How Powerful Are Graph Neural Networks?

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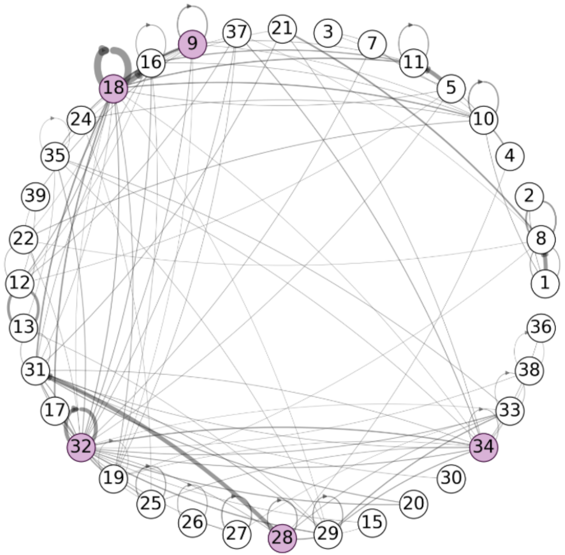
Big Picture

- What Graph Neural Net(GNN) can do and cannot do?
- Empirical success but limited theoretical research
- How expressive are different GNN architectures in capturing and distinguishing graph structures?

Motivation - US and Australian economy



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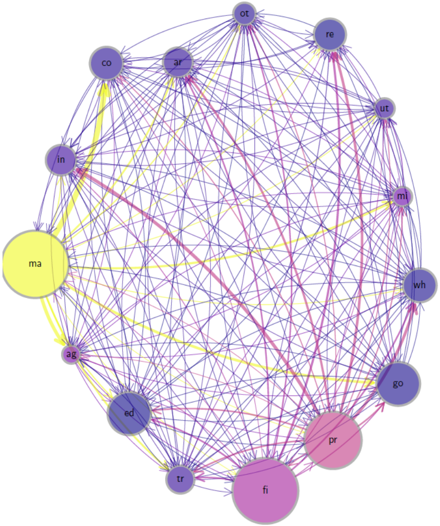

Weisfeiler-Lehman (WL) test

Algorithm *1-WL (color refinement)*

Input: $G = (V, E, X_V)$

1. $c_v^0 \leftarrow \text{hash}(X_v)$ for all $v \in V$
2. **repeat**
3. $\quad c_v^\ell \leftarrow \text{hash}(c_v^{\ell-1}, \{\!\{c_w^{\ell-1} : w \in \mathcal{N}_G(v)\}\!\})\ \forall v \in V$
4. **until** $(c_v^\ell)_{v \in V} = (c_v^{\ell-1})_{v \in V}$
5. **return** $\{\!\{c_v^\ell : v \in V\}\!\}$

What is GNN? Setup

- $G = (V, E, X_V)$
- In the k-th layer

$$h_v^k = COMBINE^{(k)}\left(h_v^{k-1}, a_v^{(k)}\right), a_v^{(k)} = AGGREGATE^{(k)}\left(\{h_u^{k-1} : u \in \mathcal{N}(v)\}\right)$$

Looks really like the iteration step in the WL test

Key Theorem

Theorem 1

No message-passing GNN can be more powerful than the 1-WL test at distinguishing graph structure.

Theorem 2

GNN can achieve this theoretical upper bound using the GIN architecture

What is GIN?

Graph Isomorphic Network

GIN:

$$h_v^{(k)} = MLP\left(\underbrace{(1+\epsilon)h_v^{(k-1)}}_{\text{center node}} + \underbrace{\sum_{u \in N(v)} h_u^{(k-1)}}_{\text{neighbors}}\right)$$

- The sum aggregator preserves multiset cardinality
- MLP(NN) has the universal approximation properties
- As powerful as 1-WL test

Discussion

- Is 1-WL good enough? (Fail to distinguish a regular graph with n nodes)

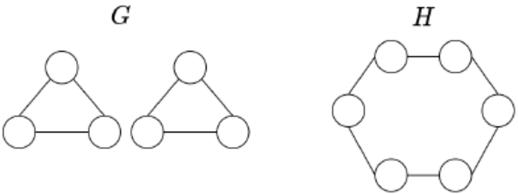

Fig. 1. Two graphs can not be distinguished by WL and 2-WL, but can be distinguished by 2-FWL.

- Difficulty lies at the tradeoff: Computational complexity and expressiveness

Future outlooks

- Perturbations: What happens if there is a shock to one nodes? How will this shock propogates through the network
- Two network are the “same” if all or random shock has the same propagation