Graph Structure Learning with Variational Information Bottleneck

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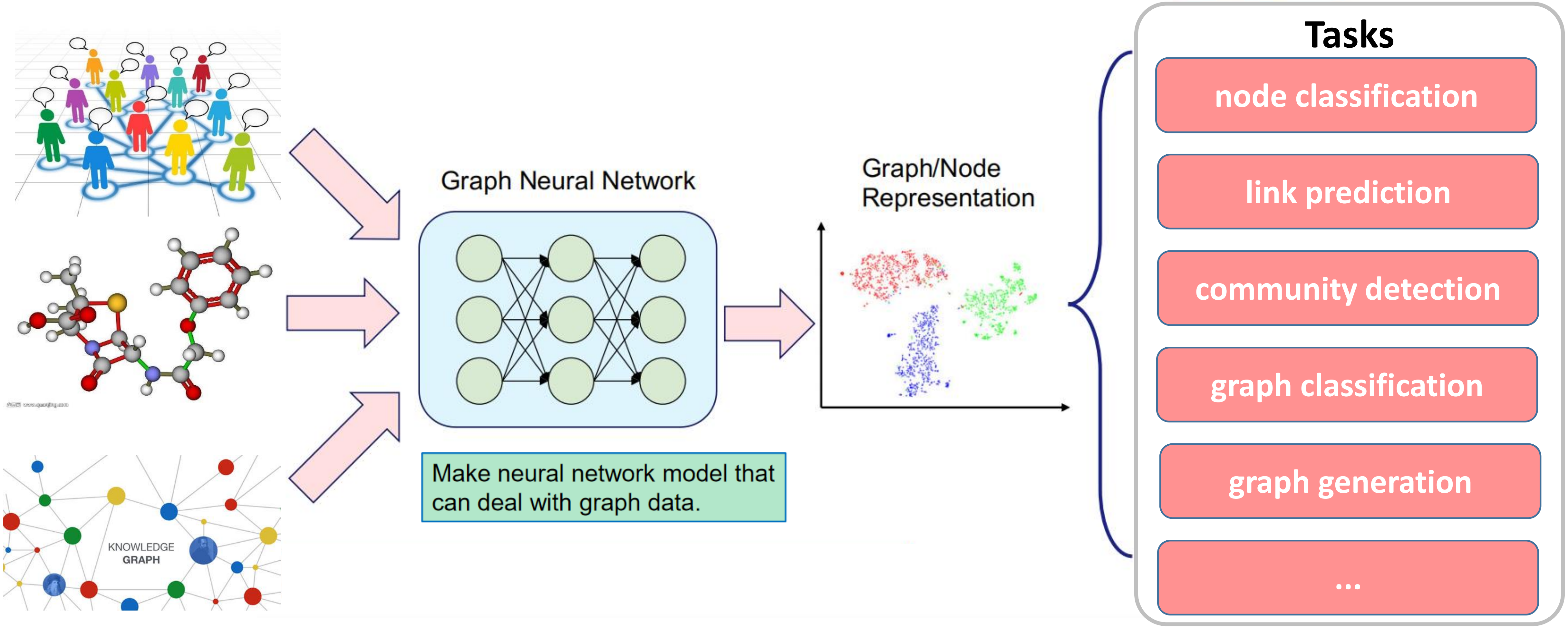
Paper: https://arxiv.org/abs/2112.08903

Graph Neural Network



Acknowledgement from https://ai.tencent.com/ailab/ml/WWW-Deep-Graph-Learning.html

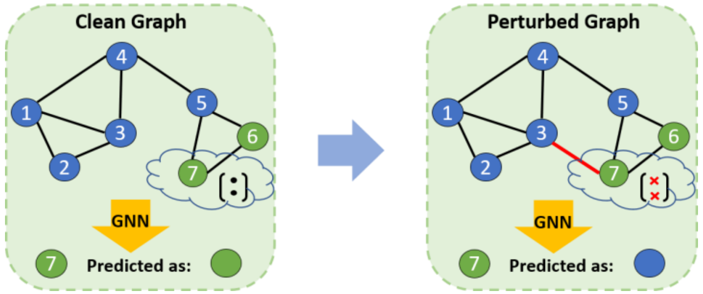
Why Graph Structure Learning?

One fundamental assumption of GNN: the observed topology is ground-truth information and consistent with the properties of GNNs.

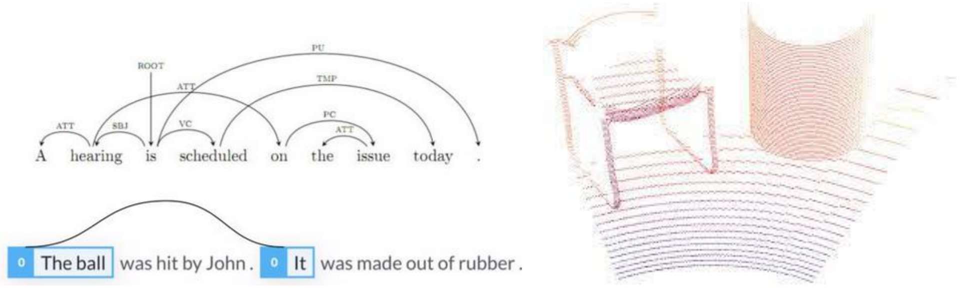
However,

- Questionable if the given intrinsic graph-structures are optimal (i.e., noisy, adversarial perturbation, incomplete) for the downstream tasks
- Many applications (e.g., NLP tasks) may only have non-graph structured data or even just the original feature matrix.

noisy social network



graph adverarial attack

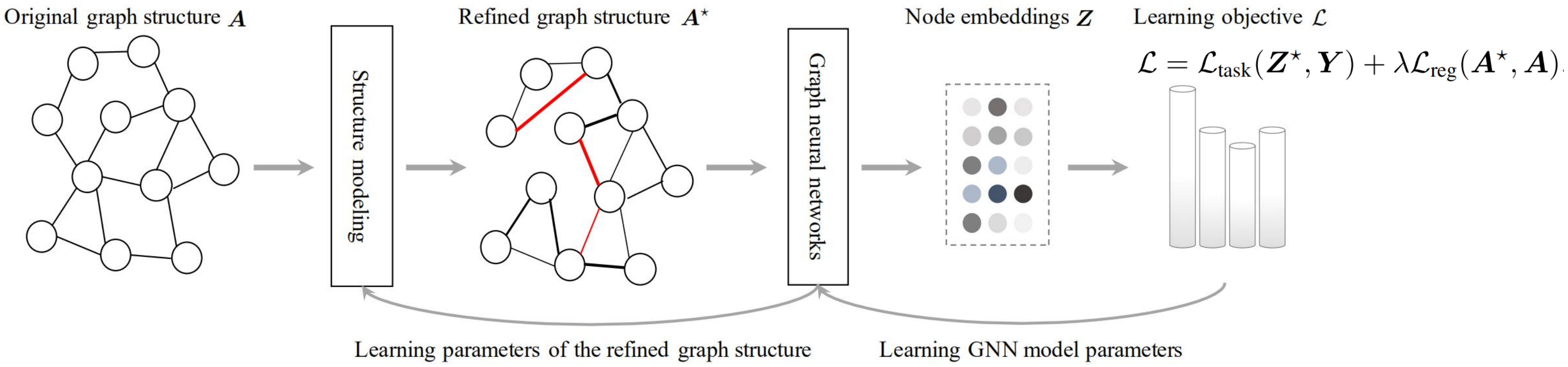


non-graph structure data

Graph Structure Learning

Graph structure learning targets jointly learning an optimized graph structure and corresponding representations to improving the robustness of GNN models.

Input: a raw graph **Output:** a refined graph structure

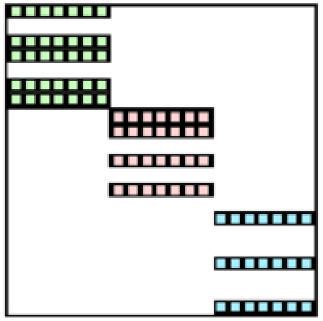


General Paradiam of GSL: Structure Modeling → Message Passing → Learning Objective

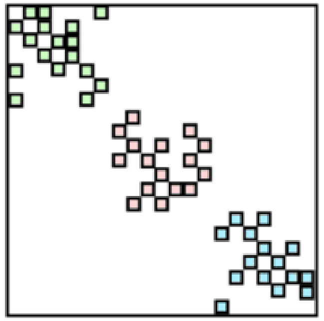
Acknowledgement from https://arxiv.org/abs/2103.03036

What is a “good” structure?

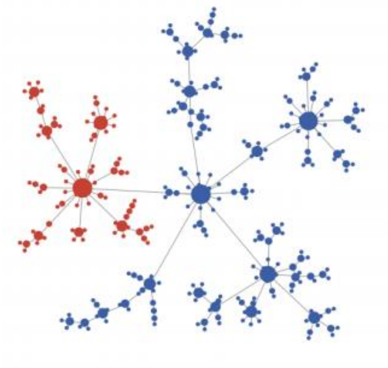
Previous works: basd on **assumptions** (e.g., homophily) or **certain constraints** (low-rank, sparse, conectted, feature-smoothing)



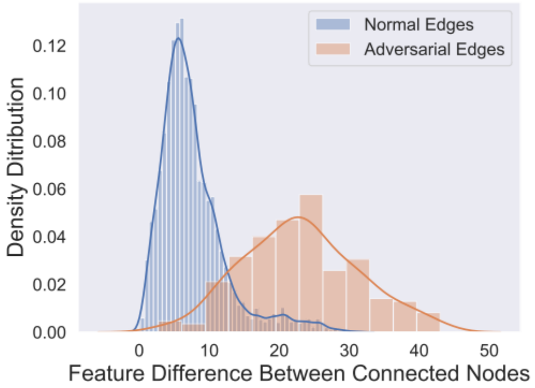
(b) low-rank



(c) sparse



absolute homophily:



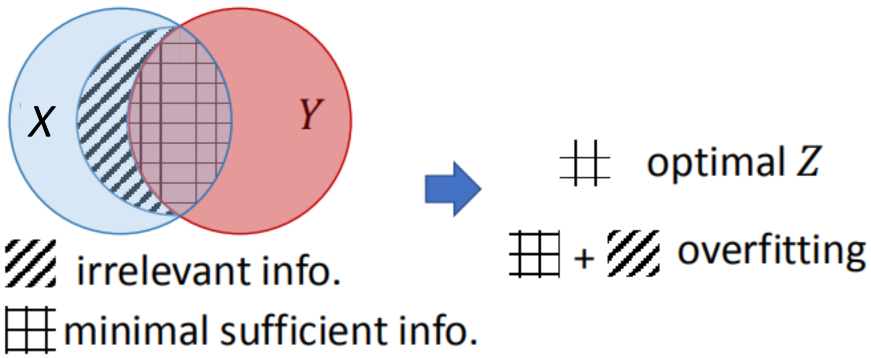
(d) Feature Smoothness

There is still a lack of a general framework that can mine underlying relations from the essence of representation learning

Acknowledgement from https://dl.acm.org/doi/abs/10.1145/3394486.3403049

Information Bottleneck (IB)

Information Bootleneck: an optimal representation **Z** should contain the **minimal** **sufficient** information for the downstream prediction task



X: data *Y: task* *Z: representation*

IB Objective: $\arg\max_{Z} I(Y,Z) - \beta I(X,Z)$

prediction term: make the prediction accurate

compression term: discourages acquiring irrelevant information

Acknowledgement from https://arxiv.org/abs/2010.12811

Our Work: Graph Structure Learning with IB

Advance IB principle for graph structure learning:

We focus on learning an optimal **IB-Graph** for G, which is compressed with minimum information loss in terms of G's properties for the downstream prediction task

Objective:

$$\underset{G_{\mathrm{IB}}}{\operatorname{argmin}} \underbrace{-I(G_{IB};Y)}_{\text{prediction term}} + \underbrace{\beta I(G_{IB};G)}_{\text{compression term}}$$

Proposition 1 (Upper bound of $-I(G_{\mathrm{IB}};Y)$). *For graph $G \in \mathbb{G}$ with label $Y \in \mathbb{Y}$ and IB-Graph G_{IB} learned from G, we have*

$$-I(Y;G_{\mathrm{IB}}) \leq -\iint p(Y,G_{\mathrm{IB}}) \log q_\theta(Y|G_{\mathrm{IB}}) dY dG_{\mathrm{IB}} + H(Y), \tag{5}$$

where $q_\theta(Y|G_{\mathrm{IB}})$ is the variational approximation of the true posterior $p(Y|G_{\mathrm{IB}})$.

Proposition 2 (Upper bound of $I(G_{\mathrm{IB}};G)$). *For graph $G \in \mathcal{G}$ and IB-Graph G_{IB} learned from G, we have*

$$I(G_{\mathrm{IB}};G) \leq \iint p(G_{\mathrm{IB}},G) \log \frac{p(G_{\mathrm{IB}}|G)}{r(G_{\mathrm{IB}})} dG_{\mathrm{IB}} dG, \tag{6}$$

where $r(G_{\mathrm{IB}})$ is the variational approximation to the prior distribution $p(G_{\mathrm{IB}})$ of G_{IB}.

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Advance IB principle for graph structure learning:

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Objective:

$$\underset{G_{\mathrm{IB}}}{\operatorname{argmin}} \underbrace{-I(G_{IB};Y)}_{\text{prediction term}} + \underbrace{\beta I(G_{IB};G)}_{\text{compression term}}$$

$$\begin{aligned} & -I(G_{\mathrm{IB}};Y)+\beta I(G_{\mathrm{IB}};G) \\ \approx & -I(Z_{\mathrm{IB}};Y)+\beta I(Z_{\mathrm{IB}};G) \\ \leq & \frac{1}{N}\sum_{i=1}^{N}\left\{-\log q_\theta(Y_i|Z_{\mathrm{IB}i})+\beta p(Z_{\mathrm{IB}i}|G_i)\log\frac{p(Z_{\mathrm{IB}i}|G_i)}{r(Z_{\mathrm{IB}})}\right\}. \end{aligned} \qquad (8)$$

Graph Structure Learning with Variational Information Bottleneck, AAAI 2022

Our Work: Graph Structure Learning with IB

Step 1: Generate IB-Graph

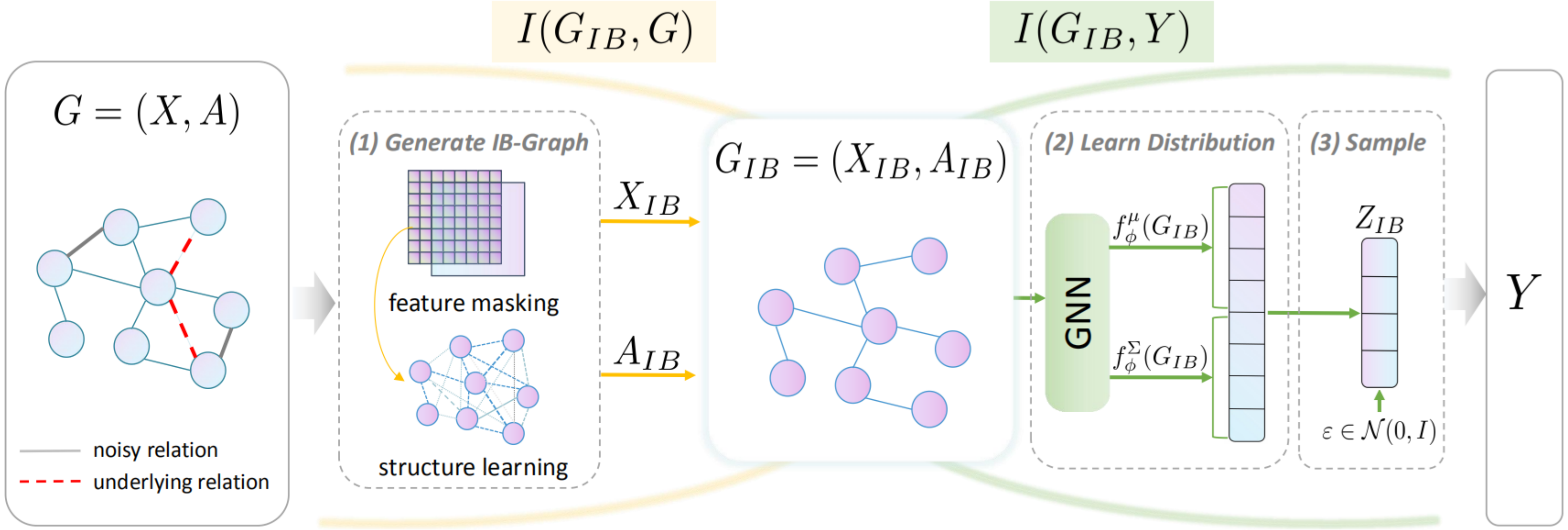
- **Feature Masking**: discretely drop features that are irrelevant to the task
- **Structure Learning**: model all edges as a set of mutually independent Bernoulli random variables parameterized by the learned attention weights

$$X_{\mathrm{IB}} = X_r + (X - X_r) \odot M,$$

$$A_{\mathrm{IB}} = \bigcup_{u,v \in V} \{a_{u,v} \sim \mathrm{Ber}(\pi_{u,v})\}$$

$$Z(u) = \mathbf{NN}(X_{\mathrm{IB}}(u)),$$

$$\pi_{u,v} = \mathrm{sigmoid}\left(Z(u)Z(v)^{\mathrm{T}}\right),$$



$$
\begin{aligned}
& -I(G_{\mathrm{IB}};Y) + \beta I(G_{\mathrm{IB}};G) \\
\approx & -I(Z_{\mathrm{IB}};Y) + \beta I(Z_{\mathrm{IB}};G) \\
\leq & \frac{1}{N}\sum_{i=1}^{N}\left\{-\log q_\theta(Y_i|Z_{\mathrm{IB}i}) + \beta p(Z_{\mathrm{IB}i}|G_i)\log\frac{p(Z_{\mathrm{IB}i}|G_i)}{r(Z_{\mathrm{IB}})}\right\}.
\end{aligned} \tag{8}
$$

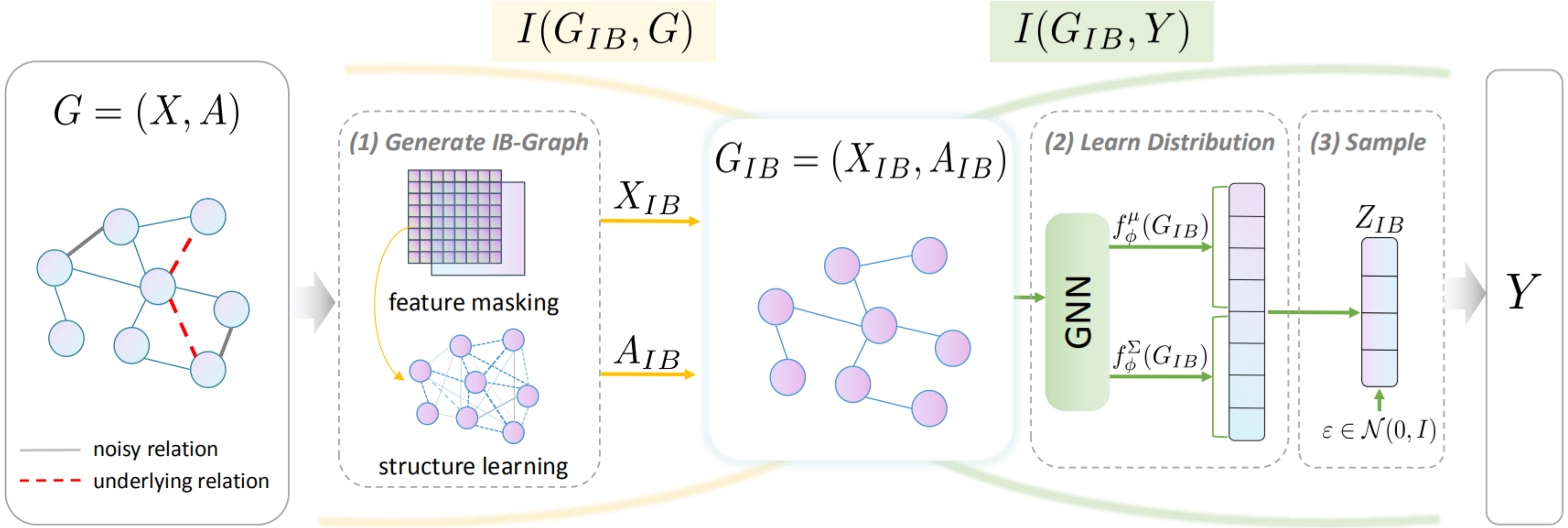
Graph Structure Learning with Variational Information Bottleneck, AAAI 2022

Our Work: Graph Structure Learning with IB

Step 2: Learn Distribution of IB-Graph Representation

- We consider a parametric Gaussian distribution as prior $r(Z_{\mathrm{IB}})$ and $p(Z_{\mathrm{IB}}|G)$i)
- We model the $f_\phi(G_{\mathrm{IB}})$ as a GNN, where $f_\phi^\mu(G_{\mathrm{IB}})$ and $f_\phi^\Sigma(G_{\mathrm{IB}})$ are the 2K-dimensional output value

$$r(Z_{\mathrm{IB}}) = \mathcal{N}(\mu_0, \Sigma_0), \qquad p(Z_{\mathrm{IB}}|G) = \mathcal{N}\left(f_\phi^\mu(G_{\mathrm{IB}}), f_\phi^\Sigma(G_{\mathrm{IB}})\right)$$



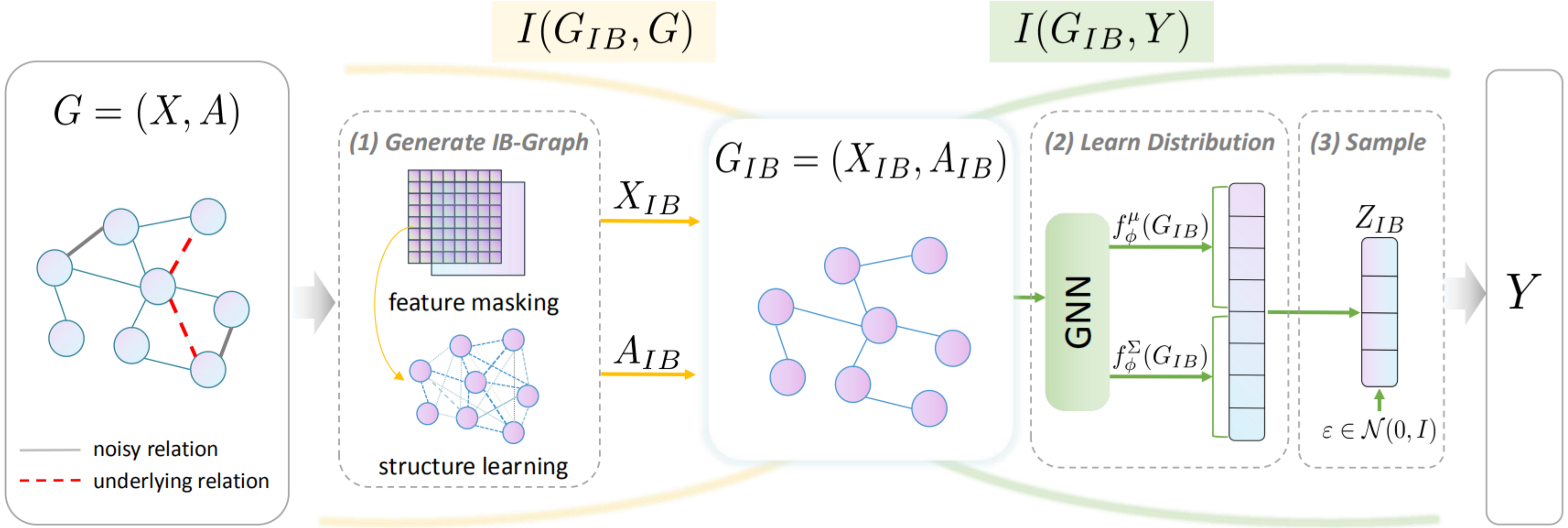
$$\begin{aligned}
&-I(G_{\mathrm{IB}};Y)+\beta I(G_{\mathrm{IB}};G)\\
\approx\ &-I(Z_{\mathrm{IB}};Y)+\beta I(Z_{\mathrm{IB}};G)\\
\leq\ &\frac{1}{N}\sum_{i=1}^{N}\left\{-\log q_\theta(Y_i|Z_{\mathrm{IB}i})+\beta p(Z_{\mathrm{IB}i}|G_i)\log\frac{p(Z_{\mathrm{IB}i}|G_i)}{r(Z_{\mathrm{IB}})}\right\}.
\end{aligned} \tag{8}$$

Our Work: Graph Structure Learning with IB

Step 3: Sample IB-Graph Representation

- We can use the reparameterization trick for gradients estimation

$$Z_{\mathrm{IB}} = f_\phi^\mu(G_{\mathrm{IB}}) + f_\phi^\Sigma(G_{\mathrm{IB}}) \odot \varepsilon,$$



$$\begin{aligned} & -I(G_{\mathrm{IB}};Y) + \beta I(G_{\mathrm{IB}};G) \\ \approx & -I(Z_{\mathrm{IB}};Y) + \beta I(Z_{\mathrm{IB}};G) \\ \leq & \frac{1}{N}\sum_{i=1}^{N}\left\{-\log q_\theta(Y_i|Z_{\mathrm{IB}i}) + \beta p(Z_{\mathrm{IB}i}|G_i)\log\frac{p(Z_{\mathrm{IB}i}|G_i)}{r(Z_{\mathrm{IB}})}\right\}. \end{aligned} \tag{8}$$

Evalauation on Graph Classification Task

- **Datasets:** Four social network datasets
- **Baselines:** Graph structure learners with different GNN backbones

Table 1: Summary of graph classification results: "average accuracy ± standard deviation" and "improvements" (%). Underlined: best performance of specific backbones, **bold**: best results of each dataset.

Structure Learner	Backbone	IMDB-B Accuracy	IMDB-B Δ	IMDB-M Accuracy	IMDB-M Δ	REDDIT-B Accuracy	REDDIT-B Δ	COLLAB Accuracy	COLLAB Δ
N/A	GCN	70.7±3.7	-	49.7±2.1	-	73.6±4.5	-	77.6±2.6	-
	GAT	71.3±3.5	-	50.9±2.7	-	73.1±2.6	-	75.4±2.4	-
	GIN	72.1±3.8	-	49.7±0.4	-	85.4±3.0	-	78.8±1.4	-
NeuralSparse	GCN	72.0±2.6	↑1.3	50.1±3.1	↑0.4	72.1±5.2	↓1.5	76.0±2.0	↓1.6
	GAT	73.4±2.2	↑2.1	53.7±3.1	↑2.8	74.3±3.1	↑1.2	75.4±5.8	0.0
	GIN	73.8±1.6	↑1.7	54.2±5.4	↑4.5	86.2±2.7	↑0.8	76.6±2.1	↓2.2
Subgraph-IB	GCN	72.2±3.9	↑1.5	51.8±3.9	↑2.1	76.7±3.0	↑3.1	76.3±2.3	↓1.3
	GAT	72.9±4.6	↑1.6	51.3±2.4	↑0.4	75.3±4.7	↑2.2	77.3±1.9	↑1.9
	GIN	73.7±7.0	↑1.6	51.6±4.8	↑1.9	85.7±3.5	↑0.3	77.2±2.3	↓1.6
IDGL	GCN	72.2±4.2	↑1.5	52.1±2.4	↑2.4	75.1±1.4	↑1.5	78.1±2.1	↑0.5
	GAT	71.5±4.6	↑0.2	51.8±2.4	↑0.9	76.2±2.5	↑3.1	76.8±4.4	↑1.4
	GIN	74.1±3.2	↑2.0	51.1±2.1	↑1.4	85.7±3.5	↑0.3	76.7±3.8	↓2.1
VIB-GSL	GCN	74.1±3.3	↑3.4	54.3±1.7	↑4.6	77.5±2.4	↑3.9	78.3±1.4	↑0.7
	GAT	75.2±2.7	↑3.9	54.1±2.7	↑3.2	78.1±2.5	↑5.0	79.1±1.2	↑3.7
	GIN	**77.1±1.4**	**↑5.0**	**55.6±2.0**	**↑5.9**	**88.5±1.8**	**↑3.1**	**79.3±2.1**	**↑0.5**

VIB-GSL can learn better graph structure to improve the representation quality

Graph Denosing and Paramete Sensitivity

- How does VIB-GSL perform on graph data with structure noise?
- How does the trade off between prediction and compression influence the performance of VIB-GSL?

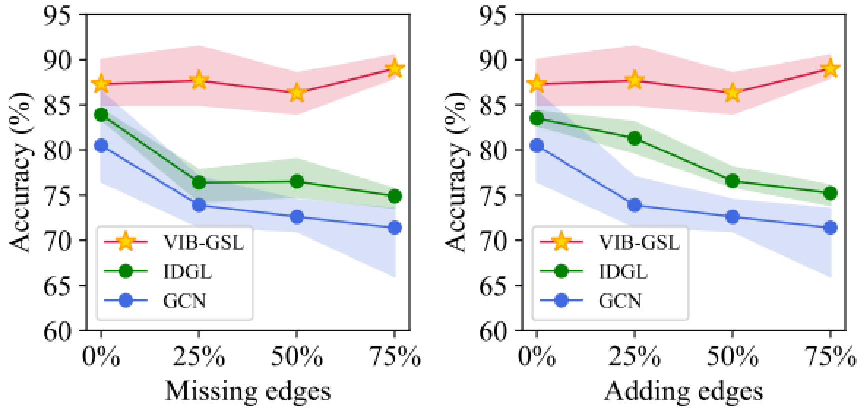


Figure 2: Test accuracy (± standard deviation) in percent for the edge attack scenarios on REDDIT-B (left: edge deletion, right: edge addition).

VIB-GSL is extremely robust to structure perturbations

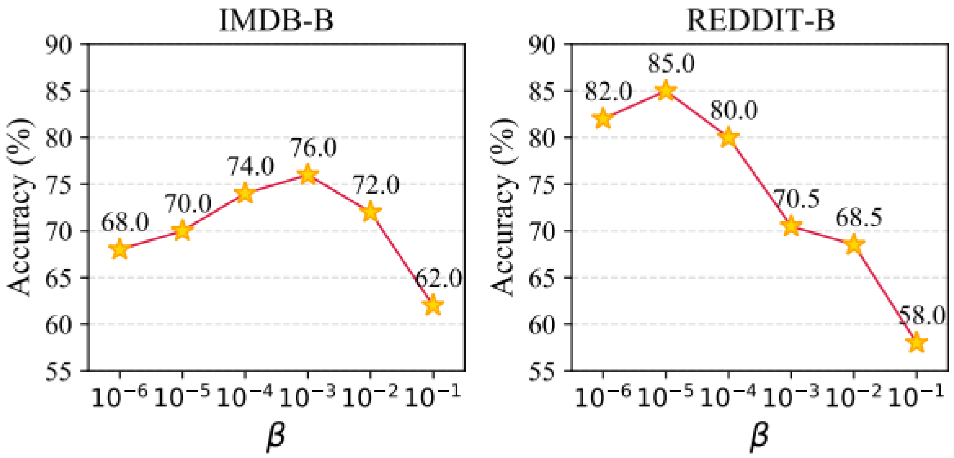


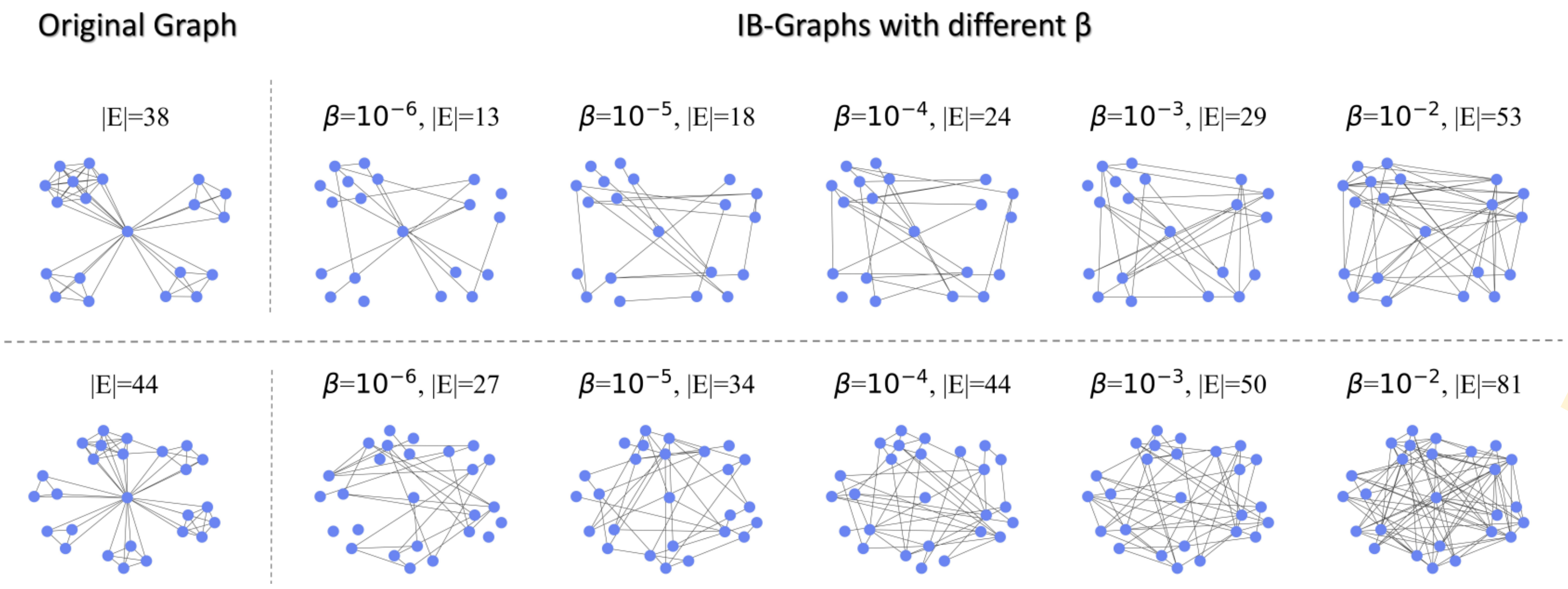
Figure 3: Impact of β on IMDB-B and REDDIT-B.

The accuracies of VIB-GSL variation across different β collapsed onto a hunchback shape

IB-Graph Visualization

How does the trade off between prediction and com-pression influence the learned IB-Graph?

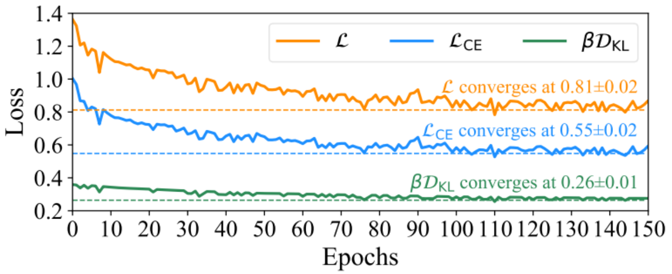
- We show original graph and IB-Graphs with different βwhen VIB-GSL achieves the same testing performance



- VIB-GSL tends to generate edges that connect nodes playing the same structure roles.
- VIB-GSL with larger β will generate a more dense graph structure.

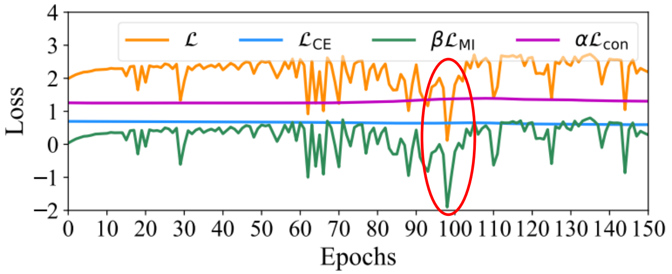
Training stability and efficiency

- **Training stability:** The tractable variational approximation for the IB objective facilitates the training stability
- **Efficiency:** Graph structure learners with different GNN backbones



(a) VIB-GSL.

VIB-GSL deduces a tractable variational approximation for the IB objective, which facilitates the training stability.



(b) Subgraph-IB.

Figure 5: Training dynamics of VIB-GSL and Subgraph-IB.

Subgraph-IB uses a bi-level optimization scheme for MI esitimation, leading to an unstable andinefficient training process

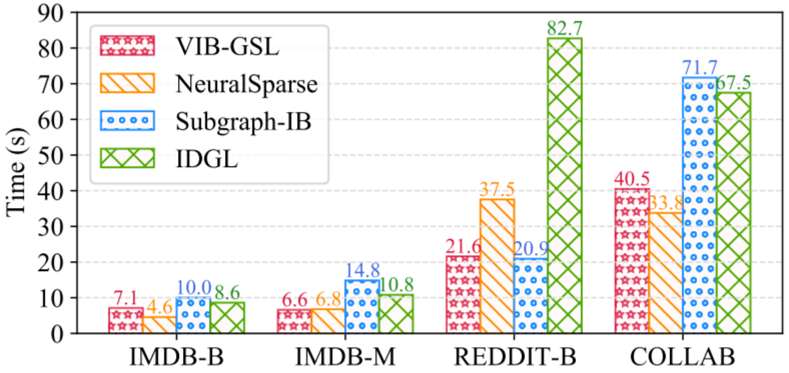


Figure 6: Training time of one epoch on various datasets.

VIB-GSL shows comparable efficiency with other methodswhen achieving the best performance

Conclusion and Future Works

- We advance the Information Bottleneck principle for graph structure learning and propose a framework named VIB-GSL, which jointly optimizes the graph structure and graph representations.
- VIB-GSL deduces a variational approximation to form a tractable IB objectivefunction that facilitates training stability and efficiency.
- Future works: A general, unified and scalable IB guided GSL framework for dfferent graph learning levels.

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