Graph Pooling via Coarsened Graph Infomax

Yunsheng Pang¹, Yunxiang Zhao², Dongsheng Li²∗
¹The University of Melbourne
²National Lab for Parallel and Distributed Processing, College of Computer, National University of Defense Technology
{yunshengp.yunxiangz}@student.unimelb.edu.au, lds1201@163.com

ABSTRACT
Graph pooling that summaries the information in a large graph into a compact form is essential in hierarchical graph representation learning. Existing graph pooling methods either suffer from high computational complexity or cannot capture the global dependencies between graphs before and after pooling. To address the problems of existing graph pooling methods, we propose Coarsened Graph Pooling (CGIPool) that maximizes the mutual information between the input and the coarsened graph of each pooling layer to preserve graph-level dependencies. To achieve mutual information neural maximization, we apply contrastive learning and propose a self-attention-based algorithm for learning positive and negative samples. Extensive experimental results on seven datasets illustrate the superiority of CGIPool comparing to the state-of-the-art methods.

CCS CONCEPTS
• Computing methodologies → Neural networks;

KEYWORDS
Graph Pooling; Graph Neural Networks; Mutual Information

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than the author(s) must be honored. Abstracting with credit is permitted. To copy otherwise, or republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from permissions@acm.org.
SIGIR '21, July 11–15, 2021, Virtual Event, Canada.
© 2021 Copyright held by the owner/authors(s). Publication rights licensed to ACM.
ACM ISBN 978-1-4503-8037-9/21/07...
https://doi.org/10.1145/3404835.3463074

1 INTRODUCTION
Graph Neural Networks (GNNs) [1–3] have shown outstanding performance in numerous graph related tasks, such as node classification [1], graph classification [4] and link prediction [5]. Recently, learning representations of entire graphs [4, 6] has attracted a lot of attention in the fields of bioinformatics [7], recommendation systems [8, 9], social network study [10], etc [11]. In graph level representation learning, graph pooling [6] that maps large graphs to smaller ones is essential for capturing a meaningful structure of the graph and reducing the computation cost simultaneously.

1Dongsheng Li is the corresponding author.

Earlier graph pooling methods use summation or neural networks to pool all the representations of nodes [4, 12, 13]. However, these methods cannot well capture graph structure information such as subgraph and hierarchy. In recent years, hierarchical pooling methods have been proposed to address the limitations of global pooling. In hierarchical pooling, graph coarsening pooling methods consider graph pooling as a node clustering problem, which merges similar nodes to a cluster and regards the cluster centers as the nodes in the coarsened graph [6, 14, 15]. These methods perform node clustering by learning a soft cluster assignment matrix [6], which cannot leverage the sparsity in the graph topology. Moreover, the high computational complexity of these methods prevents them from being applied to large graphs. Node selection pooling methods have lower complexity compared with graph coarsening [16–19]. These methods select a subset of nodes according to the importance of nodes in the graph. However, they neglect the global dependencies between graphs before and after pooling and consider nodes’ local topology [17] only when learning nodes’ importance scores. Therefore, they cannot filter out nodes that are informative locally but not essential for graph-level representation learning.

To tackle the problems of node selection pooling, we propose CGIPool that maximizes the mutual information [20–22] between the input and the coarsened graph of each pooling layer. Specifically, we first propose positive and negative coarsening modules with the self-attention mechanism to learn real and fake coarsened graphs. The real coarsened graph, which maximally reflects the input graph, is used as the positive sample. The fake coarsened graph, which contains unimportant nodes of the input graph, is used as the negative sample. Then, we train a discriminator [23, 24] to increase the score on the positive example and decrease the score on the negative example so as to achieve mutual information neural maximization. Compared with other node selection pooling models, CGIPool that considers the global dependencies between graphs before and after pooling can preserve nodes that are informative globally rather than those informative locally. We summarize the main contributions of this paper as follows:

• We propose CGIPool, which is the first node selection pooling model that captures global dependencies between the input and the coarsened graph of each pooling layer.
• We propose self-attention-based positive and negative coarsening modules to learn real and fake coarsened graphs as positive and negative samples, thus be able to achieve mutual information neural maximization via contrastive learning.
• Experimental results demonstrate that CGIPool outperforms state-of-the-art methods on six out of seven benchmark datasets. We have made the implementation of CGIPool public available³.

³The source code is public available at: https://github.com/PangYunsheng8/CGIPool
2 RELATED WORK

We review existing works on graph pooling, followed by those on mutual information neural estimation and maximization.

Graph Pooling: Graph pooling can be divided into global pooling and hierarchical pooling [18]. Global pooling models summarize a graph into a node directly [4, 12, 13]. Hierarchical pooling that captures the local substructures of graphs can be divided into graph-coarsening-based, node-selection-based methods, and a few others. (i) Graph-coarsening pooling aims to map nodes into different clusters [6, 14, 15]. (ii) Node-selection pooling adopts learnable scoring functions to drop nodes with lower scores [16–19]. Apart from (i) and (ii), [25] scores edges and merges nodes with high-scoring edges between them, and [26] proposes a memory layer to jointly learn node representations and coarsen the input graph.

Mutual information neural estimation: Mutual information (MI) measures the mutual dependencies between two random variables [20]. Deep infomax [21] simultaneously estimates and maximizes the mutual information between the pixels and overall images to learn image representations. DGI [22] maximizes the mutual information between the input graph and each of its nodes to learn informative node representations. VPool [19] leverages MI to select nodes that maximally represent their neighborhoods, which is the only graph pooling model based on mutual information maximization. Our CGIPool considers both the information from nodes’ local neighborhoods and the global dependencies between the input and the coarsened graph, which is different from VPool that considers nodes’ local neighborhoods only.

3 METHOD

We present the overall structure of the proposed CGIPool in Figure 1, where an input graph is first fed into the proposed positive and negative coarsening modules to learn the real and fake coarsened graphs. Then, the two coarsened graphs along with the input graph are encoded as the positive and negative samples. To maximize the mutual information between the input and the coarsened graph of each pooling layer can be maximized by minimizing the mutual information loss $\mathcal{L}_{MI}$:

$$\mathcal{L}_{MI} = - \frac{1}{N \cdot \text{Lp}} \sum_{i=1}^{N \cdot \text{Lp}} \sum_{j=1}^{N} \log \sigma(T_i(e_{ij}^f, e_{ij}^{l+1})) + \log(1 - \sigma(T_i(e_{ij}^f, e_{ij}^{l+1})))$$

where $\text{Lp}$ is the number of pooling layers, $N$ is the size of the training set. The yellow square in Figure 1 shows the structure of mutual information neural estimation and maximization (MINEM). In Figure 1, the overall model for graph classification repeats the graph convolution and pooling operations three times. The overall graph level representation is the sum of coarsened graphs from different pooling layers, which will be fed into an MLP layer with a softmax classifier. The overall loss is:

$$\mathcal{L} = \mathcal{L}_{CLS} + \alpha \mathcal{L}_{MI}$$

where $\alpha$ is a hyperparameter that balances the two terms. $\mathcal{L}_{CLS}$ is the graph classification loss:

$$\mathcal{L}_{CLS} = - \sum_{i=1}^{N} \sum_{j=1}^{C} y_{ij} \log \hat{y}_{ij}$$

where $y_{ij}$ is the ground-truth label and $\hat{y}_{ij}$ is the predicted probability that the graph belongs to class $i$, $C$ is the number of classes.

3.2 Positive and Negative Coarsening Module

We detail the positive and negative coarsening modules to learn real and fake coarsened graphs based on self-attention mechanism. Specifically, the positive coarsening module selects a subset of nodes in $G^l$ to form a real coarsened graph $G^{l+1}_r$ which maximally represent $G^l$, while the negative coarsening module generates a fake coarsened graph $G^{l+1}_f$ which contains unimportant nodes in $G^l$.

Then $G^{l+1}_r$ and $G^{l+1}_f$ are fed into an encoder network to obtain their representations $e^{l+1}_r$ and $e^{l+1}_f$. We also present the fusion operation that obtains the coarsened graph $G^{l+1}$ from $G^{l+1}_r$ and $G^{l+1}_f$, which is the output of $l$-th pooling layer.

In the positive and negative coarsening modules, we first adopt two parallel graph neural networks to calculate a 1D attention score between the joint distribution $P_{OZ}$ of $P_O$ and $P_Z$, and the product of marginal distribution $P_O \otimes P_Z$ [20]:

$$I(O, Z) = D_{KL}(P_{OZ} \| P_O \otimes P_Z) \geq \sup_{T \in \mathcal{T}} [E_{e_i^l, e_j^{l+1} \sim P_{OZ}}[T(e_i^l, e_j^{l+1})]]$$

where $I(O, Z)$ is the mutual information between $O$ and $Z$, and its lower bound is learned via contrastive learning [27]. Function $T \in \mathcal{T}$ maps a pair of input graph and coarsened graph to a real value, reflecting the dependency of the two graphs. $e_i^l$ and $e_j^{l+1}$ are the coarsened graphs that sampled from $P_{OZ}$ and $P_O \otimes P_Z$, respectively. In practice, we replace the KL divergence by a GAN-like divergence to achieve mutual information maximization [28]:

$$\mathcal{L}_{GAN}(O, Z) \geq \sup_{T \in \mathcal{T}} [E_{P_{OZ}}[\log \sigma(T_0(e_i^l, e_j^{l+1}))]]$$

$$+ E_{P_O, P_Z}[\log(1 - \sigma(T_0(e_i^l, e_j^{l+1})))])$$

where $\sigma$ is the sigmoid function. We parameterize $T$ in Equation 1 with a discriminator network $T_0$. Then the mutual information between the input and the coarsened graph of each pooling layer can be maximized by minimizing the mutual information loss $\mathcal{L}_{MI}$:

$$\mathcal{L}_{MI} = - \frac{1}{N \cdot \text{Lp}} \sum_{i=1}^{N \cdot \text{Lp}} \sum_{j=1}^{N} \log \sigma(T_0(e_{ij}^f, e_{ij}^{l+1})) + \log(1 - \sigma(T_0(e_{ij}^f, e_{ij}^{l+1})))$$

where $\text{Lp}$ is the number of pooling layers, $N$ is the size of the training set. The yellow square in Figure 1 shows the structure of mutual information neural estimation and maximization (MINEM). In Figure 1, the overall model for graph classification repeats the graph convolution and pooling operations three times. The overall graph level representation is the sum of coarsened graphs from different pooling layers, which will be fed into an MLP layer with a softmax classifier. The overall loss is:

$$\mathcal{L} = \mathcal{L}_{CLS} + \alpha \mathcal{L}_{MI}$$

where $\alpha$ is a hyperparameter that balances the two terms. $\mathcal{L}_{CLS}$ is the graph classification loss:

$$\mathcal{L}_{CLS} = - \sum_{i=1}^{N} \sum_{j=1}^{C} y_{ij} \log \hat{y}_{ij}$$

where $y_{ij}$ is the ground-truth label and $\hat{y}_{ij}$ is the predicted probability that the graph belongs to class $i$, $C$ is the number of classes.
vector for each node in the input graph $G^l$:
\[
y_r^{l+1} = \sigma(GN_{r}^l(H^l, A^l)) \\
y_f^{l+1} = \sigma(GN_{f}^l(H^l, A^l))
\]
where $\sigma$ is the sigmoid function, $H^l$ and $A^l$ are the node feature matrix and adjacency matrix of $G^l$, $y_r^{l+1} \in \mathbb{R}^{N \times 1}$ and $y_f^{l+1} \in \mathbb{R}^{N \times 1}$ are score vectors learned by GNN$_r$ and GNN$_f$. We then rank all nodes according to the score vectors $y_r^{l+1}$ and $y_f^{l+1}$ and select the $k$-largest values:
\[
idx_r^{l+1} = \text{top-k}(y_r^{l+1}) \\
idx_f^{l+1} = \text{top-k}(y_f^{l+1})
\]
where $k$ is the number of selected nodes, $idx_r^{l+1}$ contains the indices of nodes selected for the real coarsened graph $G_{r}^{l+1}$, and $idx_f^{l+1}$ contains the indices of nodes selected for the fake coarsened graph $G_{f}^{l+1}$. Based on $idx_r^{l+1}$ and $idx_f^{l+1}$, the adjacency matrices $A_r^{l+1}$ of $G_{r}^{l+1}$ and $A_f^{l+1}$ of $G_{f}^{l+1}$ are:
\[
A_r^{l+1} = A^l(idx_r^{l+1}, idx_r^{l+1}) \\
A_f^{l+1} = A^l(idx_f^{l+1}, idx_f^{l+1})
\]
and the feature matrices $H_r^{l+1}$ of $G_{r}^{l+1}$ and $H_f^{l+1}$ of $G_{f}^{l+1}$ are:
\[
H_r^{l+1} = H^l(idx_r^{l+1}, :) \circ y_r^{l+1}(idx_r^{l+1}, :) \\
H_f^{l+1} = H^l(idx_f^{l+1}, :) \circ y_f^{l+1}(idx_f^{l+1}, :)
\]
where $\circ$ is the broadcasted elementwise product. Then the representations of the input and two coarsened graphs are learned via weight-shared $\text{encoder}$ network:
\[
e^{l} = \text{encoder}(H^l) \\
e^{l+1}_r = \text{encoder}(H_r^{l+1}) \\
e^{l+1}_f = \text{encoder}(H_f^{l+1})
\]
We have presented the procedure to obtain $e^{l+1}_r$ and $e^{l+1}_f$ above. To force $GN_{r}^{l+1}$ and $GN_{f}^{l+1}$ learn meaningful $y_r^{l+1}$ and $y_f^{l+1}$, where the real coarsened graph $G_{r}^{l+1}$ can represent $G^l$ and the fake coarsened graph $G_{f}^{l+1}$ contains unimportant nodes in $G^l$, we propose a fusion operation:
\[
y_d^{l+1} = \sigma(y_r^{l+1} - y_f^{l+1})
\]
where $\sigma$ is the sigmoid function that normalizes the score values. Based on the self-attention mechanism, important nodes tend to have larger values in $y_r^{l+1}$ and smaller values in $y_f^{l+1}$. We then select top-$k$ nodes $idx_d^{l+1} = \text{top-k}(y_d^{l+1}, k)$ to form the coarsened graph $G_{d}^{l+1}$, and the node feature matrix $H_{d}^{l+1}$ of $G_{d}^{l+1}$ are given by:
\[
H_{d}^{l+1} = H^l(idx_d^{l+1}, :) \circ y_d^{l+1}(idx_d^{l+1}, :)
\]
Therefore, the real coarsened graph $G_{r}^{l+1}$ formed by the nodes with the $k$-largest values in $y_r^{l+1}$ can represent the input graph $G^l$, and the fake coarsened graph $G_{f}^{l+1}$ formed by the nodes with the $k$-largest values in $y_f^{l+1}$ contains unimportant nodes in $G^l$.

## 4 EXPERIMENTS

We compare CGIPool with state-of-the-art models on graph datasets for graph classification tasks. CGIPool is implemented on PyTorch and PyTorch Geometric on an NVIDIA P100 GPU.

### 4.1 Datasets and Experimental Setup

**Datasets:** We conduct extensive experiments to evaluate our proposed CGIPool on seven datasets [29], including three small molecules datasets: NCI1, NCI109 [30] and Mutagenticity [31], three social network datasets: IMDB-B, IMDB-M and COLLAB [32], and a protein graph dataset: PROTEINS [7]. Table 1 summarizes the statistics of these datasets. Since no node feature is provided in social network datasets, we use one-hot vectors to encode the degrees of nodes as features, which is the same as [19].

**Baselines:** We validate the effectiveness of the proposed method by comparing it with state-of-the-art graph pooling models, including two global pooling methods: Set2Set [13] and DGCNN [4]; DiffPool [6] which is the first differentiable graph pooling method; and four node-selection-based graph pooling methods: TopKPool [16], SAGPool [17], ASAP [18], and VIPool [19].

**Experimental setup:** We randomly split each dataset into three parts: 80% for training, 10% for validation, and 10% for testing [17]. We repeat this random splitting 20 times and take the averaged performance with standard derivation as the final results. We set the dimension of node embedding as 128, the learning rate as 0.001, the weight decays as 0.0001, and the pooling ratio $r$ as 0.8 for all datasets. We adopt Adam as the optimizer and stop the training...
when the validation loss does not decrease for 100 consecutive
epochs. The discriminator consists of a two-layer MLP followed by
a sigmoid function. The hyper-parameter α in Eq(4) is set to 1 for
the PROTEINS dataset, and 0.001 for all rest datasets. All baselines
and CGIPool are equipped with the same three-layer GCN model
as shown in Figure 1, and pooling modules are the only differences.

4.2 Results
Table 1 summarizes the accuracy of CGIPool and baselines on graph
classification. CGIPool achieves state-of-the-art performance on all
datasets except the IMDB-B dataset, where the accuracy of CGIPool
is only 0.97% lower than that of the best baseline. Moreover, the
datasets cover different domains such as social networks, bioinfor-
matics, and molecules, which reveals that CGIPool yields great per-
f ormance in different domains. Specifically, CGIPool outperforms
state-of-the-art models by up to 1.21%, 1.43%, and 0.45% on social
networks, bioinformatics, and molecules, respectively.

4.3 Ablation and Robustness study
We examine the impact of the negative coarsening module and the
mutual information maximization in CGIPool. We also examine the
robustness of CGIPool with different pooling ratios.

4.3.1 Negative coarsening module. The negative coarsening mod-
ule in CGIPool aims to learn the fake coarsened graphs. To illustrate
its impact, we implement CGIPool-RS, which is a variant of CGIPool
that replacing the negative coarsening module by Randomly Select
the same number of nodes from the input graph. The selected nodes
form a random fake coarsened graph and will be fed into the dis-

Table 1: The statistics of datasets and graph classification accuracies of different graph pooling algorithms.

| Dataset  | Small Molecules | Social Networks | Bioinformatics |
|----------|-----------------|-----------------|----------------|
|          | NCI1            | NCI109          | IMDB-B         |
| Avg # Graphs (Classes) | 4110 (2) | 4127 (2) | 4337 (2) | 1000(2) | 1500(3) | 5000(3) | 1113(2) |
| Avg # Nodes | 29.87  | 29.68  | 30.32 | 19.77  | 13.00  | 74.49  | 39.06  |
| Avg # Edges | 32.30  | 32.13  | 30.77 | 96.53  | 65.94  | 2457.78 | 72.82  |
| VIPool   | 78.62±1.04 | 77.94±1.37 | 80.65±0.79 | 72.40±0.87 | 51.45±0.65 | 80.30±0.69 | 74.10±2.31 |
| CGIPool  | 78.62±1.04 | 77.94±1.37 | 80.65±0.79 | 72.40±0.87 | 51.45±0.65 | 80.30±0.69 | 74.10±2.31 |

Table 2: Results of CGIPool and its two variants.

| Dataset     | NCI1 | NCI109 | Mutagenicity | COLLAB |
|-------------|------|--------|--------------|--------|
| CGIPool     | 78.62±1.04 | 77.94±1.37 | 80.65±0.79 | 80.30±0.69 |
| CGIPool-RS  | 77.21±1.35 | 76.33±1.58 | 80.12±0.88 | 79.14±0.82 |
| CGIPool w/o MI | 76.92±1.30 | 75.65±1.44 | 79.23±0.91 | 78.3±0.75 |

4.3.2 Mutual Information Estimation and Maximization. To demon-
strate the impact of maximizing the mutual information between
the input and the coarsened graph of each pooling layer, we re-
move the mutual information maximization in CGIPool, and denote
this variant as “CGIPool w/o MI”. In Table 2, CGIPool outperforms
CGIPool w/o MI consistently, which proves the importance of max-
imizing the mutual information between the graph before and after
each pooling layer.

4.3.3 Performance with different pooling ratio. To prove the ro-

Figure 2: The performance of four pooling models on NCI1
and IMDB-M with different pooling ratios.

5 CONCLUSION
In this paper, we propose CGIPool that maximizes the mutual infor-
mation between the input and the coarsened graph of each pooling
layer. To achieve contrastive learning for mutual information neural
maximization, we propose self-attention-based positive and nega-
tive coarsening modules to learn real and fake coarsened graphs as
positive and negative samples. Extensive experiments show that the
proposed CGIPool outperforms state-of-the-art methods on six out
of seven graph classification datasets.

6 ACKNOWLEDGMENTS
This work is sponsored in part by the National Key Research &
Development Program of China under Grant No. 2018YFB0204300,
and the National Natural Science Foundation of China under Grant
No. 62025208 and 61932001.
REFERENCES

[1] T. N. Kipf and M. Welling, "Semi-supervised classification with graph convolutional networks," arXiv preprint arXiv:1609.02907, 2016.

[2] W. Hamilton, Z. Ying, and J. Leskovec, "Inductive representation learning on large graphs," in Advances in Neural Information Processing Systems, 2017, pp. 1024–1034.

[3] P. Velickovic, G. Cucurull, A. Casanova, A. Romero, P. Lio, and Y. Bengio, "Graph attention networks," arXiv preprint arXiv:1710.10903, 2017.

[4] M. Zhang, Z. Cui, M. Neumann, and Y. Chen, "An end-to-end deep learning architecture for graph classification," in AAAI Conference on Artificial Intelligence, vol. 32, no. 1, 2018.

[5] D. Liben-Nowell and J. Kleinberg, "The link-prediction problem for social networks," Journal of the American Society for Information Science and Technology, vol. 58, no. 7, pp. 1019–1031, 2007.

[6] Z. Ying, J. You, C. Morris, X. Ren, W. Hamilton, and J. Leskovec, "Hierarchical graph representation learning with differentiable pooling," in Advances in Neural Information Processing Systems, 2018, pp. 4800–4810.

[7] A. Feragen, N. Kasenburg, J. Petersen, M. de Bruijne, and K. M. Borgwardt, "Scalable kernels for graphs with continuous attributes," in Advances in Neural Information Processing Systems, 2013, pp. 216–224.

[8] Z. Fu, Y. Xian, R. Gao, J. Zhao, Q. Huang, Y. Ge, S. Xu, S. Geng, C. Shah, Y. Zhang et al., "Fairness-aware explainable recommendation over knowledge graphs," in ACM SIGIR Conference on Research and Development in Information Retrieval, 2020, pp. 69–78.

[9] Y. Su, R. Zhang, S. Erfani, and Z. Xu, "Detecting beneficial feature interactions for recommender systems," in AAAI Conference on Artificial Intelligence, 2021.

[10] C. Zhang, N. J. Yuan, R. Song, X. Xie, and Q. Ma, "Understanding people lifestyles: Construction of urban movement knowledge graph from ggs trajectory," in International Joint Conference on Artificial Intelligence, 2017, pp. 3616–3623.

[11] Z. Lu, P. Du, and J.-Y. Nie, "Vgn-c-bert: augmenting bert with graph embedding for text classification," in European Conference on Information Retrieval, 2020, pp. 369–382.

[12] J. Atwood and D. Towsley, "Diffusion-convolutional neural networks," arXiv preprint arXiv:1511.02136, 2015.

[13] J. Gilmer, S. S. Schoenholz, P. F. Riley, O. Vinyals, and G. E. Dahl, "Neural message passing for quantum chemistry," in International Conference on Machine Learning, 2017, pp. 1263–1272.

[14] H. Yuan and S. Ji, "Structpool: Structured graph pooling via conditional random fields," in International Conference on Learning Representations, 2020.

[15] F. M. Bianchi, D. Grattarola, and C. Alippi, "Mincut pooling in graph neural networks," arXiv preprint arXiv:1907.00481, 2019.

[16] H. Gao and S. Ji, "Graph u-nets," arXiv preprint arXiv:1905.05178, 2019.

[17] J. Lee, I. Lee, and J. Kang, "Self-attention graph pooling," arXiv preprint arXiv:1904.08082, 2019.

[18] E. Ranjan, S. Sanyal, and P. Talukdar, "Asap: Adaptive structure aware pooling for learning hierarchical graph representations," in AAAI Conference on Artificial Intelligence, vol. 34, no. 04, 2020, pp. 5470–5477.

[19] M. Li, S. Chen, Y. Zhang, and I. W. Tsang, "Graph cross networks with vertex infomax pooling," arXiv preprint arXiv:2010.01804, 2020.

[20] M. I. Belghazi, A. Baratin, S. Rajeswar, O. Ozair, Y. Bengio, A. Courville, and R. D. Hjelm, "Mine: mutual information neural estimation," arXiv preprint arXiv:1801.04062, 2018.

[21] R. D. Hjelm, A. Fedorov, S. Lavoie-Marchildon, K. Grewal, P. Bachman, A. Trischler, and Y. Bengio, "Learning deep representations by mutual information estimation and maximization," arXiv preprint arXiv:1808.06670, 2018.

[22] P. Velickovic, W. Fedus, W. L. Hamilton, P. Lio, Y. Bengio, and R. D. Hjelm, "Deep graph infomax," in International Conference on Learning Representations (Poster), 2019.

[23] A. Creswell, T. White, V. Dumoulin, K. Arulkumaran, B. Sengupta, and A. A. Bharath, "Generative adversarial networks: An overview," IEEE Signal Processing Magazine, vol. 35, no. 1, pp. 53–65, 2018.

[24] Y. Zhao, J. Qi, and R. Zhang, "Obse: Corner-based building height estimation for complex street scene images," in The World Wide Web Conference, 2019, pp. 2436–2447.

[25] F. Diehl, "Edge contraction pooling for graph neural networks," arXiv preprint arXiv:1905.10990, 2019.

[26] A. H. Khasahmadi, K. Hassani, P. Moradi, L. Lee, and Q. Morris, "Memory-based graph networks," arXiv preprint arXiv:2002.09518, 2020.

[27] N. Saunshi, O. Plevrakis, S. Arora, M. Khodak, and H. Khandeparkar, "A theoretical analysis of contrastive unsupervised representation learning," in International Conference on Machine Learning, PMLR, 2019, pp. 5628–5637.

[28] K. Dzugaite, D. M. Roy, and Z. Ghahramani, "Training generative neural networks via maximum mean discrepancy optimization," arXiv preprint arXiv:1505.03906, 2015.

[29] 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.

[30] N. Shervashidze, P. Schweitzer, E. J. Van Leeuwen, K. Mehlhorn, and K. M. Borgwardt, "Graph kernels: A rigorous, economical, and fast linear time algorithm for comparing simple undirected graphs," Journal of Machine Learning Research, vol. 11, 2010.

[31] J. Kazius, R. McGuire, and R. Bursi, "Derivation and validation of toxicophores for mutagenicity prediction," Journal of Medicinal Chemistry, vol. 48, no. 1, pp. 32–320, 2005.

[32] P. Yanardag and S. Vishwanathan, "A structural smoothing framework for robust graph comparison," Advances in Neural Information Processing Systems, vol. 28, pp. 2134–2142, 2015.