Disentangling Invariant Subgraph via Variance Contrastive Estimation under Distribution Shifts

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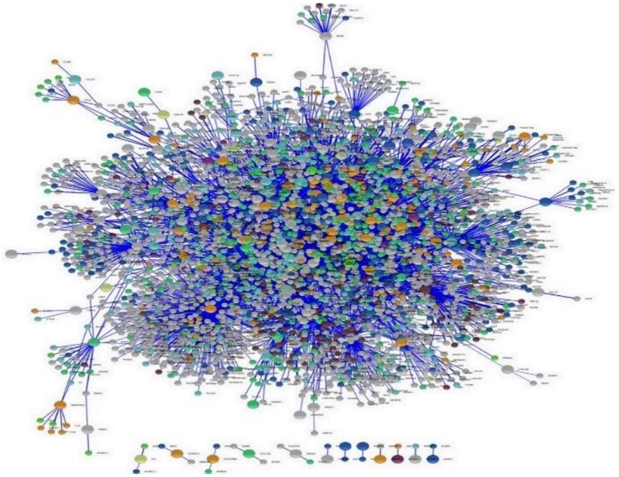
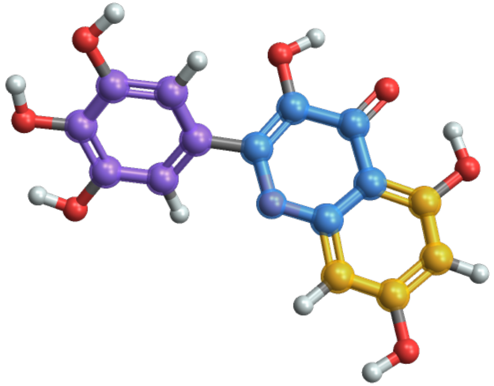
Graph Structured Data is Everywhere

Social Networks

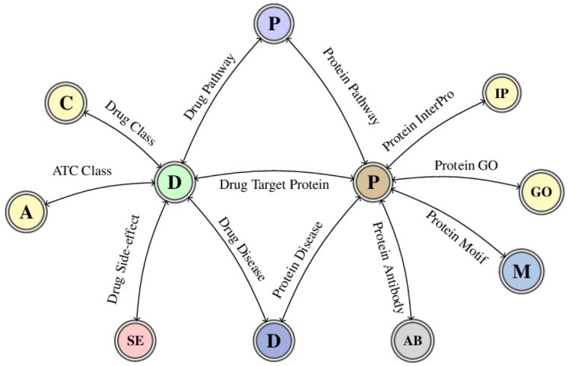
Biology Networks



Molecular Graphs

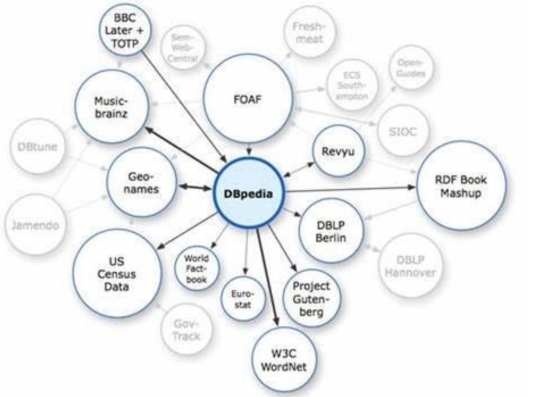


Knowledge Graphs



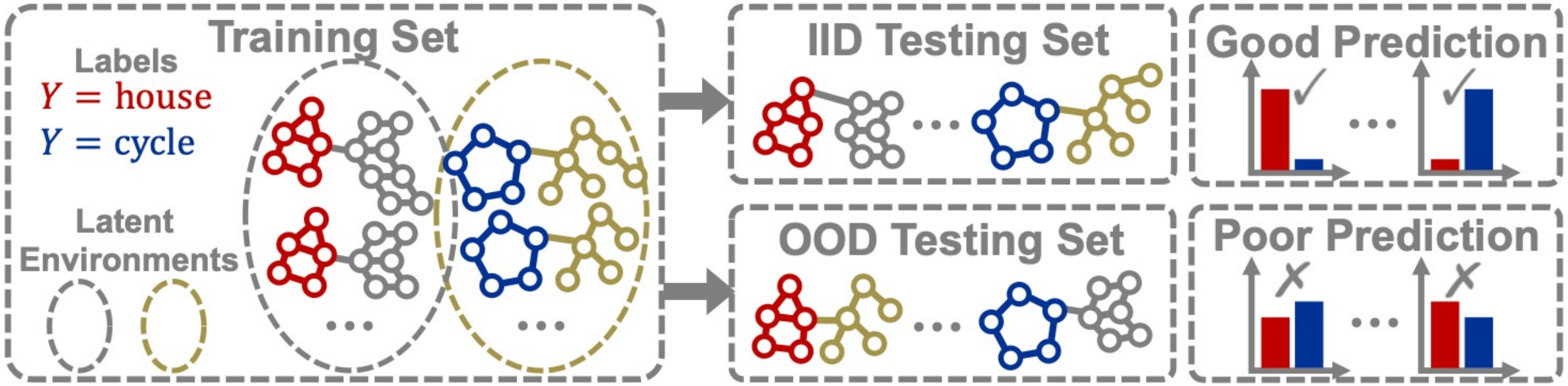
Traffic Networks

Information Networks

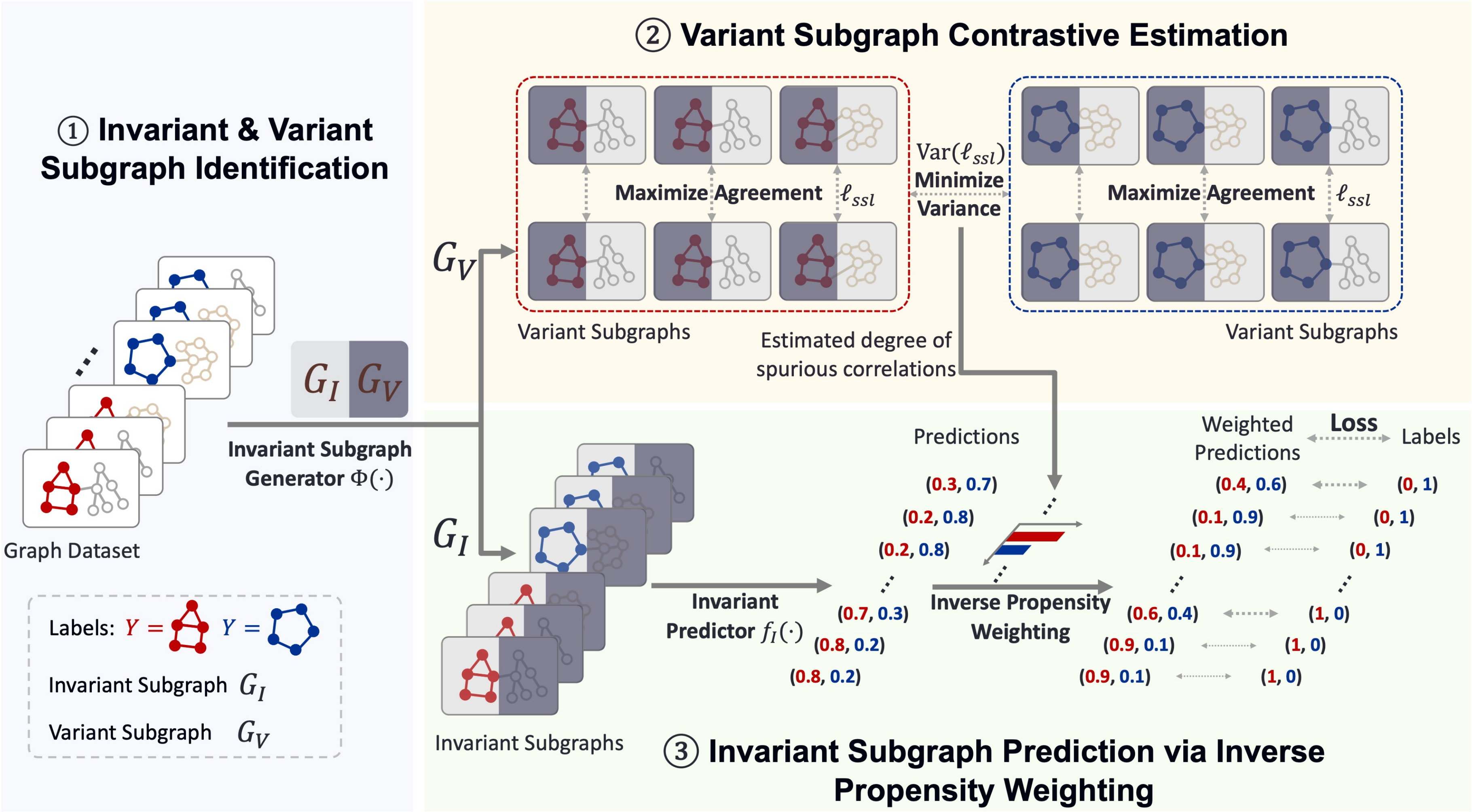


Graph Neural Networks

- **Today's graph neural networks (GNNs)**
  - GNNs built upon the in-distribution (I.D.) hypothesis fail to generalize to out-of-distribution (OOD) environments.
  - Most graph invariant learning methods heavily rely on the predefined or automatically generated environment labels, i.e., multiple training environments.
  - However, the environment labels are unavailable in most scenarios and directly annotating or generating environment labels is impractical or inaccurate.



Model Framework



Theoretical Analysis

- **Theoretical Analysis**
  - Our method can disentangle the ground-truth invariant and variant subgraphs which is a significant step towards OOD generalized predictions.

Theorem 1. *Denote the optimal invariant subgraph generator* Φ^* *that disentangles the ground-truth invariant subgraph* G_I^* *and variant subgraph* G_V^* *given the input graph* G, *where* G_I^* *satisfies Assumption 1 and denote the complement as* $G_V^* = G \backslash G_I^*$. *Assume the second variance term of Eq. (5) is minimized, we have that the first contrastive loss term is minimized iff the invariant subgraph generator* Φ *equals* Φ^*.

Experimental Results

- **Results on real-world benchmarks**

Table 1. Experimental results (%) of our method and baselines. The evaluation metric is accuracy for CMNIST, CFashion, and CKuzushiji, and ROC-AUC for MOLSIDER and MOLHIV. ± denotes the standard deviation. The best results are in bold for each row. Our **VIVACE** outperforms the baselines in all comparisons, indicating its superiority against graph distribution shifts.

Dataset	**Bias**	**Methods**							
	r	GCN	GIN	FactorGCN	DiffPool	DIR	LDD	DisC	**VIVACE**
CMNIST	0.8	50.43±4.13	57.75±0.78	72.30±1.18	73.79±0.02	9.98±0.33	64.95±1.22	82.60±0.93	**82.71±0.74**
	0.9	28.97±4.40	36.78±5.55	62.35±5.07	66.45±0.78	9.96±0.23	56.65±2.18	78.14±2.14	**79.46±1.87**
	0.95	13.50±1.38	16.04±1.14	42.50±4.91	47.12±1.04	10.03±0.27	46.83±2.88	63.47±5.65	**64.72±4.61**
CFashion	0.8	63.60±0.53	64.25±0.46	61.23±1.11	62.82±0.53	13.02±1.92	63.85±1.17	66.85±1.11	**67.09±1.23**
	0.9	57.22±0.93	58.03±0.40	53.50±1.29	57.50±0.39	12.80±1.67	64.30±0.89	65.33±4.70	**65.38±4.18**
	0.95	47.69±0.42	49.74±0.60	45.78±2.40	50.86±0.20	11.98±1.41	62.28±0.48	63.93±1.50	**63.96±1.27**
CKuzushiji	0.8	38.45±1.10	41.83±0.78	42.87±1.19	45.46±0.65	10.35±0.32	42.38±0.33	55.53±2.29	**55.58±1.87**
	0.9	28.35±0.79	30.09±0.87	32.35±2.79	36.18±0.19	10.72±0.27	38.75±0.49	48.13±2.59	**48.15±1.91**
	0.95	20.70±0.88	21.18±1.63	23.87±0.12	27.45±0.26	10.59±0.46	33.08±0.59	36.63±1.73	**37.01±1.67**
MOLSIDER		59.62±1.82	57.61±1.48	53.32±1.75	60.21±1.55	57.74±1.63	58.83±1.62	59.31±1.87	**62.15±1.10**
MOLHIV		76.13±1.01	75.63±1.41	57.18±1.54	76.32±1.48	77.05±0.57	76.91±1.81	76.97±1.03	**78.11±0.82**

Best OOD generalization performances

Thanks!

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