Do we need to improve Message Passing?

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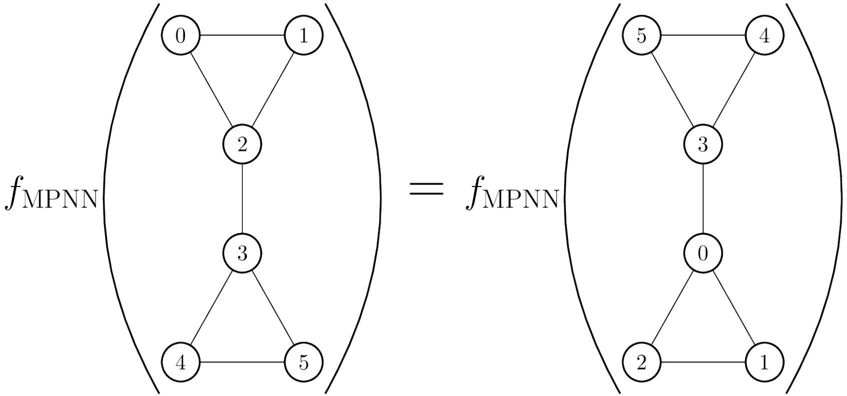
Motivation: Drug Discovery

- 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



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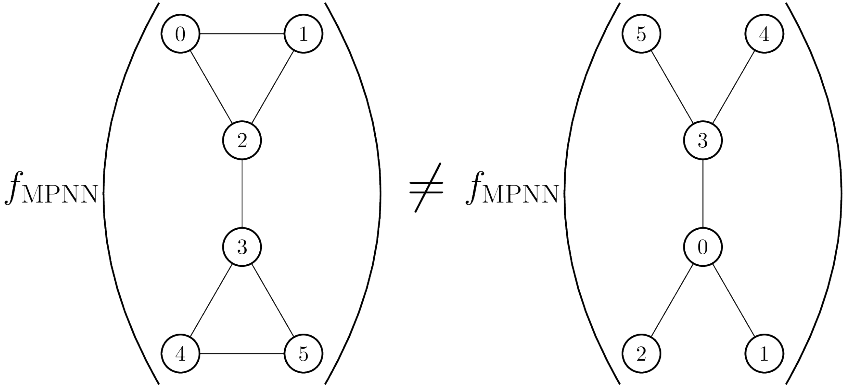

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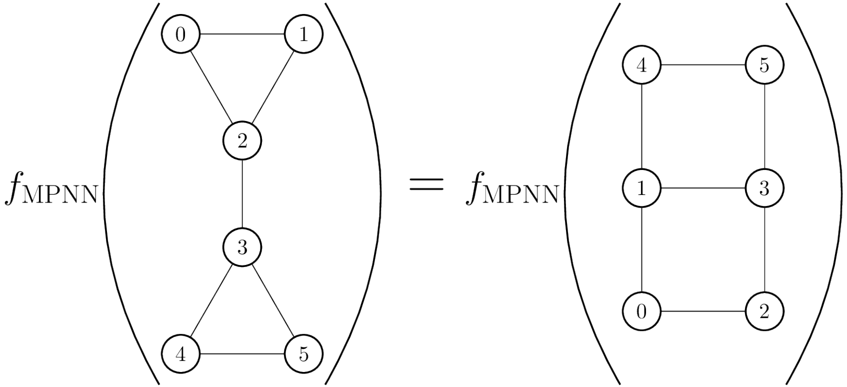
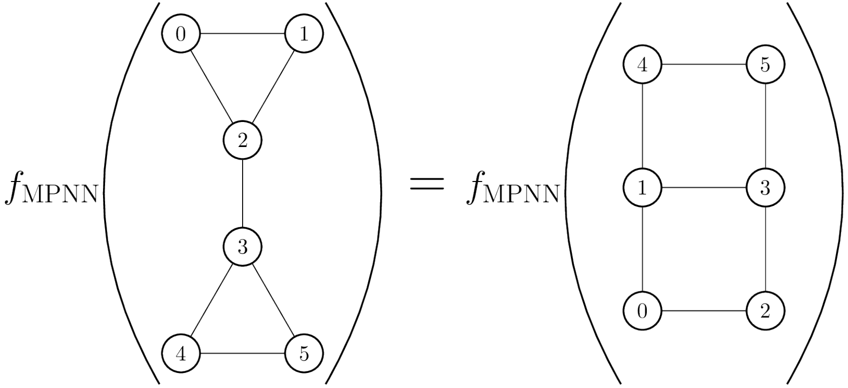


Expressiveness

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



- Formally: $G_1 \neq_{\text{iso}} G_2 \quad f_{\text{MPNN}}(G_1) = f_{\text{MPNN}}(G_2)$

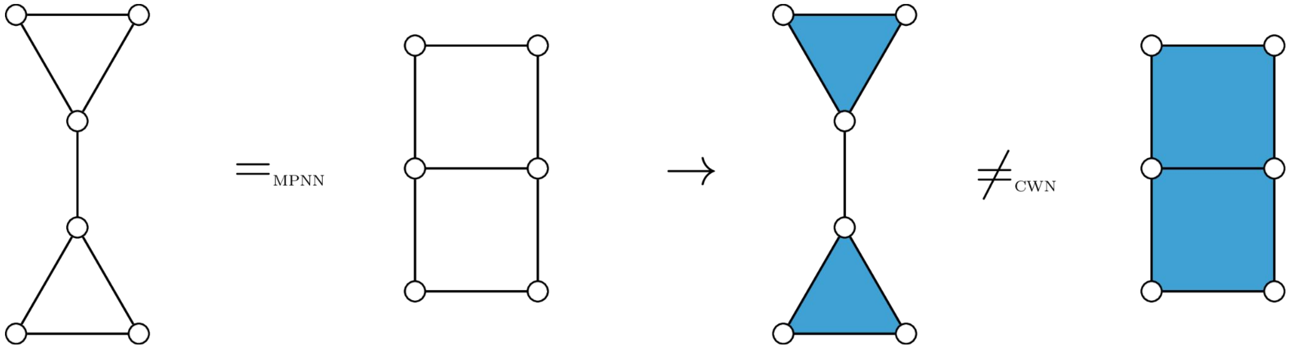
Improving Expressiveness

Problem: $G_1 \neq_{\text{iso}} G_2 \qquad f_{\text{MPNN}}(G_1) = f_{\text{MPNN}}(G_2)$

Option 1: Changing message passing

- Transform graph to different structure with T
- Improved message passing f_{NEW}
- $\rightarrow f_{\text{NEW}}(T(G_1)) \neq f_{\text{NEW}}(T(G_2))$

Example: CW Networks



Bodnar et al., *CW Networks*, NeurIPS, 2021

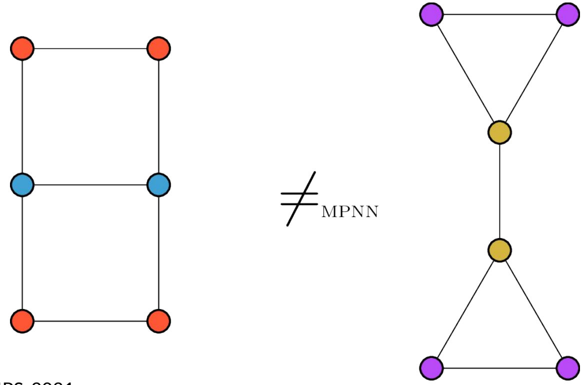
Improving Expressiveness

Problem: $G_1 \neq_{\text{iso}} G_2 \qquad f_{\text{MPNN}}(G_1) = f_{\text{MPNN}}(G_2)$

Option 2: Changing the graphs

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

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

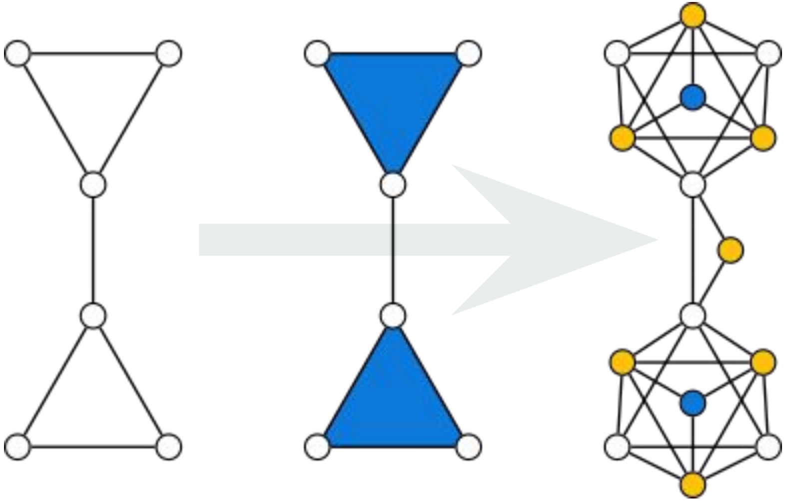
Our Work

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

- **Theorem**: All can be replaced by a graph transformation + MPNN
- **Experiments** of graph transformations + MPNN on molecule datasets

Graph Transformations

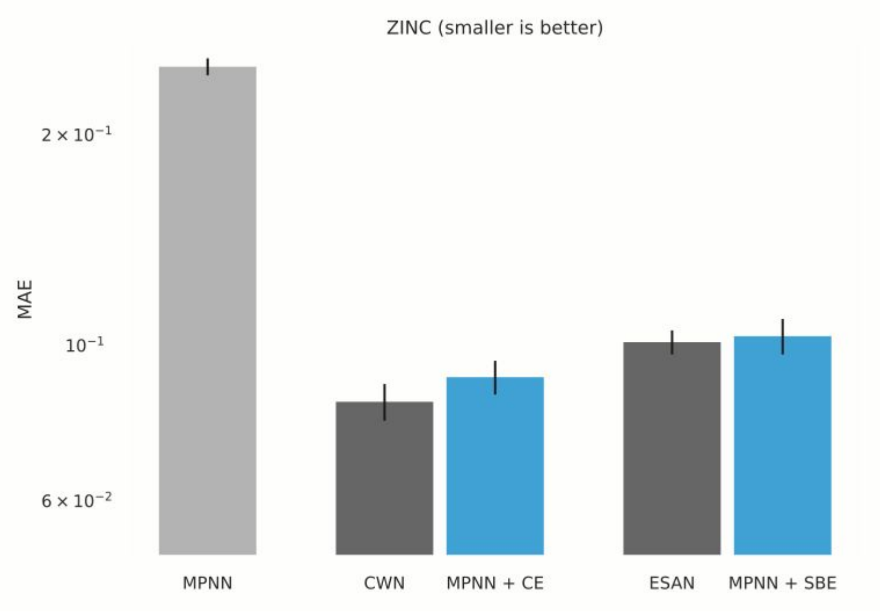
Theorem: Cell Encoding + MPNN is at least as expressive as CWN



Graph

Regular
Cell Complex

Graph



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

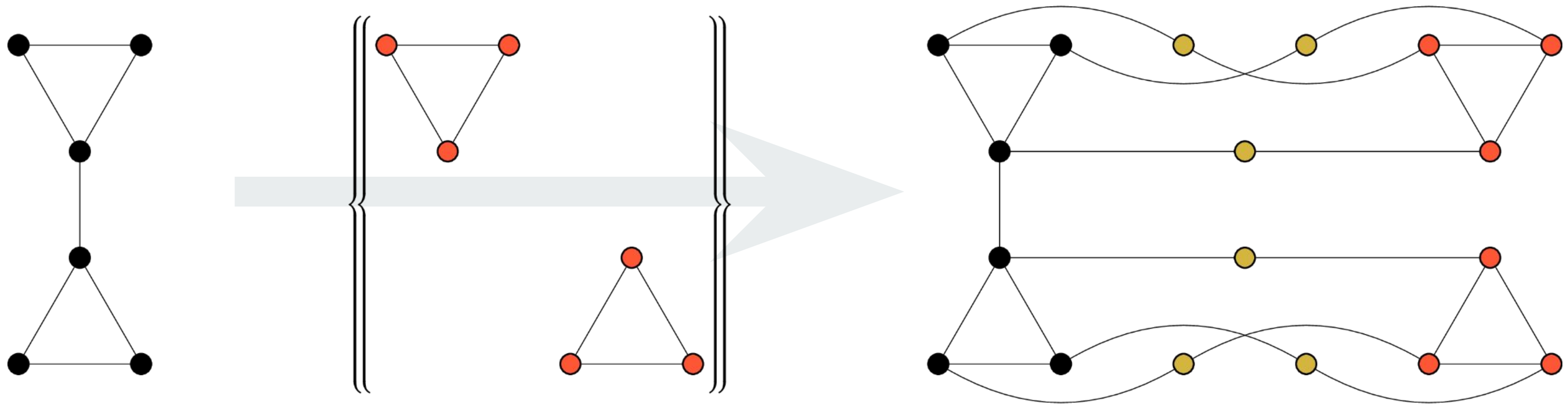
- **Future Work:**
    - How do we formalize this idea?
    - How far can we push MPNNs with graph transformations?

Conclusion

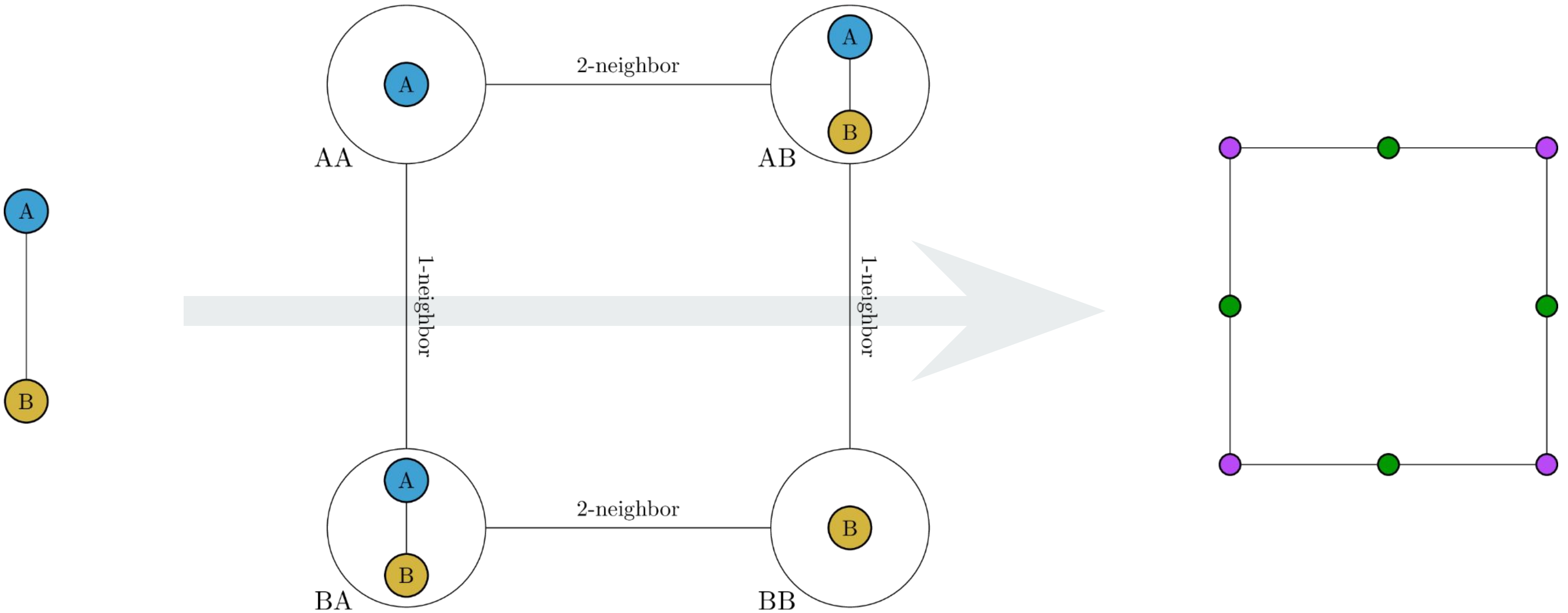
- **Publications:**
  - Jogl, Thiessen, Gärtner, Reducing Learning on Cell Complexes to Graphs, GTRL workshop at ICLR, 2022
  - Jogl, Thiessen, Gärtner, Weisfeiler and Leman Return with Graph Transformations, MLG workshop at ECML, 2022

- **Related:** Veličković, Message passing all the way up, GTRL workshop at ICLR, 2022

Bonus Graph Transformations: SBE & ESAN



Bonus Graph Transformations: δ-k GNNs / Transform.



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