v/i] = (u_1, \ldots, u_{i-1}, v, u_{i+1}, \ldots, u_k)$.
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\forall t, t' \in V^k_G : \lambda^{(i+1)}(t) = \lambda^{(i+1)}(t') \text{ if and only if } \lambda^{(j)}(t) = \lambda^{(j)}(t').
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$k$-dimensional Weisfeiler-Lehman
There are different versions of the Weisfeiler-Lehman algorithm leading to inconsistent dimension counts. We follow the version of Cai et al. (1992), as it has been adopted as the standard in the literature on graph isomorphism testing. This version is also known as folklore Weisfeiler-Lehman algorithm, and sometimes denoted as $k$-FWL.
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We will always refer to the folklore version of this algorithm in the sequel, unless stated explicitly otherwise.
A Tale of Two Graphs
Recall that for all $k \geq 2$ two graphs $G$ and $H$ satisfy the same $C^k$-sentences if and only if $(k - 1)$-WL does not distinguish them (Cai et al., 1992).
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$$\Phi(x) = \exists y, z \ E(x, y) \land E(y, z) \land E(x, z).$$
Recall that for all \( k \geq 2 \) two graphs \( G \) and \( H \) satisfy the same \( C^k \)-sentences if and only if \( (k - 1) \)-WL does not distinguish them (Cai et al., 1992).

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It is easy to see that the graph on the left hand side satisfies \( \Phi(u) \) for any node \( u \), and the graph on the right hand side does not. That is, there are \( C^3 \)-sentences, distinguishing these graphs, and so must 2-WL.
Higher-Order Graph Neural Networks
Higher-Order Message Passing
Neural Networks
Weisfeiler-Lehman: From $1$-GNNs to $k$-GNNs
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This form of message passing can capture structural information that is not visible at the node-level.
Weisfeiler-Lehman: From 1-GNNs to $k$-GNNs
3-GNNs of (Morris et al., 2019) have the same power as folklore 2-WL. For example, 3-GNNs can distinguish the two graphs shown above, by the \#triangles they contain, given by the Boolean formula in $C^3$: 
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This formula states that there are at least three triangles, which is satisfied by the graph on the left hand side but not by the graph on the right hand side. \( k \)-GNNs with \( k \geq 3 \) are strictly more powerful than MPNNs.
Hierarchical Variants
Hierarchical variants of $k$-GNNs, called $1$-$k$-GNNs, aim to combine graph representations learned at different granularities. The idea is to apply message passing starting from one-hot indicator vectors as initial features, and applying the usual node-level message passing (1-WL), and afterwards using the resulting representations to learn better representations for pairs of nodes, with a higher-order message passing (2-WL), etc., illustrated in Figure 1 of (Morris et al., 2019), as shown above.
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Figure 1: Illustration of the proposed hierarchical variant of the $k$-GNN layer. For each subgraph $S$ on $k$ nodes a feature $f$ is learned, which is initialized with the learned features of all $(k - 1)$-element subgraphs of $S$. Hence, a hierarchical representation of the input graph is learned.
Hierarchical Variants

(a) Hierarchical 1-2-3-GNN network architecture  
(b) Pooling from 2- to 3-GNN.

Figure 1: Illustration of the proposed hierarchical variant of the $k$-GNN layer. For each subgraph $S$ on $k$ nodes a feature $f$ is learned, which is initialized with the learned features of all $(k - 1)$-element subgraphs of $S$. Hence, a hierarchical representation of the input graph is learned.
In this hierarchical approach the initial messages in a $k$-GNN are based on the output of lower-dimensional GNNs, which allows the model to effectively capture graph structures of varying granularity.

Many real-world graphs inherit a hierarchical structure in this sense, and so a hierarchical message passing approach is potentially helpful — and this is empirically confirmed in the evaluation of (Morris et al., 2019).
Limitations of $k$-GNNs
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This can hurt the inductive bias, especially when node level features are very important for the task at hand!
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MPNNs are permutation-invariant:

$$\text{POOL}(\text{MPNN}(\mathbf{PAP}^\top, \mathbf{PX})) = \text{POOL}(\mathbf{P(\text{MPNN}(\mathbf{A}, \mathbf{X}))})$$

for any permutation matrix \( \mathbf{P} \), adjacency matrix \( \mathbf{A} \), and feature matrix \( \mathbf{X} \).
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MPNNs are **permutation-invariant**:  
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\text{POOL}\left(\text{MPNN}(\mathbf{P}\mathbf{A}\mathbf{P}^T, \mathbf{P}\mathbf{X})\right) = \text{POOL}\left(\mathbf{P}(\text{MPNN}(\mathbf{A}, \mathbf{X}))\right)
\]
for any permutation matrix \(\mathbf{P}\), adjacency matrix \(\mathbf{A}\), and feature matrix \(\mathbf{X}\).

MPNNs are **permutation-equivariant**:  
\[
\mathbf{P}(\text{MPNN}(\mathbf{A}, \mathbf{X})) = \text{MPNN}(\mathbf{P}\mathbf{A}\mathbf{P}^T, \mathbf{P}\mathbf{X})
\]
for any permutation matrix \(\mathbf{P}\), adjacency matrix \(\mathbf{A}\), and feature matrix \(\mathbf{X}\).
Invariant/Equivariant Graph Networks
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Formally, we consider an order $(k+1)$-tensor $\mathbf{T} \in \mathbb{R}^{|V|^k \times d}$ where the first $k$ channels of this tensor are indexed by the nodes of the graph. We write $\mathbf{P} \star \mathbf{T}$ to denote a permutation of the first $k$ channels of this tensor according the node permutation matrix $\mathbf{P}$. 
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A **linear invariant layer** can be defined as \(L : \mathbb{R}^{|V|^k \times d_1} \rightarrow \mathbb{R}^{d_2}\) such that for all permutations \(P\):

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Based on this abstraction, invariant $k$-order GNN model (Maron et al., 2019b), or $k$-IGNs, is defined as:

$$F = \text{MLP} \circ \mathcal{H} \circ \mathcal{L}_d \circ \sigma \circ \cdots \circ \sigma \circ \mathcal{L}_1,$$

where $\mathcal{L}_1, \ldots, \mathcal{L}_d$ are equivariant linear layers (with up to $k$ different channels), $\mathcal{H}$ is an invariant layer, and $\sigma$ denotes element-wise non-linearity. Figure 1 of (Maron et al., 2019c) illustrates the model.
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The input to the k-order invariant GNN is a tensor $T \in \mathbb{R}^{\lvert V \rvert^2 \times d}$, where the first two channels correspond to the adjacency matrix of the graph and the remaining channels encode the initial node features.

The model is called k-order, as it allows equivariant layers with k channels, and this directly correlates with the expressive power of the model.
Expressive Power of Invariant Graph Networks
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**Theorem 1** (Maron et al., 2019a). Given two graphs $G, G'$ that can be distinguished by the $k$-WL graph isomorphism test, there exists a $k$-order network $F$ so that $F(G) \neq F(G')$. On the other direction for every two isomorphic graphs $G, G'$ and $k$-order network $F$, $F(G) = F(G')$. 
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If we bound the size of the input graphs with $n$, measured in the number of nodes, then $n$-th order invariant networks can distinguish any pair of non-isomorphic graphs. Note that invariant networks with order-2 tensors could already be computationally challenging!
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More specifically, invariant networks are universal with tensor order $\frac{n(n-1)}{2}$. An alternative proof is given by (Keriven and Peyré, 2019), who also showed a universality result for the equivariant case.
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Indeed, $k$-IGNs are inherently designed for graph-level computations: the correspondence with node tuples, is only implicit, unlike $k$-GNNs, where tuples have representations that are explicitly maintained and updated.
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Indeed, $k$-IGNs are inherently designed for graph-level computations: the correspondence with node tuples, is only implicit, unlike $k$-GNNs, where tuples have representations that are explicitly maintained and updated.

Finally, these models are also prohibitive to run for large values of $k$, due to their very large memory and computational requirements.
Provably Powerful Graph Networks
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Figure 2: Block structure.
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PPGN works with 2 tensors, and is defined as follows:

\[ F = \text{MLP} \circ \mathcal{H} \circ \mathcal{B}_d \circ \cdots \circ \mathcal{B}_1, \]

where, as in k-IGNs, \( \mathcal{H} \) is an invariant layer, and \( \mathcal{B}_1, \ldots, \mathcal{B}_d \) are blocks have the structure shown in Figure 2 of (Maron et al., 2019a).

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Briefly, given an input $T \in \mathbb{R}^{|V| \times |V| \times d}$ the idea is to apply MLP to each feature of the input tensor independently (i.e., 3 MLPs), and then perform matrix multiplication between matching features.
Provably Powerful Graph Networks

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PPGNs have therefore the same power as 3-GNNs, but the strong point is that they maintain only $O(n^2)$ embeddings, which makes them more memory-efficient than 3-GNNs.

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Expressive Power in the Real World
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1. 1-WL edge cases typically correspond to data that is highly regular, whereas real-world data is overwhelmingly uneven and variable, e.g., knowledge graphs, where some entities are connected to hundreds of other entities, and others connect to very few, if any.

2. Real-world graphs are also typically large, and involve thousands, and potentially millions, of nodes. At this scale, the limitations of 1-WL are less likely to surface, as it is highly probable that some local substructure within the large graph can help distinguish it. In fact, 1-WL can distinguish almost all graphs as the number of graph nodes tends to infinity (Babai et al., 1980), i.e., it can distinguish these graphs with probability almost 1.
Expressive Power in Real-World Data

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This has been noted and new synthetic datasets dedicated to quantify the effect of expressive power are proposed (Abboud et al., 2020) with a detailed comparison against higher-order models, as we will see in more detail in Lecture 7.
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“In many networks it is found that if vertex A is connected to vertex B and vertex B to vertex C, then there is a heightened probability that vertex A will also be connected to vertex C. In the language of social networks, the friend of your friend is likely also to be your friend.
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where a “connected triple” means a single vertex with edges running to an unordered pair of others.”
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"In simple terms, $C$ is the mean probability that two vertices that are network neighbours of the same other vertex will themselves be neighbours." (Newman, 2013)
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The graph shown above has 1 triangle and 8 connected triples, and so has a clustering coefficient of $3/8$.

There are other ways of defining cluster coefficient but they rely on being able to detect triangles.
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For instance, protein graphs exhibit heterophily, as the proteins that interact with one another are usually different from a composition perspective.
MPNNs vs Higher-Order Models
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By contrast, higher-order models are more global, and so cannot naturally be restricted to this setting, unless empowered with some local variants.

For example, $k$-GNN, for larger $k$, would require non-uniform handling of its connected tuples, based on local neighbourhoods, and $k$-IGN processes all nodes simultaneously, and thus must learn to filter out non-local features!
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• Homophily and heterophily: MPNNs vs higher-order models

• There are other extensions of MPNNs, particularly with random features, yielding more expressive power without the need for higher-order tensors — Lecture 7.
References


• Ralph Abboud, İsmail İlkan Ceylan, Martin Grohe, Thomas Lukasiewicz, The Surprising Power of Graph Neural Networks with Random Node Initialization, arXiv:2010.01179, 2020