Extending Graph Neural Networks with Global Features

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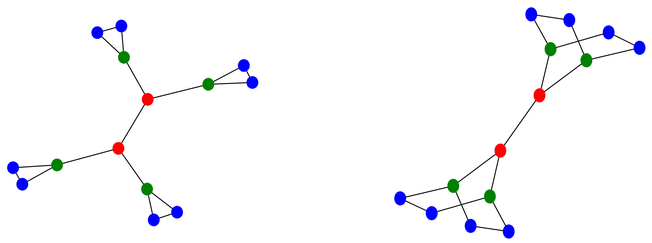
What We Do

- We enhance message passing graph neural networks (*MPNNs*) by incorporating **expressive global graph features**
- Global properties like **topological indices** have been important to *chemoinformatics* but have been overlooked by the GNN community
- Focus on features based on **node degrees**, **connectivity**, **distances**, or **spectral properties**



MPNNs cannot distinguish these two graphs, but graph features can (Wiener index, Hosoya index, independence number, maximum matching)

Global Features

Less expressive than MPNNs:

- **Circuit rank**: #edges which make graph acyclic when removed
- **Spectral radius:** largest eigenvalue of the adjacency matrix
- **Zagreb indices:**
  - M_1: sum of squares of the degrees of the nodes
  - M_2: sum of products of the degrees of pairs of adjacent nodes

More expressive than MPNNs:

- **Wiener index**: sum of lengths of all pairwise shortest paths
- **Maximum matching**: biggest set of edges with no common vertices
- **Hosoya index:** number of matchings in a graph
- **Independence number:** biggest set of non-neighboring vertices
- **2nd smallest Laplacian eigenvalue:** measures connectivity

Experiments

- Evaluate whether global graph feature can improve predictive performance of different GNNs (**GIN**, **GCN**, **CWN**) on molecular benchmark datasets
- Evaluation metrics used:
  - **ZINC**: mean absolute error (MAE) ↓
  - **ogbg-molhiv**: area under the curve (ROC-AUC) ↑
  - **QM9**: mean absolute error (MAE) ↓

ZINC

	No feature (base case)	Wiener index	All features	Constant (1's)
GIN	0.185	0.177	**0.164**	0.182
GCN	0.217	0.206	**0.203**	0.213
CWN	0.126	0.103	**0.101**	0.122

QM9

	No feature (base case)	Wiener index	All features	Constant (1's)
GIN	0.0609	0.0598	**0.0576**	0.0604
GCN	0.0768	0.0749	**0.0708**	0.0765

ogbg-molhiv

	No feature (base case)	Wiener index	Zagreb M_2	Constant (1's)
GIN	0.7674	0.7662	**0.7761**	0.7614
CWN	0.7838	0.7895	**0.7983**	0.7912

Architecture

- Concatenate the learned graph embedding of a GNN with our global graph features
- Train GNN **without** global features
- Finetune GNN with global features

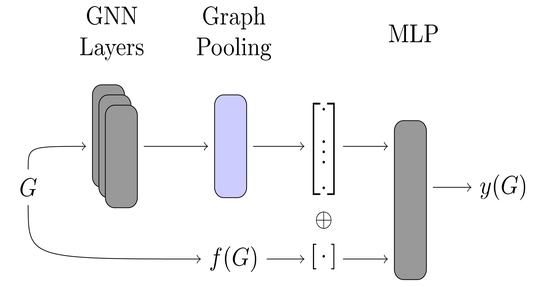


Figure 1: We concatenate global graph features to the output of the graph pooling layer after multiple GNN layers.

Conclusion

- Global graph features are underrated in the GNN community
- Fine-tuning GNNs with global graph features can boost predictive performance

Paper

Code