Higher Order Structures for Graph Explanations

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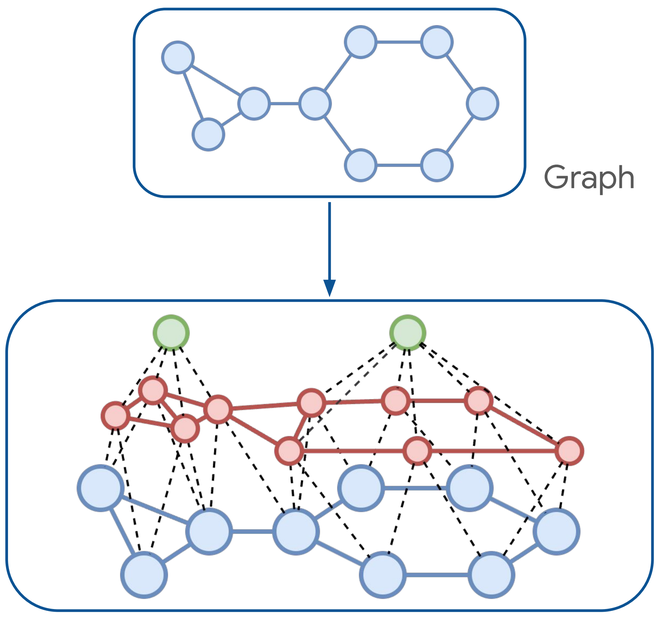
Motivation

Graphs model pairwise relationships between entities. This can overlook the **multi-node interactions** that occur in many real-world systems like molecular structures and social group dynamics.



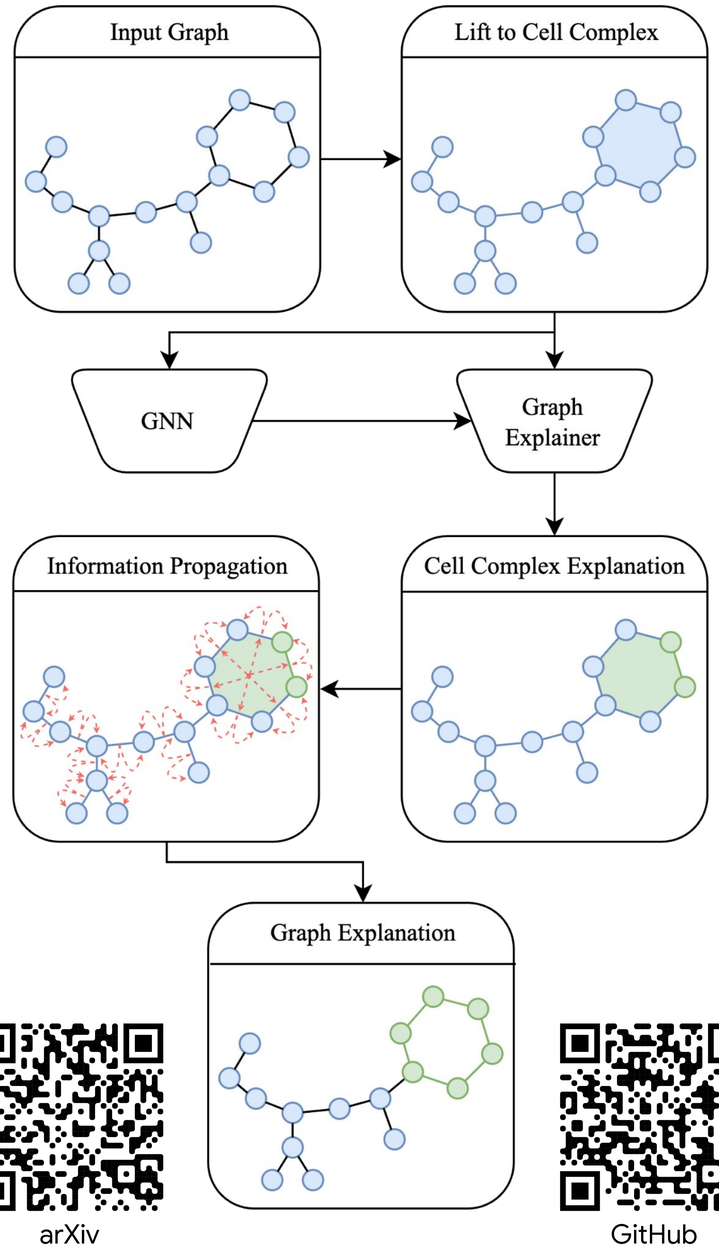
Contribution

By **leveraging higher-order structures** our framework can capture these multi-node interactions.

This leads to **more accurate and faithful explanations** of GNN predictions, ultimately increasing the model's transparency and trustworthiness.

FORGE

Framework for Higher **O**rder **G**raph **E**xplanation

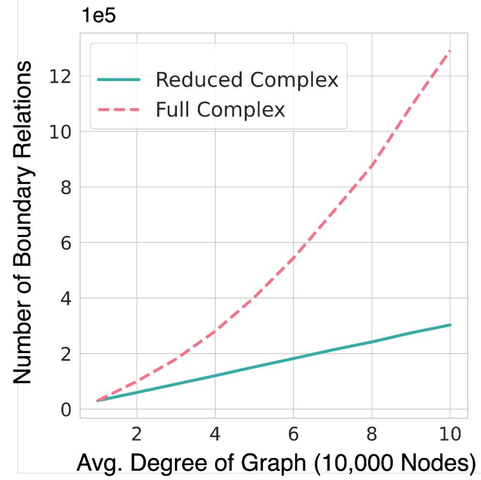


arXiv

GitHub

Results

Scalable



Accurate

Datasets	GNNExplainer B	GNNExplainer F	GraphMask B	GraphMask F	GradExplainer B	GradExplainer F
Benzene	0.456	**0.772**	0.276	0.378	0.167	0.353
AlkCarb	0.054	0.130	0.048	0.055	0.114	0.217
FluoCarb	0.207	**0.441**	0.077	0.230	0.233	0.439
Mutag	**0.380**	0.339	0.127	0.163	0.172	0.218
Bull/Square	0.126	0.433	0.082	0.241	0.179	0.298
House/Hex	0.107	0.478	0.115	0.271	0.199	0.410
Wheel/House	0.102	0.361	0.233	0.378	0.169	0.426
Cube/Wheel	0.114	0.339	0.183	0.402	0.119	**0.494**

Faithful

Explainer	GEF(↓) B	GEF(↓) F
GNNExplainer	$0.189_{\pm 0.04}$	$\mathbf{0.083_{\pm 0.02}}$
GraphMask	$0.051_{\pm 0.03}$	$\mathbf{0.028_{\pm 0.02}}$
GradExplainer	$0.389_{\pm 0.13}$	$\mathbf{0.078_{\pm 0.05}}$
PGMExplainer	$\mathbf{0.204_{\pm 0.05}}$	$0.234_{\pm 0.03}$
SubgraphX	$0.008_{\pm 0.01}$	$\mathbf{0.007_{\pm 0.00}}$
Random	$0.124_{\pm 0.04}$	-