A Appendix material

A.1   Proof of Theorem 3.1

Proof. We can expand $\mathcal{L}_{sd}(F, A)$ and obtain

$$
\begin{aligned}
\mathcal{L}_{sd}(F, A) &= \sum_{x,x'\in X} \left(\frac{A_{xx'}}{\sqrt{A_x A_{x'}}} - \mathbf{f}_x^\top \mathbf{f}_{x'} \right)^2 \\
&= \text{const} + \sum_{x,x'\in X} \left(-2A_{xx'} f(x)^\top f(x') + A_x A_{x'} \left(f(x)^\top f(x') \right)^2 \right),
\end{aligned}
\tag{1}
$$

where $\mathbf{f}_x = \sqrt{A_x} f(x)$ is a re-scaled version of $f(x)$. At a high level, we follow the proof in [1], while the specific form of loss varies with the different definitions of positive/negative pairs. The form of $\mathcal{L}_{scl}(f)$ is derived from plugging $A_{xx'}$ and A_x.

Recall that $A_{xx'}$ is defined by

$$
A_{xx'} = \alpha \sum_{c_i\in\mathcal{C}} \mathbb{E}_{x\sim\mathcal{P}_{c_i}, x'\sim\mathcal{P}_{c_i}} A_{xx'}^l + \beta \mathbb{E}_{x\sim\mathcal{P}_u, x'\sim\mathcal{P}_u} A_{xx'},
\tag{2}
$$

thus we have,

$$
\begin{aligned}
&-2\sum_{x,x'\in X} A_{xx'} f(x)^\top f(x') \\
={}&-2\alpha \sum_{c_i\in\mathcal{C}} \mathbb{E}_{x\sim\mathcal{P}_{c_i}, x'\sim\mathcal{P}_{c_i}} A_{xx'} f(x)^\top f(x') - 2\beta \mathbb{E}_{x\sim\mathcal{P}_u, x'\sim\mathcal{P}_u} A_{xx'} f(x)^\top f(x') \\
={}&-2\alpha \sum_{c_i\in\mathcal{C}} \mathbb{E}_{x\sim\mathcal{P}_{c_i}, x'\sim\mathcal{P}_{c_i}, A_{xx'}\neq 0} f(x)^\top f(x') - 2\beta \mathbb{E}_{x\sim\mathcal{P}_u, x'\sim\mathcal{P}_u, A_{xx'}\neq 0} f(x)^\top f(x') \\
={}&-2\alpha \sum_{c_i\in\mathcal{C}} \mathbb{E}_{x\sim\mathcal{P}_{c_i}, x^+\in\{x'|A_{xx'}\neq 0, x'\sim\mathcal{P}_{c_i}\}} f(x)^\top f(x^+) - 2\beta \mathbb{E}_{x\sim\mathcal{P}_u, x^+\in\{x'|A_{xx'}\neq 0, x'\sim\mathcal{P}_u\}} f(x)^\top f(x^+) \\
={}&-2\alpha \mathcal{L}_1(f) - 2\beta \mathcal{L}_2(f).
\end{aligned}
$$

The penultimate equation is derived from the following lemma:

$$
\begin{aligned}
&\mathcal{L}_{sd}(F) = \mathcal{L}(f) + \text{const} \\
&\text{where } \mathcal{L}(f) \triangleq -2 \cdot \mathbb{E}_{x,x^+}\left[f(x)^\top f(x^+) \right] + \mathbb{E}_{x,x^-}\left[\left(f(x)^\top f(x^-) \right)^2 \right].
\end{aligned}
\tag{3}
$$

Recall that A_x is given by

$$
A_x = \sum_{x'\in X} A_{xx'}
\tag{4}
$$

$$
= \alpha \sum_{c_i\in\mathcal{C}} \mathbb{E}_{x\sim\mathcal{P}_{c_i}} A_x + \beta \mathbb{E}_{x\sim\mathcal{P}_u} A_x.
\tag{5}
$$

1

thus plugging A_x and $A_{x'}$ we have,

$$\sum_{x,x'\in X} A_x A_{x'} \left(f(x)^\top f(x')\right)^2$$

$$= \sum_{x,x'\in X}\left(\alpha\sum_{c_i\in\mathcal{C}}\mathbb{E}_{x\sim\mathcal{P}_{c_i}}A_x + \beta\mathbb{E}_{x\sim\mathcal{P}_u}A_x\right)\cdot\left(\alpha\sum_{c_j\in\mathcal{C}}\mathbb{E}_{x'\sim\mathcal{P}_{c_j}}A_{x'} + \beta\mathbb{E}_{x'\sim\mathcal{P}_u}A_{x'}\right)\left(f(x)^\top f(x')\right)^2$$

$$=\alpha^2\sum_{x,x'\in X}\sum_{c_i\in\mathcal{C}}\mathbb{E}_{x\sim\mathcal{P}_{c_i}}A_x\sum_{c_j\in\mathcal{C}}\mathbb{E}_{x'\sim\mathcal{P}_{c_j}}A_{x'}\left(f(x)^\top f(x')\right)^2$$

$$+2\alpha\beta\sum_{x,x'\in X}\sum_{c_i\in\mathcal{C}}\mathbb{E}_{x\sim\mathcal{P}_{c_i}}A_x\mathbb{E}_{x'\sim\mathcal{P}_u}A_{x'}\left(f(x)^\top f(x')\right)^2$$

$$+\beta^2\sum_{x,x'\in X}\mathbb{E}_{x\sim\mathcal{P}_u}A_x\mathbb{E}_{x'\sim\mathcal{P}_u}A_{x'}\left(f(x)^\top f(x')\right)^2$$

$$=\alpha^2\sum_{c_i\in\mathcal{C}}\sum_{c_j\in\mathcal{C}}\mathbb{E}_{x\sim\mathcal{P}_{c_i},x^-\in\{x'|A_{xx'}=0,x'\sim\mathcal{P}_{c_j}\}}\left[\left(f(x)^\top f(x')\right)^2\right]$$

$$+2\alpha\beta\sum_{c_i\in\mathcal{C}}\mathbb{E}_{x\sim\mathcal{P}_{c_i},x^-\in\{x'|A_{xx'}=0,x'\sim\mathcal{P}_u\}}\left[\left(f(x)^\top f(x')\right)^2\right]$$

$$+\beta^2\mathbb{E}_{x\sim\mathcal{P}_u,x^-\in\{x'|A_{xx'}=0,x'\sim\mathcal{P}_u\}}\left[\left(f(x)^\top f(x')\right)^2\right]$$
$$=\alpha^2\mathcal{L}_3(f)+2\alpha\beta\mathcal{L}_4(f)+\beta^2\mathcal{L}_5(f).$$

$\square$

The proof of Theorem 3.1 is finished.

A.2 Additional Experiments

A.2.1 Zero-shot node classification for large-scale data

For SpeAr, the spectral contrastive loss computes the similarities between samples, with a time complexity of $O(N_s N_s^+ + N_u N_u^+ + N_s N_u + N_s N_s^- + N_u N_u^-)$. Let N_s be the count of labeled nodes, N_s^+ be the count of positive nodes of labeled nodes, and N_s^- the negative nodes. N_u is the count of unlabeled nodes, with N_u^+ and N_u^- representing the count of positive and negative nodes, respectively. This complexity reveals a substantial demand for computational resources, presenting a notable challenge for processing large-scale graph data.

Following GraphCEN [2], we validate the efficacy of the SpeAr on large-scale dataset, such as ogbn-arxiv [3]. Ogbn-arxiv has 169343 nodes, and 2484941 edges. The feature dimension is 128 and the total class number is 40. Class split I is [20/0/20], 20 seen classes as training set, 20 unseen classes as testing set. Class split II is [13/13/14], 13 seen classes as training set, 13 unseen classes as validation set, and 14 unseen classes as testing set. Confronted with memory limitations, we adopt a multi-round subgraph extraction strategy. Specifically, in each round, we extract subgraphs that encompass both seen and unseen class nodes and execute the SpeAr algorithm on these subgraphs. Through this iterative process of extraction, we aim to progressively accumulate performance gains that mirror the execution of SpeAr on the entire graph, all while maintaining computational efficiency. As shown in Table 1, our proposed method SpeAr shows significant improvement in performance metrics compared to existing methods. The comparative analysis in the table highlights the superiority of our method in capturing class-discriminative information in graph structures.

Table 1: A comparative performance analysis of DGPN, DBiGCN, and ours SpeAr for zero-shot node classification on ogbn-arxiv. (%)

	DGPN	DBiGCN	GraphCEN	SpeAr(Ours)
Class Split I	22.37	21.40	23.96	**30.45**
Class Split II	21.95	25.92	28.36	**32.20**

2

Table 2: The Comparison of zero-shot node classification accuracy (%) using the different CSDs.

	Cora			Citeseer			C-M10M		
	TEXT	LABEL	Decline rate	TEXT	LABEL	Decline rate	TEXT	LABEL	Decline rate
DAP	26.56	25.34	-4.59 %	34.01	30.01	-11.76%	38.71	32.67	-15.60%
ESZSL	27.35	25.79	-5.70%	30.32	28.52	-5.94%	37.00	35.02	-5.35%
ZS-GCN	25.73	23.73	-7.77%	28.62	26.11	-8.77%	37.89	33.32	-12.06%
WDVSc	30.62	18.73	-38.83%	23.46	19.70	-16.02%	38.12	30.82	-19.15%
Hyperbolic-ZSL	26.36	25.47	-3.38%	34.18	21.04	-38.44%	35.80	34.49	-3.66%
DGPN	33.78	32.55	-3.64%	38.02	31.83	-16.28%	41.98	35.05	-16.51%
DBiGCN	45.14	39.05	-13.49%	40.97	39.10	-3.10%	45.45	43.71	-3.83%
SpeAr(Ours)	**60.48**	**49.52**	-18.12%	**59.72**	**48.88**	-18.15%	**54.22**	**47.05**	-13.22%
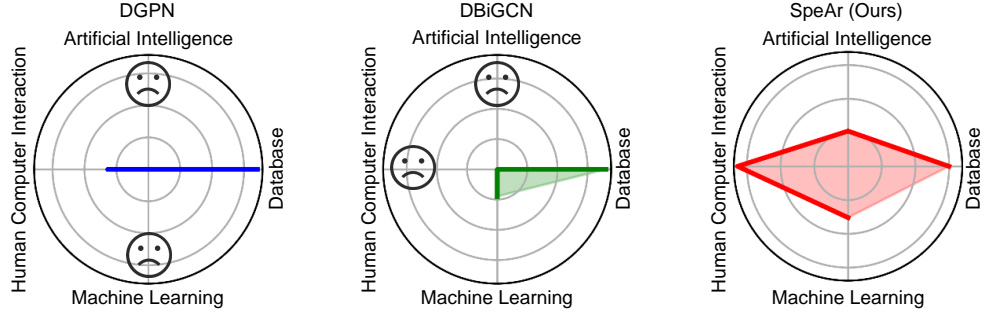
Figure 1: An example of the SpeAr model's effectiveness in mitigating prediction bias on Citeseer.

A.2.2 Discussion on Different CSVs

The impact of external knowledge from different sources on model outcomes is significantly varied. In Table 2, we individually examined the effects of LABEL-based CSVs and TEXT-based CSVs as external knowledge. Given that TEXT data encapsulates a richer set of categorical information, the SpeAr model utilizing text-based CSVs demonstrates superior performance. Indeed, when employing LABEL-based CSVs as the input external knowledge, SpeAr also outperforms existing methods, further corroborating the efficacy of the spectral contrastive loss and prototype updating mechanisms proposed in this paper for excavating and identifying categories on graphs. This series of results underscore that our approach significantly enhances the discriminability between different classes, thereby elevating the model's overall recognition capability.

A.2.3 Discussion on SpeAr model's effectiveness in mitigating prediction bias

We verify the benefits of SpeAr in mitigating prediction bias on the dataset Citeseer. As shown in Figure 1, the recall for certain classes is extremely low or even zero. For instance, the unseen classes "Human Computer Interaction" and "Artificial Intelligence" exhibit a zero recall rate when predicted by the DBiGCN. In contrast, the SpeAr model provides more accurate classification outcomes for all unseen classes.

B Limitation

Although the SpeAr model shows excellent performance on the ZNC task, its relatively high computational complexity may become a challenge when dealing with large-scale graph data. Especially in application scenarios with limited resources or high real-time requirements, the high computational cost may limit the usefulness of the model. Therefor, we effectively alleviate this problem by adopting the strategy of multi-round subgraph training. The model can gradually learn and integrate information from different subgraphs, thus realizing effective processing of large graph data while maintaining computational efficiency.

3

C Experiments Compute Resources

Computation resources: We execute our code on a computer with NVIDIA GeForce RTX 3090 (GPU) and Intel Xeon Gold 6254 (CPU).

D Societal Impacts

The introduction of SpeAr has made a significant contribution to the advancement of zero-shot node classification tasks. It demonstrates tremendous potential in the field of data analysis, aiding researchers in uncovering new insights and knowledge. There are no negative societal impacts on our work.

References

[1] Jeff Z. HaoChen, Colin Wei, Adrien Gaidon, and Tengyu Ma. Provable guarantees for self-supervised deep learning with spectral contrastive loss. In *Advances in Neural Information Processing Systems*, volume 34, pages 5000–5011, 2021.

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[3] Kuansan Wang, Zhihong Shen, Chiyuan Huang, Chieh-Han Wu, Yuxiao Dong, and Anshul Kanakia. Microsoft academic graph: When experts are not enough. *Quantitative Science Studies*, 1(1):396–413, 2020.

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