Graph Property Prediction on Open Graph Benchmark: 
A Winning Solution by Graph Neural Architecture Search

Xu Wang  
4Paradigm  
Beijing, China  
wangxu01@4paradigm.com

Huan Zhao  
4Paradigm  
Beijing, China  
zhaohuan@4paradigm.com

Lanning Wei  
4Paradigm  
Beijing, China  
weilanning18z@ict.ac.cn

Quanming Yao  
Department of Electronic Engineering, Tsinghua University  
Beijing, China  
qyaoaa@tsinghua.edu.cn

ABSTRACT
Aiming at two molecular graph datasets and one protein association subgraph dataset in OGB graph classification task, we design a graph neural network framework for graph classification task by introducing PAS (Pooling Architecture Search). At the same time, we improve it based on the GNN topology design method F^2GNN to further design the feature selection and fusion strategies, so as to further improve the performance of the model in the graph property prediction task while overcoming the over smoothing problem of deep GNN training. Finally, a performance breakthrough is achieved on these three datasets, which is significantly better than other methods with fixed aggregate function. It is proved that the NAS method has high generalization ability for multiple tasks and the advantage of our method in processing graph property prediction tasks.

KEYWORDS
Graph Neural Networks, Neural Architecture Search, Automated Machine Learning, Graph Property Prediction

1 INTRODUCTION
Graph structure has been widely used in various abstract interactive complex systems, such as social networks [5], knowledge graphs [18], molecular diagrams [26] and biological networks [1, 21]. Recently, a series of progress has been made in the application of graph related machine learning methods in various fields [28]. In order to further promote the research of machine learning on graphs, Weihua Hu team of Stanford University put forward the open graph benchmark dataset in NeurIPS 2020 [12], which is committed to promoting the research of robust and reproducible graph machine learning. OGB dataset involves many fields, and the tasks are divided into node-level, edge-level and graph-level prediction tasks.

Among them, the graph-level prediction task includes four datasets from three different application fields, including two molecular graph datasets of ogbg-molhiv and ogbg-molpcba, protein-protein association subgraph dataset ogbg-ppa, and ogbg-code, a set of source code of Python abstract syntax tree. The graph-level prediction of molecular properties is shown in Figure 1. The graph neural network is used to extract information from the atomic and chemical bond features stored on nodes and edges. The representation of the whole graph is obtained according to the updated representation of each node, so as to convert the prediction of molecular properties into graph-level classification.

Based on the first three datasets of OGB graph classification task, we design a task adaptive graph neural network architecture combined with neural architecture search (NAS) [23, 36, 37] on graph, so as to achieve further performance breakthrough on each corresponding task. Specifically, we introduce the pooling structure search scheme PAS (pooling architecture search) [23], which designs the aggregate function search space, and applies the differentiable search algorithm to the specific aggregate function and pooled structure search. At the same time, we also improve PAS based on the graph neural network topology design method F^2GNN (Feature Fusion GNN) [22], which designs the topology of graph neural network from the perspective of differentiable search.

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 ACM 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.

DLG-KDD 2022, August 14, 2022,  
© 2022 Association for Computing Machinery.
method and feature fusion, so as to overcome the problem of over smoothing (reduction of feature discrimination of adjacent nodes) in the training of deep graph neural network, and finally obtain 1st place on the first three datasets, i.e., ogbg-molhiv, ogbg-molpcba, and ogbg-ppa, in the graph-level prediction task.\footnote{Note in the second dataset, i.e., molpcba, there are two settings. We obtain the 1st place among those do not use external dataset.} Code is released in: https://github.com/AutoML-Research/PAS-OGB.

2 BACKGROUND

2.1 OGB Graph Property Prediction

ogbg-molhiv and ogbg-molpcba, provided by MoleculeNet [26], are the molecule property prediction datasets, where nodes are the atoms and the edges represents the chemical bonds in each molecule graph. The former focuses on the ability of molecules to inhibit HIV virus replication, and the latter focuses on the effectiveness of different compounds against more than 100 disease targets. These two datasets contain more than 40,000 and 400,000 molecular samples, respectively, which are the largest molecule property datasets in [26]. Therefore, it is greatly significant to utilize these two datasets to screen and develop effective drugs for many diseases.

ogbg-ppa dataset is a set of undirected protein association subgraphs extracted from the protein association networks of 1,581 different species, covering 37 broad biological taxa (including mammals, bacterioides, archaea, etc.), including more than 150,000 samples. The task requires to give a protein association subgraph and predict the source of biological taxa of the association subgraph. Successfully solving this problem is of great significance to understand the evolution of cross species protein complexes, the recombination of protein interactions over time, and the discovery of functional associations between genes. It can also have an in-depth understanding of key bioinformatics tasks, such as biological network alignment. Further details of the three datasets are shown in the appendix.

At present, a variety of GNNs have been applied to graph classification task, but there is not a general method on the three datasets that can stably achieve SOTA performance. In addition, graph-level representation learning may require long-range neighbors [25, 29], and the top schemes for two molecular datasets on the leaderboard mostly adopt deeper GNNs. However, the deep GNN model often leads to the over smoothing problem of reducing the feature distinguishability of neighbor nodes and significantly reducing the final prediction effect.

2.2 Graph Neural Architecture Search

Neural architecture search (NAS) methods were proposed to automatically find SOTA CNN architectures in a pre-defined search space and representative methods are [15, 17, 27, 37]. At the same time, most of the existing GNN designs follow the message passing framework to design the aggregation function of neighbor information and the update function of node representation [9]. Very recently, researchers tried to automatically design GNN architectures by NAS. The majority of these methods focus on designing the aggregation layers in GNNs. For example, the representative method GraphNAS [8] defines a search space that includes an attention function, the number of attention heads, and embedded size, etc. Based on the JKNet [29], SNAE [35] and SNAG [36] learn to select and fuse the characteristics in each layer. Following the paradigm of NAS, one search algorithm should be employed to select architectures from the designed search space. Some work that directly introduces reinforcement learning or evolutionary algorithm into search strategy [3, 7, 11, 35]. In order to further improve the search efficiency, some methods relax the discrete search space into a continuous search space, and then they can be optimized with the gradient descent, which is efficient in orders of magnitude than the aforementioned ones.

PAS designs the pooling architectures, including Aggregation, Pooling, Readout and Merge operations, which are essential for obtaining graph-level representations. Then it developed an effective differentiable search algorithm by a continuous relaxation of the search space. And in this way, data-specific architectures are obtained. \(^{2}\)GNN provide a feature fusion perspective in designing GNN topology and propose a novel framework to unify the existing topology designs with feature selection and fusion strategies. In this paper, we transform the search space of PAS scheme, modifies the search space of aggregation function while deleting the pooling operation search, and introduces the neural architecture search method of \(^{2}\)GNN to design network topology; so as to further improve the effect of adapting to downstream tasks after feature selection and fusion.

3 METHOD

In this section, we elaborate on the proposed novel framework PAS, which is based on NAS to search for adaptive architectures for graph classification, consisting of the novel search space and the efficient search algorithm. At the same time, we will also elaborate on the improvement scheme of PAS based on \(^{2}\)GNN method. 

Notations. We represent a graph as \(G = (A, H)\), where \(A \in \mathbb{R}^{N \times N}\) is the adjacency matrix of this graph and \(H \in \mathbb{R}^{N \times d}\) is the node features, \(N\) is the node number and \(d\) is the feature dimension. For simplicity, all the intermediate layers have the same feature dimension \(d\). The input graph is represented as \(G = (A, H^0)\) in this paper.

3.1 The Design of the Search Space

As shown in Figure 2, the proposed framework contains \(N\) SFA (Selection, Fusion and Aggregation) blocks (\(N = 4\) for example) to extract the local information, and then adds one Readout module to generate the graph representations for downstream tasks. For the \(i\)-th SFA block, Selection module determines whether to use the output characteristics of the first \(i\) block. Fusion module determines the method of intergrating these selected features. The Aggregation operation \(f_s\) update the representation of each node without changing the structure of the graph itself. Therefore, the high-level features can be generated by \(H^i = f_s(f_f((f_f(f_{l=1}(H^0)), \cdots, f_{l=i-1}(H^{i-1}))))\). Here, \(f_s\) is the selection operation and \(f_f\) is the fusion operation. At the end of the SFA blocks, we add one readout operation to generate the graph representations based on the aggregation results.

The candidate operations we used in the search space are provided in Table 1. Following \(^{2}\)GNN, two operations IDENTITY and
**Table 1: The operations used in our search space.**

| Module          | Operations                      |
|-----------------|---------------------------------|
| Selection $O_s$ | ZERO, IDENTITY                  |
| Fusion $O_f$    | SUM, MEAN, MAX, CONCAT, LSTM    |
| Aggregation $O_a$ | GCN [14], GAT [20], GIN [28], GEN [16], MF [4], ExpC [30] |
| Readout $O_r$  | GLOBAL_MEAN, GLOBAL_MAX, GLOBAL_SUM |

ZERO are provided in the Selection module, which represents the "selected" and "not selected" stages for the input feature. Five fusion operations are selected to fuse these features with the summation, average, maximum, concatenation and LSTM cell, which are denoted as SUM, MEAN, MAX, CONCAT and LSTM, respectively. For Aggregation module, apart from the widely used aggregation operations GCN [14], GAT [20] and GIN [28], we further provide three operations GEN [16], MF [4] and ExpC [30] which achieved great progress in the OGB leaderboard. Following PAS, we take the maximum, mean and summation of all node embeddings as the graph-level representations, and these three operations are denoted as GLOBAL_MEAN, GLOBAL_MAX and GLOBAL_SUM, respectively.

**Discussions.** Considering that the OGB datasets ogbg-molhiv and ogbg-molpcba are the molecule datasets where the graph structures are largely correlated with the graph property, pooling operations aiming to generate the coarse graphs may lead to information loss to some extent for these two datasets [10]. Besides, the top schemes in the leaderboard also ignore the pooling operations. Therefore, compared with PAS, we delete the Pooling module and turn to designing deep GNNs to capture the long-range dependencies in OGB datasets. In this paper, we focus on extracting the long-range dependencies for the graph classification task based on the deep GNNs rather than the pooling operations. Considering the over smoothing problem of deep GNN network training, we introduce the F^2 GNN which can alleviate this problem by utilizing the features in different ranges adaptively. This method is designed for the node classification task, and we extend it into the graph classification task which is a natural application of deep GNNs.

### 3.2 The Design of the Search Algorithm

In order to make the search algorithm continuously differentiable, we design the following relaxation function to relax the discrete search space into a continuous space in the form of weighted summation:

$$\hat{o}(x) = \sum_{i=1}^{[O]} c_i o_i(x),$$

where $c_i \in (0, 1)$ is the weight of the $i$-th operation $o(\cdot)$ in set $O$. Among them, the selection module contains two opposite operations: ZERO stands for not selecting the feature, while IDENTITY stands for selecting the input feature. Therefore, the mixed selection result of this module can be expressed as:

$$\hat{o}^f(x_i) = \sum_{k=1}^{[O]} c_0^f \cdot c_k^f (x_i) = c_0^f \cdot 0 + c_1^f \cdot x_i = c_2^f \cdot x_i,$$

since the weight of ZERO operation will be fixed multiplied by 0, there will be an error in the final result, and the error will gradually expand with the advancement of the calculation process. Therefore, we introduce a temperature coefficient $\lambda$ when calculating the operation weight, and make the weight coefficient of each operation expressed as:

$$c_k = \frac{\exp(a_k / \lambda)}{\sum_{i=1}^{[O]} \exp(a_i / \lambda)}.$$

Figure 2: The framework of our method. For the $i$-th SFA block, we have $i$ selection operations $f_s$ and one fusion operation $f_f$ to select and integrate the output of the previous block. Then one aggregation operation $f_a$ is followed to aggregated messages from the neighborhood. The last SFA block will be followed by a readout operation $f_r$ to get graph representation.

4 EXPERIMENT

All models are implemented with Pytorch (version 1.8.0) on a GPU RTX3090. In addition, in order to facilitate the implementation of various GNN variants, we use the popular GNN library: PYG [6] (Pytorch Geometric) (version 2.0.1). The experimental hyper-parameter settings on the three datasets are shown in appendix.

Most of the baselines we selected are within 5 in the OGB leaderboard (the experiments on the ogbg-molpcba do not include the introduction of extend datasets for pre-training). For the two molecular property prediction tasks, we use binary cross-entropy as the loss function, while for the multi-class classification task for ogbg-molhiv, we use cross-entropy as the loss function.

### 4.1 ogbg-molhiv

For ogbg-molhiv, we automatically designed a 14 layer GNN model according to the average diameter of the graph in its dataset, and introduced two molecular fingerprints: MorganFingerprint and MACCSFingerprint [24]. We jointly train PAS and molecular fingerprint model based on random forest, and use softmax and a learnable parameter to aggregate the two results. Considering the advantages of DeepAUC [32] in binary classification task with unbalanced samples, we introduce it into the calculation of loss function. The searched architecture is shown in Figure 3(a), it mainly

![Diagram](image-url)
includes GEN, updates the node representation in deeper GNN layer, and uses MF to combine the node degree in the last three layers, which reflects the importance of atomic degree for this task. The final experimental results are shown in Table 2. It can be seen that compared with other fixed aggregation function schemes, PAS can automatically search the aggregation function of each layer in GNN, and has achieved SOTA on this dataset.

### 4.2 ogbg-molpcba

The sample size of ogbg-molpcba is about ten times larger than that of ogbg-molhiv. Preliminary experiments show that the attention mechanism has a good performance in this task, we updated the search space in the aggregation function to several variants of GAT [36], and designed an 18 layer GNN model combined with the average diameter of the graph in the dataset. The searched architecture after introducing F²GNN is shown in Figure 3(c), compared with the connect operation of dense [13], our method is more flexible in obtaining higher-level features, and interms of effect, the final performance is shown in the Table 3. Compared with PAS, the performance on ogbg-molpcba has been significantly improved after the introduction of architecture search, and the effect of SOTA without introducing additional datasets confirm the effectiveness of the scheme in the prediction of molecular graph properties.

#### Table 2: Performance on ogbg-molhiv dataset. ROC-AUC is used as the metric of this binary-class classification task.

| Method                  | Test AUC  | Validation AUC |
|-------------------------|-----------|----------------|
| Graphormer + FPs [31]   | 0.8225 ± 0.0001 | 0.8396 ± 0.0001 |
| CIN [2]                 | 0.8094 ± 0.0057 | 0.8277 ± 0.0099 |
| GMAN + FPs [33]         | 0.8244 ± 0.0033 | 0.8329 ± 0.0039 |
| DeepAUC [32]            | 0.8352 ± 0.0054 | 0.8238 ± 0.0061 |
| PAS+FPs                 | 0.8420 ± 0.0015 | 0.8238 ± 0.0028 |

#### Table 3: Performance on ogbg-molpcba dataset. Average Precision (AP) is used as the metric of this multiple binary classification task.

| Method                  | Test AP  | Validation AP |
|-------------------------|----------|---------------|
| GIN [28]                | 0.2834 ± 0.0038 | 0.2912 ± 0.0026 |
| CRAWLI [19]             | 0.2986 ± 0.0025 | 0.3075 ± 0.0020 |
| GINE + bot [33]         | 0.2994 ± 0.0019 | 0.3094 ± 0.0023 |
| Nested GIN [34]         | 0.3007 ± 0.0037 | 0.3059 ± 0.0056 |
| PAS                     | 0.3012 ± 0.0039 | 0.3151 ± 0.0047 |
| PAS+F²GNN               | 0.3147 ± 0.0015 | 0.3258 ± 0.0017 |

#### Table 4: Performance on ogbg-ppa dataset.

| Method                  | Test Accuracy | Validation Accuracy |
|-------------------------|---------------|---------------------|
| DeeperGCN [16]          | 0.7752 ± 0.0069 | 0.7484 ± 0.0052 |
| PAS                     | 0.7828 ± 0.0024 | 0.7523 ± 0.0028 |
| ExpC [30]               | 0.7976 ± 0.0072 | 0.7518 ± 0.0080 |
| ExpC² [33]              | 0.8140 ± 0.0028 | 0.7811 ± 0.0012 |
| PAS+F²GNN               | 0.8201 ± 0.0019 | 0.7720 ± 0.0023 |

Figure 3: The searched results on ogbg-molhiv, ogbg-molpcba and ogbg-ppa datasets. The last yellow blocks indicate readout operations. (a) For ogbg-molhiv, the result of aggregate functions searched for PAS, not involving topology search. (b) For ogbg-ppa, fixed the aggregate function to ExpC and search the topology. (c) For ogbg-molpcba, fixed the aggregate function to the variety of GAT and search the topology.

### 4.3 ogbg-ppa

The ogbg-ppa dataset has no initial node characteristics, and its graph specification is about 10 times higher than the first two datasets, and the training cycle is significantly increased. Considering the good performance of ExpC [30] in the graph property prediction task without initial node characteristics, we fixed it in the aggregation module, and design GNN topology based on SFA block.

The searched architecture after introducing F²GNN is shown in Figure 3(b), and the final performance on ogbg-ppa is shown in the Table 4. After introducing the topology search based on f2gnn, this scheme is significantly higher than the original schemes of expc.
and PAS, which verifies the importance of GNN topology and the advantages of topology adaptive design of this scheme.

5 CONCLUSION

For the three datasets of OGB graph classification task, we build our method based on two existing neural architecture search methods, i.e., pooling architecture search PAS, and GNN topology search $P^2$GNN. The results show that our approach has made a performance breakthrough in three tasks, which demonstrates the advantages of NAS methods for GNN. For future work, we will further explore the topology search problem of deeper GNN framework, and further apply the method to real-world, especially bioinformatic, applications.

REFERENCES

[1] Albert-Laszlo Barabasi and Zoltan N Oltvai. 2004. Network biology: understanding the cell’s functional organization. Nature reviews genetics 5, 2 (2004), 101–113.
[2] Cristian Bodnar, Fabrizio Frasca, Nina Otter, Yuguang Wang, Pietro Lio, Guido F Montufar, and Michael Bronstein. 2021. Weisfeiler and Lehman go cellular: CW networks. Advances in Neural Information Processing Systems 34 (2021), 2625–2640.
[3] Jiamin Chen, Jianliang Gao, Yibo Chen, Moctard Babatounde Oloulade, Tengfei Liu, and Hao Li. 2021. Graphpa: Parallel architecture search for graph neural networks. In Proceedings of the 44th International ACM SIGIR Conference on Research and Development in Information Retrieval. 2182–2186.
[4] David K Duvenaud, Dougal Maclaurin, Jorge Ibarzguirre, Rafael Bombarell, Timothy Hirzel, Alan Aspuru-Guzik, and Ryan P Adams. 2015. Convolutional networks on graphs for learning molecular fingerprints. Advances in neural information processing systems 28 (2015).
[5] David Easley and Jon Kleinberg. 2010. Networks, crowds, and markets: Reasoning about a highly connected world. Cambridge university press.
[6] Matthias Fey and Jan Eric Lenssen. 2019. Fast graph representation learning with PyTorch Geometric. arXiv preprint arXiv:1903.02428 (2019).
[7] Yang Gao, Hong Yang, Peng Zhang, Chuan Zhou, and Yue Hu. 2019. Graphnas: Graph neural architecture search with reinforcement learning. arXiv preprint arXiv:1904.09981 (2019).
[8] Yang Gao, Hong Yang, Peng Zhang, Chuan Zhou, and Yue Hu. 2020. Graph Neural Architecture Search. In ICJAI. Vol. 20. 1403–1409.
[9] Justin Gilmer, Samuel S Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. 2017. Neural message passing for quantum chemistry. In International Conference on machine learning. PMLR, 1263–1272.
[10] Daniele Grattarola, Daniele Zambon, Filippo Maria Bianchi, and Cesare Aliatti. 2021. Understanding Pooling in Graph Neural Networks. NeurIPS (2021).
[11] Zichao Guo, Xiangyu Zhang, Haoyuan Mu, Wen Heng, Chunxiao Liu, and Liang Lin. 2018. SNAS: stochastic neural architecture search. arXiv preprint arXiv:1812.09926 (2018).
[12] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. 2018. How powerful are graph neural networks? arXiv preprint arXiv:1810.08620 (2018).
[13] Keyulu Xu, Chengtao Li, Yonglong Tian, Tomohiro Sonobe, Ken-ichi Kawazabayashi, and Stefanie Jegelka. 2018. Representation learning on graphs with jumping knowledge networks. In International Conference on Machine Learning, PMLR, 5453–5462.
[14] Mingyi Yang, Yanning Shen, Heng Qi, and Baocai Yin. 2020. Breaking the Expressive Bottlenecks of Graph Neural Networks. CoRR abs/2012.07219 (2020).
[15] Zhenqin Wu, Bharat Rambhia, Evan N Feinberg, Joseph Gomes, Caleb Giesen, Anesh S Pappu, Karl Leswing, and Vijay Pande. 2018. MolecularNet: A benchmark for molecular machine learning. Chemical science 9, 2 (2018), 513–530.
[16] Zirui Xie, Hehui Zheng, Chunxiao Liu, and Liang Lin. 2018. SNAS: stochastic neural architecture search. arXiv preprint arXiv:1812.09926 (2018).
[17] Chengxuan Ying, Tielei Cai, Shengjie Luo, Shuxin Zheng, Guolin Ke, Di He, Yanning Shen, and Tie-Yan Liu. 2021. Do Transformers Really Perform Badly for Graph Representation? Advances in Neural Information Processing Systems 34 (2021).
[18] Zhourong Yuan, Yan Yan, Milan Sonka, and Tianbao Yang. 2020. Large-scale RNN-based deep AUC maximization: A New Surrogate Loss and Empirical Studies on Medical Image Classification. arXiv preprint arXiv:2012.03173 (2020).
[19] Hao Zhang, Jiaxin Gu, and Pengcheng Shen. 2021. $\Delta$MAN and bag of tricks for graph classification. https://github.com/PierreHao/YouGraph/tree/main/report.
[20] Maham Zang and Pan Li. 2021. Nested Graph Neural Networks. Advances in Neural Information Processing Systems 34 (2021).
[21] Huan Zhao, Lanning Wei, and Kwangmoon Yoo. 2020. Simplifying architecture search for graph neural network. arXiv preprint arXiv:2010.15621 (2020).
[22] Huan Zhao, Quanming Yao, and Weisure Tu. 2021. Search to aggregate neighborhood for graph neural network. arXiv preprint arXiv:2104.06088 (2021).
[23] Barret Zoph and Quoc V Le. 2016. Neural architecture search with reinforcement learning. arXiv preprint arXiv:1611.01578 (2016).
[24] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. 2017. Graph attention networks. arXiv preprint arXiv:1710.10903 (2017).
[25] XU Wang, Huan Zhao, Weisure Tu, Hao Li, Yu Sun, and Xiaochen Bo. 2022. Graph Neural Networks for Double-Strand DNA Breaks Prediction. arXiv preprint arXiv:2201.01855 (2022).
[26] Lanning Wei, Huan Zhao, and Zhiqiang He. 2022. Designing the Topology of Graph Neural Networks: A Novel Feature Fusion Perspective. In Proceedings of the ACM Web Conference 2022. 1381–1391.
[27] Lanning Wei, Huan Zhao, Quanming Yao, and Zhiqiang He. 2021. Pooling architecture search for graph classification. In Proceedings of the 30th ACM International Conference on Information & Knowledge Management. 2091–2100.
[28] Shanzhuo Zhang Weibin Li and Zhengjie Huang Lihang Liu. 2021. Molecule Representation Learning by Leveraging Chemical Information. https://github.com/PaddlePaddle/PaddleHelix/blob/dev/competition/ogbg_molhiv/Molecule_Representation_Learning_by_Leveraging_Chemical_Information.pdf.
[29] Zichao Guo, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. 2018. How powerful are graph neural networks? arXiv preprint arXiv:1810.08620 (2018).
[30] Keyulu Xu, Chengtao Li, Yonglong Tian, Tomohiro Sonobe, Ken-ichi Kawazabayashi, and Stefanie Jegelka. 2018. Representation learning on graphs with jumping knowledge networks. In International Conference on Machine Learning, PMLR, 5453–5462.
[31] Mingyi Yang, Yanning Shen, Heng Qi, and Baocai Yin. 2020. Breaking the Expressive Bottlenecks of Graph Neural Networks. CoRR abs/2012.07219 (2020).
[32] Zhenqin Wu, Bharat Rambhia, Evan N Feinberg, Joseph Gomes, Caleb Giesen, Anesh S Pappu, Karl Leswing, and Vijay Pande. 2018. MolecularNet: A benchmark for molecular machine learning. Chemical science 9, 2 (2018), 513–530.
A TASK DETAIL AND EXPERIMENT SETTINGS

The specific details of OGB graph property prediction datasets are shown in the Table 5. *ogbg-molhiv* is a single binary-class classification task, and ROC-AUC(Receiver Operating Characteristic-Area Under the Curve) is used as the evaluation metric. *ogbg-molpcba* is a multiple binary-class classification task, with AP(Average Precision) as the metric. The last dataset *ogbg-ppa* is a multi-class classification task, and the diameter rises sharply. All graph samples have no node features, only edge features, and accuracy is used as the evaluation metric.

The hyperparametric search space of our method on three datasets is shown in the Table 6. It should be noted that gamma is a hyperparameter of the introduced DeepAUC [32]. This method is only applicable to binary classification tasks, so gamma only appears in *ogbg-molhiv* dataset.

### Table 5: Introduction of OGB Graph Property Prediction Datasets.

| Dataset | # Graphs | # Nodes per graph | # Edges per graph | # Tasks | Task Type          | Metric     |
|---------|----------|-------------------|-------------------|---------|--------------------|------------|
| odbg-molhiv | 41,127   | 25.5              | 27.5              | 1       | Binary classification | ROC-AUC    |
| odbg-molpcba  | 437,929  | 26.0              | 28.1              | 128     | Binary classification | AP         |
| odbg-ppa     | 158,100  | 243.4             | 2,266.1           | 1       | Multi-class classification | Accuracy  |

### Table 6: Hyper-parameter search space.

|                      | odbg-molhiv | odbg-molpcba | odbg-ppa |
|----------------------|-------------|--------------|----------|
| learning rate        | [5e-3, 1e-2, 3e-2, 5e-2, 1e-1] | [5e-4, 1e-3, 3e-3, 5e-3, 1e-2] | [-] |
| batch size           | [128, 256, 512] | [256, 512, 1024] | [128, 256, 512] |
| hidden size          | [256, 512] | [512, 1024] | [256, 512] |
| dropout              | [0.1, 0.2, 0.3] | [0.1, 0.2, 0.3] | [0.1, 0.2, 0.3] |
| gamma                | [500, 700, 1000] | [-] | [-] |
| virtual node         | [True, False] | [True, False] | [True, False] |