1. Introduction:

1) Formulation of the problem

2) Solution. Use GNN. Its inherent structure is natural for molecules.

3) Current GNN models (on molecular feature prediction)

Concise survey of existing methods for solving this problem.

However, not interpretable.

4) Explainer!

Include more node features instead of simple one-hot coding

2. Method:

1) GNN models: GCN, …

Metrics: MSE

2) Explainers: GNNExplainer, integrated gradient, PGExplainer

Metrics: MSE, synthesized dataset

3. Experiments:

Node features -> Explainer -> Subset of node features –> GNN (Valent)

Comparison using diff node features

Diff dataset. HIV -> subgraph

Diff tasks, classification and regression.

GNN + Explainer

4. Conclusion

GNN + Explainer (Performance) MSE +

Explanation of the result

5. Future work

Homogenous -> Hetero

Bond -> Function group

Consideration of bond types. Not explicitly presented in the data for training.