Graph Neural Network Symposium 2021

Graph Contrastive Learning Recent Progress and Outlook

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Joint work with Yichen XU, Feng YU, Qiang LIU, Shu WU, and Liang WANG

Outline

- 1. Preamble
- 2. Deep Graph CL: GRACE
- 3. Adaptive Augmentation: GCA
- 4. Experiments
- 5. Concluding Remarks

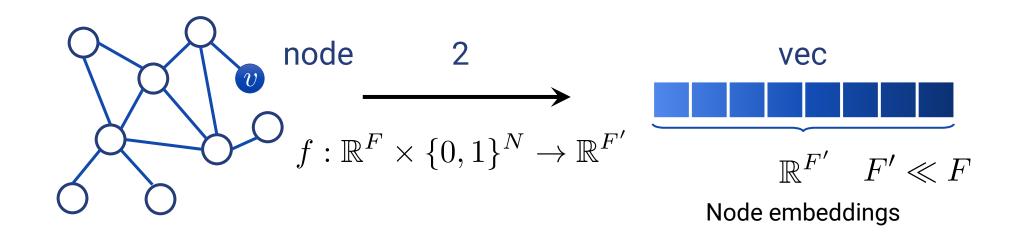
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Representation Learning on Graphs

- Goal: efficient feature learning for machine learning on graphs
- Low-dimensional node embeddings encode both structural and attributive information.



Self-supervised learning comes to rescue!

- Most GNN models are established in a supervised manner.
 - It is often expensive to obtain high-quality labels at scale in real world.
 - Supervised models learn the inductive bias encoded in labels, instead of reusable, task-invariant knowledge.

"Labels are the opium of the machine learning researcher."

--- Jitendra Malik

"The future is self-supervised!"

--- Yann LeCun

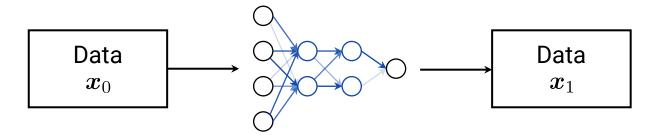
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 - It is often expensive to obtain high-quality labels at scale in real world.
 - Supervised models learn the inductive bias encoded in labels, instead of reusable, task-invariant knowledge.
- Self-supervised methods employ proxy tasks to guide learning the representations.
 - The proxy task is designed to predict any part of the input from any other observed part.
 - Typical proxy tasks for visual data include corrupted image restoration, rotation angle prediction, reorganization of shuffled patches, etc.

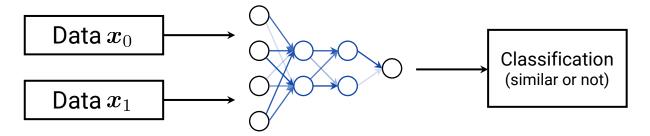
[Jing et al., 2020] L. Jing and Y. Tian, Self-supervised Visual Feature Learning with Deep Neural Networks: A Survey, TPAMI, 2020.

Taxonomy of Self-Supervised Learning

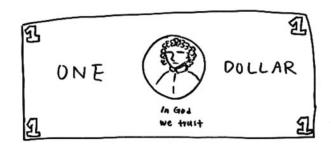
• (a) Generative/predictive: loss measured in the output space



• (b) Contrastive: loss measured in the latent space



An analogy to brain's memory...







Drawing subsequently made with a dollar bill present

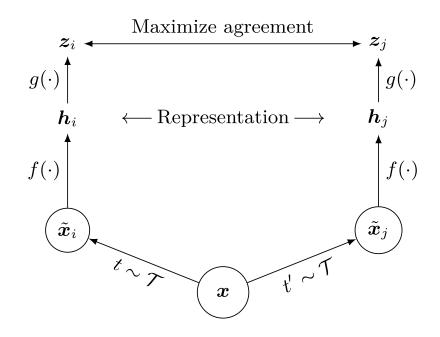
- We only need to retain several features to distinguish one bill from others!
 - Similarly, representation learning algorithms do not need to concentrate on pixel-level details. Encoding high-level features is sufficient enough to distinguish different objects.

[Epstein, 2016] R. Epstein, Your brain does not process information and it is not a computer, Aeon, 2016.

The Contrastive Learning Paradigm

 Contrastive learning aims to maximize the agreement of latent representations under stochastic data augmentation.

- Three main components:
 - Data augmentation pipeline ${\mathcal T}$
 - Encoder f and representation extractor g
 - Contrastive objective ${\cal L}$



[Chen et al., 2020] T. Chen, S. Kornblith, M. Norouzi, and G. E. Hinton, A Simple Framework for Contrastive Learning of Visual Representations, in *ICML*, 2020.

Contrastive Learning Objectives

A common pattern:

$$s(f(\boldsymbol{x}), f(\boldsymbol{x}^+)) \gg s(f(\boldsymbol{x}), f(\boldsymbol{x}^-))$$

- $f(\cdot)$ is the encoder, e.g., CNN and GNN.
- $s(\cdot, \cdot)$ measures similarity between two embeddings.
- Usually implemented with an *n*-way softmax function:

$$\mathcal{L} = -\mathbb{E}_X \left[\log \frac{\exp(s(\boldsymbol{x}, \boldsymbol{x}^+))}{\exp(s(\boldsymbol{x}, \boldsymbol{x}^+)) + \sum_{j=1}^{n-1} \exp(s(\boldsymbol{x}, \boldsymbol{x}_j))} \right]$$

- Commonly referred to as the InfoNCE loss.
- The critic function can be simply implemented as $s(x, y) = g(x)^{\top} g(y)$.

[Oord et al., 2018] A. van den Oord, Y. Li, and O. Vinyals, Representation Learning with Contrastive Predictive Coding, arXiv.org, vol. cs.LG. 2018.

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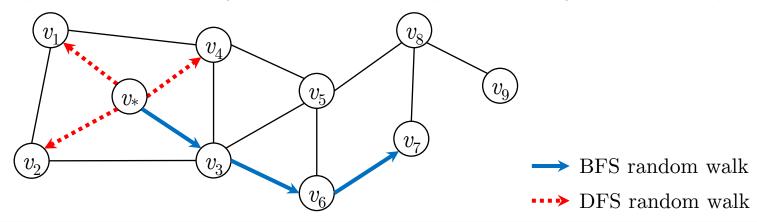
$$\mathcal{L} = -\mathbb{E}_X \left[\log \frac{\exp(s(\boldsymbol{x}, \boldsymbol{x}^+))}{\exp(s(\boldsymbol{x}, \boldsymbol{x}^+)) + \sum_{j=1}^{n-1} \exp(s(\boldsymbol{x}, \boldsymbol{x}_j))} \right]$$

Distinguish a pair of representations from two augmentations of the same sample (positives) apart from (n-1) pairs of representations from different samples (negatives).

[Oord et al., 2018] A. van den Oord, Y. Li, and O. Vinyals, Representation Learning with Contrastive Predictive Coding, arXiv.org, vol. cs.LG. 2018.

Traditional Graph Contrastive Learning

- Traditional work of network embedding inherently follows a contrastive paradigm originated in the skip-gram model.
 - Nodes appearing on the same random walk are considered as positive samples and are encouraged to share similar embeddings.
 - Network embedding schemes could be regarded as reconstructing a preset graph proximity matrix, having difficulty of leveraging attributes.



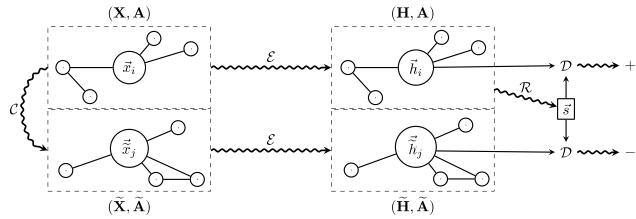
[Grover et al., 2016] A. Grover and J. Leskovec, node2vec: Scalable Feature Learning for Networks, in KDD, 2016.

Deep Graph Contrastive Learning

- GNNs employ more powerful encoders for learning representations by aggregating information from neighborhood.
- GNN-based contrastive learning studies are in their infancy.
 Existing work primarily differs in contrastive objectives and data augmentation techniques.
 - Contrastive objective: defines which embeddings to pull together or push apart.
 - Data augmentation: transforms the original graphs to congruent counterparts.

Deep Graph Infomax

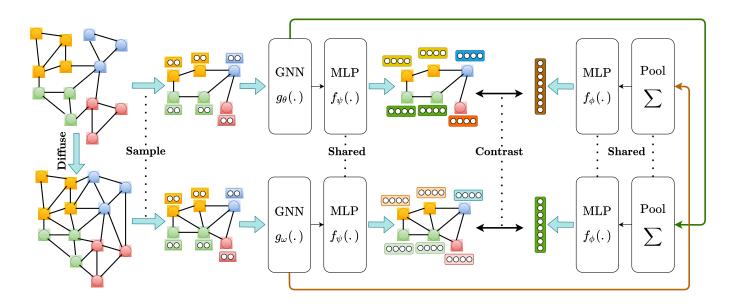
- Capture similarities using mutual information $I(h_i; s)$.
 - s is a graph summary vector.
- Optimize MI using a binary classifier \mathcal{D} .
 - Generate negative examples (nodes not belonging to the graph) via an explicit corruption function $\mathcal C$ which randomly shuffles the adjacency matrix. (X,A) (H,A)



[Veličković et al., 2019] P. Veličković, W. Fedus, W. L. Hamilton, P. Liò, Y. Bengio, and R. D. Hjelm, Deep Graph Infomax, in *ICLR*, 2019.

Multiview Graph Contrastive Learning

- Generate another view by applying diffusion kernels.
- Simultaneously optimize embeddings in two views to distill more global information.



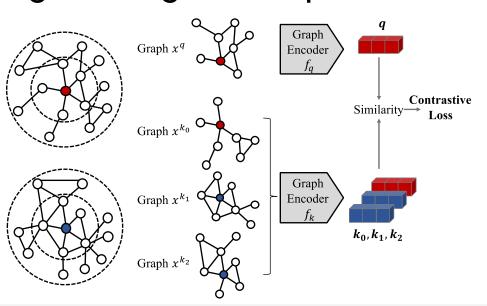
[Hassani et al., 2020] K. Hassani and A. H. Khasahmadi, Contrastive Multi-View Representation Learning on Graphs, in ICML, 2020.

Graph Contrastive Coding

 Generate a series of positives and negatives by sampling subgraphs within a batch.

Employ feature engineering techniques for transferable node

representations.



[Qiu et al., 2020] J. Qiu, Q. Chen, Y. Dong, J. Zhang, H. Yang, M. Ding, K. Wang, and J. Tang, GCC: Graph Contrastive Coding for Graph Neural Network Pre-Training, in *KDD*, 2020.

Interlude: Contrastive Objectives

- Global-local contrastive objective:
 - DGI [Veličković et al., 2019] and MVGRL [Hassani et al., 2020] maximize the agreement between node- and graph-level representations.
 - The graph readout function should be injective [Xu et al., 2019], which is hard to fulfill. Otherwise, it is not guaranteed to distill enough information from node-level embeddings.
- Local-local contrastive objective:
 - Follow-up work GCC [Qiu et al., 2020], GRACE [Zhu et al., 2020], and GraphCL [You et al., 2020] eschew the need of an injective readout function and directly maximize the agreement of node embeddings across two augmented views.

Interlude: Augmentation for Graph CL

- Existing studies mostly adopt a bi-level augmentation scheme:
 - Structure-level augmentation
 - Shuffling the adjacency matrix [Veličković et al., 2019]
 - Adding / dropping edges [You et al., 2020; Zhu et al., 2020]
 - Sampling subgraphs [Hassani et al., 2020; Qiu et al., 2020; You et al., 2020]
 - Generating global view via diffusion kernels [Hassani et al., 2020]
 - ...
 - Attribute-level augmentation
 - Dropping / masking features [You et al., 2020; Zhu et al., 2020]
 - Adding Gaussian noise
 - ...

Outline

1. Preamble

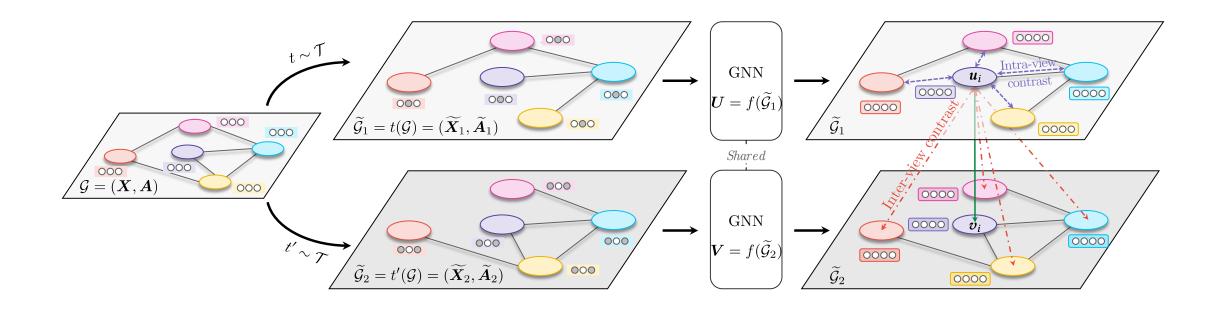
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3. Adaptive Augmentation: GCA

4. Experiments

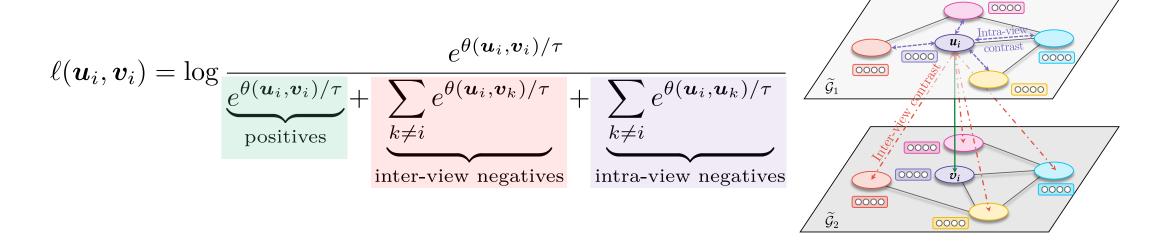
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The Proposed Approach



Graph Contrastive Learning Across Views

- Firstly, we generate two correlated graph views by randomly augmenting the structure and features.
- Then, we train the model using a contrastive loss to maximize the agreement between node embeddings in the latent space.



Hybrid Graph View Generation

- We corrupt the original graph at both structure and attribute levels to construct diverse node contexts.
- Removing edges: randomly remove a portion of edges in the original graph.

$$\widetilde{\boldsymbol{R}}_{ij} \sim \mathrm{Bern}(1-p_r), \quad \text{if } \boldsymbol{A}_{ij} = 1,$$

$$\widetilde{\boldsymbol{A}} = \boldsymbol{A} \circ \widetilde{\boldsymbol{R}}.$$

 Masking node features: randomly mask a fraction of dimensions with zeros in node features.

$$\widetilde{\boldsymbol{x}}_i \sim \operatorname{Bern}(1-p_m), \quad \forall i,$$

$$\widetilde{\boldsymbol{X}} = [\boldsymbol{x}_1 \circ \widetilde{\boldsymbol{m}}; \ \boldsymbol{x}_2 \circ \widetilde{\boldsymbol{m}}; \ \cdots; \ \boldsymbol{x}_N \circ \widetilde{\boldsymbol{m}}]^\top.$$

Theoretical Groundings

Definition 1. Mutual Information (MI).

• Mutual information I(X;Y) is a measure of the mutual dependence between the two random variables X and Y, determining how different the joint distribution of the pair P(X,Y) is to the marginal P(X)P(Y).

Definition 2. InfoMax Principle.

• A function that maps a set of input values I to a set of output values O should be learned so as to maximize the MI between I and O.

[Linsker, 1998] R. Linsker, Self-Organization in a Perceptual Network, IEEE Computer, 1988.

Theoretical Groundings (cont.)

Theorem 1. Connections to MI maximization.

- Let $X_i = \{x_k\}_{k \in \mathcal{N}(i)}$ be the neighborhood of node v_i that collectively maps to its output embedding, where $\mathcal{N}(i)$ denotes the set of neighbors of node v_i specified by GNN architectures, and X be the corresponding random variable with a uniform distribution p(X) = 1/N.
- Given two random variables ${m U}, {m V} \in \mathbb{R}^{F'}$ being the embedding in the two views, with their joint distribution denoted as $P({m U}, {m V})$, our objective ${\mathcal J}$ is a lower bound of MI between input ${m X}$ and node representations in two graph views ${m U}, {m V}$:

$$\mathcal{J} \leq I(\boldsymbol{X}; \boldsymbol{U}, \boldsymbol{V}).$$

Theoretical Groundings (cont.)

Theorem 2. Connections to the triplet loss.

• When the projection function g is the identity function, and we measure embedding similarity by simply taking the inner product, i.e. $s(u, v) = u^{\top}v$, and further assuming that positive pairs are far more aligned than negative pairs, i.e. $u_i^{\top}v_k \ll u_i^{\top}v_i$ and $u_i^{\top}u_k \ll u_i^{\top}v_i$, minimizing the pairwise objective $\ell(u_i, v_i)$ coincides with maximizing the triplet loss, as given in the sequel

$$-\ell(m{u}_i,m{v}_i) \propto 4 au + \sum_{j
eq i} \left(\|m{u}_i - m{v}_i\|^2 - \|m{u}_i - m{v}_j\|^2 + \|m{u}_i - m{v}_i\|^2 - \|m{u}_i - m{u}_j\|^2
ight).$$

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Adaptive Augmentation in CL

- How to integrate augmentation schemes into graph CL is still an empirical choice.
- In essence, CL seeks to learn representations that are insensitive to perturbation induced by augmentation schemes.
 - Simple random augmentation in either structural or attribute domain is not sufficient.
 - Discrepancy in the impact of nodes and edges exists. Augmentation should preserve important structural and attribute information of graphs.

[Wu et al., 2020] M. Wu, C. Zhuang, M. Mosse, D. Yamins, and N. Goodman, On Mutual Information in Contrastive Learning for Visual Representations, arXiv.org, vol. cs.LG. 27-May-2020.

[Xiao et al., 2020] T. Xiao, X. Wang, A. A. Efros, and T. Darrell, What Should Not Be Contrastive in Contrastive Learning, arXiv.org, vol. cs.CV. 13-Aug-2020.

Adaptive Augmentation on Graphs

- Data augmentation should be adaptive to the given graph.
 - We propose to keep important structures and attributes unchanged and perturb possibly unimportant links and features.
- Bi-level augmentation: remove edges (topology-level) and mask features (attribute-level)
 - Removing or masking probabilities are skewed for unimportant edges or features.
 - From an amortized perspective, we emphasize important structures and attributes over randomly corrupted views.

Topology-level Augmentation

ullet We sample a modified edge subset $\widetilde{\mathcal{E}}$ with probability

$$P\{(u,v) \in \widetilde{\mathcal{E}}\} = 1 - p_{uv}^e.$$

- In network science, **node centrality** $\varphi_c(\cdot)$ is a widely-used measure that quantifies the influence of a node in the graph.
- The **edge importance** w_{uv}^e for edge (u,v) can be defined based on the centrality of two connected nodes.
 - Directed graphs: $w_{uv}^e = \varphi_c(v)$
 - Undirected graphs: $w_{uv}^e = (\varphi_c(u) + \varphi_c(v))/2$

[Newman, 2018] M. E. J. Newman, Networks: An Introduction (Second Edition), Oxford University Press, 2018.

Topology-level Augmentation (cont.)

Alleviate the nodes with heavily dense connections:

$$s_{uv}^e = \log w_{uv}^e.$$

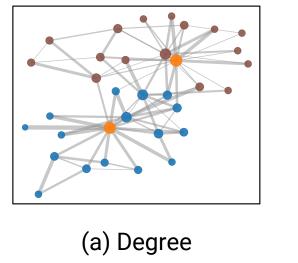
Normalize to avoid overly high removal probabilities:

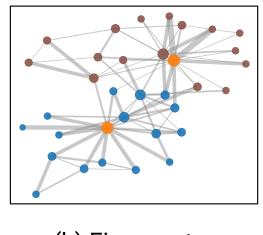
$$p_{uv}^e = \min\left(\frac{s_{\text{max}}^e - s_{uv}^e}{s_{\text{max}}^e - \mu_s^e} \cdot p_e, \ p_\tau\right),\,$$

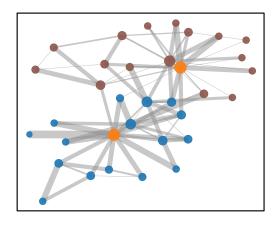
- p_e is a hyperparameter that controls the overall removing probability.
- s_{max}^e and μ_s^e is the maximum and average of s_{uv}^e .
- $p_{\tau} < 1$ is a cut-off probability.

Centrality Measures

We consider three widely-used centrality measures:







(b) Eigenvector

(c) PageRank

- Visualized on the Karate club dataset.
- The three measures all highlight connection around the central nodes (two coaches) and exhibit negligible performance difference.

Attribute-level Augmentation

 We add noise to node attributes via randomly masking a fraction of dimensions with zeros in node features:

$$\widetilde{\boldsymbol{x}}_i \sim \operatorname{Bern}(1 - p_i^f), \quad \forall i,$$

$$\widetilde{\boldsymbol{X}} = [\boldsymbol{x}_1 \circ \widetilde{\boldsymbol{m}}; \ \boldsymbol{x}_2 \circ \widetilde{\boldsymbol{m}}; \ \cdots; \ \boldsymbol{x}_N \circ \widetilde{\boldsymbol{m}}]^\top.$$

- The importance for each dimension of node features can be derived from node centrality scores.
 - Assumption: feature dimensions frequently appearing in influential nodes should be important.

$$w_i^f = \sum_{u \in \mathcal{V}} x_{ui} \cdot \varphi_c(u),$$

• $x_{ui} \in \{0,1\}$ indicate the occurrence of dimension i in node u.

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Datasets

Dataset	#Nodes	#Edges	#Features	#Classes
Wiki-CS	11,701	216,123	300	10
Amazon-Computers	13,752	$245,\!861$	767	10
Amazon-Photo	7,650	119,081	745	8
Coauthor-CS	18,333	81,894	$6,\!805$	15
Coauthor-Physics	$34,\!493$	247,962	$8,\!415$	5

Baselines

- Network embedding methods:
 - DeepWalk [Perozzi et al., 2014] and node2vec [Grover et al., 2016]
- Unsupervised GNNs:
 - Recontraction-based methods: GAE, VGAE [Kipf et al., 2016], and GraphSAGE [Hamilton et al., 2017]
 - Contrastive learning methods: DGI [Veličković et al., 2019], GMI [Peng et al., 2020], and MVGRL [Hassani et al., 2020]
- Supervised GNNs:
 - GCN [Kipf et al., 2017] and GAT [Veličković et al., 2018]

Experimental Configurations

- Linear evaluation: unsupervised training followed by employing a simple ℓ_2 -reguarlized logistic regression model.
- Evaluation metrics: node classification accuracy.
- Base model: we employ a two-layer GCN as the encoder for all baselines.

$$\mathrm{GC}_i(\boldsymbol{X}, \boldsymbol{A}) = \sigma\left(\hat{\boldsymbol{D}}^{-\frac{1}{2}}\hat{\boldsymbol{A}}\hat{\boldsymbol{D}}^{-\frac{1}{2}}\boldsymbol{X}\boldsymbol{W}_i\right),$$
 $f(\boldsymbol{X}, \boldsymbol{A}) = \mathrm{GC}_2(\mathrm{GC}_1(\boldsymbol{X}, \boldsymbol{A}), \boldsymbol{A}).$

Overall Performance

Method	Training Data	Wiki-CS	Computers	Photo	CS	Physics
Raw features	X	71.98	73.81	78.53	90.37	93.58
node2vec	$oldsymbol{A}$	71.79	84.39	89.67	85.08	91.19
DeepWalk	$oldsymbol{A}$	74.35	85.68	89.44	84.61	91.77
DeepWalk + features	$oldsymbol{X},oldsymbol{A}$	77.21	86.28	90.05	87.70	94.90
GAE	$oldsymbol{X}, oldsymbol{A}$	70.15	85.27	91.62	90.01	94.92
VGAE	$\boldsymbol{X},\boldsymbol{A}$	75.63	86.37	92.20	92.11	94.52
$\overline{\mathrm{DGI}}$	$\boldsymbol{X},\boldsymbol{A}$	75.35	83.95	91.61	92.15	94.51
GMI	$\boldsymbol{X},\boldsymbol{A}$	74.85	82.21	90.68	OOM	OOM
MVGRL	$\boldsymbol{X},\boldsymbol{A}$	77.52	87.52	91.74	92.11	95.33
GRACE	$oldsymbol{X},oldsymbol{A}$	78.19	86.25	92.15	92.93	95.26
$\mathbf{GCA}\text{-}\mathbf{DE}$	$oldsymbol{X},oldsymbol{A}$	78.30	87.85	92.49	93.10	95.68
$\mathbf{GCA} ext{-}\mathbf{PR}$	$oldsymbol{X},oldsymbol{A}$	78.35	87.80	92.53	93.06	95.72
GCA-EV	$oldsymbol{X},oldsymbol{A}$	78.23	87.54	92.24	92.95	95.73
GCN	$oldsymbol{X}, oldsymbol{A}, oldsymbol{Y}$	77.19	86.51	92.42	93.03	95.65
GAT	$oldsymbol{X}, oldsymbol{A}, oldsymbol{Y}$	77.65	86.93	92.56	92.31	95.47

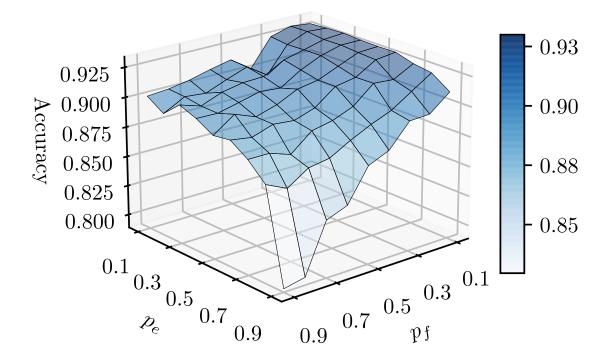
Ablation Studies

- GCA-T-A (GRACE): uniform augmentation.
- GCA-T and GCA-A: substitute the topology and the attribute augmentation scheme with uniform sampling respectively.

Variant	Topology	Attribute	Wiki-CS	Computers	Photo	CS	Physics
GCA-T-A	Uniform	Uniform	78.19	86.25	92.15	92.93	95.26
GCA-T	Uniform	Adaptive	78.23	86.72	92.20	93.07	95.59
GCA-A	Adaptive	Uniform	78.25	87.66	92.23	93.02	95.54
\mathbf{GCA}	Adaptive	Adaptive	78.30	87.85	92.49	93.10	95.68

Sensitivity Analysis

 Vary the removal and masking probabilities from 0.1 to 0.9 to see the robustness under different magnitudes of perturbation.



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Wrapping Up

- 1. We have developed a novel graph CL framework GRACE and its extension GCA with adaptive augmentation.
- 2. Local-local contrastive objective enables better distillation of nodelevel representations.
- 3. Augmentation schemes on both structural and attributive levels are critical for graph CL.
- 4. Important nodes/attributes, identified using centrality measures, should be preserved during augmentation to force the model learn intrinsic patterns of graphs.
- 5. Our proposed method achieves SOTA performance and bridges the gap between unsupervised and supervised learning.

Graph SSL: Retrospect and Prospect

- Graph self-supervised learning (SSL) is a promising way to learn graph embeddings without human annotations.
- Graph CL stems from traditional network embedding approaches and has established a new paradigm for unsupervised representation learning on graphs.
- However, the development of graph CL remains nascent, yet calls for a principled understanding of it.
 - Utilization of both topology and attribute spaces
 - Data augmentation and positive/negative sampling on graphs
 - Contrastive objectives

• ...

Useful Resources

- A curated list of must-read papers, survey, and talks
 - http://bit.ly/GraphSSL



- Graph contrastive learning library for PyTorch
 - To be released in late March
 - http://bit.ly/GraphCL



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[Chen et al., 2020] T. Chen, S. Kornblith, M. Norouzi, and G. E. Hinton, A Simple Framework for Contrastive Learning of Visual Representations, in *ICML*, 2020.

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