

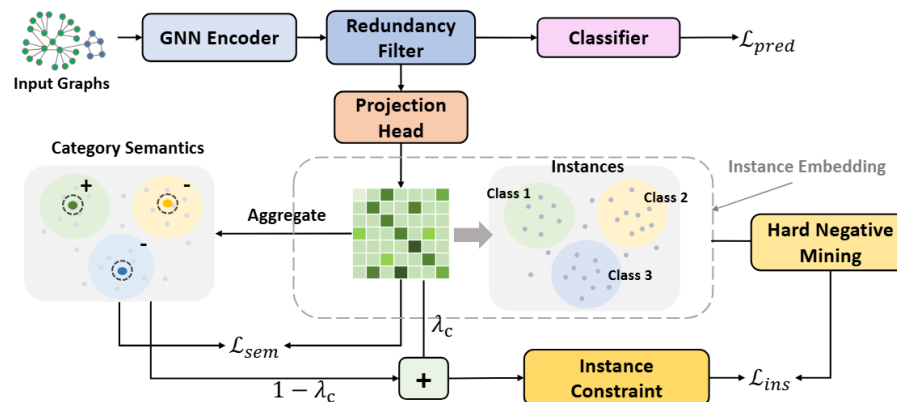
Invariant Graph Learning Meets Information Bottleneck for Out-of-Distribution Generalization

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Problems & Ideas

- Problems of conventional graph invariant learning approaches:
 - Suffer from the complex graph structure.
 - Data augmentation approaches suffer from disruptions to invariance during the graph manipulation process.
- Causal intervention faces reliability issues due to a lack of supervised signals for causal parts.
- Ideas: Invariant Graph Learning based on Information bottleneck, combining a redundancy filter and multi-level contrastive learning.



The training graphs are fed into the GNN encoder and attention mechanism~\cite{sui2022causal,brody2021attentive}. After being projected to another space, instance embeddings are aggregated to semantics. Then semantic-level and instance-level contrastive learning are optimized jointly, along with instance constraint and hard negative mining to avoid model collapse.

Main Contributions

- Contributions:
 - We propose a novel framework, (InfoIGL), to extract the invariant features of graphs and enhance models' generalization ability to unseen distributions.
 - To satisfy the invariance and sufficiency conditions of invariant learning, we compress redundant information from spurious features with redundancy filter and maximize mutual information of graphs with multi-level contrastive learning
 - Extensive experiments demonstrate the superiority of InfoIGL, highlighting its potential for real-world applications.

	Motif		HIV		Molbbbp		CMNIST
	size	base	size	scaffold	size	scaffold	color
InfoIGL(ours)	85.53 ^{+2.37}	92.51 ^{+0.16}	93.15 ^{+0.77}	72.37 ^{+1.63}	83.39 ^{+2.76}	77.05 ^{+2.24}	38.93 ^{+1.11}
improvement	↑ 12.22%	↑ 8.80%	↑ 9.82%	↓ 1.07%	↑ 2.57%	↑ 7.33%	↑ 5.09%

Performance of different methods on synthetic (Motif) and real-world (HIV, Molbbbp, CMNIST) datasets. Our method demonstrates a significant improvement on state-of-the-art.