INVERSE PROBLEMS OVER TRAINED GRAPH NEURAL NETWORKS

OPTIMIZATION, SYMMETRY-BREAKING, AND APPLICATIONS

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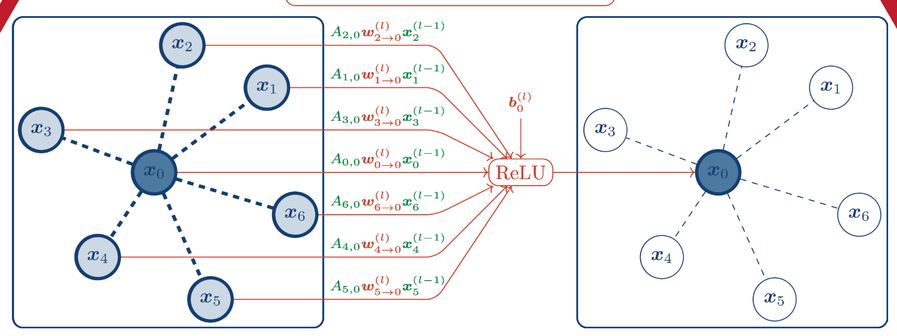
Optimization

A GNN layer with unknown graph:

$(l-1)^{th}$ layer

$$x_v^{(l)} = \mathrm{ReLU}\left(\sum_{u \in V} A_{u,v} w_{u \to v}^{(l)} x_u^{(l-1)} + b_v^{(l)}\right)$$

l^{th} layer



How to encode a GNN to an optimization problem? (without doing math and programming)

PyG → OMLT → PYOMO

OMLT automatically encodes a trained GNN to its corresponding optimization formulation

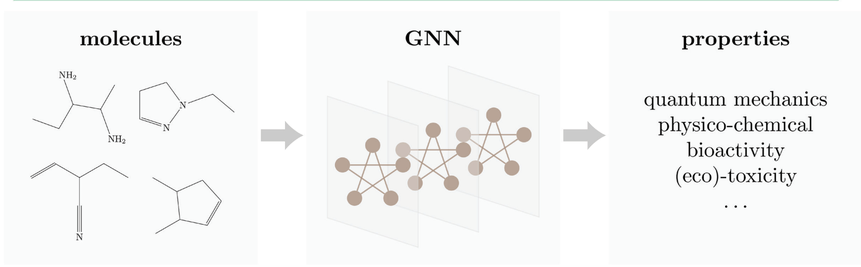
Molecular Design

How to find desired molecules?

$$\min_{X,A} \; GNN(X, A), \; s.t. \; f(X, A) \le 0$$

predictive model; molecular feasibility; features, graph

Prediction (Forward): What are the properties for a given molecule?



Optimization (Backward): What is the optimal molecule with desired properties?

Part I: Optimal molecular design

data-driven, property-oriented
structure-exploited, validity-ensured

Part II: Molecular generation

try Limeade!
end-to-end, lightweight generator

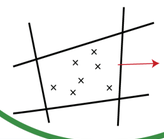
Requirements

- size of molecules
- types of atoms
- composition of molecules
- substructure inclusion
- substructure exclusion
- .....

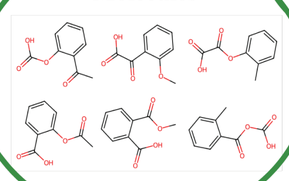
LIMEADE

Optimization

- Variables (binary): features
- Constraints (linear): requirements



Molecules



Symmetry Breaking

Symmetry issue!

One graph with N nodes has N! different indexing

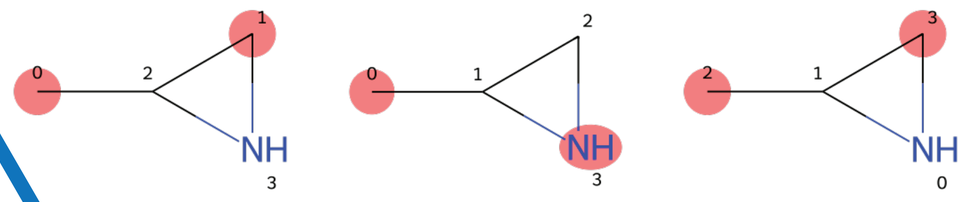
Symmetry-breaking constraints

(S1): The subgraph induced by nodes {0,1,…,v} is connected.

(S2): Node 0 has the most special features.

(S3): Node v has neighbors with smaller indexes compared to v+1.

Solutions removed by (S1) – (S3):



Generally applicable

suitable for any symmetry issue caused by graph isomorphism

Empirically powerful

remove >98% symmetries for molecular benchmarks

Theoretically guaranteed

at least one indexing is feasible given any graph

AI Safety

GNNs are vulnerable!

Small input changes could lead to wrong predictions

How to certify the robustness of a GNN?

$$m(c^*, c) := \min_{(X,A)} \; GNN_{c^*}(X, A) - GNN_c(X, A)$$

attack label; correct prediction; wrong prediction; true label

$$s.t. \; X \in \mathcal{P}(X^*), \; A \in \mathcal{P}(A^*)$$

perturb feature; perturb graph

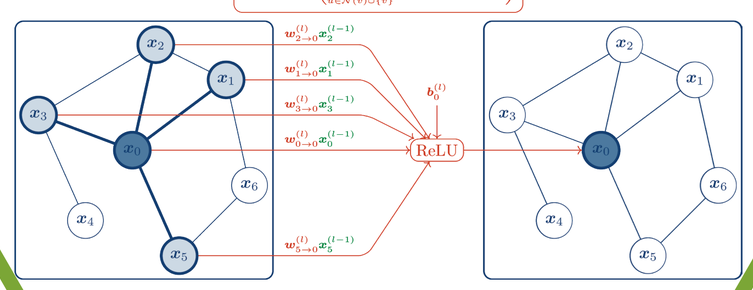
$m(c^*, c) \ge 0 \Leftrightarrow$ robust

$m(c^*, c) < 0 \Leftrightarrow$ non-robust

$(l-1)^{th}$ layer

$$x_v^{(l)} = \mathrm{ReLU}\left(\sum_{u \in \mathcal{N}(v) \cup \{v\}} w_{u \to v}^{(l)} x_u^{(l-1)} + b_v^{(l)}\right)$$

l^{th} layer



Topology-based bounds tightening

more attacks, tighter bounds, faster verification

IMPERIAL

computational optimisation group

BASF We create chemistry

IConIC Innovative Continuous Manufacturing of Industrial Chemicals

Sargent Centre for Process Systems Engineering