EGonc: Energy-based Open-Set Node Classification with substitute Unknowns

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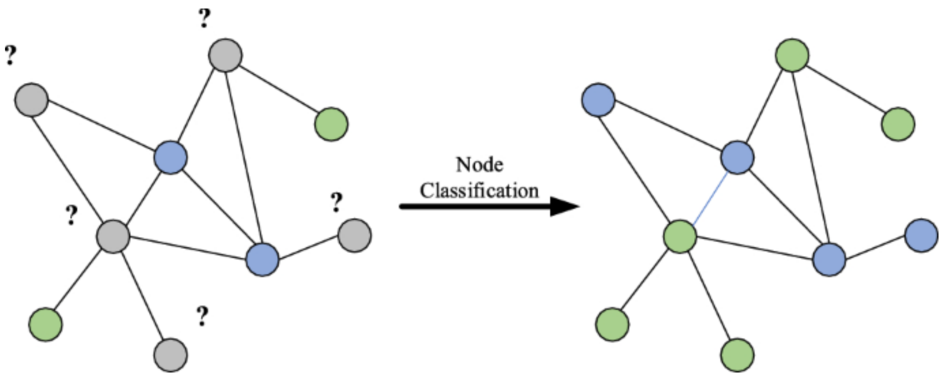
Introduction

Background

- Node classification is the task of predicting the labels of unlabeled nodes in a graph.
- SOTA methods based on graph neural networks achieve excellent performance when all labels are available during training.
- But in real-life, models are often applied on data with new classes, which can lead to massive misclassification and thus significantly degrade performance.
- Hence, developing open-set classification methods is crucial to resolve this issue.



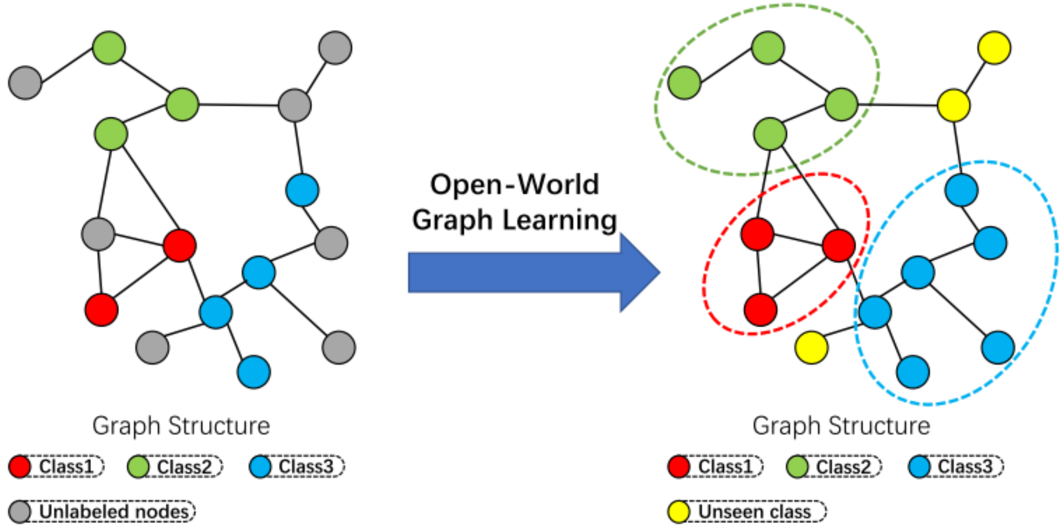
Introduction

■ Motivation

Major challenges in Graph Learning:

mostly based on closed-world assumptions, lacking generalization ability

- Restricting the category space to remain consistent between the training and the testing stages.
- Most methods based on the open-world assumption adhere to a transductive setting.
- Most open-set node classification methods on graphs are based on discriminative or generative models, lacking new approaches.



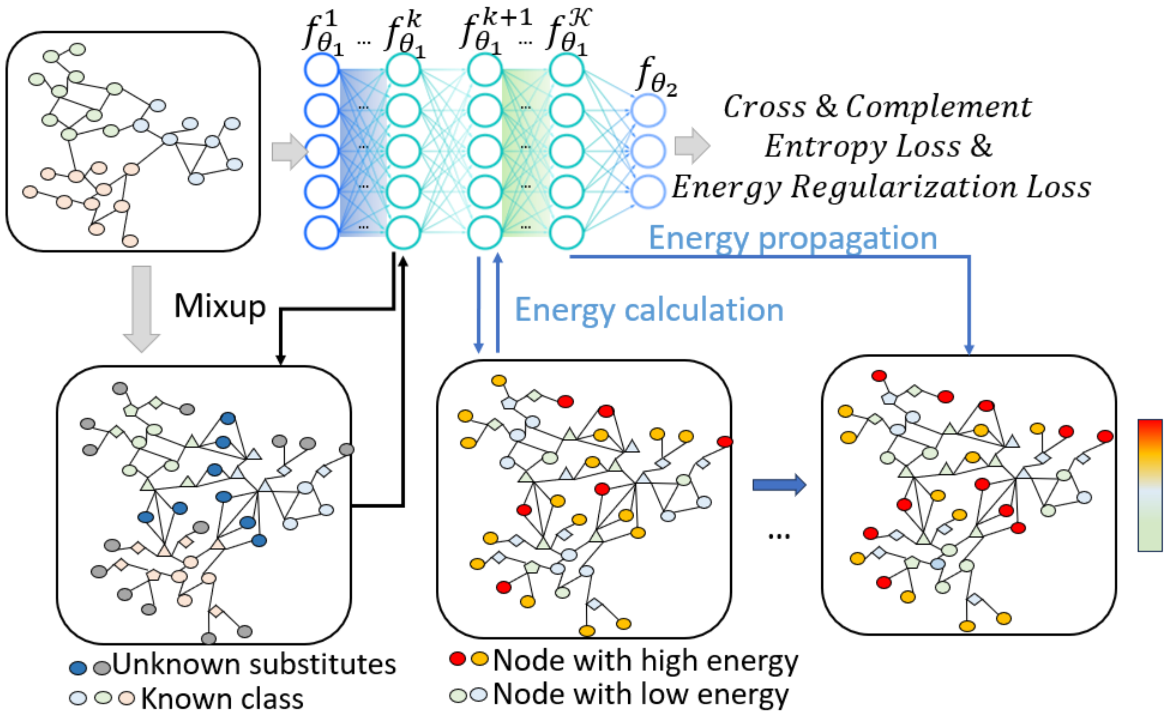
Introduction

Contribution

- A novel method, $EGonc$, for open-set node classification is proposed by redefining the open-world graph learning paradigm based on the energy model and elaborate unknown-substitute generation.
- $EGonc$ has nice theoretical properties that guarantee an overall distinguishable margin between the detection scores for IND and OOD samples.
- No open-set data (samples of unknown classes or any side information of unknown classes) is required during training and validation.
- $EGonc$ is agnostic to specific GNN architecture and demonstrates robust generalization capabilities.

Model

■ Overview of $EGonc$ model.



Our model is mainly consists of three components:

- ➢ Substitute Unknowns Generation
  - ➢ An effective way for generating Substitute unknown nodes
  - ✓ Inter-Class Unknown substitute
  - ✓ External Unknown substitute
- ➢ Energy Propagation
  - ➢ An bridge between the energy function and an open-set classifier
- ➢ Open-Set Classifier Learning
  - ➢ An learing module to guarantee the classification of known classes and the rejection of the unknown class.

Model

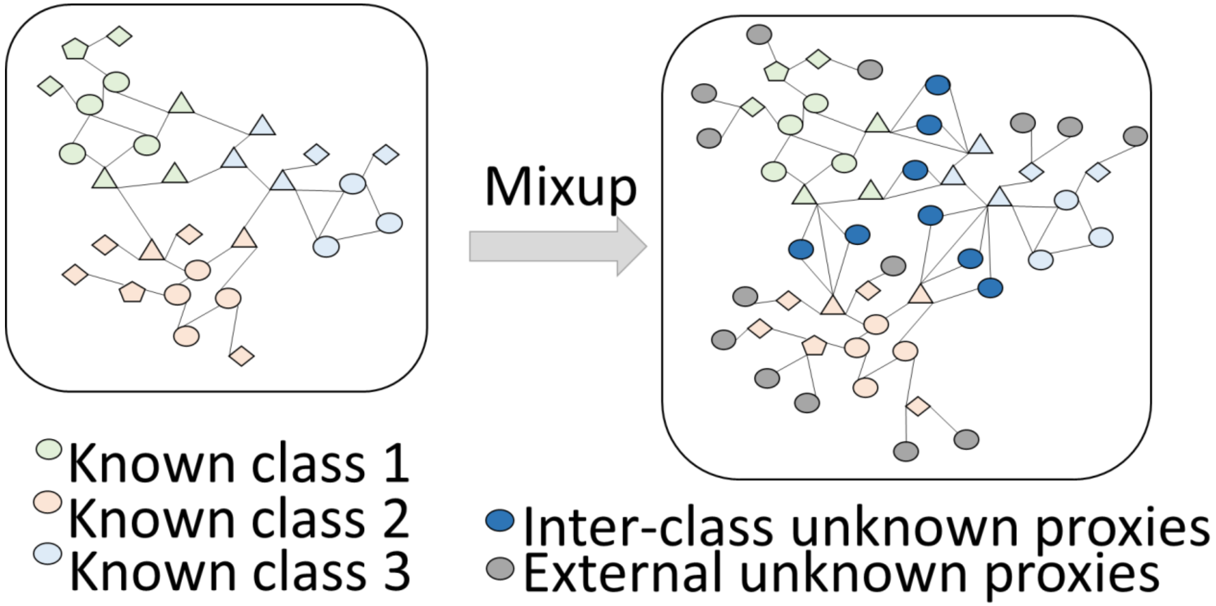
Inter-Class Unknown substitutes

$$\begin{cases} \tilde{x}_i = \alpha h_i^k(\theta_1; x_i, A) + (1-\alpha) h_j^k(\theta_1; x_j, A) \\ \tilde{y}_i = C + 1 \end{cases}$$

External Unknown Substitutes

$$h_{(c)}^k = \frac{1}{|X^c|} \sum_{x_i \in X^c} h_i^k(\theta_1; x_i, A)\,,\, c = 1, \dots, C$$

$$\begin{cases} \tilde{x}_i = \beta h_i^k(\theta_1; x_i, A) + (-\gamma\, h_{(y_i)}^k) \\ \tilde{y}_i = C + 1 \end{cases}$$

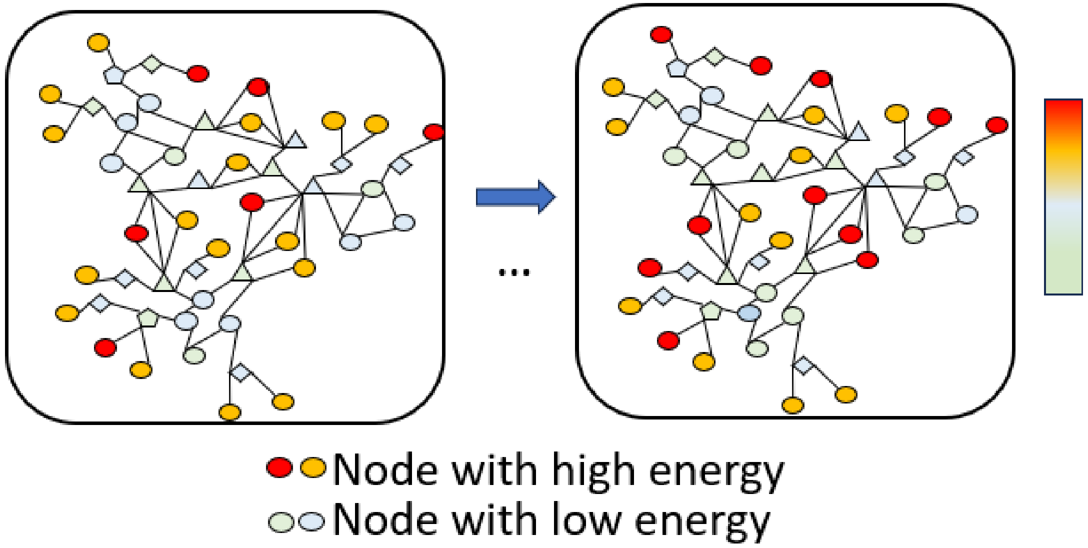


Model

Energy Propagation

$$E^{(k)} = kE^{(k-1)} + (1-k)D^{-1}\hat{A}E^{(k-1)}$$

$$\hat{A} = D^{-1/2}AD^{-1/2}$$
$$E^{(k)} = [E_i^{(k)}]$$



Model

Algorithm 1 EGonc: open-set node classification

```
Require: : G = (V, E, X): a graph with links and features;
    D_tr = {G, Y}: train set with labeled nodes;
    X_te = S ∪ U: test set where S are the known classes appeared in training and U are the unknown
    classes;
Ensure: f(X_te → 𝒴), 𝒴 ∈ {1, ..., C, unknown}.
Obtain the inter-class node pairs {(x_i, y_i), (x_j, y_j)} ∈ D_tr  s.t. y_i ≠ y_j & a_ij = 1
Obtain the peripheral nodes that are leaf nodes and low confident nodes.
while not convergence do
    For the first m = 1, ... k layer:
        h_i^m = f^m(θ_1; h_i^{m-1}, h_j^{m-1}, j ∈ N_i), ∀x_i ∈ D_tr
    At the k-th layer:
        Create unknown substitutes X_sub using Eq. (8) & (9)
        Augment the substitutes to known class samples:
        D̄_tr = D_tr ∪ (X_sub, Y_C+1)
    For the m = k + 1, ..., k_1 − 1 layers:
        h_i^m = f^m(θ_1; h_i^{m-1}, h_j^{m-1}, j ∈ N_i), ∀x_i ∈ D̄_tr
    For the m = k_1, ..., K layers:
        h_i^m = f^m(θ_1; h_i^{m-1}, h_j^{m-1}, j ∈ N_i), ∀x_i ∈ D̄_tr
        E_i^m = f^m(E_i^{m-1}, E_j^{m-1}, j ∈ N_i), ∀x_i ∈ D̄_tr
    For open-set classifier layer:
        Obtain cross entropy loss as Eq. (11)
        Obtain complement entropy loss as Eq. (12)
        Obtain energy regularization loss as Eq. (13)
    Back-propagate loss gradient using Eq. (14) and update weights
    if early stopping condition is satisfied then
        Terminate
    end if
end while
```

- ✓ $l_1 = \sum_{(x_i,y_i)\epsilon D_{tr}} l_{CrE}(\hat{y}_i, y_i) + \lambda_1 \sum_{x_i \epsilon X_{sub}} l_{CrE}(\hat{y}_i, C+1)$
- ✓ l_1 use $l_{CrE}(\hat{y}_i, y_i) = -y_i log \hat{y}_i$ to maximize data likelihood
- ✓ $l_2 = \sum_{(x_i,y_i)\epsilon D_{tr}} l_{CrE}(\hat{y}_i / y_i, C+1) + \sum_{x_i \epsilon X_{sub}} l_{CoE}(\hat{y}_i, y_i)$
- ✓ $l_{CoE} = -\sum_{c=1, c\neq y_i}^{C+1} \frac{\hat{y}_{i,c}}{1-\hat{y}_{i,y_i}} log \frac{\hat{y}_{i,c}}{1-\hat{y}_{i,y_i}}$
- ✓ l_2 use l_{CoE} and to l_{CrE} to eliminate the effects of complement classes
- ✓ $l_3 = k_1 \left(\sum_{(x_i,y_i)\epsilon D_{tr}} \sigma(E_{ind}(x_i)) + \sum_{x_j \epsilon X_{sub}} \sigma\left(E_{ood}(x_j)\right) \right)$
- ✓ $+k_2 \left(\sum_{(x_i,y_i)\epsilon D_{tr}} \sigma(E_{ind}(x_i))^2 + \sum_{x_j \epsilon X_{sub}} \sigma\left(E_{ood}(x_j)\right)^2 \right)$
- ✓ And the loss function is $l_{total} = l_1 + \lambda_2 l_2 + \lambda_3 l_3$

Experiment

Table 5: Statistics of the experimental datasets.

Dataset	Nodes	Edges	Features	Labels
Cora	2708	5429	1433	7
Citeseer	3312	4732	3703	6
DBLP	17716	105734	1639	4
PubMed	19717	44325	500	3
Ogbn_arxiv	169343	1166243	128	40

We select five real-world datasets.

- ✓ Cora
- ✓ Citeseer
- ✓ DBLP
- ✓ PubMed
- ✓ Ogbn_arxiv

Table 1: Near open-set classification on five citation network datasets with one unknown class (u=1) in the *inductive learning setting*. Numbers reported are all percentage (%).

Methods	Cora		Citeseer		DBLP		Pubmed		Ogbn_arxiv		Average	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1
GCN_soft	70.6	67.6	44.6	38.9	63.8	59.2	28.9	29.9	49.8	17.5	51.5	42.6
GCN_sig	69.2	64.7	45.3	44.5	63.5	58.7	28.9	29.8	48.8	9.5	51.1	41.4
GCN_soft_τ	73.6	73.8	57.3	54.5	65.0	62.4	49.7	48.6	47.3	20.6	58.6	52.0
GCN_sig_τ	79.7	80.1	62.1	54.6	69.2	68.2	45.1	46.0	46.0	8.3	60.4	51.4
Openmax	74.6	75.1	56.2	54.5	67.2	67.2	49.1	48.7	45.5	16.3	58.5	52.4
DOC	77.8	78.1	66.0	56.7	69.9	69.2	45.6	46.2	46.7	20.7	61.2	52.2
PROSER	83.2	83.7	73.7	63.6	71.7	72.6	71.0	58.4	53.0	31.1	70.5	61.9
OpenWGL	78.1	78.9	64.1	60.8	71.4	72.2	65.3	63.4	45.4	20.7	64.9	60.2
GNNSAFE	79.6	81.0	69.8	60.3	72.5	74.1	70.1	66.8	51.2	24.2	68.6	61.3
$\mathcal{G}^2Pxy$	84.3	84.8	75.5	71.0	77.3	79.0	73.7	70.2	62.7	**33.0**	74.7	67.6
EGonc	**84.5**	**84.9**	**75.8**	**71.5**	**79.1**	**80.8**	**80.2**	**75.5**	**63.0**	**33.0**	**76.5**	**69.1**

- ✓ Our method consistently **outperforms** baseline methods for all datasets.

- ✓ Specifically, Our method is **better** than GNNSAFE, g^2pxy and OpenWGL in the inductive learning setting, which are the state-of-the-art method.

Experiment

1. As shown in Table 8, our proposed method consistently **outperforms** the baselines in terms of Acc and F1 on different datasets in the transductive learning setting.

2. As shown in Table 3, when compared under far open-set classification setting, our model consistently outperforms them **in all metrics**.

Table 8: Near open-set classification on five citation network datasets with one unknown class (u=1) under in the *transductive learning setting*. Numbers reported are all percentage (%).

Methods	Cora		Citeseer		DBLP		Pubmed		Ogbn_arxiv		Average	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1
GCN_soft	70.8	68.2	44.7	38.9	62.9	57.0	29.2	29.7	50.2	18.4	51.6	42.4
GCN_sig	68.8	64.5	44.6	40.1	63.4	59.2	29.0	29.5	46.8	8.4	50.5	40.3
GCN_soft_τ	78.1	78.9	67.3	57.0	67.3	67.7	68.9	27.2	49.6	19.0	66.2	50.0
GCN_sig_τ	78.3	78.5	65.4	55.3	71.4	71.5	69.0	27.2	45.9	7.7	66.0	48.0
Openmax	77.2	76.9	57.5	56.7	69.0	70.6	55.0	52.1	49.2	18.9	61.6	55.0
DOC	77.3	77.9	65.1	55.3	71.7	72.0	68.4	34.2	49.9	19.4	66.5	51.8
PROSER	84.7	83.6	74.3	66.6	75.3	71.6	72.8	60.8	55.0	30.7	72.4	62.7
OpenWGL	83.3	83.5	70.0	65.4	74.3	74.2	71.2	68.0	46.0	20.0	69.0	62.2
GNNSAFE	80.7	81.9	73.1	62.2	74.2	75.8	73.5	69.9	52.8	24.1	70.8	62.8
$\mathcal{G}^2Pxy$	90.7	89.7	76.3	71.8	77.5	79.5	78.0	73.4	63.7	31.4	77.2	69.2
EGonc	**91.2**	**90.4**	**77.2**	**72.9**	**79.4**	**80.7**	**86.5**	**80.5**	**63.8**	**31.6**	**79.6**	**71.2**

Table 3: Accuracy and macro-F1 for far open-set classification on benchmark datasets. Numbers reported are all percentage (%).

Methods	Co_Ci		Ci_DB		DB_Pub		Average	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1
GCN_soft	43.0	58.9	38.4	42.5	41.9	53.7	41.1	51.7
GCN_sig	41.6	57.5	36.3	42.1	41.6	45.2	39.8	48.3
GCN_soft_τ	81.2	77.6	86.2	71.1	85.0	**75.6**	84.1	74.8
GCN_sig_τ	69.4	51.8	68.7	48.0	79.8	69.1	72.6	56.3
Openmax	56.2	55.1	69.6	60.3	69.6	58.7	65.1	58.0
DOC	69.4	57.8	75.5	62.3	78.0	70.7	74.3	63.6
PROSER	78.5	79.1	81.5	66.4	78.6	69.0	79.5	71.5
OpenWGL	80.6	76.7	44.6	11.9	84.6	70.7	69.9	53.1
GNNSAFE	79.3	79.9	80.9	65.9	80.0	65.0	80.1	70.3
$\mathcal{G}^2Pxy$	81.3	80.5	87.5	74.4	86.5	72.3	85.1	75.7
EGonc	**81.7**	**81.0**	**88.1**	**75.2**	**87.2**	72.8	**85.7**	**76.3**

Experiment

Table 2: Accuracy and macro-F1 scores of EGonc and its variants with respect to different losses and generation strategies.

Components				Cora		Citeseer		DBLP		Pubmed		O_arxiv		Average	
l_1		l_2	l_3	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1
✓				84.2	84.7	75.2	69.0	76.5	77.7	70.1	47.3	61.9	**34.1**	73.6	62.6
✓		✓		84.3	84.8	75.5	71.0	77.3	79.0	73.7	70.2	62.7	33.0	74.7	67.6
✓		✓	✓	**84.5**	**84.9**	**75.8**	**71.5**	**79.1**	**80.8**	**80.2**	**75.5**	**63.0**	33.0	**76.5**	**69.1**
X_{far}	X_{rand}	X_{int}	X_{ext}	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1
				82.7	83.2	73.5	69.6	69.5	71.3	70.4	67.2	60.1	30.0	71.2	64.3
✓				83.7	84.0	75.5	66.9	72.3	72.7	71.8	68.5	62.3	29.3	73.1	64.3
	✓			81.3	82.2	74.6	63.7	71.2	71.5	70.0	66.9	61.9	32.3	71.8	63.3
		✓		84.2	84.7	75.3	70.8	75.3	76.9	73.4	68.7	62.3	31.4	74.1	66.5
			✓	84.1	84.6	75.4	70.9	75.5	74.8	71.4	66.9	61.5	29.5	73.6	65.3
✓	✓			84.0	84.4	75.7	71.2	72.0	71.7	73.0	69.1	61.9	32.0	73.3	65.7
		✓	✓	**84.5**	**84.9**	**75.8**	**71.5**	**79.1**	**80.8**	**80.2**	**75.5**	**63.0**	**33.0**	**76.5**	**69.1**

1. As shown in Table 2, we compare variants of $EGonc$ **with respect to the generative strategy and different losses** to demonstrate its effect.

Experiment

Table 4: Accuracy and macro-F1 scores of open-set classification methods with different backbone neural network. Numbers reported are all percentage (%).

Methods	Cora		Citeseer		Dblp		PubMed		Ogbn_arxiv	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1
GCN_soft_τ	73.6	73.8	57.3	54.5	65.0	62.4	49.7	48.6	47.3	20.6
GCN_DOC	77.8	78.1	66.0	56.7	69.9	69.2	45.6	46.2	46.7	20.7
GCN_Openmax	74.6	75.1	56.2	54.5	67.2	67.2	49.1	48.7	45.5	16.3
GCN_$\mathcal{G}^2Pxy$	84.3	84.8	75.5	71.0	77.3	79.0	73.7	70.2	62.7	**33.0**
GCN_EGonc	**84.5**	**84.9**	**75.8**	**71.5**	**79.1**	**80.8**	**80.2**	**75.5**	**63.0**	**33.0**
GAT_soft_τ	71.6	69.2	58.9	51.1	65.4	66.6	43.2	43.7	49.1	16.7
GAT_DOC	71.1	72.6	62.4	59.5	64.2	61.8	42.1	42.9	48.3	16.2
GAT_Openmax	66.3	63.4	48.6	48.9	62.5	56.9	48.6	47.0	32.2	8.4
GAT_$\mathcal{G}^2Pxy$	80.4	81.0	75.2	70.9	72.9	73.7	71.7	47.0	53.7	22.6
GAT_EGonc	**80.8**	**81.3**	**75.3**	**71.0**	**73.1**	**74.0**	**74.3**	**63.6**	**56.1**	**24.5**
Graphsage_soft_τ	72.7	72.9	63.5	51.2	64.3	64.0	46.6	46.9	51.5	16.0
Graphsage_DOC	76.0	75.4	63.6	59.9	68.9	72.2	44.6	45.7	49.5	14.7
Graphsage_Openmax	71.1	70.6	47.9	48.7	62.3	56.9	44.4	45.1	43.2	8.0
Graphsage_$\mathcal{G}^2Pxy$	87.2	**87.3**	78.6	76.9	74.4	74.7	72.8	64.9	62.8	36.5
Graphsage_EGonc	**87.3**	**87.3**	**79.5**	**77.4**	**78.0**	**79.6**	**73.0**	**65.0**	**63.4**	**38.4**

1. As shown in Table 4, the proposed model $EGonc$ **is agnostic to specific GNN architecture** and demonstrates robust generalization capabilities.

Conclusion

- In this paper, we propose a novel energy-based generative open-set node classification method, $EGonc$, by estimating the underlying density of the training data to decide whether a given input is close to the IND data.

- Two kinds of substitute unknowns are generated to mimic the distribution of real open-set samples.

- Under constraint of cross entropy loss, complement entropy loss, and energy regularization loss, $EGonc$ achieves superior effectiveness for unknown class detection and known class classification, which is validated by experiments on benchmark graph datasets.

- Moreover, $EGonc$ also has good generalization since it has no specific requirement on the GNN architecture.

$EGonc: Energy-based\ Open-Set\ Node\ Classification\ with\ substitute\ Unknowns$

Thank you!

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