- The **anchor-neighborhood alignment (ANA)** leverages graph diffusion to achieve weighted alignment between central anchor and neighbors, enhancing the adequacy of graph structure exploration and improving the model's topological awareness. Moreover, ANA aligns representations of the same node from different views, enabling the extraction of invariant information across multiple views.
- The **isotropic constraints (IC)** is employed to overcome dimensional collapse issues and enhance representation diversity.
- Throughout the paper, we elaborate on the motivation and functionality of the two modules in multiple places:

Abstract:

neural model. As a cornerstone module, an anchor-neighborhood alignment strategy, which utilizes graph diffusion to construct the probability distribution of positive samples based on the structural context of the anchor node, enables sufficient exploration of graph topology and endows the neural model with stronger structure-aware ability. To enhance diversity of node representations, a scheme of isotropic constraints is introduced to encourage representations to exhibit consistent distribution along any direction in space, which compels data points to be scattered throughout the whole representation space and naturally solves the notorious dimensional collapse in self-supervised learning. Owing to no re-

Introduction:

logical relationships within the graph. Subsequently, the positive samples with diffusion weights are derived from the constructed distribution to realize weighted anchor-neighborhood alignment in representation space to endow the model with stronger structure-aware ability. Furthermore, it is imperative to eliminate collapse

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tions (referred to as anisotropy), as depicted in Figure 2. In light of our observations, we introduce an approach of isotropic constraints to mitigate dimensional collapse, encouraging representations to exhibit a consistent distribution across all spatial directions and achieve diversity. Our research advances the study of dimensional

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- A strategy of anchor-neighborhood alignment is put forward to enhance the comprehensive exploration of unlabeled graph data and reinforce topological awareness of neural models, whose core is an ingenious positive sampling scheme based on structural context distribution.
- We reexamine another manifestation of dimension collapse, namely, anisotropic distributions. Correspondingly, an innovative scheme of isotropic constraints is proposed to mitigate collapse issues and enhance representation diversity, independent of existing methods such as negative sampling, channel decorrelation, and asymmetric architectures.

Related Workd:

alleviate collapse issues by decoupling various channels. Diverging from previous research, our approach enforces isotropic constraints on representations, which provides a natural solution to address collapse issues and parallels current literature.

Method:

3.2 Anchor-Neighborhood Alignment:

However, in the context of graph self-supervised learning, naively treating two nodes from different augmented views as a positive pair is suboptimal. *On the one hand*, the graph harbors a wealth of structural information that characterizes the relationships between nodes, which can offer guidance for modeling the distribution of positive samples. Disregarding the potential role of the topological structure in shaping self-supervised objectives and treating it solely as a regulator of message passing in GNNs lead to inadequate utilization of graph information. *On the other hand*, the positive sample pair is only acquired from various augmented versions of the same node, which poses a challenge in determining the strength of augmentation. The related studies have shown that increasing data augmentation can improve the quality of self-supervised representations, but overly strong augmentations introducing excessive disturbances result in a decline in performance [32]. In other words, this *strict alignment* exhibits limited resilience to data augmentation and results in weak robustness.

3.3 Isotropic Constraints:

Our research focuses on fully unleashing the potential of graph self-supervised learning, which inherently necessitates enhancing expressive capacity of the models and diversity of node representations. Under-expressed representations fail to adequately span the entire representation space, giving rise to the notorious issue of dimension collapse in the realm of self-supervised learning. In existing literature, a prevailing viewpoint on dimensional collapse is that distinct dimensions manifest significant correlations, which inevitably convey coupled and redundant information. Beyond this prevalent opinion, as depicted in Figure 2, another potential manifestation of dimensional collapse is that the representations exhibit certain distributional disparities along various directions. Along

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3.4 Overall Objective Function:

ANA serves as a cornerstone module, endowing the neural model with the ability to learn augmentation-invariant representations and capture structural information. IC can reinforce the expressive power of the model and improve the diversity of representations. The two terms complement each other, forming a comprehensive self-supervised objective:

Some new experiments demonstrating the robustness of ANA toward strong augmentation:

Table 7: Performance with ANA-IC under strong augmentation ($p_e = 0.9, p_f = 0.9$). $K = 0$ denotes no ANA.

K	0	1	2	3	4	5
Computers	79.81	87.17	87.71	87.92	87.97	88.10
Pubmed	75.7	78.8	79.2	80.3	80.2	80.3
Citeseer	67.3	70.3	70.7	70.4	70.2	69.8

E.1.4 Robustness and Resilience toward Strong Augmentation. As mentioned earlier, when $K = 0$ in Eq. (3), the anchor-neighborhood alignment degenerates into strict alignment between various augmented views of the same instance. Here, we conduct experiments to illustrate the anchor-neighborhood alignment is more robust to strong augmentations than the strict alignment. Specifically, both edge removal ratio p_e and feature masking ratio p_f are set to 0.9 and various values of K are validated. The experimental results are summarized in Table 7 where the performance under $K > 0$ are consistently better than those under $K = 0$ with considerable margin, which demonstrates that the proposed anchor-neighborhood alignment strategy has greater robustness and resilience in the face of strong augmentation. ANA can still capture valuable information from structural context for self-supervised learning, even with unreasonable data augmentation. The great robustness can make our approach more stable in real-world scenario applications.

In summary,

- ANA serves as a **cornerstone module** for extracting invariant information across views and mining structural information within the graphs.
- IC, as an **enhancement module**, increases information amount, enhances model expressiveness, and diversifies representations.
- In our paper, we demonstrate the roles of two modules through extensive experiments, such as t-SNE visualization in Figure 10.