Combating Bilateral Edge Noise for Robust Link Prediction

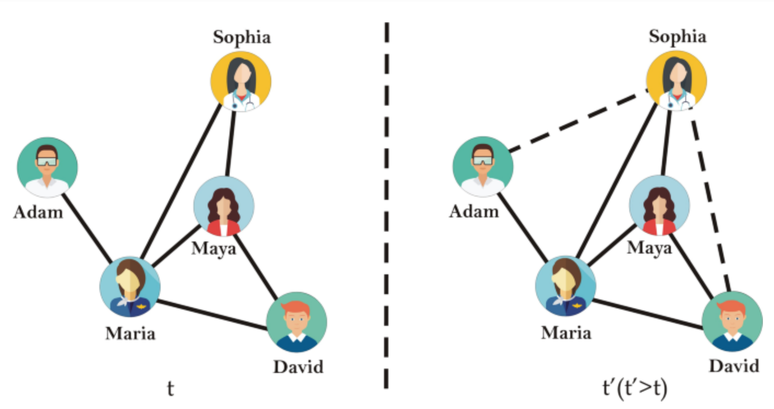
Zhanke Zhou, Jiangchao Yao, Jiaxu Liu, Xiawei Guo,
Quanming Yao, Li He, Liang Wang, Bo Zheng, Bo Han

香港浸會大學 HONG KONG BAPTIST UNIVERSITY · Alibaba.com · 清華大學 Tsinghua University · 上海交通大學 SHANGHAI JIAO TONG UNIVERSITY

NEURAL INFORMATION PROCESSING SYSTEMS · TMLR TRUSTWORTHY MACHINE LEARNING AND REASONING

Paper Code

Problem: Link Prediction with Noise

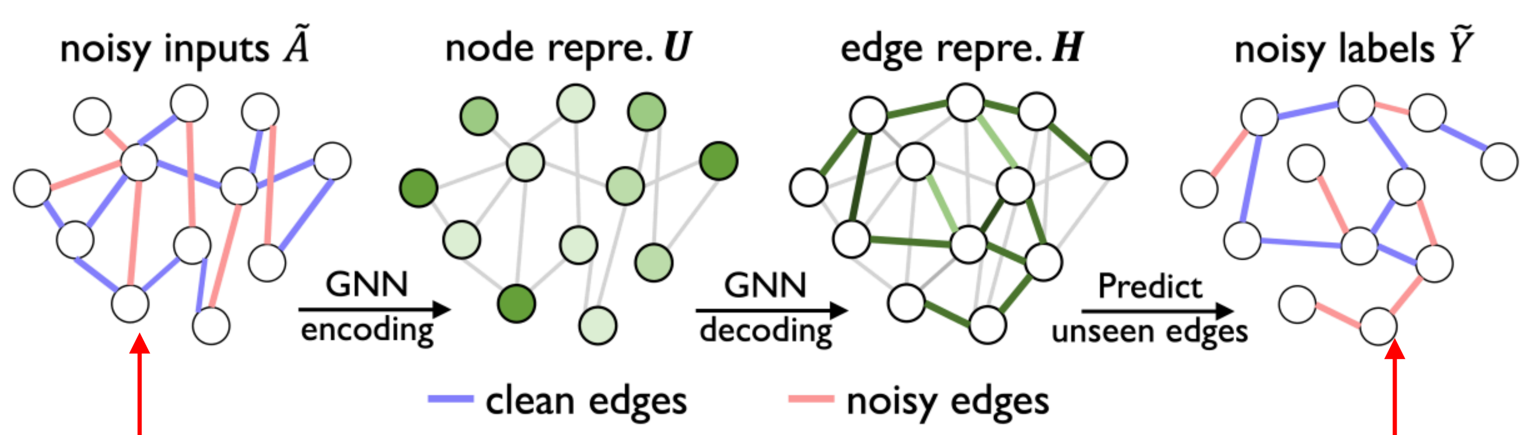


The link prediction task:
- based on the **observed** links
- to predict the **latent** links

The Bilateral Edge Noise

Existing graph benchmarks are generally **clean**.

However, graph data can be **noisy** in practical scenarios:
- the **observed** graph is often with noisy edges (**input noise**)
- the **predictive** graph often contains noisy labels (**label noise**)
- these two kinds of noise can exist at the same time (by random split)

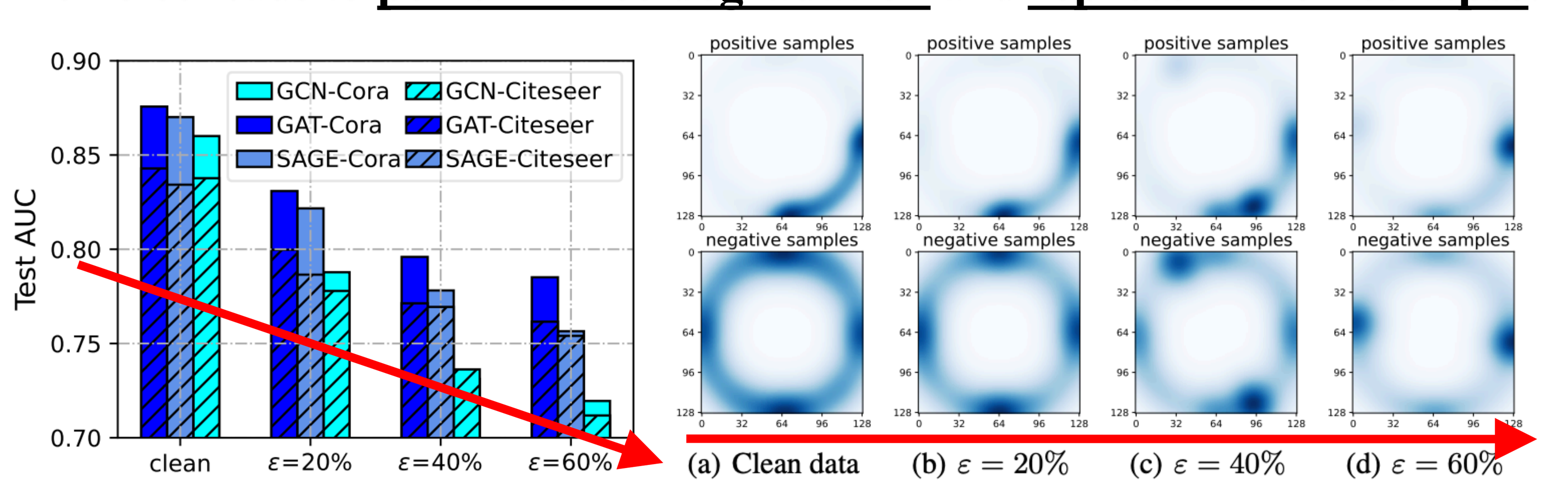


We call this kind of noise as the "**bilateral edge noise**"

Definition 3.1 (Bilateral edge noise). *Given a clean training data, i.e., observed graph $\mathcal{G}=(A,X)$ and labels $Y\in\{0,1\}$ of query edges, the noisy adjacence $\tilde{A}$ is generated by directly adding edge noise to the original adjacent matrix A while keeping the node features X unchanged. The noisy labels $\tilde{Y}$ are similarly generated by adding edge noise to the labels Y. Specifically, given a noise ratio ε_a, the noisy edges A' ($\tilde{A}=A+A'$) are generated by flipping the zero element in A as one with the probability ε_a. It satisfies that $A'\odot A=O$ and $\varepsilon_a=|\texttt{nonzero}(\tilde{A})|-|\texttt{nonzero}(A)|/|\texttt{nonzero}(A)|$. Similarly, noisy labels are generated and added to the original labels, where $\varepsilon_y=|\texttt{nonzero}(\tilde{Y})|-|\texttt{nonzero}(Y)|/|\texttt{nonzero}(Y)|$.*

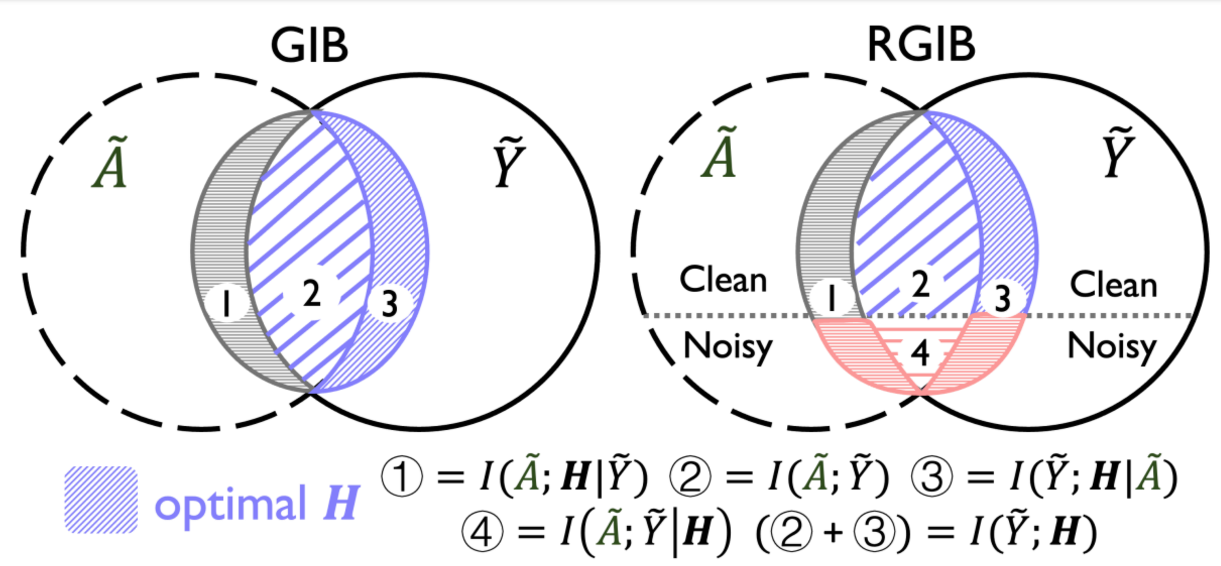
The Effects of Bilateral Edge Noise

The noise leads to <u>performance degradation</u> and <u>representation collapse</u>:



➔ How to improve the robustness of GNNs under edge noise? 🤔

Method: Robust Graph Information Bottleneck



$$\min \mathrm{GIB} \triangleq -I(\boldsymbol{H};\tilde{Y}),\ \text{s.t. } I(\boldsymbol{H};\tilde{A})<\gamma,$$

➔ **GIB** is vulnerable to label noise for its maximum label supervision

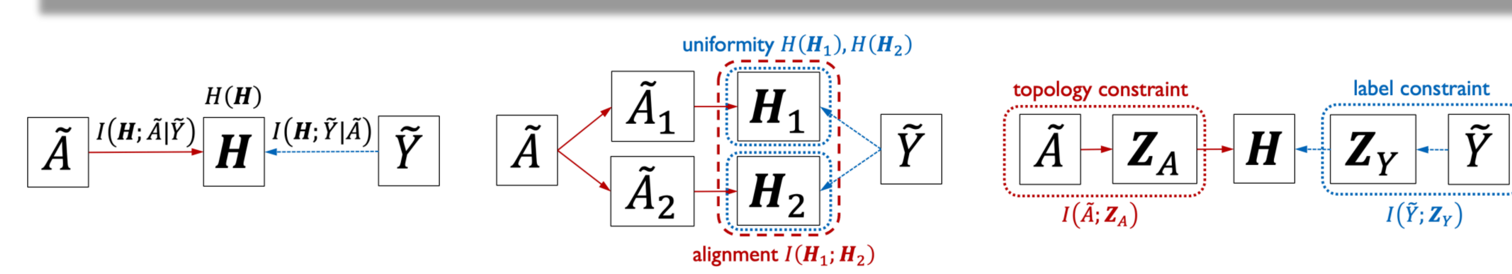
In this work, we further balance the mutual dependence
- among graph topology $\tilde{A}$, target labels $\tilde{Y}$, and representation $\boldsymbol{H}$
- build a new learning objective RGIB for robust representation

Definition 4.1 (Robust Graph Information Bottleneck). *Based on the above analysis, we propose a new learning objective to balance informative signals regarding $\boldsymbol{H}$, as illustrated in Fig. 5(a), i.e.,*

$$\min RGIB \triangleq -I(\boldsymbol{H};\tilde{Y}),\quad s.t.\ \gamma_H^-<H(\boldsymbol{H})<\gamma_H^+, I(\boldsymbol{H};\tilde{Y}|\tilde{A})<\gamma_Y,\ I(\boldsymbol{H};\tilde{A}|\tilde{Y})<\gamma_A. \tag{2}$$

Specifically, constraints on $H(\boldsymbol{H})$ encourage a diverse $\boldsymbol{H}$ to prevent representation collapse ($>\gamma_H^-$) and also limit its capacity ($<\gamma_H^+$) to avoid over-fitting. Another two MI terms, $I(\boldsymbol{H};\tilde{Y}|\tilde{A})$ and $I(\boldsymbol{H};\tilde{A}|\tilde{Y})$, mutually regularize posteriors to mitigate the negative impact of bilateral noise on $\boldsymbol{H}$. The complete derivation of RGIB and a further comparison of RGIB and GIB are in Appendix B.2.

Instantiation: RGIB-SSL and RGIB-REP



RGIB **RGIB-SSL** **RGIB-REP**

$$\min \text{RGIB-SSL} \triangleq -\underbrace{\lambda_s(I(\boldsymbol{H}_1;\tilde{Y})+I(\boldsymbol{H}_2;\tilde{Y}))}_{\text{supervision}}-\underbrace{\lambda_u(H(\boldsymbol{H}_1)+H(\boldsymbol{H}_2))}_{\text{uniformity}}-\underbrace{\lambda_a I(\boldsymbol{H}_1;\boldsymbol{H}_2)}_{\text{alignment}}.$$

RGIB-SSL optimizes the representation with **self-supervised learning** to achieve a **tractable approximation** of the MI terms
- integrate a uniformity term and an alignment term with graph augmentation
- adopt the contrastive learning technique and contrast pair of samples

$$\min \text{RGIB-REP} \triangleq -\underbrace{\lambda_s I(\boldsymbol{H};\boldsymbol{Z}_Y)}_{\text{supervision}}\ \underbrace{+\lambda_A I(\boldsymbol{Z}_A;\tilde{A})+}_{\text{topology constraint}}\ \underbrace{\lambda_Y I(\boldsymbol{Z}_Y;\tilde{Y})}_{\text{label constraint}}.$$

RGIB-REP purifies the noisy signals with **reparameterization mechanism**
- latent variables $\boldsymbol{Z}_Y$ and $\boldsymbol{Z}_A$ are clean signals extracted from noisy $\tilde{Y}$ and $\tilde{A}$
- $\mathrm{I}(\boldsymbol{H};\boldsymbol{Z}_Y)$ measures the supervised signals with selected samples $\boldsymbol{Z}_Y$
- $\mathrm{I}(\boldsymbol{Z}_A;\tilde{A})$ and $\mathrm{I}(\boldsymbol{Z}_Y;\tilde{Y})$ help to select the clean information from noisy $\tilde{A},\tilde{Y}$

Experiments

➔ RGIB performs the best in all six datasets under the bilateral noise:

method	Cora 20%	Cora 40%	Cora 60%	Citeseer 20%	Citeseer 40%	Citeseer 60%	Pubmed 20%	Pubmed 40%	Pubmed 60%	Facebook 20%	Facebook 40%	Facebook 60%	Chameleon 20%	Chameleon 40%	Chameleon 60%	Squirrel 20%	Squirrel 40%	Squirrel 60%
Standard	.8111	.7419	.6970	.7864	.7380	.7085	.8870	.8748	.8641	.9829	.9520	.9438	.9616	.9496	.9274	.9432	.9406	.9386
DropEdge	.8017	.7423	.7303	.7635	.7393	.7094	.8711	.8482	.8354	.9811	.9682	.9473	.9568	.9548	.9407	.9439	.9377	.9365
NeuralSparse	.8190	.7318	.7293	.7765	.7397	.7148	.8908	.8733	.8630	.9825	.9638	.9456	.9599	.9497	.9402	.9494	.9309	.9297
PTDNet	.8047	.7559	.7388	.7795	.7423	.7283	.8872	.8733	.8623	.9725	.9674	.9485	.9607	.9514	.9424	.9485	.9326	.9304
Co-teaching	.8197	.7479	.7030	.7533	.7238	.7131	.8943	.8760	.8638	.9820	.9526	.9480	.9595	.9516	.9483	.9461	.9352	.9374
Peer loss	.8185	.7468	.7018	.7423	.7345	.7104	.8961	.8815	.8566	.9807	.9536	.9430	.9543	.9533	.9267	.9457	.9345	.9286
Jaccard	.8143	.7498	.7024	.7473	.7324	.7107	.8872	.8803	.8512	.9794	.9579	.9428	.9503	.9538	.9344	.9443	.9327	.9244
GIB	.8198	.7485	.7148	.7509	.7388	.7121	.8899	.8729	.8544	.9773	.9608	.9417	.9554	.9561	.9321	.9472	.9329	.9302
SupCon	.8240	.7819	.7490	.7554	.7458	.7299	.8853	.8718	.8525	.9588	.9508	.9297	.9561	.9531	.9467	.9473	.9348	.9301
GRACE	.7872	.6940	.6929	.7632	.7242	.6844	.8922	.8749	.8588	.8899	.8865	.8315	.8978	.8987	.8949	.9394	.9380	.9363
RGIB-REP	.8313	.7966	.7591	.7875	.7519	.7312	.9017	.8834	.8652	**.9832**	**.9770**	.9519	**.9723**	**.9621**	**.9519**	**.9509**	**.9455**	**.9434**
RGIB-SSL	**.8930**	**.8554**	**.8339**	**.8694**	**.8427**	**.8137**	**.9225**	**.8918**	**.8697**	.9829	.9711	**.9643**	.9655	.9592	.9500	.9499	.9426	.9425

➔ RGIB consistently surpasses all the baselines under the unilateral noise:

input noise	Cora 20%	Cora 40%	Cora 60%	Citeseer 20%	Citeseer 40%	Citeseer 60%	Pubmed 20%	Pubmed 40%	Pubmed 60%	Facebook 20%	Facebook 40%	Facebook 60%	Chameleon 20%	Chameleon 40%	Chameleon 60%	Squirrel 20%	Squirrel 40%	Squirrel 60%
Standard	.8027	.7856	.7490	.8054	.7708	.7583	.8854	.8759	.8651	.9819	.9668	.9622	.9608	.9433	.9368	.9416	.9395	.9411
DropEdge	.8338	.7826	.7454	.8025	.7730	.7473	.8682	.8456	.8376	.9803	.9685	.9531	.9567	.9433	.9432	.9426	.9376	.9358
NeuralSparse	.8534	.7794	.7637	.8093	.7809	.7468	.8931	.8720	.8649	.9712	.9691	.9583	.9609	.9540	.9348	.9469	.9403	.9417
PTDNet	.8433	.8214	.7770	.8119	.7811	.7638	.8903	.8776	.8609	.9725	.9668	.9493	.9610	.9457	.9360	.9469	.9400	.9379
Co-teaching	.8045	.7871	.7530	.8059	.7753	.7668	.8931	.8792	.8606	.9712	.9707	.9714	.9524	.9446	.9447	.9462	.9425	.9306
Peer loss	.8051	.7866	.7517	.8106	.7767	.7653	.8917	.8811	.8643	.9758	.9703	.9622	.9558	.9482	.9412	.9362	.9386	.9336
Jaccard	.8200	.7838	.7617	.8176	.7776	.7725	.8987	.8764	.8639	.9784	.9702	.9638	.9507	.9436	.9364	.9388	.9345	.9240
GIB	.8002	.8099	.7741	.8070	.7717	.7798	.8932	.8808	.8618	.9796	.9647	.9650	.9605	.9521	.9416	.9390	.9406	.9397
SupCon	.8349	.8301	.8025	.8076	.7767	.7655	.8867	.8739	.8558	.9647	.9517	.9401	.9606	.9536	.9468	.9372	.9343	.9305
GRACE	.7877	.7107	.6975	.7615	.7151	.6830	.8810	.8795	.8593	.9015	.8833	.8395	.8994	.9007	.8964	.9392	.9378	.9363
RGIB-REP	.8624	.8313	.8158	.8299	.7996	.7771	.9008	.8822	.8687	**.9833**	**.9723**	**.9682**	**.9705**	**.9604**	.9480	**.9495**	**.9432**	.9405
RGIB-SSL	**.9024**	**.8577**	**.8421**	**.8747**	**.8461**	**.8245**	**.9126**	**.8889**	**.8693**	.9821	.9707	.9668	.9658	.9570	**.9486**	.9479	.9429	**.9429**

label noise	Cora 20%	Cora 40%	Cora 60%	Citeseer 20%	Citeseer 40%	Citeseer 60%	Pubmed 20%	Pubmed 40%	Pubmed 60%	Facebook 20%	Facebook 40%	Facebook 60%	Chameleon 20%	Chameleon 40%	Chameleon 60%	Squirrel 20%	Squirrel 40%	Squirrel 60%
Standard	.8281	.8054	.8060	.7965	.7850	.7659	.9030	.9039	.9070	.9882	.9880	.9886	.9686	.9580	.9362	.9720	.9720	.9710
DropEdge	.8363	.8273	.8148	.7937	.7853	.7632	.9313	.9201	.9240	.9673	.9771	.9776	.9580	.9579	.9578	.9608	.9603	.9698
NeuralSparse	.8524	.8246	.8211	.7968	.7921	.7752	.9272	.9136	.9089	.9781	.9781	.9784	.9583	.9583	.9571	.9633	.9626	.9625
PTDNet	.8460	.8214	.8138	.7968	.7765	.7622	.9219	.9099	.9093	.9879	.9880	.9783	.9585	.9576	.9665	.9633	.9623	.9626
Co-teaching	.8446	.8209	.8157	.7974	.7877	.7913	.9315	.9291	.9319	.9762	.9797	.9638	.9642	.9650	.9533	.9675	.9641	.9655
Peer loss	.8325	.8036	.8069	.7991	.7990	.7751	.9126	.9101	.9210	.9769	.9750	.9734	.9621	.9501	.9569	.9636	.9694	.9696
Jaccard	.8289	.8064	.8148	.8061	.7887	.7689	.9098	.9135	.9096	.9702	.9725	.9758	.9603	.9659	.9557	.9529	.9512	.9501
GIB	.8337	.8137	.8157	.7986	.7852	.7649	.9037	.9114	.9064	.9742	.9703	.9771	.9651	.9582	.9489	.9641	.9628	.9601
SupCon	.8491	.8275	.8256	.8024	.7983	.7807	.9131	.9108	.9162	.9647	.9567	.9553	.9584	.9580	.9477	.9516	.9595	.9511
GRACE	.8531	.8237	.8193	.7909	.7630	.7737	.9234	.9252	.9255	.8913	.8972	.8887	.9053	.9074	.9075	.9171	.9174	.9166
RGIB-REP	.8554	.8318	.8297	.8083	.7846	.7945	.9357	.9343	.9332	**.9884**	**.9883**	**.9889**	**.9785**	**.9797**	**.9785**	**.9735**	**.9733**	**.9737**
RGIB-SSL	**.9314**	**.9224**	**.9241**	**.9204**	**.9218**	**.9250**	**.9594**	**.9604**	**.9613**	.9857	.9881	.9857	.9730	.9752	.9744	.9727	.9729	.9726

➔ the graph representation has obvious improvement in distribution:

Table 5: Comparison of alignment. Here, std. is short for *standard training*, and SSL/REP are short for RGIB-SSL/RGIB-REP, respectively.

dataset / method	Cora std.	Cora REP	Cora SSL	Citeseer std.	Citeseer REP	Citeseer SSL
clean	.616	.524	**.475**	.445	.439	**.418**
$\varepsilon=20\%$	.687	.642	**.543**	.586	.533	**.505**
$\varepsilon=40\%$	.695	.679	**.578**	.689	.623	**.533**
$\varepsilon=60\%$	.732	.704	**.615**	.696	.647	**.542**

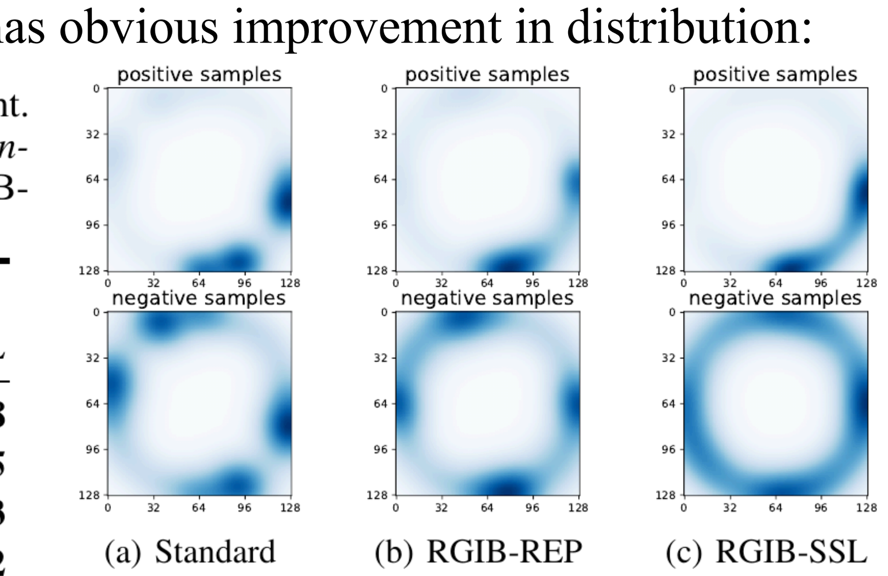


Figure 6: Uniformity distribution on Citeseer with $\varepsilon=40\%$.

Future Directions

New instantiations of RGIB, e.g., approximation of the MI terms
New scenarios with noise, e.g., feature noise, other structural noise
New graph learning tasks, e.g., node classification, graph classification
New theoretical analysis, e.g., information theory, graph generation model