GraphCoCo: Graph Complementary Contrastive Learning

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Abstract

Graph Contrastive Learning (GCL) has shown promising performance in graph representation learning (GRL) without the supervision of manual annotations. GCL can generate graph-level embeddings by maximizing the Mutual Information (MI) between different augmented views of the same graph (positive pairs). However, we identify a barrier that the optimization of InfoNCE loss only concentrates on a few embedding dimensions, limiting the distinguishability of embeddings in downstream graph classification tasks. This paper proposes an effective graph complementary contrastive learning approach named GraphCoCo to tackle the above issue. Specifically, we set the embedding of the first augmented view as the anchor embedding to localize “highlighted” dimensions (i.e., the dimensions contribute most in similarity measurement). Then remove these dimensions in the embeddings of the second augmented view to discover neglected complementary representations. Therefore, the combination of anchor and complementary embeddings significantly improves the performance in downstream tasks. Comprehensive experiments on various benchmark datasets are conducted to demonstrate the effectiveness of GraphCoCo, and the results show that our model outperforms the state-of-the-art methods.

1 Introduction

Over the past few years, Graph Representation Learning (GRL) has been increasingly popular for ubiquitous graph-structured data in various domains, including traffic \cite{yu2018}, social network \cite{fan2019}, and knowledge graph \cite{schlichtkrull2018}. Graph Neural Networks (GNNs) \cite{kipf2017, xu2019} are utilized as backbones of GRL to learn low-dimensional embeddings of nodes or graphs while maintaining structure and attribute information. Most GNN models are trained in the (semi-)supervised learning setting requiring abundant manually-annotated labels. In case of sufficient data labels, recent Contrastive Learning (CL) based on Information Maximization (InfoMax) principle \cite{linsker1988} has shown promising performance for self-supervised learning with success across fields including computer vision \cite{chen2020, he2020} and natural language processing \cite{yang2021}. These CL methods maximize the Mutual Information (MI) between different augmented views of the same instance while minimizing the MI between those of the different instances.

Inspired by the above CL models, Deep Graph InfoMax (DGI) \cite{velivckovic2019} applies the InfoMax principle to graph representation learning, which relies on maximizing the mutual information between one graph’s patch-level and global-level representations. Following SimCLR \cite{chen2020}, a series of graph contrastive learning methods \cite{hassani2020, you2020} enforce the embedding of positive pair (i.e., augmented views of the same graph) to be close and the embedding of negative pair (i.e., augmented views of different graphs) to be distant in Euclidean space. GCC \cite{qiu2020} referring to MoCo \cite{he2020} contrasts graph-level embedding with momentum encoder and maintain the queue of data samples.

However, recent studies \cite{tschannen2020, chen2020} have pointed out that there are gaps between the InfoMax principle and the performance of embeddings in the downstream tasks. Unlike contrastive learning in the computer vision literature, the usage of augmentation can result in a large discrepancy between the embeddings of the two augmented views while keeping the semantic information. Nevertheless, we experimentally observe that this discrepancy can be limited in graph contrastive learning, as shown in Fig. 1. In particular, we further notice that in graph con-
The similarity between embeddings is mainly controlled by these prominent elements which become more significant during training by influencing the direction of gradient descent. Therefore, the concentration of information on a few dimensions weakens the distinguishability of embeddings in the downstream tasks.

To tackle the above problem, we propose a novel Graph Complementary Contrastive Learning (GraphCoCo) approach with non-maximum erasing for graph-level self-supervised representation learning. The key idea of GraphCoCo is to learn the complementary embedding of graphs with two augmented views, inspired by non-maximum suppression which is widely used in visual object detection [Zhang et al., 2018]. In particular, we first generate two augmentations of the same graph and encode them into low-dimensional embeddings with GNNs. The first embedding identifies the most significant dimensions and then erases these dimensions in the second embedding to learn complementary information on other dimensions, which boosts the downstream classification tasks. Finally, we optimize the model with a prevalent contrastive loss where the non-maximum erasing operation is not performed on negative pairs. We conduct a series of experiments on various bioinformatics and social networks datasets to demonstrate the effectiveness of GraphCoCo. Our contributions are as follows:

1) We identify and theoretically analyze an obstacle of graph contrastive learning that the embeddings of positive pairs share common “highlighted” dimensions whose values can be much larger than others, which limits the expressiveness of embeddings in downstream classification tasks.

2) We propose a novel graph complementary contrastive learning approach (GraphCoCo) for self-supervised graph classification tasks. Our model effectively encourages the encoder to learn complementary representation in pre-text tasks using non-maximization erasing operation.

3) Experiments across multiple datasets show that GraphCoCo outperforms state-of-the-art self-supervised methods on graph classification tasks and achieves competitive performance on node classification tasks.

2 Related Work

Graph neural networks. Graph Neural Networks (GNNs) have attracted growing attention for analyzing graph-structured data in recent years. Generally, GNNs are categorized into spatial-domain and spectral-domain approaches. Based on the spectral graph theory, [Bruna et al., 2014] first defines the graph convolution in the spectral domain through the eigen-decomposition of the graph Laplacian, defectively causing high computational cost. Graph Convolution Network [Kipf and Welling, 2017] utilizes the 1-st approximation of the Chebyshev expansion to simplify the calculation. Spatial-based approaches follow a message passing scheme [Abu-El-Haija et al., 2019], where each node collects the information from its neighbors iteratively. GraphSAGE [Hamilton et al., 2017] aggregates the information from randomly sampled neighborhoods to scale to large graphs. GAT [Veličković et al., 2018] introduces the attention mechanism to assign scores for each node pair. GIN [Xu et al., 2019] generalizes the Weisfeiler-Lehman test and reaches the most expressive power among GNNs.

Graph contrastive learning. As one of the main approaches of self-supervised representation learning, contrastive learning has raised a surge of attraction in computer vision [He et al., 2020; Chen et al., 2020] and natural language processing [Yang et al., 2019]. Contrastive learning is based on the mutual information (MI) maximization principle by encouraging the agreement between two augmented views of the same instance and the disagreement between augmented views of different instances. Inspired by visual contrastive learning, a series of graph contrastive learning methods are devised. Deep Graph InfoMax (DGI) [Veličković et al., 2019] first applies the InfoMax principle to graph representation learning. DGI relies on maximizing the mutual information between the patch-level and global-level representation of one graph. MVGRL [Hassani and Khasahmadi, 2020] generates two augmented graph view via graph diffusion and subgraph sampling. Based on SimCLR [Chen et al., 2020], GraphCL [You et al., 2020] enforces the embedding of positive pair (i.e., augmented views of the same graph) to be close and the embedding of negative pair (i.e., augmented views of different graphs) to be distant in Euclidean space. CuCo [Chu et al., 2021] further utilizes the curriculum learning to select the negative samples. AD-GCL [Susheel et al., 2021] optimizes adversarial graph augmentation to prevent learning redundant information. JOAO [You et al., 2021] automatically and adaptively select the augmentation for specific dataset.

3 Problem Definition

Let $G = (\mathcal{V}, \mathcal{E})$ denote a graph, where $\mathcal{V} = \{v_1, v_2, \cdots, v_N\}$, $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$ denote the node set and the edge set, respectively. The adjacency matrix containing the connectivity of nodes is denoted as $A \in \{0, 1\}^{N \times N}$, where the entry $A_{ij} = 1$ if $(v_i, v_j) \in \mathcal{E}$. The feature matrix is denoted as $\mathcal{X} \in \mathbb{R}^{N \times F}$, where the $i$-th entry $x_i \in \mathbb{R}^F$ is the $F$-dimensional feature vector of node $v_i$. For self-supervised graph-level representation learning, given a set of graphs $\mathcal{G} = \{ G_1, G_2, \cdots \}$ without class information, our objective is to learn a GNN encoder $g_0(\mathcal{X}, A) \in \mathbb{R}^{F'}$ which encodes each graph $G$ into a $F'$-dimensional vector $z_G \in \mathbb{R}^{F'}$. These low-dimensional embeddings can be used in downstream tasks, such as node and graph classification.

4 Motivation

Previous work [Chen and Li, 2020] states that the InfoNCE loss, a widely used objective function in contrastive learning [Chen et al., 2020; You et al., 2020], can not guarantee to avoid shortcut solutions that only capture easy-to-learn features. The image augmentation such as color distortion and rotation, can obtain a totally pixel-level different image while
keeping semantic information. On the contrary, the graph-
data augmentation is local and limited due to the perturbation-
invariance of the adjacency matrix and lack of diversity of features. Although augmentation is applied to obtain two views of the same graph, the difference between embeddings of two augmented views is narrow, as shown in Fig. 1. Thus the contribution of the encoder when pulling positive pairs close is marginal. Additionally, we observe that a portion of elements are much larger than others in both embeddings and these larger elements share the same positions. We define the position of these much larger elements as “highlighted” dimensions. We then analyze how “highlighted” dimensions hurt the performance of the downstream tasks from the perspective of the gradient of InfoNCE shown in Proposition 1 with derivation in Appendix A.

**Proposition 1.** Given embeddings of positive pair \((u, v^+)\) and negative pairs \((u, v^-)\), the InfoNCE loss is defined as:

\[
\mathcal{L}_{\text{NCE}} = -\log \frac{\exp((u, v^+)/\tau)}{\exp((u, v^+)/\tau) + \sum_{v^-} \exp((u, v^-)/\tau)}.
\]

Then the gradient of InfoNCE w.r.t embeddings of positive pairs are:

\[
\frac{\partial \mathcal{L}_{\text{NCE}}}{\partial u} = -\frac{1}{\tau} \frac{\exp((u, v^+)/\tau)}{1 - \sum_{v^-} \exp((u, v^-)/\tau)} - \frac{1}{\tau} \sum_{v^-} \frac{\exp((u, v^-)/\tau)}{1 - \sum_{v^-} \exp((u, v^-)/\tau)} \cdot v^+.
\]

where \(p_v = \frac{\exp((u, v)/\tau)}{\exp((u, v^+)/\tau) + \sum_{v^-} \exp((u, v^-)/\tau)} \) and \(\tau\) is the temperature parameter.

Note that the value of the gradient of InfoNCE in each direction w.r.t. \(v^+\) is proportional to the value of \(u\) in each direction. Minimization of InfoNCE loss mainly lies in “highlighted” dimensions. Intuitively, contrastive learning aiming at maximizing the similarity between positive pairs leads to a shortcut that only a few dimensions to be relatively much larger. Thus, these “highlighted” dimensions are prominent to represent features of augmented graphs and suppress the expressiveness of other dimensions. Consequently, the downstream classification performance mainly depends on “highlighted” dimensions and neglects the leverage of other dimensions.

5 Method

This section presents the proposed graph complementary contrastive learning (GraphCoCo) approach. As shown in Fig. 2, given the input graph \(G\), we first generate two augmented graph views \(\tilde{G}_1\) and \(\tilde{G}_2\). Then each augmented view is encoded into low-dimensional embeddings with one shared encoder. After that, for positive pairs (i.e., two augmented views of the same graph), the embedding of the first augmented view conducts the erasing operation described in Section 5.3 on the embedding of the second one, to prevent the shortcut that focuses on optimizing “highlighted” dimensions to maximize the similarity. Since the negative pairs (i.e., augmented views of the different graph) do not share the same “highlighted” dimensions, the erasing operation is not applied to the negative pairs. Finally, the parameters of the encoder \(\theta\) are learned with contrastive objectives.

5.1 Graph Augmentation

One of the critical components in contrastive learning is graph augmentation which generates noise versions of graphs to be passed into the contrastive loss as positive pairs. Given a graph \(G\), we define the \(i\)-th augmented view as \(\tilde{G}^{(i)} = t_i(G)\), where \(i = \{1, 2\}\), \(t_i\) is selected from a group of predefined graph augmentation \(T\). Motivated by image augmentations, various graph augmentation are proposed and categorized into two types: structure-based and feature-based. We leverage the optimal combinations reported in GraphCL [You et al., 2020] for each dataset from following graph augmentation methods: 1) NodeDrop: randomly discards certain portion of nodes with their edges and features. 2) EdgeAdd and EdgeDrop: randomly adds or drops certain portion of edges in graphs. 3) FeatureMasking: randomly masks a portion of dimensions in node features with zero. 4) Subgraph: generates a subgraph with Random Walk. The details for the used augmentation approaches are given in Appendix B.

5.2 Encoder

We leverage the classic GNN [Kipf and Welling, 2017; Xu et al., 2019] as the encoder to extract the low-dimensional graph-level representation \(g_{\theta}^{(i)}\) for each augmented graphs.
\[ \hat{G}^{(1)} \]. Formally, given an augmented graphs \( \hat{G}^{(1)} \) with adjacency matrix \( A \) and high-dimensional node features \( \mathcal{X} \), where \( x_{vn} = \mathcal{X}[n, \cdot]^{T} \) is the feature vector of node \( vn \), the \( l \)-th layer of GNN first updates each node’s representation in a message passing manner:

\[
\begin{align*}
\mathbf{a}_{n}^{(1)} &= \text{AGGREGATE}^{(l)} \left( \{ \mathbf{h}_{m}^{(l-1)} : v_{m} \in \mathcal{N}(v_{n}) \} \right), \\
\mathbf{h}_{n}^{(1)} &= \text{COMBINE}^{(l)} \left( \mathbf{h}_{n}^{(l-1)}, \mathbf{a}_{n}^{(1)} \right),
\end{align*}
\]

(2)

where \( \mathbf{h}_{n}^{(l)} \) is the representation of the node \( v_{n} \) in the \( l \)-th layer of GNN with \( \mathbf{h}_{n}^{(0)} = x_{vn}, \mathcal{N}(v_{n}) \) is the set of neighbors of node \( v_{n} \), \text{AGGREGATE}^{(l)}(\cdot) \) can be the sum or average operation, and \text{COMBINE}^{(l)}(\cdot) \) can be concatenation or average operation. Then the graph-level embedding of \( \hat{G}^{l} \) can be obtained through the READOUT function of GNN, which is similar to pooling operation in CNN, as follows:

\[
r_{l} = \text{READOUT}(\{h_{n}^{k-1} : v_{n} \in \mathcal{N}, k = 1, 2, \ldots, K \}),
\]

(3)

where \( K \) is the number of layers of the GNN model.

### 5.3 Erasing Operation

The key innovation of our proposed GraphCoCo approach is the erasing operation which forces the encoder to learn complementary embeddings. GraphCoCo aims at mining information of inconspicuous dimensions rather than being restricted to scarce common “highlighted” dimensions through an adversarial manner. After the GNN encoder encodes two augmented views \( \{\hat{G}^{(1)}, \hat{G}^{(2)}\} \) into embeddings \( \{r^{(1)}, r^{(2)}\} \), the embedding of the second augmented view \( r^{(2)} \) are erased with the guidance of \( r^{(1)} \). The first embedding \( r^{(1)} \) recognizes the “highlighted” dimensions whose values are larger than a pre-defined threshold. The corresponding dimensions of \( r^{(2)} \) are then erased through masking values with zeros. Note that the erasing operation is performed only on positive pairs but not on negative pairs.

Formally, the augmented views of the input graph are transformed by the GNN encoder \( g_{\theta}() \) into a pair of embeddings \( r^{(i)} \in \mathbb{R}^{K \times F'} \), where \( i \in \{1, 2\} \), \( K \) is the number of layer of GNN, and \( F' \) is the number of output dimensions in each layer. Then normalize the \( r^{(1)} \) to the range \([0, 1]\) with min-max scaling and denote it as \( \breve{r}^{(1)} \),

\[
\breve{r}^{(1)} = \frac{r^{(1)} - \min (r^{(1)})}{\max (r^{(1)}) - \min (r^{(1)})}.
\]

We recognize dimensions whose values are larger than the hyper-parameter threshold \( \delta \) as “highlighted” dimensions. Then a binary mask matrix \( M \in \{0, 1\}^{K \times F'} \) is created to conduct the erasing operation on the embedding of second augmented view \( r^{(2)} \) as follows:

\[
M_{ij} = \begin{cases} 0, & \text{if } \breve{r}_{ij}^{(1)} > \delta \\ 1, & \text{otherwise} \end{cases}
\]

(4)

The erased embedding \( \hat{r}^{(2)} \) as the complementary embedding can be obtained,

\[
\hat{r}^{(2)} = r^{(2)} \odot M,
\]

where \( \odot \) is the Hadamard product. A projection head \( h(\cdot) \) composed of 2-layer MLP and ReLU non-linearity is applied on all embeddings for optimization objective.

\[
z_{\pm}^{(1)} = h(r^{(1)}), \quad z_{\pm}^{(2)} = h(\hat{r}^{(2)}), \quad \hat{z}^{(2)} = h(r^{(2)}),
\]

where \( \pm \) denotes positive and negative pairs.

### 5.4 Model Training

We follow [You et al., 2020] and train the GraphCoCo end-to-end by maximizing the agreement between positive pairs \( \{z_{+}^{(1)}, z_{+}^{(2)}\} \) via a contrastive loss. We use the Info Noise-Contrastive Estimation (InfoNCE) [Oord et al., 2018] which is a lower bound of the mutual information as the training objective. Specifically, given a minibatch of \( n \) graphs \( \{G_{j}, \eta_{j} \}_{j=1}^{n} \), let \( \tilde{z}_{j}^{(1)} = h(g_{\theta}(t_{1}(G_{j}))), \quad \tilde{z}_{j}^{(2)} = h(g_{\theta}(t_{2}(G_{j}))) \), and \( \tilde{z}_{j}^{(2)} = h(g_{\theta}(t_{2}(G_{j}))), \) where \( t_{1}(\cdot) \) is the augmentation function, \( g_{\theta}(\cdot) \) is the GNN encoder, \( h(\cdot) \) is the projection header, \( M \) is the masking matrix in Eq. 4, and \( \{\cdot, \cdot\} \) stands for positive or negative pairs. With \( \text{sim}(\cdot, \cdot) \) denoting the cosine similarity, the loss for the mini-batch with size \( B \) is:

\[
L = -\frac{1}{n} \sum_{j=1}^{B} \sum_{k \in \{1, 2\}} \log \frac{\exp(\text{sim}(\tilde{z}_{j}^{(1)}, z_{j}^{(1)}))/\tau}{\exp(\text{sim}(\tilde{z}_{j}^{(1)}, z_{j}^{(2)})/\tau) + \sigma_{-}}.
\]

(5)

where \( \sigma_{-} = \sum_{j=1}^{B} \sum_{k \neq j, q \in \{1, 2\}} \exp(\text{sim}(z_{j}^{(k)}, \tilde{z}_{q}^{(q)})/\tau) \).

The training process is described in Algorithm 1.

### 6 Experiment

#### 6.1 Protocol

**Task and datasets.** We compare state-of-the-art methods in the settings of unsupervised graph classification tasks and

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**Algorithm 1 Training algorithm of GraphCoCo**

**Input:** Training set \( G = \{G_{j}\}_{j=1}^{G} \), GNN encoder \( g_{\theta}(\cdot) \), augmentation distribution \( T \), threshold \( \delta \), mask matrix \( M \), batch size \( B \)

**Output:** The pre-trained encoder \( g_{\theta}(\cdot) \)

1: Randomly initialize parameters \( \theta \) of the GNN encoder and set all elements of \( M \) to be 0.
2: for each minibatch \( B \) sampled from \( G \) do
3: \hspace{1em} for \( k = 1, 2, \ldots, B \) do
4: \hspace{2em} Select two augmentation methods \( t_{1}, t_{2} \) from \( T \)
5: \hspace{2em} \( \tilde{g}_{k}^{(1)} \leftarrow t_{1}(G_{k}), \quad \tilde{g}_{k}^{(2)} \leftarrow t_{2}(G_{k}) \)
6: \hspace{2em} \( r_{k}^{(1)} \leftarrow g_{\theta}(\tilde{g}_{k}^{(1)}), \quad r_{k}^{(2)} \leftarrow g_{\theta}(\tilde{g}_{k}^{(2)}) \)
7: \hspace{2em} \( M_{pq} = 1 \) if \( |r_{k}^{(1)}|_{pq} > \delta \) where \( p, q \) are indexes of elements in tensors.
8: \hspace{2em} \( r_{k}^{(2)} \leftarrow r_{k}^{(2)} \odot M \)
9: \hspace{2em} \( z_{k, +}^{(1)} \leftarrow h(r_{k}^{(1)}), \quad z_{k, +}^{(2)} \leftarrow h(\hat{r}_{k}^{(2)}), \quad z_{k, -}^{(2)} \leftarrow h(r_{k}^{(2)}) \)
10: \hspace{2em} Computer the loss \( L \) via Eq. 5.
11: \hspace{2em} Update the parameters of \( g_{\theta}(\cdot) \) and \( h(\cdot) \) with adam optimizer by minimizing \( L \).
12: end for
13: end for
14: return The GNN encoder \( g_{\theta}(\cdot) \)
benchmark datasets [Morris et al., 2020]. We conduct experiments on nine
datasets: Coauthor-CS, Amazon-Photo, Amazon-Computer) for node
classification tasks. Details of datasets are in Appendix C.

Table 1: Unsupervised graph classification result comparison (% with standard deviation) of GraphCoCo and baselines.

| Datasets          | PTC-MR   | PROTEINS | NCI1 | DD  | COLLAB | IMDB-B | IMDB-M | RDT-B | RDT-MSK |
|-------------------|----------|----------|------|-----|--------|--------|--------|-------|---------|
| GCN               | 64 ± 2.3 | 76.2 ± 2.8 | 80.2 ± 2.0 | 76.2 ± 1.4 | 79.0 ± 1.8 | 74.0 ± 3.4 | 51.9 ± 3.8 | < 50.0 | < 20.0 |
| GIN               | 64 ± 7.0 | 76.6 ± 3.2 | 82.7 ± 1.7 | 78.9 ± 1.3 | 80.2 ± 1.9 | 75.1 ± 5.1 | 52.4 ± 2.8 | 92.4 ± 2.5 | 57.0 ± 1.7 |

Table 2: Unsupervised graph classification result comparison (% with standard deviation) of GraphCoCo and baselines.

| Datasets          | Pubmed   | CS       | Photo   | Computer   |
|-------------------|----------|----------|---------|------------|
| GCN               | 79.0 ± 0.3 | 91.8 ± 0.1 | 87.3 ± 1.0 | 86.5 ± 0.5 |
| GAT               | 79.0 ± 0.3 | 90.5 ± 0.7 | 86.2 ± 1.5 | 86.9 ± 0.3 |

Self-supervised Methods

| Datasets          | DGI      | MVGRL    | GCA     | CCA-SSG   |
|-------------------|----------|----------|---------|-----------|
| DGI               | 77.3 ± 0.6 | 90.0 ± 0.3 | 83.1 ± 0.5 | 83.9 ± 0.5 |
| MVGRL             | 80.1 ± 0.7 | 92.1 ± 0.1 | 87.3 ± 0.3 | 87.5 ± 0.1 |
| GCA               | 80.7 ± 0.2 | 92.95 ± 0.12 | 92.24 ± 0.21 | 87.85 ± 0.31 |
| CCA-SSG           | 81.6 ± 0.4 | 93.31 ± 0.22 | 93.14 ± 0.14 | 88.74 ± 0.28 |
| GraphCoCo         | 82.23 ± 0.54 | 91.67 ± 0.33 | 92.79 ± 0.17 | 87.49 ± 0.35 |

We leverage the graph isomorphism network (GIN) [Xu et al., 2019] as the encoder due to its powerful expressiveness in distinguishing the structure of graphs to obtain the graph-level representations, specifically, we adopt a three-layer GIN with 32 hidden units in each layer and a sum pooling readout function. Then the embeddings generated by the encoder are fed into the downstream SVM classifier. The threshold δ in the erasing operation is set to 0.7. We utilize the 10-fold cross-validation to train the SVM and record mean accuracy with the standard variation of five-time trials on the test set. Other hyper-parameters remain consistency with the GraphCL [You et al., 2020]. For node classification tasks, we follow settings of DGI [Veličković et al., 2019] which uses the GCN as the encoder and logistic regression downstream classifier. More details of the experimental setup can be found in Appendix C.

6.2 Experimental Results

The results of self-supervised graph classification are reported in Tab. 1. We can see contrast-based methods generally exceed both the graph kernel methods and traditional unsupervised methods, indicating the advantages of contrastive learning. GraphCoCo outperforms other unsupervised representation learning baselines with significant improvement across eight of nine datasets, especially on sparse-graph, demonstrating the superiority of our approach. For example, GraphCoCo achieves 82.07% accuracy on dense-graph dataset DD, surpassing GraphCL by 3.45% accuracy and GCoCo by 2.87% accuracy individually. Meanwhile, the GraphCoCo achieves 73.83% accuracy on sparse-graph dataset IMDB-B, exceeding the GraphCL by 2.69% and AD-GCL by 2.34% accuracy, respectively. The results are attributed to the key component in our approach: the non-maximization erasing operation, which allows information to be represented in all dimensions of embeddings rather than concentrating on a small number of the highlighted dimensions. The similarity between two embeddings is no longer dominated only by “highlighted” dimensions in both embeddings as in previous works. Finally, with a more uniform distribution of information, all dimensions of the embeddings contribute when performing downstream classification tasks, bringing about a notable improvement. Tab. 2 reports the results of node classification. The GNN encoder in the graph classification task has one readout layer, which is not in the encoder of the node classification task. We design our approach from the gradient of InfoNCE loss w.r.t the graph-level embeddings which is the output of the readout layer. Thus our approach is more suitable for graph-level classification.

Even so, results show that our method extended to node classification achieves competitive performance compared to the
SOTA self-supervised node classification methods.

6.3 Ablation Study

Comprehensive ablation studies on graph classification are conducted to verify the superiority of our non-maximization erasing operation for learning complementary embeddings. We design following 4 variants of the proposed GraphCoCo: (1) GraphCoCo (w/o EO): removes the erasing operation component. Note that this variant is the same as GraphCL which maximizes the similarity between embeddings of positive pairs. (2) GraphCoCo-rand: for positive pairs, randomly mask some dimensions of embedding of the second augmented view with zeros, which is equivalent to applying a dropout function. To make sure the ratio of masked dimensions in the variant is the same as in GraphCoCo with the optimal hyper-parameter threshold $\delta$, as shown in Fig. 4, we implement the GraphCoCo-rand by randomly shuffling $M$ in Eq. 4. (3) GraphCoCo-non-min: for positive pairs, the dimensions of the second embedding to be erased are the smallest dimensions of the first embedding instead of the largest ones. (4) GraphCoCo-bi: bi-directional erasing operation, i.e., for positive pair, each embedding of augmented view conducts the non-max erasing operation on the other.

Fig. 3 compares the results of GraphCoCo and its variants, from which we make the following observations. First, the classification results decrease if the non-maximization erasing operation is removed, verifying the efficacy of learning the complementary embedding. GraphCoCo-rand improves the GraphCL but does not outperform the GraphCoCo. GraphCoCo-bi has the similar performance with GraphCoCo. Lastly, the non-min erasing operation can hardly improve and even hurts the model.

### 6.4 Parameter Sensitivity Study

**Sensitivity study w.r.t. the erasing threshold $\delta$.** We vary the values of the import hyper-parameter threshold $\delta$ in the erasing operation in Eq. 4 from 0.0 to 1.0 on four datasets, and the results are shown in Fig. 4. Surprisingly, even if the second embedding is completely erased when $\delta = 0$, we can still optimize the encoder by repulsing negative pairs and get a barely satisfactory result. In general, we find that when the threshold $\delta$ is less than 0.7, the classification accuracy grows with the increase of the threshold. The optimal value of $\delta$ is 0.7 or 0.8 for most datasets, with the exception of dataset NCI1, where the optimal value is 0.4.

**Effect of intensity of augmentations.** Since the sparsity of augmented views affects the common highlighted dimensions of both embeddings, we vary the ratio of nodes, edges or features discarded in graph augmentation including NodeDrop, EdgeDrop and FeatureMasking on four datasets. From the results in Figure 5, we observe that classification performance degenerates as the intensity of augmentation grows overly high. The optimal modification probability for most datasets is 0.1 to 0.3. These results are in record with the observation that graph-data are sparse and hard to be recovered after discarding information.

### 6.5 Transfer Learning Study

We conduct experiments on four large-scale datasets to evaluate the transferability in predicting the molecular property. The encoder is pre-trained on the ZINC dataset without label and fine-tuned on other datasets, where all settings follow [Hu et al., 2020]. We select baselines including no-pretrained GIN, GraphCL [You et al., 2020] and strategies used in [Hu et al., 2020] including EdgePred, AttrMasking and ContextPred. The experiment result is shown in Tab. 3 evaluated with mean and standard deviation of ROC-AUC score for five trials. GraphCoCo achieves the best performance on three of four datasets and outperforms GraphCL on all datasets. Detailed setup of transfer learning is in Appendix C.

### 7 Conclusion

This paper investigates the gaps between contrastive loss and downstream tasks (graph/node classification) performance and proposes the graph complementary contrastive learning in a self-supervised manner named GraphCoCo. In GraphCoCo, the first embedding of positive pairs discovers the most significant dimensions and erases these dimensions of the second embedding, which is regarded as the complement of the first. The complementary embedding helps the encoder learn neglected information and enhance the distinguishability of the embedding. Extensive experiments show that GraphCoCo significantly outperforms the state-of-the-art self-supervised methods.

| Datasets | BBP | ToxCast | SIDER | ClinTox |
|----------|-----|---------|-------|---------|
| Pre-train |     |         |       |         |
| ZINC 2M  |     |         |       |         |
| No pre-train | 61.8 ± 4.5 | 64.4 ± 0.6 | 57.3 ± 1.6 | 58.0 ± 4.4 |
| EdgePred | 67.3 ± 2.4 | 64.1 ± 0.6 | 60.4 ± 0.7 | 64.1 ± 3.7 |
| AttrMasking | 64.3 ± 2.8 | 64.2 ± 0.5 | 61.0 ± 0.7 | 71.8 ± 4.1 |
| ContexPred | 68.9 ± 2.0 | 63.9 ± 0.6 | 60.9 ± 0.6 | 65.9 ± 3.8 |
| GraphCL | 69.68 ± 0.67 | 62.40 ± 0.57 | 60.53 ± 0.88 | 75.99 ± 2.65 |

GraphCoCo: 70.34 ± 1.21 | 63.04 ± 0.92 | 61.45 ± 1.63 | 76.92 ± 1.91

Table 3: Transfer learning comparison by ROC-AUC.
References

[Abu-El-Haija et al., 2019] S. Abu-El-Haija, B. Perozzi, A. Kapoor, N. Alipourfard, K. Lerman, H. Harutyunyan, Greg Ver S., and A. Galstyan. Mixhop: Higher-order graph convolutional architectures via sparsified neighborhood mixing. In ICML, 2019.

[Adhikari et al., 2018] B. Adhikari, Y. Zhang, N. Ramakrishnan, and B. A. Prakash. Sub2vec: Feature learning for subgraphs. In PAKDD, 2018.

[Bruna et al., 2014] J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun. Spectral networks and locally connected networks on graphs. In ICML, 2014.

[Chen and Li, 2020] T. Chen and L. Li. Intriguing properties of contrastive losses. arXiv preprint arXiv:2011.02803, 2020.

[Chen et al., 2020] T. Chen, S. Kornblith, M. Norouzi, and G. Hinton. A simple framework for contrastive learning of visual representations. In ICML, 2020.

[Chu et al., 2021] G. Chu, X. Wang, C. Shi, and X. Jiang. Cuco: Graph representation with curriculum contrastive learning. In IJCAI, 2021.

[Fan et al., 2019] W. Fan, Y. Ma, Q. Li, Y. He, E. Zhao, J. Tang, and D. Yin. Graph neural networks for social recommendation. In WWW, 2019.

[Hamilton et al., 2017] W. L. Hamilton, R. Ying, and J. Leskovec. Inductive representation learning on large graphs. In NIPS, 2017.

[Hassani and Khasahmadi, 2020] K. Hassani and A. H. Khasahmadi. Contrastive multi-view representation learning on graphs. In ICML, 2020.

[He et al., 2020] K. He, H. Fan, Y. Wu, S. Xie, and R. Girshick. Momentum contrast for unsupervised visual representation learning. In CVPR, 2020.

[Hu et al., 2020] W. Hu, B. Liu, J. Gomes, M. Zitnik, P. Liang, V. Pande, and J. Leskovec. Strategies for pre-training graph neural networks. In ICLR, 2020.

[Kipf and Welling, 2017] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. In ICLR, 2017.

[Linsker, 1988] R. Linsker. Self-organization in a perceptual network. Computer, 21(3):105–117, 1988.

[Morris et al., 2020] C. Morris, N. M. Kriege, F. Bause, K. Kersting, P. Mutzel, and M. Neumann. Tudataset: A collection of benchmark datasets for learning with graphs. arXiv preprint arXiv:2007.08663, 2020.

[Narayanan et al., 2017] A. Narayanan, M. Chandramohan, R. Venkatesan, L. Chen, Y. Liu, and S. Jaiswal. graph2vec: Learning distributed representations of graphs. arXiv preprint arXiv:1707.05005, 2017.

[Oord et al., 2018] A. Oord, Y. Li, and O. Vinyals. Representation learning with contrastive predictive coding. arXiv preprint arXiv:1807.03748, 2018.

[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.

[Schlichtkrull et al., 2018] M. Schlichtkrull, T. N. Kipf, P. Bloem, R. Van Den Berg, I. Titov, and M. Welling. Modeling relational data with graph convolutional networks. In ESWC, 2018.

[Shervashidze et al., 2011] N. Shervashidze, P. Schweitzer, E. J. Van Leeuwen, K. Mehlhorn, and K. M. Borgwardt. Weisfeiler-lehman graph kernels. JMLR, 12(9), 2011.

[Sun et al., 2020] F. Sun, J. Hoffman, V. Verma, and J. Tang. Infograph: Unsupervised and semi-supervised graph-level representation learning via mutual information maximization. In ICLR, 2020.

[Susheel et al., 2021] P Susheel, P Li, C. Hao, and J. Neville. Adversarial graph augmentation to improve graph contrastive learning. In NIPS, 2021.

[Tschannen et al., 2020] M. Tschannen, J. Djolonga, P. K. Rubenstein, S. Gelly, and M. Lucic. On mutual information maximization for representation learning. In ICLR, 2020.

[Veličković et al., 2018] P. Veličković, G Cucurull, A Casanova, A Romero, P Liò, and Y Bengio. Graph attention networks. In ICLR, 2018.

[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.

[Xu et al., 2019] K Xu, W Hu, J. Leskovec, and S. Jegelka. How powerful are graph neural networks? In ICLR, 2019.

[Yanardag and Vishwanathan, 2015] P. Yanardag and S.V.N. Vishwanathan. Deep graph kernels. In KDD, pages 1365–1374, 2015.

[Yang et al., 2019] Z. Yang, Y. Cheng, Y. Liu, and M. Sun. Reducing word omission errors in neural machine translation: A contrastive learning approach. In ACL, 2019.

[Yang et al., 2021] N. Yang, F. Wei, B. Jiao, D. Jiang, and L. Yang. XMOCO: Cross momentum contrastive learning for open-domain question answering. In ACL, 2021.

[You et al., 2020] Y. You, T. Chen, Y. Sui, T. Chen, Z. Wang, and Y. Shen. Graph contrastive learning with augmentations. In NIPS, 2020.

[You et al., 2021] Y. You, T. Chen, Y. Shen, and Z. Wang. Graph contrastive learning automated. In ICML, 2021.

[Yu et al., 2018] B. Yu, H. Yin, and Z. Zhu. Spatio-temporal graph convolutional networks: a deep learning framework for traffic forecasting. InIJCAI, 2018.

[Zhao et al., 2018] X. Zhang, Y. Wei, J. Feng, Y. Yang, and T. S. Huang. Adversarial complementary learning for weakly supervised object localization. In CVPR, 2018.

[Zhao et al., 2021] H. Zhang, Q. Wu, J. Yan, D. Wipf, and P. S. Yu. From canonical correlation analysis to self-supervised graph neural networks. NIPS, 2021.

[Zhu et al., 2021] Y. Zhu, Y. Xu, F. Yu, Q. Liu, Shu Wu, and L. Wang. Graph contrastive learning with adaptive augmentation. In WWW, 2021.