Do we need to improve Message Passing?

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Motivation: Drug Discovery

- Need to learn relevant graph structures (e.g. cycles)
- Often Message Passing Graph Neural Network (MPNN) is used for this task
Message Passing Graph Neural Networks

- Compute node representations via message passing
- Permutation invariant
- Can solve some graph isomorphism problems
Message Passing Graph Neural Networks

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\[ f_{\text{MPNN}} = f_{\text{MPNN}} \]
Expressiveness

- A is at least as expressive as B: A can distinguish every pair of graphs B can distinguish.
- MPNNs have limited expressiveness:

Formally: \( G_1 \not\sim_{iso} G_2 \quad f_{MPNN}(G_1) = f_{MPNN}(G_2) \)
Improving Expressiveness

Problem: \( G_1 \not\cong_{iso} G_2 \quad f_{MPNN}(G_1) = f_{MPNN}(G_2) \)

Option 1: Changing message passing

- Transform graph to different structure with \( T \)
- Improved message passing \( f_{NEW} \)
- \( f_{NEW}(T(G_1)) \not\cong f_{NEW}(T(G_2)) \)

Example: CW Networks
Improving Expressiveness

Problem: \( G_1 \not\equiv_{iso} G_2 \quad f_{\text{MPNN}}(G_1) = f_{\text{MPNN}}(G_2) \)

Option 2: Changing the graphs

- Transform graphs \( T^* \)
- \( f_{\text{MPNN}}(T^*(G_1)) \neq f_{\text{MPNN}}(T^*(G_2)) \)

Example: Add information about graph structures to vertex features

Barceló et al., Graph Neural Networks with Local Graph Parameters, NeurIPS, 2021
Bouritsas et al., Improving Graph Neural Network Expressivity via Subgraph Isomorphism Counting, GRL+ Workshop at ICML, 2020
Do we need to improve message passing or are graph transformations enough?

**Claim:** Graph transformations are enough.*

* in most cases
Our Work

- Investigate algorithms with improved message passing:
  - CW Networks (CWN)
  - Equivariant Subgraph Aggregation Networks (ESAN)
  - (Local) $\delta$-$k$ dimensional GNNs ($\delta$-$k$ GNNs)

- **Theorem:** All can be replaced by a graph transformation + MPNN

- **Experiments** of graph transformations + MPNN on molecule datasets
Theorem: Cell Encoding + MPNN is at least as expressive as CWN
Conclusion

- MPNNs struggle with distinguishing graphs
- Fixed by graph transformations or improved message passing
- **Claim**: graph transformations are enough
  - Proven this for CWN, ESAN, δ-k-GNNs
  - Experiments show this can work in practice

**Future Work:**
- How do we formalize this idea?
- How far can we push MPNNs with graph transformations?
Conclusion

- **Publications:**
  - Jogl, Thiessen, Gärtner, Reducing Learning on Cell Complexes to Graphs, GTRL workshop at ICLR, 2022
  - Jogl, Thiessen, Gärtner, Weisfeiler and Leman Return with Graph Transformations, MLG workshop at ECML, 2022

- **Related:** Veličković, Message passing all the way up, GTRL workshop at ICLR, 2022
Bonus Graph Transformations: SBE & ESAN
Bonus Graph Transformations: $\delta$-k GNNs / Transform.
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