Graph Self-Contrast Representation Learning

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Abstract—Graph contrastive learning (GCL) has recently emerged as a promising approach for graph representation learning. Some existing methods adopt the 1-vs-K scheme to construct one positive and K negative samples for each graph, but it is difficult to set K. For those methods that do not use negative samples, it is often necessary to add additional strategies to avoid model collapse, which could only alleviate the problem to some extent. All these drawbacks will undoubtedly have an adverse impact on the generalizability and efficiency of the model. In this paper, to address these issues, we propose a novel graph self-contrast framework GraphSC, which only uses one positive and one negative sample, and chooses triplet loss as the objective. Specifically, self-contrast has two implications. First, GraphSC generates both positive and negative views of a graph sample from the graph itself via graph augmentation functions of various intensities, and use them for self-contrast. Second, GraphSC uses Hilbert-Schmidt Independence Criterion (HSIC) to factorize the representations into multiple factors and proposes a masked self-contrast mechanism to better separate positive and negative samples. Further, Since the triplet loss only optimizes the relative distance between the anchor and its positive/negative samples, it is difficult to ensure the absolute distance between the anchor and positive sample. Therefore, we explicitly reduced the absolute distance between the anchor and positive sample to accelerate convergence. Finally, we conduct extensive experiments to evaluate the performance of GraphSC against 19 other stateof-the-art methods in both unsupervised and transfer learning settings.

Index Terms—graph representation learning, contrastive learning

I. INTRODUCTION

Graph self-supervised learning (GSSL) [1]–[3] has attracted significant attention in recent years. Compared with traditional semi-supervised and supervised graph learning [4]–[6], GSSL seeks to employ supervision extracted from data itself, which can effectively circumvent the need for costly annotated data. In particular, one of the main types of GSSL is graph contrastive learning (GCL) [3], [7], whose core idea is to minimize the distance between representations of different augmented views

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Fig. 1. A toy example to show the influence of the number of negative samples K on the model performance. In our experiments, we set K = B - 1 in GraphCL and K = 1 in our model GraphSC, where B is the batch size.

of the same graph ("positive pairs"), and maximize that of augmented views from different graphs ("negative pairs").

According to whether negative samples are used by the model or not, most existing graph-level GCL methods fall into one of two classes. On the one hand, some approaches construct one positive sample and K negative samples for each graph [3], [8], [9], and formulate their objectives based on the normalized temperature-scaled cross entropy loss (NT-Xent) [10], such as GraphCL [3]. However, these methods are easily affected by K and an appropriate K value is usually set empirically, which lacks theoretical supports. When K is small, the model might not learn sufficient information to discriminate positive and negative samples; otherwise, there could lead to a large number of false-negative samples and slow convergence. In these methods, for each graph in a batch, other graphs in the same batch are considered as its negative samples, i.e., K = B - 1, where B is the batch size. As shown in Fig. 1, the performance of GraphCL is significantly affected by Kon the COLLAB dataset. In particular, when K is small, the performance of GraphCL drops drastically. On the other hand, the second type of methods propose to not use negative samples. However, these methods could suffer from a degenerate solution [11], where all outputs "crash" to an undesired constant. To avoid such model collapse, additional strategies have to be applied, such as asymmetric dual encoders [12], [13]. Recently, some studies [14] have showed that although these training strategies can avoid collapse to some extent, they may still cause collapse in partial dimensions of the representation, which leads to worse performance. The main reason for the model collapse is the complete non-use of negative samples. Therefore, a research question arises: *To avoid the problem of K selection and the degenerate solution, can we develop a GCL model that constructs only one positive sample and one negative sample for each graph?*

Given one positive sample and one negative sample for each graph, a straightforward framework is to use triplet loss as objective function. However, triplet loss is hard-to-train and mainly suffers from poor local optima and slow convergence, partially due to that the loss function employs only one negative example while not interacting with other negative classes per update [10]. In short, there are two difficulties: one is to find a valid negative sample and the other is to solve the hard-to-train problem.

For the first difficulty, hard negative sample mining [15]-[19] has been proposed. However, most existing methods applied to graphs are node-level sampling, and very few is for graph-level sampling. Recently, Cuco [20] proposes curriculum contrastive learning, which ranks negative samples from easy to hard and trains them in order. CGC [21] proposes to obtain reliable counterfactual negative samples by pretraining to help contrastive learning. However, this introduces additional computational overhead that limits the performance of GCL. Inspired by the fact that some substances change their properties in response to external conditions, we propose a simple yet effective method to obtain negative samples from graph themselves. For example, an enzymatic protein could become a non-enzymatic one after some perturbations. Since the non-enzymatic protein is directly generated from the enzymatic protein, they can share structural similarities to some degree, which makes the negative sample discriminatively difficult, thereby achieving a similar effect to hard negative sampling.

To address the hard-to-train problem, we consider multiple facets of each graph to construct masked embedding vectors for its positive/negative samples. Then the self-contrast is performed not only between the whole embedding vectors, but also between masked embedding vectors corresponding to each facet. The masked contrast can be used to provide more information and speed up the model convergence. Further, optimizing the triplet loss essentially maximizes the distance between positive and negative samples. This amplifies the margin between different classes but cannot ensure lowdimensional representations for each class compact. Therefore, we further shorten the absolute distance between anchor and positive sample, which can make each class more compact and make the distance between similar samples in the feature space closer. It can also provide shortcuts for model convergence (we will show the experimental results in Section V).

In this paper, we study graph contrastive learning and propose a novel Graph Self-Contrast framework GraphSC, which follows the pattern of generating positive and negative samples from the samples themselves and conducting selfcontrast. For each graph, GraphSC first generates one positive sample and one negative sample from the graph itself, and then self-contrasts the graph with its positive/negative samples as well as their masked embeddings. Inspired by the assumption in [3] that the semantics of a graph will not change for a certain perturbation strength, we move forward and assume that the semantics of a graph will change under strong perturbations. Specifically, we propose to generate two different (positive and negative) views of a graph via graph augmentation functions of various intensities. After that, the original graph and two generated views of the graph are fed into a shared GNN encoder, after which sum pooling is used to derive graphlevel representations. In particular, we use the representation of the original graph as anchor, and the representations of views generated by weak and strong perturbations as a positive sample and a negative sample, respectively. Further, to implement masked self-contrast, we perform a division on the embeddings of positive/negative samples, and divide each representation vector into multiple factors by Hilbert-Schmidt Independence Criterion (HSIC) [22]. In addition to the contrast between the whole embedding vectors, we mask each factor separately and perform masked self-contrast between corresponding representations. Moreover, we use Mean Square Error (MSE) loss/Barlow Twins loss (BT) [23] as a regularization to shorten the absolute distance between anchor and positive sample. This leads to better convergence in implementation. Finally, we summarize the contributions as follows:

- We propose a novel graph self-contrast representation learning framework GraphSC.
- We present a simple yet effective method to construct negative samples from graphs themselves in graph-level representation learning.
- We use triplet loss in graph contrastive learning and address the hard-to-train problem of triplet loss by putting forward a masked self-contrast mechanism and directly shortening the absolute distance for positive pairs.
- We conduct extensive experiments to evaluate the performance of GraphSC in both unsupervised learning and transfer learning settings. Experimental results show that GraphSC performs favorably against other state-of-thearts.

II. RELATED WORK

A. Graph self-supervised learning

Graph self-supervised learning [1]–[3] aims to extract informative knowledge from graphs through pre-designed pretext tasks without relying on manual labels. They can be used to alleviate the annotation bottleneck that is one of the main barriers for practical deployment of deep learning today. According to the objectives of pretext tasks, existing graph self-supervised learning methods can be broadly divided into four categories: (1) generation-based methods [1], which aim to reconstruct the input graph data and use the input data as their supervision signals; (2) auxiliary-property-based methods [24], which attempt to obtain graph-related properties from the graph and further take them as supervision signals, such as pseudo labels of unlabeled data; (3) contrast-based methods [2], [3], which construct positive and negative pairs for contrast. These methods follow the core idea of maximizing the mutual information (MI) [25] between positive pairs and minimizing that between negative pairs. (4) hybrid methods [26], which integrate various pretext tasks together in a multi-task learning fashion. Our proposed method GraphSC is contrast-based and we next introduce contrast-based methods in detail. For a comprehensive survey on graph self-supervised learning, see [27].

B. Graph contrastive learning

According to the contrast mode, graph contrastive learning can be mainly divided into three categories: node-node contrast, node-graph contrast and graph-graph contrast.

For node-node contrast, the representative model GRACE [28] first generates two contrastive views of a graph via graph augmentation, and then pulls close the representations of samples in positive pairs while pushing away that of samples in inter-view and intra-view negative pairs. GCA [29] further introduces an adaptive augmentation by incorporating various priors for topological and semantic aspects of the graph, which results in a more competitive performance. GCC [30] utilizes random walk as augmentations to extract the contextual information. BGRL [31] maximizes the MI between node representations from online and target networks.

There also exist methods [2], [7], [32]–[34] that are based on node-graph contrast. For example, DGI [2] learns both local and global semantic information in graphs by contrasting nodelevel embeddings with the graph-level representation. After that, GIC [32] seeks to additionally capture cluster-level information by first clustering nodes based on their embeddings, and then maximizing the MI between nodes in the same cluster. MVGRL [33] first generates two graph views via graph diffusion and subgraph sampling. Then it trains graph encoders by contrasting node embeddings in a view and the graph-level representation in another view. Further, SUBG-CON [34] uses triplet loss as objective function. For each node, it first extracts the top-k most informative neighbors to form a subgraph. Then it pulls close the distance between the representations of the node and the subgraph, and pushes away that between the representations of the node and a randomly selected subgraph.

The third type of methods are based on graph-graph contrast. The early model GraphCL [3] designs four types of graph augmentation (node dropping, edge perturbation, attribute masking and subgraph extraction), and then adopts the NT-Xent loss to learn the graph-level representation. Further, JOAO [35] proposes a unified bi-level optimization framework to automatically select data augmentations. AD-GCL [36] uses adversarial graph augmentation strategies that enables GNNs to avoid capturing redundant information during training. Inspired by Invariant Rationale Discovery (IRD), RGCL [9] puts forward rationale-aware augmentations for graph contrastive learning to preserve the critical information in the graph. There are also methods that do not need data augmentations. For example, SimGRACE [8] feeds the original graph into a GNN encoder and achieves data augmentation through perturbation of the encoder.

III. PRELIMINARY

In this section, we introduce basic concepts used in this paper.

A. Graph Neural Networks (GNNs)

Let $G = (\mathcal{V}, \mathcal{E})$ denote an undirected graph, where $\mathcal{V} = \{v_1, v_2, \cdots, v_N\}$ is the node set and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ represents the edge set. We use $X \in \mathbb{R}^{N \times F}$ to denote the node feature matrix, where F is the dimension of node features. Generally, given a GNN model $f(\cdot)$, message propagation in the *l*-th layer can be divided into two operations: one is to aggregate information from a node's neighbors while the other is to update a node's embedding. Taking node v_i as an example, we formally define these two operations as:

$$a_i^{(l)} = \operatorname{AGGREGATE}^{(l)} \{ h_j^{(l-1)}, \forall v_j \in \mathcal{N}(v_i) \}, \qquad (1)$$

$$h_i^{(l)} = \text{COMBINE}\{h_i^{(l-1)}, a_i^{(l)}\},$$
 (2)

where $h_i^{(l)}$ is the embedding of node v_i in the *l*-th layer and $\mathcal{N}(v_i)$ is a set of nodes adjacent to v_i . AGGREGATE^(l)(·) and COMBINE^(l)(·) are two functions in each GNN layer. After *L* propagation layers, the output embedding for *G* is summarized on node embeddings via the READOUT function, which is formulated as:

$$f(G) = \text{READOUT}\{h_i^{(L)}, \forall v_i \in \mathcal{V}\}.$$
(3)

B. Hilbert-Schmidt Independence Criterion

The Hilbert-Schmidt Independence Criterion (HSIC) [22] is a kernel-based measure of dependence between probability distributions. Let \mathcal{F} be a Hilbert space of real-value functions from a set \mathcal{X} to \mathbb{R} . We say \mathcal{F} is a Reproducing Kernel Hilbert Space (RKHS) if $\forall x \in \mathcal{X}$, the Dirac evaluation operator $\delta_x :$ $\mathcal{F} \to \mathbb{R}$, which maps $f \in \mathcal{F}$ to $f(x) \in \mathbb{R}$, is a bounded linear functional. In RHKS, $\forall x \in \mathcal{X}$, there is a mapping $\phi(x) \in \mathcal{F}$ and there also exists a unique definite kernel $u : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, such that $\langle \phi(x), \phi(x') \rangle_{\mathcal{F}} = u(x, x')$.

Assume that we have two separable RKHSs \mathcal{F} , \mathcal{G} and a joint measure p_{xy} over $(\mathcal{X} \times \mathcal{Y}, \Gamma \times \Lambda)$, where Γ is the Borel sets on set \mathcal{X} and Λ is the Borel sets on set \mathcal{Y} . Then the Hilbert-Schmidt Independence Criterion (HSIC) is defined as the squared Hilbert-Schmidt norm of the associated cross-covariance operator C_{xy} :

$$HSIC(p_{xy}, \mathcal{F}, \mathcal{G}) := ||C_{xy}||_{HS}^2, \tag{4}$$

where the Hilbert-Schmidt norm is $||A||_{HS} = \sqrt{\sum_{i,j} a_{ij}^2}$, and the cross-covariance operator is given as follows:

$$C_{xy} := \mathbf{E}_{x,y}[(\phi(x) - \mu_x) \otimes (\varphi(y) - \mu_y)], \tag{5}$$

Here, \otimes is tensor product, and $\phi(\cdot)$, $\varphi(\cdot)$ are functions that map $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ to RKHSs \mathcal{F} and \mathcal{G} w.r.t. the kernel functions $u(x,y) = \langle \phi(x), \phi(y) \rangle$ and $s(x,y) = \langle \varphi(x), \varphi(y) \rangle$, respectively. Accordingly, given i.i.d. m samples $(X,Y) = \{(x_1, y_1), \cdots, (x_m, y_m)\}$ drawn from the joint distribution of p_{xy} , the empirical version of HSIC is given as:

$$HSIC(X,Y) = (m-1)^{-2}tr(UHSH),$$
 (6)

where $U, S, H \in \mathbb{R}^{m \times m}$, $U_{ij} := u(x_i, x_j)$, $S_{ij} := s(y_i, y_j)$ and $H_{ij} := I - m^{-1}$.

IV. METHOD

In this section, we introduce the GraphSC framework. Given a graph, GraphSC first generates two augmented views as positive and negative samples via weak and strong perturbation, respectively (Step 1). Then the graph and its augmented views are fed into a GNN encoder with shared parameters to obtain corresponding graph-level representations (Step 2). After these representations have been mapped, they are self-contrasted (Step 3). At the same time, considering each graph has multifacet features, GraphSC first factorizes the representations of positive and negative samples by using HSIC, and then masks each factor sequentially to generate multiple masked views (Step ④). The representations of anchors and the masked representations of positive and negative samples are contrasted after a projection head (Step 5). Finally, GraphSC shortens the absolute distance between an anchor and its positive sample (Step 6). The overall framework of GraphSC is given in Fig. 2.

A. Data augmentation

To construct positive and negative pairs, most existing graph contrastive learning methods [3], [36] first perform data augmentations on graphs, such as node dropping and edge perturbation. After that, for each graph, its augmented views of graphs form positive samples while that of other graphs in the same mini-batch are considered as negative samples. Despite the success, these methods can be easily affected by the number of negative samples K. To mitigate the influence of K on the model performance and reduce the number of false negative samples selected, using hard negative samples could be a feasible solution. However, general hard negative sample mining strategies are either not suitable for graph data [37] or computationally costly [20].

Inspired by the assumption in GraphCL [3] that the semantics of a graph will not change for a certain perturbation strength, we further assume that the semantics of a graph will change under strong perturbations. Based on these two assumptions, we generate positive and negative pairs from graphs themselves via graph augmentation functions of various intensities. Specifically, given a graph G, the generated view of the graph with weak perturbation is considered as a positive sample G^+ , while that generated by strong perturbation is taken as negative sample G^- . Formally, for any graph augmentation function $\mathcal{A}(\cdot)$ and two different perturbation rates r_a , r_b , where $(r_a < r_b)$, we have

$$G^+ = \mathcal{A}(G; r_a), G^- = \mathcal{A}(G; r_b).$$
⁽⁷⁾

In this way, since negative samples are directly constructed from graphs themselves, they can share similarities with the original graphs to some degree. Therefore, these negative samples can play the role of hard negative, which can boost the model performance.

B. Model architecture

Self-contrast: Given a graph G_i and its augmentations G_i^+ and G_i^- , we first feed them into a shared GNN encoder $f(\cdot;\theta)$ to learn graph-level representation vectors h_i, h_i^+, h_i^- , respectively. We denote

$$h_i = f(G_i), h_i^+ = f(G_i^+), h_i^- = f(G_i^-).$$
(8)

After that, as suggested in [38], the projection head, a non-linear transformation, can be used to map these representations to another latent space, which can enhance the model performance. Therefore, we further define a projection head $g_1(\cdot; \phi_1)$ and derive:

$$y_i = g_1(h_i), y_i^+ = g_1(h_i^+), y_i^- = g_1(h_i^-),$$
 (9)

where $y_i, y_i^+, y_i^- \in \mathbb{R}^d$. These vectors characterize the overall feature information of samples, which can be used for contrast.

Masked self-contrast: Further, since each graph has multifacet features, in order to pull apart positive pairs from negative pairs, we can perform contrastive learning from masked views. Specifically, we first factorize the representations y_i^+, y_i^- of positive and negative samples into n independent factors $y_i^+ = [c_{i1}^+, c_{i2}^+, \cdots, c_{in}^+]$ and $y_i^- = [c_{i1}^-, c_{i2}^-, \cdots, c_{in}^-]$, respectively. Then we sequentially mask each factor and generate n views. For the m-th masked view, the corresponding embeddings of positive and negative samples are denoted as:

$$y_{im}^{+} = [c_{i1}^{+}, \cdots, c_{i(m-1)}^{+}, c_{0}, c_{i(m+1)}^{+}, \cdots, c_{in}^{+}] \text{ and} y_{im}^{-} = [c_{i1}^{-}, \cdots, c_{i(m-1)}^{-}, c_{0}, c_{i(m+1)}^{-}, \cdots, c_{in}^{-}],$$
(10)

where $c_0 \in \mathbb{R}^{d_c}$ is an all-zero vector and $d_c = d/n$. We further feed y_i, y_{im}^+, y_{im}^- into the second projection head $g_2(\cdot; \phi_2)$ to obtain their projected embeddings:

$$q_i = g_2(y_i), q_{im}^+ = g_2(y_{im}^+), q_{im}^- = g_2(y_{im}^-).$$
 (11)

These projected embeddings can be used for masked contrast across various views.

Shorten the absolute distance: Finally, since triplet loss can only capture the relative distance between an anchor and its positive/negative sample, we explicitly shorten the absolute distance between an anchor and its positive distance. To achieve the goal, we introduce the third projection head $g_3(\cdot; \phi_3)$ and generate

$$z_i = g_3(h_i), z_i^+ = g_3(h_i^+), \tag{12}$$

where $z_i, z_i^+ \in \mathbb{R}^{d_h}$. Then we explicitly pull close z_i and z_i^+ .



Fig. 2. The overall framework of GraphSC. For details of each step, see Section IV.

C. Contrastive loss

In the training process, we randomly select B graphs from the whole dataset of N graphs as a mini-batch. For each graph G_i in the mini-batch, we apply two different strengths of perturbation, which generates a triple (G_i, G_i^+, G_i^-) . Further, we derive the corresponding representations (h_i, h_i^+, h_i^-) through a shared GNN encoder.

Self-contrast: To implement self-contrast between complete representations, we put (h_i, h_i^+, h_i^-) into a projection head to get (y_i, y_i^+, y_i^-) , and use triplet margin loss to enlarge the relative distance between positive and negative sample pairs:

$$\mathcal{L}_{se} = \frac{1}{B} \sum_{i=1}^{B} \max(||y_i - y_i^+||^2 - ||y_i - y_i^-||^2 + \epsilon, 0), \quad (13)$$

Note that ϵ is the margin.

Masked self-contrast:For masked self-contrast, we first use Hilbert-Schmidt Independence Criterion (HSIC) [22] to factorize y_i^+ and y_i^- into *n* factors:

$$\mathcal{L}_{fa} = \frac{1}{B} \sum_{i=1}^{B} \sum_{j \neq k}^{n} [\text{HSIC}(c_{ij}^{+}, c_{ik}^{+}) + \text{HSIC}(c_{ij}^{-}, c_{ik}^{-})]. \quad (14)$$

This process ensures that factors are as independent as possible from each other, which helps reduce the dependence between multiple partial representations. After that, we sequentially mask each factor to generate a set of masked representations $\{y_{im}^+\}_{m=1}^n$ and $\{y_{im}^-\}_{m=1}^n$, respectively. When a factor is masked, it is still expected that the positive sample can be close to the anchor while the negative sample is distant. Therefore, we formulate the masked contrastive loss as:

$$\mathcal{L}_{ma} = \frac{1}{B} \sum_{i=1}^{B} \sum_{m=1}^{n} w_{im} \cdot \max(\|q_i - q_{im}^+\|^2 - \|q_i - q_{im}^-\|^2 + \epsilon, 0), \quad (15)$$

where

$$w_{im} = \left(1 - \frac{exp(e_{im})}{\sum_{i=1}^{n} exp(e_{im})}\right) \cdot \frac{1}{n-1},\tag{16}$$

$$e_{im} = q_i \cdot (q_{im}^+ - q_{im}^-)^T.$$
(17)

Here, we introduce the weight w_{im} for the *m*-th factor and $\sum_{m=1}^{n} w_{im} = 1$. For the factor that leads to a small relative distance, our model will assign a large weight and thus pay more attention to the corresponding optimization process.

Shorten the absolute distance: To shorten the absolute distance between positive pairs, which can make each class more compact, we propose two models GraphSC and GraphSC-MSE, which use Barlow Twins loss and MSE loss as regularization terms, respectively.

(1) **GraphSC:** GraphSC pulls close the representations of the anchor and the positive sample after the third projection head g_3 , and we formulate the objective function \mathcal{L}_{ab} as:

$$\mathcal{L}_{ab} = \frac{1}{B} \sum_{i} (1 - C_{ii})^2 + \beta \sum_{i} \sum_{j \neq i} C_{ij}^2, \qquad (18)$$

$$C_{ij} = \frac{\sum_{b=1}^{B} z_{b,i} z_{b,j}^{+}}{\sqrt{\sum_{b=1}^{B} (z_{b,i})^2} \sqrt{\sum_{b=1}^{B} (z_{b,j}^{+})^2}}.$$
 (19)

Here, Barlow Twins loss can additionally reduce the redundancy between components of embedding vectors, which can also boost the model performance. (2) GraphSC-MSE: GraphSC-MSE no longer structurally needs the third projection head g_3 , and the regularization term \mathcal{L}_{ab} can be written as:

$$\mathcal{L}_{ab} = \frac{1}{B} \sum_{i=1}^{B} ||y_i - y_i^+||^2, \qquad (20)$$

Note that the MSE loss is a widely used distance measure, and we can use GraphSC-MSE to verify the necessity and effectiveness of shortening the absolute distance between the anchor and the positive sample. Finally, our objective function is summarized as:

$$\min \mathcal{L} = \underbrace{\mathcal{L}_{se} + \lambda_1 \cdot \mathcal{L}_{ma} + \lambda_2 \cdot \mathcal{L}_{fa}}_{relative \ term} + \underbrace{\lambda_3 \cdot \mathcal{L}_{ab}}_{absolute \ term}, \quad (21)$$

where λ_1 , λ_2 and λ_3 are hyper-parameters that are used to balance the term importance.

V. EXPERIMENTS

In this section, we conduct experiments on multiple benchmark datasets to evaluate the performance of GraphSC through answering the following research questions.

- **RQ1.** (Generalizability) Does GraphSC outperform other competitors in unsupervised settings?
- **RQ2.(Transferability**) Can GNNs pre-train with GraphSC show better transferability than competitors?
- **RQ3.** (Effectiveness) Are the individual components of GraphSC really valid for the model ?
- **RQ4.** (Convergence) What is the effect of \mathcal{L}_{ma} , \mathcal{L}_{ab} and the proposed negative sample generation strategy on the convergence of the model?
- **RQ5.** (Hyperparameters Sensitivity) Is the proposed GraphSC sensitive to hyperparameters like perturbation intensity r_a , r_b and the term weight λ_1 , λ_2 , λ_3 ?

A. Experimental Setup

Datasets: For unsupervised learning, we use 8 datasets from the benchmark TU dataset [39], including graph data for various biochemical molecules (i.e., NCI1, PROTEINS, DD, MUTAG) and social networks (i.e., COLLAB, REDDIT-BINARY, REEDIT-MULTI-5K and IMDB-BINARY). For transfer learning, we perform pre-training on ZINC-2M which samples 2 million unlabeled molecules from ZINC15 [40] and fine-tune the model with 8 datasets including BBBP, Tox21,

 TABLE I

 DATASETS STATISTICS FOR UNSUPERVISED LEARNING.

Dataset	Category	Graph Num. Avg. Node Avg. Edge				
NCI1	Biochemical Molecules	4110	29.87	32.30		
PROTEINS	Biochemical Molecules	1113	39.06	72.82		
DD	Biochemical Molecules	1178	284.32	715.66		
MUTAG	Biochemical Molecules	188	17.93	19.79		
COLLAB	Social Networks	5000	74.49	2457.78		
RDT-B		2000	429.63	497.75		
RDB-M	Social Networks	4999	508.52	594.87		
IMDB-B	Social Networks	1000	19.77	96.53		

ToxCast, SIDER, ClinTox, MUV, HIV and BACE. More details can be seen in the Table I and Table II.

Baselines: For unsupervised learning, we compare GraphSC with three kernel-based methods including graphlet kernel (GL) [41], Weisfeiler-Lehman kernel (WL) [42], and deep graph kernel (DGK) [43]. Furthermore, we compare GraphSC with other state-of-the-art methods: sub2vec [44], graph2vec [45], InfoGraph [7], GraphCL [3], JOAO(v2) [35], AD-GCL [36], SimGRACE [8], RGCL [9] and LaGraph [46]. We also take GraphSC-MSE as our baseline. For transfer learning, we adopt DGI [2], EdgePred [47], AttrMasking [47], ContextPred [47], GraphCL [3], JOAO(v2) [35], AD-GCL [36], SimGRACE [8], GraphLoG [48] and RGCL [9], which are the state-of-the-art pre-training paradigms in this area, as our baselines.

Evaluation Protocols: Following the settings of previous works [3], [9], [47], we evaluate the performance and generalizability of the learned representations on both unsupervised and transfer learning settings. In unsupervised setting, we train GraphSC using the whole dataset to learn graph representations and feed them into a downstream SVM classifier with 10-fold cross-validation, report the mean accuracy with standard deviation after 5 runs. For transfer learning, we pre-train and fine-tune GNN encoder in different datasets to evaluate the transferability of the pre-training scheme. The fine-tuning procedure is repeated for 10 times with different random seeds and we evaluate the mean and standard deviation of AUROC scores on each downstream dataset, which is consistent with our baselines.

Implementation details: We implement GraphSC using PyTorch. The model is initialized by Xavier initialization [49] and trained by Adam [50]. As suggested in [19], we set ϵ in (13) and (15) to 0.2. Similarly, we set β in (18) to 0.013 according to [23]. For other hyperparameters, we fine-tune them by grid search. For unsupervised learning, we first fine-tune learning rate from $\{0.001, 0.005, 0.01\}$. For the augmentation functions $A(\cdot)$, we choose from four augmentations and some of their combinations, which are in line with GraphCL [3]. For the perturbation rates r_a and r_b , we fine-tune them from {0.05, 0.1, 0.15, 0.2} and {0.15,0.2,0.25,0.3,0.35,0.4} respectively. In addition, we fine-tune λ_1 , λ_2 and λ_3 from {0.001, 0.01, 0.1, 1, 10, 100 }. In transfer learning, we pre-trained the GNN encoder on the ZINC-2M dataset, and we set learning rate to 0.001, the number of epochs to 80, r_a to 0.1, r_b to 0.25, λ_1 to 1, λ_2 to 0.01 and λ_3 to 0.01. In addition, we use the combination of subgraph and node dropping as augmentation function, which is the same as GraphCL [3]. In the process of fine-tuning, we adjust the two hyperparameters learning rate and epoch, and the grid search range is $\{0.0001, 0.0005, 0.001\}$ and $\{20, 40, 0.000\}$ 60, 80, 100} respectively. Since most results of baselines are publicly available, we directly report these results from their original papers. For the results of AD-GCL and GraphLoG, we report these results from RGCL [9]. For fairness, we run all the experiments on a server with 128G memory and a single NVIDIA 2080Ti GPU. We provide our code and data here: https://anonymous.4open.science/r/GraphSC-8360.

Datasets	Category	Utilization	Graph Num.	Avg. Node	Avg.Degree
ZINC-2M	Biochemical Molecules	PRE-TRAINING	2,000,000	26.62	57.72
BBBP	Biochemical Molecules	FINETUNING	2,039	24.06	51.90
TOX21	Biochemical Molecules	FINETUNING	7,831	18.57	38.58
TOXCAST	Biochemical Molecules	FINETUNING	8,576	18.78	38.52
SIDER	Biochemical Molecules	FINETUNING	1,427	33.64	70.71
CLINTOX	Biochemical Molecules	FINETUNING	1,477	26.15	55.76
MUV	Biochemical Molecules	FINETUNING	93,087	24.23	52.55
HIV	Biochemical Molecules	FINETUNING	41,127	25.51	54.93
BACE	Biochemical Molecules	FINETUNING	1,513	34.08	73.71

TABLE II DATASETS STATISTICS FOR TRANSFER LEARNING.

B. Unsupervised learning (RQ1)

For unsupervised representation learning, we take the onehot representations of node labels and degrees as node feature vectors for molecular datasets and social network datasets, respectively. We summarize the experimental results in Table III. From the table, we see that GraphSC ranks first on 5 out of 8 datasets and has competitive results on the other three. For example, the accuracie of GraphSC on the COLLAB datasets is 78.90%, which is > 1.2% higher than the runner-up. Moreover, GraphSC also leads in the other four datasets (i.e. NCI1, PROTEINS, RED-B and RED-M5K) by 0.3%-0.8%. Further, the average ranking of GraphSC across all the datasets is 1.5, much better than the runner-up's, which is 2.8. We also notice that GraphSC-MSE, which utilizes the MSE loss to minimize the absolute distance between anchor and positive sample, is the runner-up among all the methods. This further verifies the effectiveness of our proposed self-contrast framework, which is not simply originated from the Barlow Twin loss regularization.

C. Transfer learning (RQ2)

In transfer learning, we first pre-train a backbone model on Zinc-2M, and fine-tune the model on 8 multi-task binary classification datasets. All the results w.r.t. the area under receiver operating characteristic (AUROC) on downstream tasks are presented in Table IV, as well as the average scores. From the table, we see that GraphSC achieves the highest average score compared with other baselines, and also the best performances on the BBBP and Toxcast datasets. For other cases where GraphSC is not the winner, the gap between GraphSC's score and the winner's is small. For example, the gaps between GraphSC and the winner on the SIDER and MUV datasets are only 0.89% and 0.35%, respectively. Further, let us take a closer look at GraphCL, which uses the same augmentation functions as GraphSC. Specifically, GraphSC leads GraphCL by > 6% on both ClinTox and MUV datasets, and has an average score on all datasets that is 2.6% higher than GraphCL.

D. Ablation Study (RQ3)

We conduct an ablation study on GraphSC to understand the characteristics of its main components. One variant randomly selects an augmented view of another sample as a negative sample. This is different from GraphSC, which uses a negative sample that is directly constructed from the graph sample itself (see Section IV-A). We call this variant **GraphSC_rd** (random), which helps us evaluate the validity of our negative generation strategy. Another variant trains model without considering masked self-contrast. This helps us understand the importance of masked self-contrast. Finally, to show the importance of the Barlow Twins loss regularization term, We remove \mathcal{L}_{ab} from the objective function and call this variant **GraphSC_nB** (no Barlow Twins). The results are given in Table V and we observe:

(1) GraphSC achieves better performance than GraphSC_rd. Since GraphSC_rd randomly selects an augmented view of other sample as a negative, the performance gaps between GraphSC and GraphSC_rd show that GraphSC's negative generation strategy is very effective in selecting a valid negative sample to improve classification accuracy.

(2) GraphSC clearly outperforms GraphSC_nm on all datasets. GraphSC_nm, which removes \mathcal{L}_{ma} from the objective function, does not perform masked self-contrast. This leads to significant performance degradation due to the ignorance of the fact that graph-structured data generally contains multiple aspects of information.

(3) GraphSC beats GraphSC_nB across all datasets. In particular, GraphSC significantly outperforms GraphSC_nB on MUTAG and COLLAB. This shows that the Barlow Twins loss regularization is particularly important for model training. When using Barlow Twins loss regularization, the model can explicitly shorten the absolute distance between the anchor and the positive sample. This effectively compensates for the inherent weakness of triplet loss.

TABLE III

UNSUPERVISED REPRESENTATION LEARNING ON TU DATASETS. ALL THE BASELINES ARE COMPARED IN THE SAME EXPERIMENT SETTING W.R.T. THE CLASSIFICATION ACCURACY(%). <u>Bold</u> indicates the best performance on each dataset. A.R. denotes average rank. - indicates that results are not available in published papers. Results for SOTA methods are as published.

Dataset	NCI1	PROTEINS	DD	MUTAG	COLLAB	RDT-B	RDT-M5K	IMDB-B	A.R.
GL	-	-	-	81.66 ± 2.11	-	77.34 ± 0.18	41.01 ± 0.17	65.87 ± 0.98	13.3
WL	80.01 ± 0.50	72.92 ± 0.56	-	80.72 ± 3.00	-	68.82 ± 0.41	46.06 ± 0.21	72.30 ± 3.44	7.9
DGK	80.31 ± 0.46	73.30 ± 0.82	-	87.44 ± 2.72	-	78.04 ± 0.39	41.27 ± 0.18	72.30 ± 3.44	6.4
sub2vec	52.84 ± 1.47	53.03 ± 0.55	-	61.05 ± 15.80	-	71.48 ± 0.41	36.68 ± 0.42	55.26 ± 1.54	14.5
graph2vec	73.22 ± 1.81	73.30 ± 2.05	-	83.15 ± 9.25	-	75.78 ± 1.03	47.86 ± 0.26	71.10 ± 0.57	11.5
InfoGraph	76.20 ± 1.06	74.44 ± 0.31	72.85 ± 1.78	89.01 ± 1.13	70.65 ± 1.13	82.50 ± 1.42	53.46 ± 1.03	73.03 ± 0.87	7.9
GraphCL	77.87 ± 0.41	74.39 ± 0.45	78.62 ± 0.40	86.80 ± 1.34	71.36 ± 1.15	89.53 ± 0.84	55.99 ± 0.28	71.14 ± 0.44	7.8
JOAO	78.07 ± 0.47	74.55 ± 0.41	77.32 ± 0.54	87.35 ± 1.02	69.50 ± 0.36	85.29 ± 1.35	55.74 ± 0.63	70.21 ± 3.08	8.9
JOAOv2	78.36 ± 0.53	74.07 ± 1.10	77.40 ± 1.15	87.67 ± 0.79	69.33 ± 0.34	86.42 ± 1.45	56.03 ± 0.27	70.83 ± 0.25	8
AD-GCL	73.91 ± 0.77	73.28 ± 0.46	75.79 ± 0.87	88.74 ± 1.85	72.02 ± 0.56	90.07 ± 0.85	54.33 ± 0.32	70.21 ± 0.68	8.5
SimGRACE	79.12 ± 0.44	75.35 ± 0.09	77.44 ± 1.11	89.01 ± 1.31	71.72 ± 0.82	89.51 ± 0.89	55.91 ± 0.34	71.30 ± 0.77	5.6
RGCL	78.14 ± 1.08	75.03 ± 0.43	$\textbf{78.86} \pm \textbf{0.48}$	87.66 ± 1.01	70.92 ± 0.65	90.34 ± 0.58	56.38 ± 0.40	71.85 ± 0.84	5.1
LaGraph	79.9 ± 0.5	75.2 ± 0.4	78.1 ± 0.4	$\underline{90.2\pm1.1}$	77.6 ± 0.2	90.4 ± 0.8	56.4 ± 0.4	73.7 ± 0.9	3
GraphSC-MSE	80.39 ± 0.62	75.58 ± 0.23	78.32 ± 0.77	88.04 ± 1.56	77.64 ± 0.26	90.26 ± 0.80	56.38 ± 0.60	$\textbf{74.34} \pm \textbf{0.72}$	2.8
GraphSC	$\underline{\textbf{81.12}\pm\textbf{0.40}}$	$\underline{\textbf{75.92} \pm \textbf{0.15}}$	78.32 ± 1.07	89.19 ± 1.83	$\underline{\textbf{78.90} \pm \textbf{0.32}}$	$\underline{\textbf{91.08} \pm \textbf{0.56}}$	$\underline{\textbf{56.71} \pm \textbf{0.30}}$	$\overline{74.28\pm0.76}$	<u>1.5</u>

TABLE IV

TRANSFER LEARNING ON DOWNSTREAM GRAPH CLASSIFICATION TASKS. WE COMPARED ALL THE METHODS W.R.T. THE AUROC SCORE(%). <u>Bold</u> INDICATES THE BEST PERFORMANCE ON EACH DATASET. - INDICATES THAT RESULTS ARE NOT AVAILABLE IN PUBLISHED PAPERS. RESULTS FOR SOTA METHODS ARE AS PUBLISHED.

Dataset	BBBP	Tox21	ToxCast	SIDER	ClinTox	MUV	HIV	BACE	AVG.
No Pre-Train	65.8 ± 4.5	74.0 ± 0.8	63.4 ± 0.6	57.3 ± 1.6	58.0 ± 4.4	71.8 ± 2.5	75.3 ± 1.9	70.1 ± 5.4	66.96
DGI	68.8 ± 0.8	75.3 ± 0.5	62.7 ± 0.4	58.4 ± 0.8	69.9 ± 3.0	75.3 ± 2.5	76.0 ± 0.7	75.9 ± 1.6	70.29
EdgePred	67.3 ± 0.24	76.0 ± 0.6	64.1 ± 0.6	60.4 ± 0.7	64.1 ± 3.7	74.1 ± 2.1	76.3 ± 1.0	79.9 ± 0.9	70.28
AttrMasking	64.3 ± 2.8	$\textbf{76.7} \pm \textbf{0.4}$	64.2 ± 0.5	61.0 ± 0.7	71.8 ± 4.1	74.7 ± 1.4	77.2 ± 1.1	79.3 ± 1.6	71.15
ContextPred	68.0 ± 2.0	$\overline{75.7\pm0.7}$	63.9 ± 0.6	60.9 ± 0.6	65.9 ± 3.8	75.8 ± 1.7	77.3 ± 1.0	79.6 ± 1.2	70.89
GraphCL	69.68 ± 0.67	73.87 ± 0.66	62.40 ± 0.57	60.53 ± 0.88	75.99 ± 2.65	69.80 ± 2.66	$\textbf{78.47} \pm \textbf{1.22}$	75.38 ± 1.44	70.77
JOAO	70.22 ± 0.98	74.98 ± 0.29	62.94 ± 0.48	59.97 ± 0.79	81.32 ± 2.49	71.66 ± 1.43	$\overline{76.73 \pm 1.23}$	77.34 ± 0.48	71.9
JOAOv2	71.39 ± 0.92	74.27 ± 0.62	63.16 ± 0.45	60.49 ± 0.74	80.97 ± 1.64	73.67 ± 1.00	77.51 ± 1.17	75.49 ± 1.27	72.12
AD-GCL	68.26 ± 1.03	73.56 ± 0.72	63.10 ± 0.66	59.24 ± 0.86	77.63 ± 4.21	74.94 ± 2.54	75.45 ± 1.28	75.02 ± 1.88	70.90
SimGRACE	71.25 ± 0.86	-	63.36 ± 0.52	60.59 ± 0.96	-	-	-	-	-
GraphLoG	71.04 ± 1.86	74.65 ± 0.60	62.32 ± 0.51	57.86 ± 1.44	78.72 ± 2.58	74.95 ± 1.96	75.12 ± 1.98	$\textbf{82.6} \pm \textbf{1.25}$	72.16
RGCL	71.42 ± 0.66	75.20 ± 0.34	63.33 ± 0.17	$\underline{\textbf{61.38} \pm \textbf{0.61}}$	$\underline{\textbf{83.38}\pm\textbf{0.91}}$	$\textbf{76.66} \pm \textbf{0.99}$	77.90 ± 0.80	$\overline{76.03\pm0.77}$	73.16
GraphSC	$\textbf{72.16} \pm \textbf{1.42}$	$\overline{75.58\pm0.56}$	$\underline{64.27 \pm 0.23}$	60.49 ± 0.41	82.29 ± 1.21	$\overline{76.31\pm0.71}$	$\overline{77.08\pm0.83}$	$\overline{78.82 \pm 1.38}$	73.37

 TABLE V

 Ablation study for GraphSC on unsupervised learning datasets.

Dataset	NCI1	PROTEINS	DD	MUTAG	COLLAB	RDT-B	RDT-M5K	IMDB-B	AVG.
GraphSC_rd	80.44 ± 0.43	74.90 ± 0.70	77.60 ± 0.56	86.36 ± 1.93	77.60 ± 0.32	90.02 ± 0.96	56.18 ± 0.66	73.22 ± 0.77	77.04
GraphSC_nm	80.79 ± 0.31	74.98 ± 0.73	77.39 ± 0.33	87.66 ± 0.95	77.46 ± 0.37	89.89 ± 0.65	56.17 ± 0.56	73.66 ± 0.54	77.25
GraphSC_nB	79.61 ± 0.36	75.19 ± 0.36	77.27 ± 0.84	86.68 ± 1.94	77.24 ± 0.30	89.80 ± 0.48	56.12 ± 0.34	73.66 ± 0.84	76.95
GraphSC	$\underline{\textbf{81.12}\pm\textbf{0.40}}$	$\underline{\textbf{75.92} \pm \textbf{0.15}}$	$\underline{\textbf{78.32} \pm \textbf{1.07}}$	$\underline{\textbf{89.19} \pm \textbf{1.83}}$	$\underline{\textbf{78.90} \pm \textbf{0.32}}$	$\underline{\textbf{91.08} \pm \textbf{0.56}}$	$\underline{\textbf{56.71} \pm \textbf{0.30}}$	$\underline{\textbf{74.28} \pm \textbf{0.76}}$	<u>78.19</u>

E. Convergence analysis (RQ4)

We next show how different components of GraphSC can address the hard-to-train due to the usage of triplet loss objective. To show the difficulty in training triplet loss based objective, we further consider a variant of GraphSC that randomly selects an augmented view of another sample as a negative sample and uses the triplet loss to train GNN encoder. We call it **GraphSC_rdt** (random selection and triplet loss). We take it as a reference and show the convergence results of GraphSC variants on four datasets in Fig. 3. From the figure, we observe that: (1) The accuracy of GraphSC_rdt does not increase with more training epochs on all four datasets. This shows that GraphSC_rdt is hard-to-train due to the triplet loss objective.

(2) GraphSC converges faster than GraphSC_nm. Specifically, on the COLLAB and REDDIT-BINARY datasets, GraphSC_nm converges with more than 60 epochs, while GraphSC uses only 20 epochs. In addition, GraphSC_nm trains very unsteadily on REDDIT-MULTI-5K. The convergence speed gaps between GraphSC and GraphSC_nm show that GraphSC's masked self-contrast is very effective in accelerating model convergence.



Fig. 3. Convergence curves for GraphSC and its variants on NCI1, COLLAB, REDDIT-BINARY and REDDIT-MULTI-5K datasets



Fig. 4. Accuracy difference between GraphSC and GraphCL versus various perturbation intensity pairs in unsupervised learning settings. Since $r_a < r_b$, we fill in the parts of the diagram that violate this condition with blanks.



Fig. 5. GraphSC 's sensitivity analysis w.r.t. the hyperparameters λ_1 , λ_2 and λ_3 in unsupervised learning settings.

(3) Compared with GraphSC, GraphSC_nB converges slower and performs worse. GraphSC_nB, which only consider relative distances between anchor and positive sample, might not pull close positive sample pairs well. By explicitly shortening the absolute distance for positive sample pairs, GraphSC converges faster and performs better.

(4) GraphSC also achieves faster convergence than GraphSC_rd. This shows that the negative generation strategy is particularly important for model training. When using our proposed negative generation strategy, the model can obtain informative negative samples, which accelerates convergence.

F. Hyperparameter sensitivity analysis (RQ5)

We end this section with a sensitivity analysis on the hyperparameters of GraphSC. In particular, we study four key hyperparameters: the perturbation intensities r_a, r_b , and the term weights $\lambda_1, \lambda_2, \lambda_3$. We evaluate the performance of GraphSC on unsupervised settings. We vary one hyperparameter each time with others fixed. Experimental results are given in Fig. 4 and Fig. 5.

• **Perturbation intensity**: As shown in Fig. 4, we calculate the accuracy difference between GraphSC and GraphCL for different combinations of perturbation strengths. Although the

best settings of perturbations are different for each dataset, GraphSC performs very well over various perturbation strength combinations. This demonstrates the stability of the model.

• Term weight λ_1 , λ_2 and λ_3 : As can be observed in Fig. 5, for the term weight λ_1 , λ_2 and λ_3 , GraphSC gives very stable performances over a wide range of parameter values. This also shows the robust performance of GraphSC.

VI. CONCLUSIONS

In this paper, we studied graph-level representation learning and proposed GraphSC, a graph contrastive learning framework, which uses triplet loss as objective. GraphSC first uses graph augmentation functions of different intensities to obtain a positive and negative view of a graph sample from the graph itself. Further, it factorizes the graph representations into multiple factors and then presented a self-contrast mechanism to separate positive and negative samples. Moreover, GraphSC tries to shorten the absolute distance between an anchor and its positive sample, which addresses the problem of triplet loss in optimizing only the relative distance between the anchor point and its positive/negative samples. We conducted extensive experiments in both unsupervised and transfer learning settings, and experimental results demonstrate the effectiveness and transferability of the proposed framework.

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